

Phase Transitions and Critical Phenomena

Volume 3
Series
Expansions for
Lattice Models

Edited by

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General Preface

The discontinuities in physical behaviour which occur when a system undergoes a phase transition have claimed the attention of scientists for many years. Particular interest has been focused on phenomena associated with critical points such as that of liquid-vapour equilibrium, or ferromagnetism (the Curie point). It was recognised at an early stage that the discontinuities were associated with interactions between the microscopic constituents of the system, but an exact treatment by means of statistical mechanics appeared prohibitively difficult. During the latter part of the 19th and the earlier part of the 20th century, phenomenological explanations were devised which seemed to account adequately for the discontinuities and to provide insight into their detailed character.

The modern era in phase transitions started in 1944 when Onsager succeeded in carrying out an exact statistical mechanical calculation for a simple interacting atomic model, the two-dimensional Ising model. His solution showed that the previous "classical" theories were unreliable in their quantitative predictions, and provided a great stimulus to explore the true behaviour near discontinuities and critical points. The problems to be faced in extending Onsager's work were formidable, and at first progress was slow. However, there were many different aspects to be investigated and a number of alternative lines of theoretical approach to be pursued. The field began to attract new experimentalists and theoreticians of ability.

During the 1960's there was considerable progress towards a greater understanding of phase transitions and critical phenomena, and the research literature grew rapidly. Much of this literature is of ephemeral value and has been rendered obsolete by new developments. However, a body of established results has accumulated steadily, but remains scattered in the literature. After discussions with many of those engaged in active research in the field, we felt that the time was ripe for an attempt to incorporate these results into a publication which could then serve as a basic text. The aim of the publication would be to present a coherent account of all that is definitely known about phase transitions and critical phenomena, and to provide a standard reference for some time to come, particularly for graduate students.

We therefore listed a number of topics of major importance, and contacted an expert who had been particularly concerned with each topic with the request that he should contribute an article. We were gratified by the favourable response, and by the calibre of the manuscripts we received.

It soon became clear that several volumes would be needed to achieve our objective. In fairness to contributors who produced their manuscripts on time, we have tried to avoid unnecessary delay in publication, but at the same time we have endeavoured as far as possible to maintain coherence in the contents of individual volumes. Volume 1 deals with exact results and solutions, Volume 3 with series expansions, and Volume 4 with critical correlations; Volume 2 contains a number of different articles each throwing its own light on phase transitions and critical phenomena, and related topics are grouped together.

We are well aware of the many gaps which still remain even after the publication of these 4 volumes. We shall endeavour to cover them in later volumes of the publication.

February, 1972

C. Domb
M. S. Green

Preface to Volume 3

In Volumes 1 and 2 a good deal of space was devoted to the discussion of exact solutions of models which give rise to phase transitions and critical points. However, these solutions are confined to two dimensions if realistic physical interactions between the microscopic constituents of the system are used. They can only be extended to three dimensions if an unphysical interaction is introduced.

The present volume is devoted to the series expansion method of exploring critical behaviour, which has provided the most significant information so far on three dimensional models with realistic interactions. The series considered are perturbation expansions in an interaction parameter; starting from an initial non-interacting state they represent a change in behaviour from a smooth analytic function to one with characteristic singularities or discontinuities. A rigorous characterization of such singularities is possible only if the general term in the series is known exactly, or at least asymptotically. In practice only a finite number of terms of the series is available.

From the strictly mathematical point of view, therefore, nothing can be said about the singularities, and all the suggestions put forward in this volume about critical behaviour are in the nature of conjectures. But they are conjectures with a sound physical basis, which draw heavily on the experience of the exact solutions referred to above; indeed a number of the conjectures were confirmed rigorously by exact solutions which became available subsequently.

For any particular model there are two distinct problems to be tackled. The first is the technical problem of developing series expansion of as great length as possible for different models of physical interest. For this purpose techniques have been evolved by different research groups introducing many simplifications and making effective use of computers. Although this is a specialized art, we have endeavoured to provide sufficient detail in the description to enable a non-specialist to understand the calculations, and if necessary to pursue them for himself. This has sometimes required the reproduction of material not available in the published literature, and we have left to the discretion of individual authors exactly how much to include for the discussion of their particular model.

The resulting numerical values of coefficients in series expansions are an

important source of exact information relating to the models discussed, and we have encouraged authors to reproduce these primary data in as complete a form as practicable. Where a number of parameters are involved and tables would be too lengthy reference has been given to original publications.

The second problem is the use of numerical coefficients to assess critical behaviour of thermodynamic functions. This is discussed in general terms in Chapter 4 by Gaunt and Guttman who describe available methods and illustrate them by suitably chosen examples. In the individual chapters dealing with specific models, we have suggested to authors that whilst they should provide full details of their conclusions about critical behaviour, they need only summarize briefly the analysis on which these conclusions are based. Our aim has therefore been to provide for the non-specialist or experimentalist a coherent account of what the experts who have been investigating a particular model think about its critical properties. For a more careful assessment of how much confidence to place in the conjectures, reference should then be made to the original literature.

The first four chapters are concerned with features common to all models. Modern formulations of perturbation expansions lean heavily on the terminology and ideas of graph theory, and Chapter 1 by Domb begins with an elementary account of those aspects which are of importance in the statistical mechanics of interacting particles. The classical cluster integral theory of a condensing gas is then summarized in a form suitable for application to lattice models. The latter part of the chapter is devoted to the theory of "lattice constants" or embeddings, which are the number of ways in which different types of graph can be constructed from the bonds on a given lattice; these have played a central role in the technical problem of deriving series expansions for lattice models.

In the early period of development of series expansions in the 1950s lattice constants were calculated by hand with the aid of a number of theorems which served as short-cuts. When high speed computers had developed sufficiently, it became clear that by careful programming the enumerations could be pursued much further, and nowadays computers are a major factor in the calculations. It is important that the programme should be efficient so as to obtain the maximum possible number of terms in the computer time available. In Chapter 2 J. L. Martin, who was one of the pioneers in this application of computers, describes typical programmes which he has devised for enumerating the lattice constants of different types of graph. We hope that this article will fill a gap in the literature since little has been published elsewhere on the design of programmes.

An alternative approach to series expansions which does not make use of lattice constants was formulated in 1959 by Brout and developed by Englert, Horwitz, Callen and others. Basing itself on free random walks rather than

the non-intersecting walks which arise in the theory of lattice constants, the formalism parallels that of quantum field theory. For several years this approach did not yield practical results of significance because of the large number of diagrams which needed to be taken into account. An important breakthrough took place in the late 1960s when Wortis and his research group devised a mechanical procedure for taking account of the vast majority of the diagrams, leaving relatively few to be tackled individually. The method is now a powerful practical alternative to that of lattice constants, and it is described by Wortis in Chapter 3.

As mentioned above, Chapter 4 by Gaunt and Guttmann tackles the problem of assessing the analytic behaviour of a function in a region of particular interest from a finite number of terms of its power series expansion. The ratio method first used by Domb and Sykes in 1957 was effective for power series which are consistent in sign. The Padé approximant introduced into this field by Baker in 1961 could be applied more widely; various other methods introduced subsequently were designed to deal with specific difficulties. Extrapolations are treated with reserve and scepticism by statisticians. It is worth pointing out, therefore, that in the above treatments the physicist uses his general knowledge and intuition to postulate for the quantity under investigation an analytic form with a number of parameters. He then uses the numerical data to test the consistency of the postulate and obtain good estimates of the parameters.

The remaining five chapters are concerned with specific models. The Heisenberg model of a ferromagnet is the model for which high temperature series expansions were first used (by Opechowski in 1937 following a suggestion of Kramers). In many respects it is the most difficult model to deal with because of the non-commutation of spin operators. Chapter 5 by Rushbrooke, Baker and Wood gives a comprehensive account of the problems which need to be tackled and of the results achieved.

By contrast the Ising model discussed by Domb in Chapter 6 is the simplest model with a realistic physical interaction. The combinatorial problems are straightforward and both high temperature and low temperature series expansions can be derived; also exact solutions for certain properties are available in two dimensions. The model has served as a pioneer in the exploration of critical behaviour, since a more detailed investigation has been possible than for any other model. The literature on the Ising model is extensive, and we hope that this review and precis will be useful to theoreticians and experimentalists in the field.

When the spin of the Heisenberg model is allowed to become infinite, a model of classical interacting vectors is obtained. This represents a considerable simplification since the non-commutation has been removed. The model can be generalized by allowing the spins to interact in D dimensions

as was first suggested by Stanley; he showed that when $D \rightarrow \infty$ the solution becomes identical with that of the spherical model for which exact results are available (Joyce, Volume 2, Chapter 10). In Chapter 7 Stanley discusses the critical behaviour of the model as a function of lattice dimension d and spin dimension D . It has been conjectured that for short-range force models all patterns of critical behaviour can be covered by suitable choice of d and D . Following the terminology introduced by Kadanoff, Stanley calls the Hamiltonian for this model the *Universality Hamiltonian*.

If the spin dimension of the standard Heisenberg model is reduced to two, the $X-Y$ model results. This model has a number of features of particular interest which have been studied in detail by Betts and his collaborators. The Ising and $X-Y$ models represent different cases of extreme anisotropy for a general three dimensional spin exchange interaction. Chapter 8 by Betts deals with the model and its applications. The $X-Y$ model differs in one respect from the other models mentioned above, namely that the order parameter does not commute with the Hamiltonian. Because of this unusual property the model is particularly useful for studying dynamical aspects of critical behaviour. Although these form the subject of a special article in Volume 5, a brief discussion of certain dynamical features of the $X-Y$ model is included in Chapter 8.

Finally Chapter 9 by Nagle is concerned with ferroelectric models whose exact solutions in two dimensions were discussed by Lieb and Wu in Volume 1, Chapter 8. Nagle had estimated the entropy of ice in two dimensions by series methods before Lieb succeeded in calculating the result exactly; the closeness of the estimate to the exact result has served as a vindication of the series method, and gives confidence in the corresponding three dimensional estimates.

In a number of instances the same topics have been discussed by different authors, for example Padé approximants, the universality hypothesis, crossover exponents. Although each author had a different application in mind, a few brief paragraphs of introduction were provided. The editors took no action to modify these sections since they felt that the small amount of duplication which has arisen is offset by the advantage that each chapter is reasonably self-contained.

Whilst the present volume was in preparation a development of major importance in the theory of critical phenomena has occurred. The application of the renormalization group in this field by K. G. Wilson has enabled direct calculations to be made of critical exponents and other features of critical behaviour in terms of the parameter $\varepsilon = 4 - d$. The excellent qualitative agreement between these calculations and the estimates in the present volume based on series expansions enhances our confidence in both methods. There are, however, non-negligible differences in the values of the exponents

obtained by the two methods. It is yet to be seen whether further improvements in the renormalization group approach (or in the series expansion method) will bring these two approaches in complete agreement. One possibility is that Wilson's method and the series expansion method apply to two different physical systems, i.e. fluids and lattices. This subject is a matter of active investigation at the present time. Brief references to the results of the renormalization group method will be found in the present volume, but the true impact will be reflected in subsequent volumes of the publication. In fact we plan to devote Volume 6 completely to the renormalization group and its wide range of applications.

The time lag between the appearance of Volumes 2 and 3 has been larger than we intended when we approached authors for their contributions. A number of factors have combined to cause the delay and we apologise in particular to those authors who produced their manuscripts very promptly. We thank them for their patience and forbearance.

December, 1973

C. Domb
M. S. Green

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Volume 6 (The Renormalization Group and its Applications)

1. Graph Theory and Embeddings

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I. General Introduction

Perturbation expansions have been used widely in astronomy and physics to calculate the effect of small changes in problems for which exact solutions are available. However, for physical phenomena in which an interaction completely changes the character of the solution, it is necessary to derive substantial numbers of terms of such perturbation expansions, and if possible to estimate the asymptotic behaviour of the coefficients. Such expansions have attracted particular attention in statistical mechanics, and have led to important progress in the theory of critical behaviour.

In classifying the contributions of higher order terms, one is naturally led to a description in terms of linear graphs. The first systematic development of this approach was the cluster integral theory of a condensing gas by Mayer and his collaborators (1937–1939) (paralleled by Yvon, 1937). Formally, this was a great step forward since it provided a closed form expression for the general virial coefficient of a gas in terms of intermolecular forces. Also,

there was a particular elegance associated with the development, which could be divided into two stages; in the first stage it was shown that by calculating the logarithm of the partition function instead of the partition function, all contributions corresponding to disconnected graphs were eliminated (for graph terminology see Section II.A); in the second stage it was shown that by changing the expansion variable from the activity to the density, an additional class of contributions was eliminated, and only contributions corresponding to multiply connected graphs survived.

During the 1950's Uhlenbeck initiated a series of researches into the theory of linear graphs and its relationship to the cluster integral development. He was able to derive Mayer's results by a simple application of a general theorem of Polya (1937), and he used this theorem to enumerate the various types of graph which arose in the expansion. Unfortunately, this investigation led to the conclusion that the gain in proceeding to the second stage above was confined to the first few terms. Asymptotically, there was little difference between the number of graphs entering at the first or second stage, and this number increased with extraordinary rapidity. As a result there seemed little hope of evaluating a sufficient number of cluster integrals to determine the asymptotic behaviour of the virial coefficients.

The use of perturbation expansions to investigate lattice models of interacting systems achieved a more promising start. Preliminary work by Kramers and Wannier (1941) for the Ising model and by Opechowski (1937) for the Heisenberg model, showed how such expansions could be derived. Onsager's exact solution of the two-dimensional Ising model in zero field (1944) provided closed form expressions which could be expanded as power series and used as a basis for comparison. Domb (1949, 1952), Wakefield (1951) and Domb and Sykes (1956, 1957a) were able to derive lengthy series expansions for the Ising model from which they drew definite conclusions regarding critical behaviour. The same method was used for a number of different interacting lattice models, several of which form the subject of chapters in this volume. In fact, the series expansion method has so far proved the most effective tool in exploring detailed behaviour in the critical region. Even the most exciting recent use of the renormalization group (Wilson, 1972) has tested the accuracy of its conclusions by comparison with predictions based on series expansions (Wilson and Fisher, 1972).

The Ising model is equivalent to a lattice gas, (see this volume, Chapter 6) and the Mayer development can be applied with an especially simple form of potential (Fuchs 1942, Yvon 1945, 1948; Rushbrooke and Scoins, 1953). However, instead of evaluating cluster integrals we need to calculate the numbers of configurations of various types which can be embedded in the lattice using bonds which correspond to interactions. These numbers have been termed "lattice constants" (Domb and Sykes, 1957b) and correspond

to "embeddings" in the terminology of graph theory (Sykes *et al.* 1966). The same numbers enter in calculations of series expansions for all lattice models.

One of the aims of the present chapter is to provide an elementary introduction to the graph theoretical concepts needed in the development of series expansions. We shall be concerned with explaining the content and significance of the various theorems we discuss rather than with their rigorous proof, but we hope to give sufficient references for anyone interested to pursue the subject further. In the same spirit, we shall summarize the main results of the Mayer theory so that they can then be applied to lattice systems. We shall discuss theoretical developments connected with lattice constants and their enumeration. Extensive tables of lattice constants have been constructed in the past few years, and we shall endeavour to describe what is available.

A more comprehensive general discussion of perturbation expansions is given in Chapter 3 of the present volume (by M. Wortis) which is complementary to the present chapter. The approach described by Wortis follows the development of perturbation expansions in quantum field theory, and the two stages in the Mayer development are paralleled by linked-cluster expansions and vertex renormalizations. This development does not make use of embeddings in the lattice but of free graphs corresponding to random walks on the lattice. The two methods developed independently, and Wortis discusses in detail the relation between them. Both have contributed effectively to our knowledge of critical behaviour as will be seen from the results quoted in various chapters of this Volume and in Vol. 4 of this publication.

II. Linear Graphs

Graph theory is an area with a substantial communication gap between the mathematician and the physicist or chemist. Various attempts have been made to bridge this gap, and the present writer would recommend for preliminary reading, "An Introduction to Combinational Analysis" by Riordan (1958), papers by Uhlenbeck and his collaborators (see Uhlenbeck and Ford, 1962), and the paper by Essam and Fisher (1970) as a reference text for basic definitions. Some general references on graph theory are Berge (1958), Busacker and Saaty (1965), Harary (1967, 1969), König (1936), Ore (1962) and Tutte (1966). For some general references on topology see Kelley (1955), Patterson (1963) and Veblen (1931).

A. Graph terminology

1. Elementary definitions

A linear graph G is a collection of p points (or *vertices*) with l lines (or *edges*) between certain pairs of points. Only the connections between the

points are significant, not the shape of the connecting lines. Two graphs which can be put into 1-1 correspondence so that the points and connections correspond are termed *isomorphic*. For applications with which we are concerned they can be regarded as identical.

A graph is *simple* if

- (a) two points are connected by at most one line,
- (b) there are no loops (see Fig. 1)

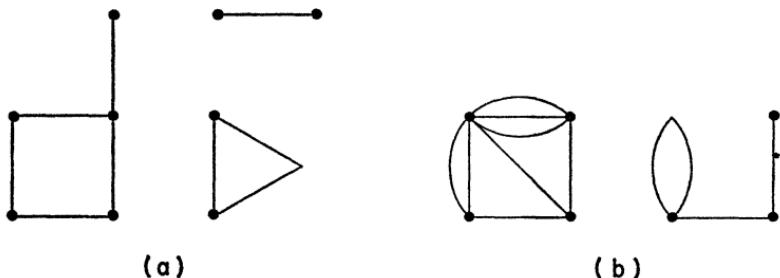


FIG. 1. (a). Simple graphs. (b). Non-simple graphs.

In cluster integral theory and subsequent applications to the Ising model we shall be directly concerned with simple graphs. However, we shall need non-simple graphs as a classifying tool. Diagrammatic expansions of the type used in quantum field theory also contain non-simple graphs.

A graph C is said to be *connected* if there is at least one path between any two points; otherwise it is *disconnected* (Fig. 2).

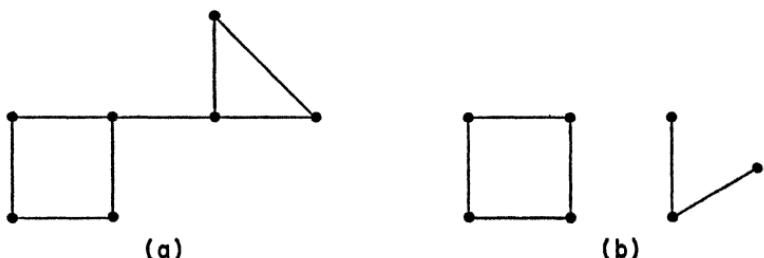


FIG. 2. (a). Connected graphs. (b). Disconnected graphs.

An *articulation* or *cutting point* is a point which if omitted would cause the graph to fall into disconnected parts (Fig. 3). A graph with an articulation point is called an *articulated graph*.

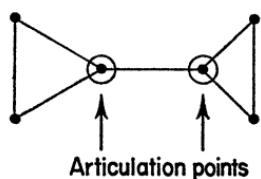


FIG. 3. Articulated graph.

A *star S* (or *multiply connected graph*) is a graph with no articulation point. Between any two points of the graph there are at least two independent paths (i.e. having no intermediate point in common) (Fig. 4.).



FIG. 4. Stars.

By convention it is convenient to classify a single line with two points as a two point star.

A *Cayley tree* is a graph with no closed cycles (Fig. 5).

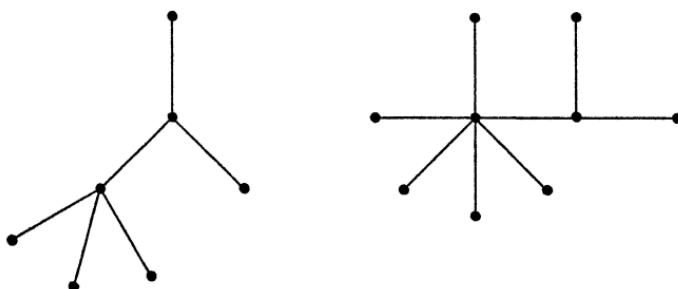


FIG. 5. Cayley trees.

A *Husimi tree* is a graph constructed of simple polygons attached by articulation points. It is *pure* if only one type of polygon enters, otherwise it is *mixed*; when the polygons are all triangles it is a *cactus* (Fig. 6).

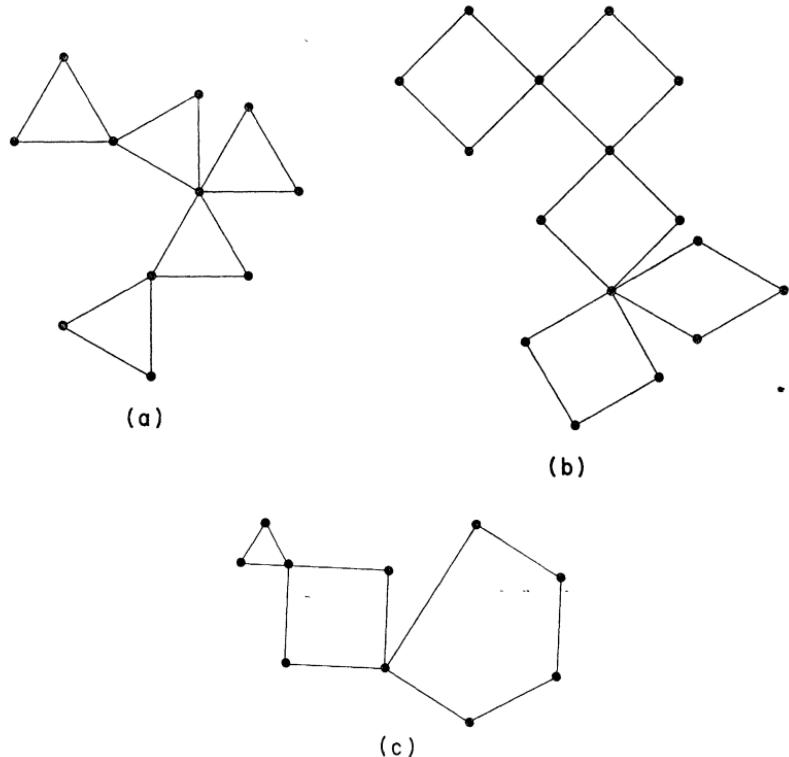


FIG. 6. (a). Cactus. (b). Pure Husimi tree. (c). Mixed Husimi tree.

A *star tree* is a graph constructed of stars attached by articulation point (Fig. 7).

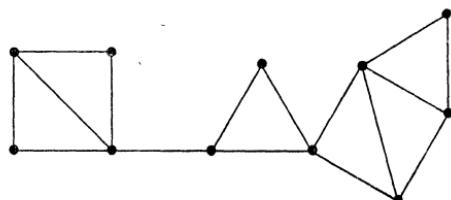


FIG. 7. Star tree

2. Labelled graphs

So far we have not distinguished between the points from which the graph was constructed. The graphs we have discussed have been *free* or *topological*. However, for many applications it is important to regard the points of the graph as distinguishable. For each free graph there will be a number v of labelled graphs. To take an elementary example the graph Fig. 8 has $p = 3$ and $v = 3$.

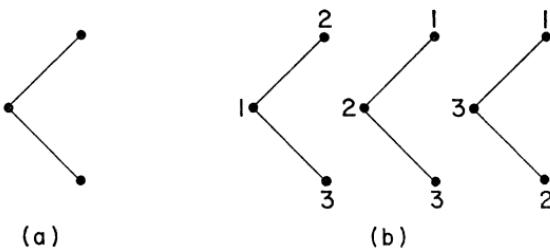


FIG. 8. (a). Free graph. (b). Labelled graph.

It is clear that v is related to the *symmetry* of the graph. There are $p!$ different possible permutations of the labelled points, but because of symmetry, groups of different labellings have identical connections. We can define the group Γ of a labelled graph as the set of permutations which leave the connections invariant. The order of this group, g , is called the *symmetry number* of the graph, and it is easy to see that $v = p!/g$. We illustrate by the example in Fig. 9 for which $g = 4$, $v = 6$ and $\Gamma \equiv (1), (13), (24), (13)(24)$.

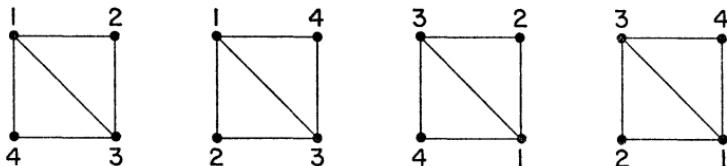


FIG. 9. Graph group and symmetry number.

3. Rooted graphs

We may also wish to single out one or more points of the graph as roots (which we denote by open circles). Let us first consider inserting roots into a free graph. From a single free graph we will obtain a number w_r of rooted free graphs; to take the above simple example we obtain two graphs with a

single root, three with two roots, and two with three roots (Fig. 10). Labelling can be introduced into rooted graphs as before. Rooting usually reduces the symmetry, and for example with a single root introduced above we have in both cases $g = 2$, $v = 12$.

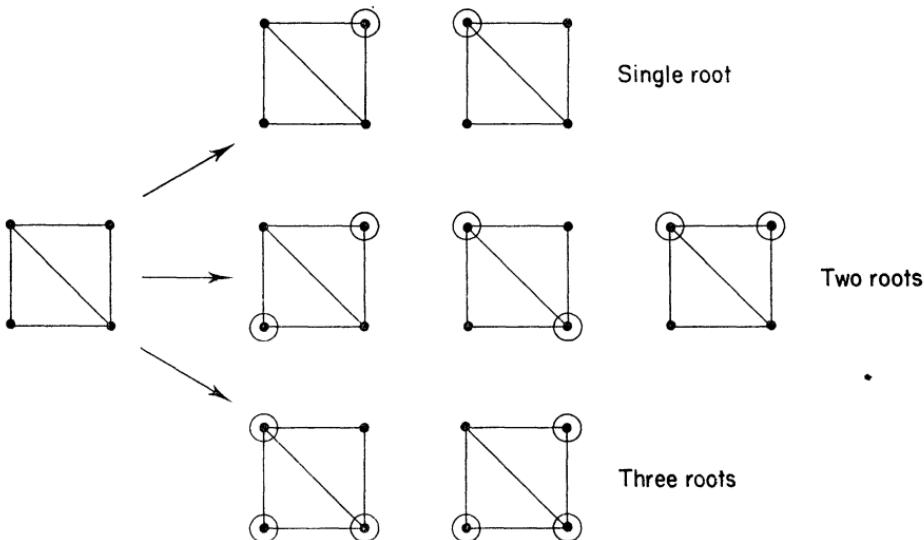


FIG. 10. Rooting of unlabelled graphs.

4. Different species

Another useful generalization is to allow the points of the graph to belong to different species, (conveniently represented by different colours). For example with two species our total p will be divided into p_a and p_b ($p = p_a + p_b$), and there are three types of line $a-a$, $b-b$ $a-b$. For each possible p_a and p_b and a given free graph we will obtain a new set w_p of free or topological graphs by selecting the vertices to belong to species one or two. Taking our previous graph as an example with $p_a = p_b = 2$ we obtain the three graphs shown in Fig. 11.

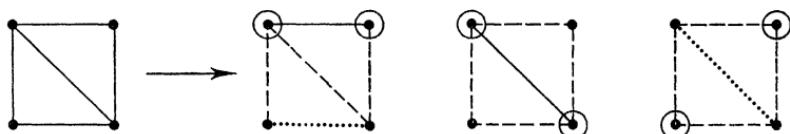


FIG. 11. Different species (coloured vertices).

For each new topological graph we can now introduce appropriate labellings with a new symmetry number obtained by running through all $p_a! p_b!$ possible permutations.

Instead of colouring the points we can colour the lines of the graph, for example we can divide l into l_a and l_b ($l = l_a + l_b$) and we obtain a set w_l of new graphs. Taking $l_a = 2$, $l_b = 3$ in the above example we obtain $w_l = 4$ (Fig. 12). If we run through the $p!$ labelling permutations we find that the symmetry number is reduced again as indicated.

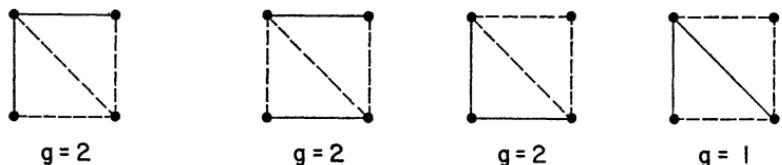


FIG. 12. Coloured edges.

5. Cyclomatic number and homeomorphic graphs

The cyclomatic number c of a connected graph C is defined by

$$c(C) = l - p + 1. \quad (2.1)$$

It represents the number of independent cycles in the graphs and is an important parameter in graph classification. Graphs with no closed cycles (Cayley trees Fig. 5) have $c = 0$, polygons have $c = 1$, and Fig. 13 gives a number of illustrations of more complex graphs and their cyclomatic numbers.

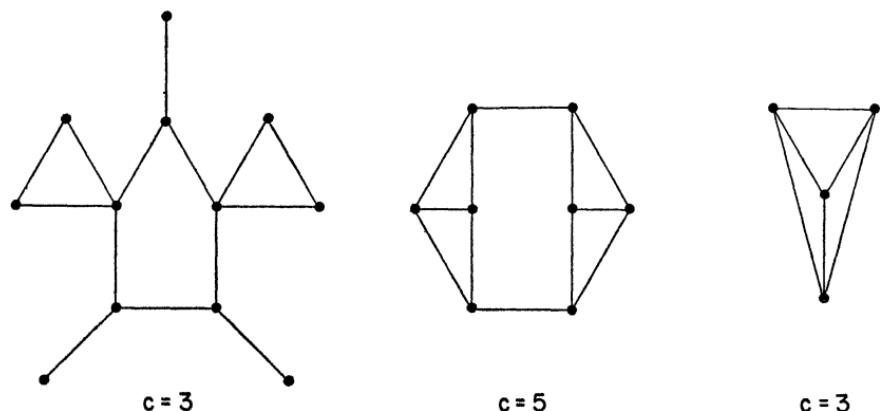


FIG. 13. Cyclomatic numbers of graphs.

The cyclomatic number of a graph C consisting of two disconnected parts C_1 and C_2 joined by an articulation is given by

$$c(C) = c(C_1) + c(C_2). \quad (2.2)$$

When dealing with disconnected graphs G , we use $n(G)$ to denote the number of connected components, and $c(G)$ is defined by

$$c(G) = l - p + n. \quad (2.3)$$

We then have for a disconnected graph G made up of connected components C_1 and C_2 ,

$$c(G) = c(C_1) + c(C_2). \quad (2.4)$$

Disconnected graphs can be classified by means of their connected components. If we have a list of all connected graphs with up to p points in a dictionary order, we can immediately list *all* graphs with up to p points by simple partitioning. In a rather similar manner articulated graphs can be classified by means of their star components, but the symmetry of the com-

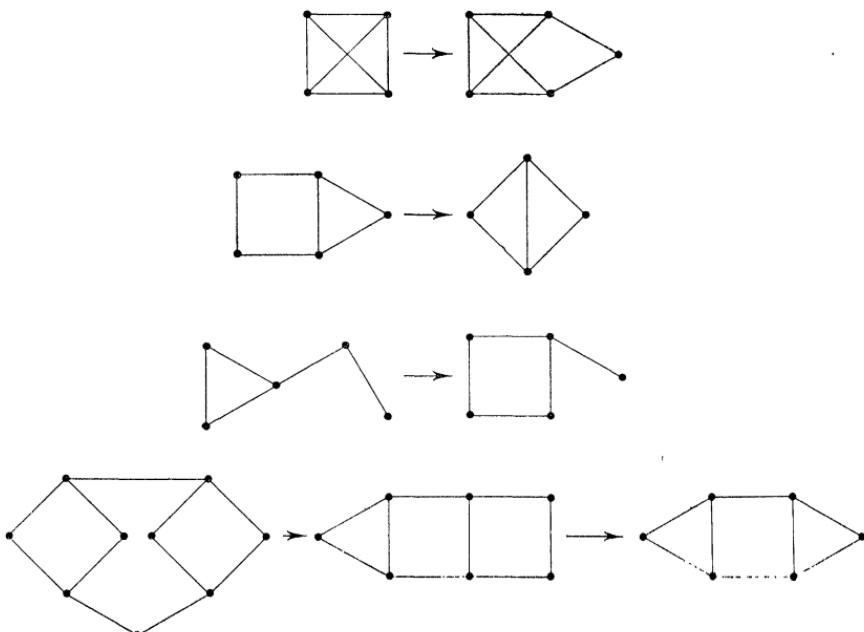


FIG. 14. Homeomorphic graphs.

ponent stars must be taken into account to ensure that no graph is listed more than once. Hence we see that stars form the basic "bricks" out of which complex graphs are constructed, and a good deal of attention has been devoted to their classification.

To discuss this in more detail we first define the *degree* or *valence* (or *coordination number*) of a vertex as the number of edges incident on the vertex. A vertex of degree greater than 2 is called a *node* or *principal point* of the graph; a vertex of degree 2 or 1 is called an *antinode*.

If G is any graph and A a vertex of degree 2, we define the *suppression* of the vertex A to be the deletion of A from the vertex set of G and the identification of the two edges incident on A . The reverse process of replacing an edge BC by two edges AB, AC by the creation of a new vertex A is called the *insertion* of a second order vertex on the edge BC .

If G is any graph and G' a graph derived from G by the insertion or suppression of any number of vertices of degree 2, then G and G' are said to be *homeomorphic* and each is a *homeomorph* of the other. Fig. 14 gives some illustrative examples.

Homeomorphs have the same cyclomatic number, since the insertion of a vertex of degree 2 adds 1 to both l and p . They are graphs with the same basic topology, and constitute a useful sub-grouping of connected or star graphs. When all vertices of degree 2 have been removed we refer to the homeomorphs as *irreducible*. Typical irreducible homeomorphs are *tadpoles*, *dumbbells* and *figure eights* (Fig. 15).

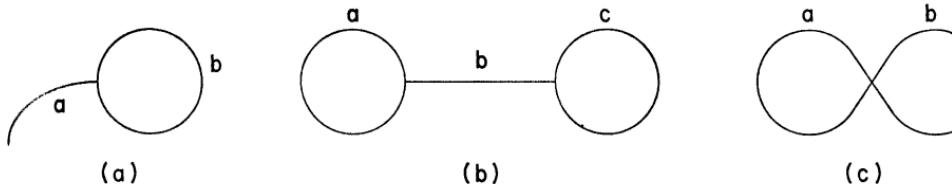
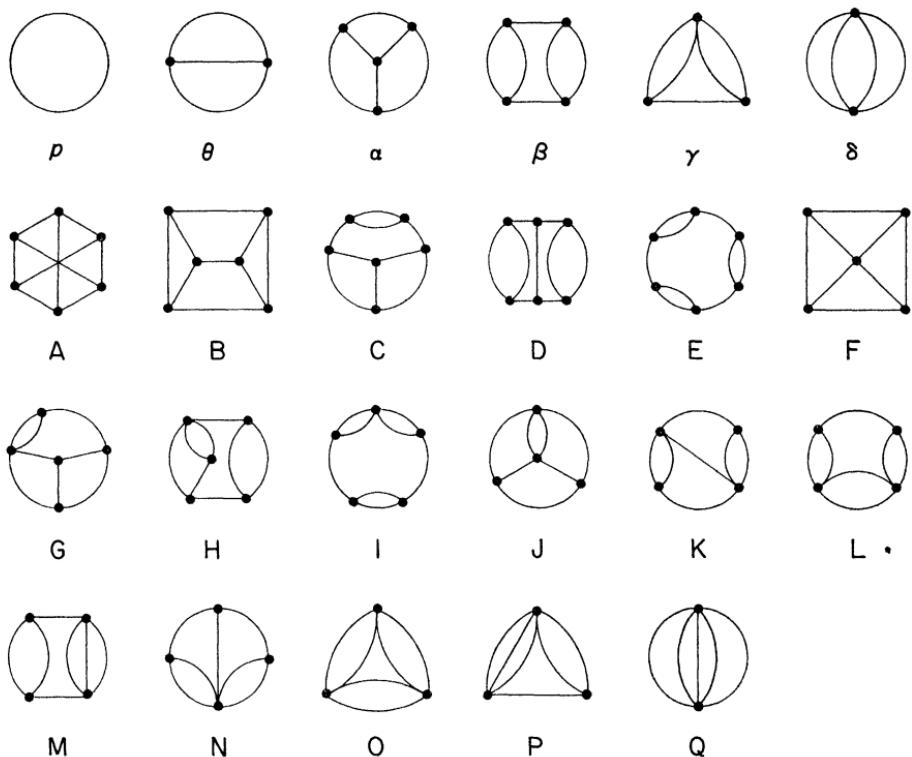


FIG. 15. Some typical homeomorphs. (a). Tadpole *t*. (b). Dumbbell *d*. (c). Figure eight *e*.

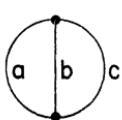
The classification of stars by means of cyclomatic number was first undertaken by Sykes *et al.* (1966) and we shall now discuss their procedure.

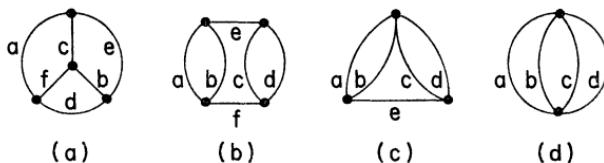
Homeomorphically irreducible stars (HI stars) for $c = 1, 2, 3, 4$ are reproduced in Fig. 16 (the case $c = 4$ was first introduced in Essam and Sykes, 1966). If we now wish to list all simple stars with p vertices and l edges homeomorphic to a given type we must consider in how many different ways

FIG. 16. HI stars with cyclomatic number $c = 1, 2, 3, 4$ (after Sykes *et al.*, 1966).

vertices of degree 2 can be inserted so that the total number of edges is l . When $c = 2$ there is only one HI star, the θ type, and the simple stars correspond to the number of possible non-zero a, b , and c satisfying (Fig. 17)

$$a + b + c = l = p + 1 \quad (a \leq b \leq c; b, c \geq 2). \quad (2.5)$$

FIG. 17. θ -graph.

FIG. 18. (a). α graph. (b). β graph. (c). γ graph. (d). δ graph.

There are 4 HI stars corresponding to $c = 3$ which are designated α , β , γ and δ types. They are labelled according to the scheme in Fig. 18 and give rise to the following simple stars

$$\delta: a + b + c + d = l = p + 2 \quad (a \leq b \leq c \leq d; b, c, d \geq 2) \quad (2.6)$$

$$\gamma: a + b + c + d + e = l \quad (a \leq b, c \leq d, a \leq c; b, d \geq 2) \quad (2.7)$$

$$\beta: a + b + c + d + e + f = l \quad (a \leq b, c \leq d, e \leq f, a \leq c; b, d \geq 2) \quad (2.8)$$

$$\alpha: a + b + c + d + e + f = l \quad (a \leq b, c \leq d, a \leq c, c \leq \min(e, f)) \quad (2.9)$$

The first three are straightforward; the α -type needs a little more discussion. For a given tetrahedron, the pairs (a, b) (c, d) and (e, f) are written in dictionary order; the lines (a, b) and (c, d) can then be uniquely characterised but there is still freedom to choose (e, f) or (f, e) to characterise the tetrahedron completely. We shall give some numerical illustrations of this procedure when we discuss the enumeration of stars in Section II.B and the lattice constants for these graphs in Section IV.

There are 17 HI stars corresponding to $c = 4$, 118 corresponding to $c = 5$ (Heap, 1966), and 1198 corresponding to $c = 6$ (Heap, 1969). We shall discuss their enumeration in Section II.B4.

Sykes *et al.* (1966) introduced the following notation for these stars which can be generalized to higher orders:

$$\begin{aligned}
 c = 1 & \quad (l)_p \\
 c = 2 & \quad (a, b, c)_\theta \\
 c = 3 & \quad (a, b; c, d; e, f)_\alpha \\
 & \quad (a, b; c, d; e, f)_\beta \\
 & \quad (a, b; c, d; e, f)_\gamma \\
 & \quad (a, b; c, d; e, f)_\delta.
 \end{aligned} \quad (2.10)$$

In actual fact the notation was introduced for the *weak lattice constant* of the star (see Section IV.A2). However where there is no risk of confusion we shall also use it to denote the star itself.

6. Adjacency matrix

Even when two graphs or HI stars are drawn in full it is a sophisticated problem to determine whether they are isomorphic or not. This is illustrated in Fig. 19 where two isomorphic simple stars are presented but one immedi-

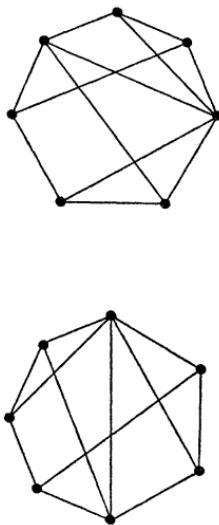


FIG. 19. Example of isomorphic graphs.

ately notes that their general appearance is quite different.[†] A useful characterization of a simple *labelled* graph is provided by its *incidence matrix* **A** which has

$$\begin{aligned} a_{ij} &= 1 \text{ if } i \text{ and } j \text{ are connected} \\ a_{ij} &= 0 \text{ otherwise.} \end{aligned} \tag{2.11}$$

For non-simple graphs (and for HI stars) the corresponding *adjacency* matrix **B** has

$$\begin{aligned} b_{ij} &= v_{ij} \text{ if } i \text{ and } j \text{ are connected} \\ b_{ij} &= 0 \text{ otherwise} \end{aligned} \tag{2.12}$$

where v_{ij} is the number of lines joining i and j .

It is clear that as the labelling is changed the matrix is transformed. For a graph with p points there are $p!$ possible labellings and matrices and the problem of determining whether two graphs are isomorphic reduces to that

[†] I am grateful to Dr. F. M. Sykes for providing this example.

of determining whether their incidence matrices can be transformed into one another by re-labelling. A necessary condition is that these matrices should have the same eigenvalues, and this can readily be checked numerically by forming the traces of successive powers. However, the condition is not sufficient (Baker, 1966; Fisher, 1966) and Fig. 20 shows the smallest pair of graphs ($p = 6$) whose incidence matrices have the same eigenvalues (isospectral).

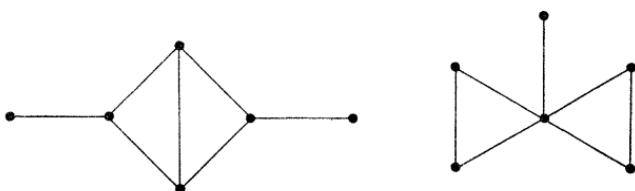


FIG. 20. The smallest pair of isospectral graphs.

A useful procedure for ordering and identifying graphs and HI stars was suggested by Nagle (1966) by selecting a particular labelling as *canonical* for a given graph. We shall illustrate Nagle's approach for HI stars.

A k -tuple, Q , is an ordered set of k integers (Q_1, Q_2, \dots, Q_k) . The k -tuple Q is regarded as greater than the k -tuple Q' if there exists an r ($1 \leq r \leq k$) such that $Q_i = Q'_i$ for $1 < i < r$ and $Q_r > Q'_r$. For example, $(5, 4, 4, 3)$ precedes $(4, 5, 4, 3)$ and $(4, 4, 4, 4)$, and $(6, 5, 3)$ precedes $(3, 5, 6)$ and $(6, 4, 4)$ so that this ordering corresponds to standard numerical ordering.

Now consider the degrees of the vertices of the graph and from them form the *degree-tuple* of the graph $d = (d_1, d_2, \dots, d_p)$ where d_i is the degree of the vertex. Relabel the vertices so that this degree-tuple is a maximum with $d_1 \geq d_2 \dots \geq d_p$.

In general, this labelling will not be unique. The multiple edges of the graph can now be taken into account by considering each vertex of degree d_i in detail. Suppose it is made up of d_{i1} single edges, d_{i2} double edges, d_{i3} triple edges, etc. Then each d_i can be expressed as a k -tuple *degree specification* $(d_{i1}, \dots, d_{i2}, d_{i1})$ where $k = d_1$, and

$$d_i = \sum_{r=1}^{d_i} r d_{ir}. \quad (2.13)$$

The graph can now be relabelled so that if there are two vertices of the same degree the one having the larger degree specification is assigned the lower label.

The labelling may still not be unique. In order to complete the specification we now turn to the adjacency matrices of all labellings which are not differentiated. Each matrix can be regarded as a p^2 -tuple.

$$B = (b_{11}, b_{12}, \dots, b_{1p}, b_{21}, \dots, b_{2p}, \dots, b_{p1}, \dots, b_{pp})$$

and the final labelling is taken as the one which makes this a maximum. This is called canonical labelling and the corresponding adjacency matrix is called the *canonical matrix*.

The comprehensive enumeration by Heap (1969) of all HI stars with $c \leq 6$ tabulates the stars by means of their adjacency matrices ordered in accordance with the above procedure.

B. Enumeration

In developing perturbation expansions, it is important to devise a systematic method of enumerating all the terms which enter at a particular stage. Since these terms can conveniently be described by linear graphs, we are led to the problem of enumerating linear graphs of various types which can be constructed with p points and l lines. The first stage in the enumeration is the calculation of the total number of graphs. This is a problem in combinatorial analysis, and its solution draws heavily on the most powerful tool of combinatorial analysis, the generating (or counting) function. For a general introduction to the subject of combinatorial analysis we strongly recommend Riordan (1958) and the classic treatise by Macmahon (1915, 1916).

The earliest results on graphical enumeration were derived by Cayley (1889–1897), who was concerned with the tree configurations which were subsequently named after him. A powerful general technique which could be applied to a large variety of enumerative problems was introduced by Polya in 1937, and much of the subsequent development has consisted in applying Polya's theorem to different situations. However Stein and Stein (1963) have pointed out that Polya was anticipated by Redfield (1927) who gave a precise prescription for dealing with a class of enumeration problems of which that of linear graphs is a special case, and they based their own extensive enumerations on his work (see also Harary, 1960).

The proof of Polya's theorem can be found in the literature in a number of places [e.g. Riordan (1958), p. 131; Uhlenbeck and Ford (1962), Chapter 4; Harary (1969), p. 180] and we do not therefore feel the need to reproduce it at length here. Instead, we shall endeavour to show how the theorem has been applied to problems arising in statistical mechanics.

1. Labelled graphs

Let $N(p, l)$ be the total number of linear graphs among p labelled points with l lines, let $C(p, l)$ be the number of connected graphs and $S(p, l)$ the number of

stars. By means of two theorems Riddell and Uhlenbeck (1953) showed how $C(p, l)$ and $S(p, l)$ could be derived from $N(p, l)$; the latter can immediately be written down as the number of ways of selecting l lines out of $p(p - 1)/2$ lines, i.e.

$$\binom{p(p-1)/2}{l} \quad (2.14)$$

Our treatment will follow that of Uhlenbeck (1960), since this enables the Mayer theory to be derived at the same time.

(a) *Theorem I. Decomposition of general graphs into connected graphs*

With each graph G_n , define a weight $w(G_N)$ having the following properties:

- (i) $w(G_n)$ is independent of the labelling of the points
- (ii) For a disconnected graph G_n consisting of connected parts (C_p) , $w(G_n) = \pi$ (all C_p) $w(C_p)$.

Let $F_n = \sum_{(G_n)} w(G_n)$ over all graphs of n points

$f_p = \sum_{(C_p)} w(C_p)$ over all connected graphs of p points.

Define

$$F(x) = \sum_{n=1}^{\infty} F_n x^n / n! \quad (2.15)$$

as the generating function for all graphs, and

$$f(x) = \sum_{p=1}^{\infty} f_p x^p / p! \quad (2.16)$$

as the generating function for connected graphs. Then

$$1 + F(x) = \exp f(x). \quad (2.17)$$

The theorem hinges of the *product property* of the generating functions of two independent collections of labelled graphs. Consider two independent collections of graphs among labelled points A, B with generating functions $I^{(A)}(x)$ and $F^{(B)}(x)$. Join the collection together, i.e. allow graphs to be made up of a part from each collection. Then any graph with n_1 points from the first collection and n_2 points from the second collection will carry a factor $(n_1 + n_2)! / n_1! n_2!$ because of the re-labelling of the $(n_1 + n_2)$ points. Hence, since the generating function is defined with the x^n divided by $n!$ we see that

$$F^{(A+B)}(x) = F^{(A)}(x) F^{(B)}(x). \quad (2.18)$$

The definition of the generating function (2.15), (2.16) with the factorial in the denominator is thus essential whenever we are dealing with labelled points (Riordan, 1958).

We now decompose the general graph into mutually exclusive sets consisting of one connected part, two separate connected parts, ... m separate parts with generating functions $F_1(x)$, $F_2(x)$... $F_m(x)$... so that

$$F(x) = \sum_{m=1}^{\infty} F_m(x). \quad (2.19)$$

Using the product property (2.18) we find that

$$F_m(x) = [f(x)]^m / m! \quad (2.20)$$

where $m!$ is required because the m parts are chosen from the same collection of connected graphs, and any permutation of the m parts leads to the same disjoint graph. From (2.19) and (2.20) we immediately derive (2.12).

The theorem applies to any weight $w(G_n)$ satisfying conditions (i) and (ii) above. For counting purposes we take

$$w(G_N) = y^l \quad (2.21)$$

where l is the number of lines in the graph. (The perturbation expansion of a condensing gas requires a different $w(G_N)$ which will be discussed in Section III.A.) We then find that

$$\begin{aligned} 1 + F_y(x) &= 1 + x + \frac{x^2}{2!}(1+y) + \frac{x^3}{3!}(1+y)^3 + \frac{x^4}{4!}(1+y)^6 \\ &\quad + \dots \frac{x^p}{p!}(1+y)^{\frac{1}{2}p(p-1)} + \dots \end{aligned} \quad (2.22)$$

Taking the logarithm and expanding we obtain

$$\begin{aligned} f_y(x) &= x + \frac{x^2}{1!}y + \frac{x^3}{3!}(3y^2 + y^3) + \frac{x^4}{4!}(16y^3 + 15y^4 + 6y^5 + y^6) + \frac{x^5}{5!}(125y^4 + 222y^5 + 205y^6 + 120y^7 + 45y^8 + 10y^9 + y^{10}) + \dots \end{aligned} \quad (2.23)$$

from which the values of $C(p, l)$ can be obtained. Tables of $C(p, l)$ for p up to 7 are given in Uhlenbeck and Ford (1962).

We can write down an exact formula as follows:

$$C(p, l) = \sum_{r=1}^p \frac{(-1)^{r-1}}{r} \sum'_{(p_i)} \frac{p!}{p_1! p_2! \dots p_r!} \sum_{l=1}^r \binom{\frac{1}{2} p_i (p_i - 1)}{l}, \quad (2.24)$$

where in \sum' all the p_i are ≥ 1 , and $p_1 + p_2 + \dots + p_r = p$. The largest term corresponds to $r = 1$, and it is easy to write down the first two terms,

$$C(p, l) = \binom{\frac{1}{2}p(p-1)}{l} - p \binom{\frac{1}{2}(p-1)(p-2)}{l} + \dots . \quad (2.25)$$

If p is large this can be written

$$C(p, l) = \binom{\frac{1}{2}p(p-1)}{l} \left\{ 1 - p \left[1 - \frac{2l}{p(p-1)} \right] \right\}^p. \quad (2.26)$$

Hence if $l > p \ln p$ the correction term is negligible. It can be shown rigorously that the sum of all other correction terms is negligible, and $C(p, l)$ is asymptotically equal to $N(p, l)$ (Riddell and Uhlenbeck 1953).

(b). *Theorem II. Decomposition of connected graphs into stars*

Every connected graph is made up of constituent stars (Fig. 21), and the second theorem enables us to count the total number of connected graphs in terms of the star constituents.

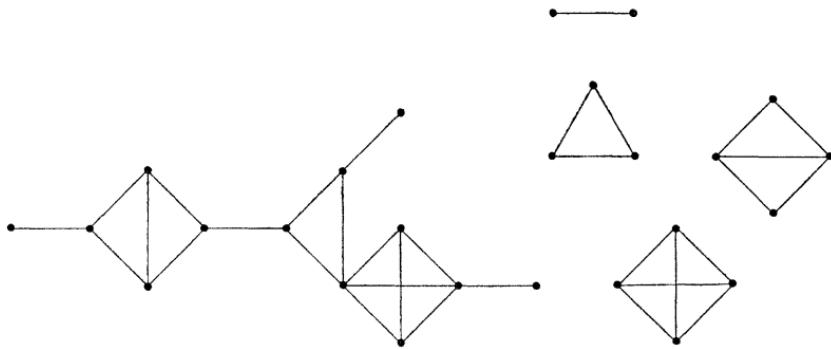


FIG. 21. General connected graph composed of stars.

With each connected graph C_p define a weight $w(C_p)$ having the following properties:—

- (i) $w(C_p)$ is independent of labelling
- (ii) For a connected graph C_p made up of stars S_m ,

$$w(C_p) = \prod_{(\text{all } S_m)} w(S_m).$$

Let $s_q = \sum_{(S_m)} w(S_m)$ over all stars of m points.

Define

$$S(x) = \sum_{q=2}^{\infty} \frac{S_q x^q}{q!} \quad (2.27)$$

as the generating function for stars. Let

$$R(x) = x \frac{\partial f}{\partial x} = \sum_{p=1}^{\infty} p f_p x^p / p! \quad (2.28)$$

Then

$$\frac{R(x)}{x} = \exp S' [R(x)]. \quad (2.29)$$

This theorem again hinges on a product property, analogous to (2.18), but in order to build up connected graphs from their constituents, we need to deal first with *rooted graphs* in which a particular point is singled out as the root. Connection between different constituent graphs will be made at their roots. The function $R(x)$ in (2.28) is the generating function for rooted connected graphs. If we now have two collections of rooted graphs with generating functions $R^{(A)}(x)$ and $R^{(B)}(x)$, and we join the collections together by merging the roots (Fig. 22) then

$$R^{(A+B)}(x) = \frac{R^{(A)}(x) R^{(B)}(x)}{x}. \quad (2.30)$$

When we merge the roots we lose one point and we divide the number of labellings by the total number of points, and this is taken into account correctly in (2.30).

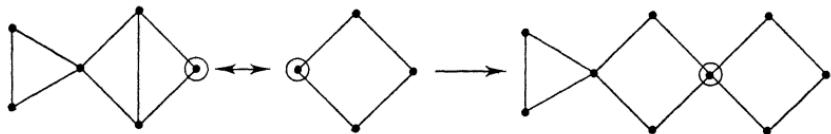


FIG. 22. Merging two collections of rooted graphs.

We shall illustrate the method of decomposition by considering first the simpler problem of enumerating rooted *Cayley trees*. We can decompose these into mutually exclusive sets with one line at the root, two lines at the root, ... m lines at the root; we call these *main leaves* meeting at the root. Let $T_1(x)$ be the generating function for a rooted single main leaf. Then it is not difficult to see that the generating function for trees with m main leaves meeting at the root is

$$T_m(x) = \frac{x}{m!} \left[\frac{T_1(x)}{x} \right]^m. \quad (2.31)$$

The powers of x enter since m separate roots are merged into one. Hence the generating function $T(x)$ for rooted Cayley trees is given by

$$T(x) = x \exp T_1(x)/x. \quad (2.32)$$

If we now investigate the structure of $T_1(x)$ we find that if we separate off the line leading to the root we are left with a general rooted Cayley tree. Hence we can use the product property to derive the relation

$$T_1(x) = xwT(x) \quad (w = \text{weight at a line}). \quad (2.33)$$

From (2.31) and (2.32) we have the functional relation

$$T(x) = x \exp wT(x). \quad (2.34)$$

Using Lagrange's Theorem for the reversion of series (Edwards, 1896) we find that the coefficient of $x^p/p!$ is the expansion of T is

$$\frac{d^{p-1}}{du^{p-1}} [\exp pwu]_0 = (pw)^{p-1}. \quad (2.35)$$

Thus the number of rooted Cayley trees is p^{p-1} , and the number of Cayley trees by (2.28) is p^{p-2} .

We now proceed to enumerate *mixed Husimi trees* (Husimi, 1950) in the same way. Equations (2.31) and (2.32) remain valid, but in investigating the structure of $T_1(x)$ the configuration leading to the root can either be a line, or a triangle, or a quadrilateral, ... or an m -gon. Instead of (2.33) we therefore have

$$T_1(x) = x \left[w_2 T + \frac{w_3 T^2}{2} + \frac{w_4 T^3}{2} + \dots + \frac{w_m T^{m-1}}{2} + \dots \right] \quad (T = T(x)). \quad (2.36)$$

Here we have differentiated the weights corresponding to the different polygons for the time being so that we can take account of their individual numbers; the factor $\frac{1}{2}$ arises from the symmetry of a rooted polygon about an axis through the root. If we write

$$S(x) = \frac{x^2 w_2}{2} + \frac{x^3 w_3}{6} + \frac{x^4 w_4}{8} + \dots \quad (2.37)$$

then (2.36) is equal to $xS'(T)$, and from (2.34)

$$\frac{T(x)}{x} = \exp S'(T), \quad (2.38)$$

which is exactly of the form (2.29).

We can apply Lagrange's theorem to (2.38) to obtain the coefficient of $x^p/p!$ as

$$\frac{d^{p-1}}{du^{p-1}} \left[\exp p w_2 u \exp \frac{p}{2} w_3 u^2 \exp \frac{p}{2} w_4 u^3 + \dots \right]_0. \quad (2.39)$$

The number of *rooted* trees with n_2 single lines, n_3 triangles, n_4 quadrilaterals, ... is the coefficient of $w_2^{n_2} w_3^{n_3} \dots$ in (2.39) and is easily written down as

$$\frac{(p-1)!}{n_2! 2^{n_3} n_3! 2^{n_4} n_4! \dots} p^{n_2+n_3+n_4+\dots} \quad (2.40)$$

$$(p-1 = n_2 + 2n_3 + 3n_4 + \dots).$$

To obtain the number of trees we divide by p as before.

We are now in a position to deal with the general enumeration of *rooted connected graphs* which are in fact *rooted star trees*. We replace $T(x)$ by $R(x)$ and derive in the same way as (2.32) the relation

$$R(x) = x \exp R_1(x)/x. \quad (2.41)$$

When we investigate the structure of $R_1(x)$ the configuration leading to the root can be a general star; if its symmetry number is g then we must divide by g to obtain the number of different configurations arising from labelled trees hung on its vertices. When we root the star and differentiate the root point from all the others we multiply this by q the number of vertices (q/g is the analogue of the $\frac{1}{2}$ which arose for simple polygons). Hence all trees corresponding to this star at the root will satisfy

$$R_1(x) = \frac{x q w_s}{g} R^{q-1} \quad (2.42)$$

where $w_s = w(S_q)$ = weight of the star S_q . But, in fact, the total number of *labelled* stars corresponding to a given free star is $q!/g$ so that

$$\frac{S_q}{q!} = \sum_{\substack{\text{all different} \\ \text{q point free stars}}} \frac{w(S_q)}{g}. \quad (2.43)$$

Thus, if we take into account all possible stars at the root we obtain

$$\frac{R_1(x)}{x} = \sum_{q=2}^{\infty} \frac{q S_q}{q!} R^{q-1} = S'(R). \quad (2.44)$$

From (2.41) and (2.44) we derive (2.29). If we wish we can enumerate star trees in the same manner as Husimi trees, and we will obtain a formula similar to (2.40) with the symmetry numbers g/q replacing the 2's in the denominator.

For the purpose of determining $S(p, l)$ we use the same weight as in (2.21), $w(C_p) = y^l$ (the appropriate weight for the perturbation expansion will be discussed in Chapter 3). From (2.23) and (2.28) we derive the first terms of $R_y(x)$

$$\begin{aligned} \frac{R_y(x)}{x} &= 1 + \frac{xy}{1!} + \frac{x^2}{2!} (3y^2 + y^3) + \frac{x^3}{3!} (16y^3 + 15y^4 + 6y^5 + y^6) \\ &+ \frac{x^4}{4!} (125y^4 + 222y^5 + 205y^6 + 120y^7 + 45y^8 + 10y^9 + y^{10}) + \dots \end{aligned} \quad (2.45)$$

The logarithm of (2.45) must be equated to $S_y'(R)$ or

$$s_2 R_y + s_3 R_y^2 / 2! + s_4 R_y^3 / 3! + s_5 R_y^4 / 4! \dots \quad (2.46)$$

Using the formulae in Riordan (1958, p. 37 and p. 49 Table 3), we find that

$$\begin{aligned} S_y(x) &= \frac{x^2 y}{2!} + \frac{x^3 y^3}{3!} + \frac{x^4}{4!} (16y^3 + 15y^4 + 6y^5 + y^6) \\ &+ \frac{x^5}{5!} (125y^4 + 222y^5 + 205y^6 + 120y^7 + 45y^8 \\ &+ 10y^9 + y^{10}) + \dots . \end{aligned} \quad (2.47)$$

By combinatorial arguments similar to (2.24) Riddell (1951) showed that

$$S(p, l) = \binom{\frac{1}{2}p(p-1)}{l} - p \binom{\frac{1}{2}(p-1)(p-2)}{l} - p(p-1) \binom{\frac{1}{2}(p-1)(p-2)}{l-1} \quad (2.48)$$

For large p and $l > p \ln p$ the first term in (2.48) dominates and hence $N(p, l)$, $C(p, l)$ and $S(p, l)$ are asymptotically equal.

2. Unlabelled graphs

We shall be guided by the notation of Uhlenbeck and Ford (1962), denoting the total number of linear graphs among p unlabelled points with l lines by $\pi(p, l)$, the number of connected graphs by $\gamma(p, l)$, and the number of stars by $\sigma(p, l)$. We denote the corresponding generating functions, *defined without the factorials* by $\pi(x, y)$, $\gamma(x, y)$ and $\sigma(x, y)$. Thus,

$$\begin{aligned} \pi(x, y) &= \sum_{p=1}^{\infty} \pi_p(y) x^p \\ \pi_p(y) &= \sum \pi(p, l) y^l. \end{aligned} \quad (2.49)$$

(a) Rooted Cayley trees

The enumeration of free graphs is much more complicated as will be seen if we try the simplest problem of rooted unlabelled Cayley trees. Denote the generating function by $\tau(x)$. We can again decompose the trees into mutually exclusive sets with m main leaves having generating function $\tau_m(x)$, so that as before

$$\tau(x) = 1 + \sum_{m=1}^{\infty} \tau_m(x). \quad (2.50)$$

However, when we try to decompose $\tau_m(x)$ we find that the symmetry of the configurations plays a much more significant role. When we consider $\tau_1(x)$ we still have the relation analogous to (2.33),

$$\tau_1(x) = x \tau(x). \quad (2.51)$$

But when we proceed to $\tau_2(x)$, the coefficient of $\tau_2^{(n)}$ of x^n differs when n is odd from when n is even because of the possibility of equivalent configurations

$$\tau_2^{(n)} = \tau_1 \tau_{2q-2} + \tau_2 \tau_{2q-3} + \dots \tau_q \tau_{q-1} \quad (n = 2q) \quad (2.52a)$$

$$\tau_2^{(n)} = \tau_1 \tau_{2q-1} + \tau_2 \tau_{2q-2} + \dots \tau_{q-1} \tau_{q-1} + \frac{\tau_q(\tau_q + 1)}{2} \quad (n = 2q + 1). \quad (2.52b)$$

The last term in (2.52b) arises from the equivalent configurations, and is the number of ways of selecting two configurations identical or non-identical from τ_q . Hence instead of (2.31) we now have

$$\frac{\tau_2(x)}{x} = \frac{1}{2} [\tau(x)]^2 + \frac{1}{2} [\tau(x^2)]. \quad (2.52)$$

We can now proceed to $\tau_3(x)$ and obtain the appropriate relation analogous to (2.52)

$$\frac{\tau_3(x)}{x} = \frac{1}{3!} [\tau(x)]^3 + \frac{1}{2} \tau(x^2) \tau(x) + \frac{1}{3} \tau(x^3). \quad (2.53)$$

If we can manage to cope with the combinatorial analysis for general r , we will be led to the Polya relation

$$\tau(x) = x \exp \left[\tau(x) + \frac{\tau(x^2)}{2} + \frac{\tau(x^3)}{3} + \dots \frac{\tau(x^r)}{r} + \dots \right]. \quad (2.54)$$

A simpler and more direct method of obtaining this result (Riordan, 1958 p. 127) is to generalize (2.52a, b) to m lines at the root in a partition $(1^{k_1} 2^{k_2} \dots (n-1)^{k_{n-1}})$ where

$$\left. \begin{aligned} k_1 + k_2 + \dots + k_{n-1} &= m \\ k_1 + 2k_2 + \dots + (n-1)k_{n-1} &= n \end{aligned} \right\}. \quad (2.55)$$

This gives

$$\tau_m(n) = \sum \binom{\tau_1 + k_1 - 1}{k_1} \binom{\tau_2 + k_2 - 1}{k_2} \dots \binom{\tau_{n-1} + k_{n-1} - 1}{k_{n-1}} \quad (2.56)$$

and leads to the Cayley relation

$$\tau(x) = x(1-x)^{-\tau_1}(1-x^2)^{-\tau_2}(1-x^3)^{-\tau_3}\dots(1-x^r)^{-\tau_r}\dots. \quad (2.57)$$

From (2.57) it is easy to derive (2.54).

(b) Polya's theorem

This elementary discussion serves as a natural introduction to Polya's Theorem which provides the appropriate form of "product property" (like (2.52) or (2.53)) for a problem of general symmetry. To describe the theorem we require:

(i). A *generating function* $f(x)$ which counts the *figures* with which we build our configurations. For example the figures could be labelled connected graphs, or free connected graphs, or rooted labelled Cayley trees, or rooted free Cayley trees (with one main leaf). The corresponding generating functions would be $f_y(x)$, $\gamma(x, y)$, $T_1(x)/x$, $\tau_1(x)/x$ used above; the *content* of any figure would be the number of points and lines (p, l), and the generating function counts the number of figures with a given content. As a second example we could consider the colouring of the vertices or edges of a given graph. A figure would correspond to a colour and the generating function would then enumerate the possible colours available; for example for three colours we would require a three variable generating function

$$f(x, y, z) = x + y + z, \quad (2.58)$$

each variable corresponding to one possible colour.

(ii). A *store* from which we can draw an arbitrary number of copies of any figure.

(iii). A set of q *points* and a group \mathbf{G} of permutations of these points.

We obtain a *configuration* by hanging figures from the store on the q points. Two configurations are said to be *equivalent* if there is a permutation of \mathbf{G} taking one into the other. Polya's theorem provides a prescription for deriving the *configuration generating function* which counts *inequivalent* configurations from the known figure generating function, and hence of enumerating *configurations* with a given content.

To formulate this prescription we need to define the *cycle index* of a permutation group. Every element of such a group can be broken down into its constituent cycles. Let g_{j_1, j_2, \dots, j_q} be the number of elements of \mathbf{G} with j_1 cycles of length 1, j_2 of length 2, ... j_q of length q . Then the cycle index of \mathbf{G} is defined as

$$Z(\mathbf{G}) = \frac{1}{g} \sum_{j_1, \dots, j_q} g_{j_1, j_2, \dots, j_q} t_1^{j_1} t_2^{j_2} \dots t_q^{j_q} \quad (2.59)$$

where

$$j_1 + 2j_2 + \dots + qj_q = q. \quad (2.60)$$

We give some typical examples (Riordan 1958).

Identity Group

$$Z(\mathbf{E}_q) = t_1^q. \quad (2.61)$$

Symmetric Group

$$Z(\mathbf{S}_q) = \frac{1}{q!} \sum_{j_1, \dots, j_q} \frac{q!}{1^{j_1} j_1! 2^{j_2} j_2! \dots q^{j_q} q!} t_1^{j_1} t_2^{j_2} \dots t_q^{j_q}. \quad (2.62)$$

This has the useful enumerative property that

$$H[u, Z(\mathbf{S}_q)] = 1 + \sum_1^\infty u^q Z(\mathbf{S}_q) = \exp(ut_1 + u^2 t_2/2 + \dots + u^r t_r/r \dots). \quad (2.63)$$

Cyclic Group

$$Z(\mathbf{C}_q) = \sum_k \phi(k) t_k^{q/k} \quad (2.64)$$

where the sum is taken over all divisors k of q , and $\phi(k)$ is the number of numbers less than k and prime to k .

Dihedral Group

$$2qZ(\mathbf{D}_q) = \sum_k \phi(k) t_k^{q/k} + qt_1 t_2^{(q-1)/2} \quad (q \text{ odd}) \quad (2.65)$$

$$2qZ(\mathbf{D}_q) = \sum_k \phi(k) t_k^{q/k} + \frac{q}{2} t_2^{((q/2)-1)} (t_1^2 + t_2) \quad (q \text{ even}). \quad (2.66)$$

Define $Z[\mathbf{G}; f(x, y)]$ as equal to the right-hand side of (2.59) with t_k replaced by $f(x^k, y^k)$. Then Polya's theorem states that

$$F(x, y) = Z[\mathbf{G}; f(x, y)] \quad (2.67)$$

where $F(x, y)$ is the configuration generating function.

(c). *Applications of Polya's theorem*

(i). *Labelled graphs*

All of the enumerations of Section II.B.1 are related to the identity group E_q , and formulae like (2.31) result from (2.67) and (2.61).

(ii). *Rooted Cayley trees (unlabelled)*

With free graphs we are concerned with the symmetric group S_q and formulae like (2.52) and (2.53) follow from (2.67) using (2.62) for S_2 and S_3 , respectively. The main result (2.54) can readily be deduced using (2.63).

(iii). *Colouring the vertices of a graph*

Consider colouring the vertices of free graphs shown in Fig. 9 with two colours. The cycle index of Γ is

$$Z(\Gamma) = \frac{1}{4}(t_1^4 + 2t_1^2t_2 + t_2^2). \quad (2.68)$$

Hence the generating function for the coloured vertex graphs is

$$Z(\Gamma; x + y) = \frac{1}{4}[(x + y)^4 + 2(x + y)^2(x^2 + y^2) + (x^2 + y^2)^2]. \quad (2.69)$$

Putting $x = y = 1$, we find that the total number of different coloured vertex graphs is 9. Taking the coefficient of x^2y^2 we find that the number of graphs with 2 vertices each colour is 3; this is exactly what we found by direct counting in Fig. 11.

We may note that Uhlenbeck and Ford (1962) list the groups of all linear graphs up to $p = 7$, and this is of great practical help in colouring problems.

(iv). *Colouring the edges of a graph*

When we wish to deal with edge colouring we must use the edge permutation group corresponding to the interchange of edges which is induced by the change of vertices. For example, with the graph in Fig. 9, if we denote the edges (12) (23) (34) (41) (13) by 1, 2, 3, 4, 5, respectively, it is easy to derive this group Γ'

$$\Gamma' \equiv (1)(2)(3)(4)(5); (12)(34)(5), (14)(23)(5), (13)(24)(5). \quad (2.70)$$

Its cycle index is given by

$$Z(\Gamma') = \frac{1}{4} (t_1^5 + 3t_1 t_2^2), \quad (2.71)$$

and hence the generating function for colouring edges with two colours is

$$Z(\Gamma'; x + y) = (x + y)^5 + 3(x + y)(x^2 + y^2)^2. \quad (2.72)$$

Hence putting $x = y = 1$, we find that the total number of coloured edge graphs is 14. Taking the coefficient of $x^2 y^3$ the number of graphs with 2 black and 3 white edges is 4; this again agrees with the result of direct counting (Fig. 12).

(v). Total number of unlabelled graphs

To determine $\pi_p(y)$ we take as our figure a line joining two points. The figure generating function is then $1 + y$, since there can only be 0 or 1 lines joining a pair of points. We hang the figures on the $\frac{1}{2}p(p - 1)$ pairs of points, and the group G is the edge permutation group of these $\frac{1}{2}p(p - 1)$ pairs induced by the symmetric group S_p (called the *point pair* group). The cycle index of this group, denoted by $Z_2(S_p)$ was first calculated by Polya (unpublished result) and a derivation is given in Uhlenbeck and Ford (1962, p. 179).

The result is

$$\begin{aligned} Z_2(S_p) = \frac{1}{p!} \sum_{(j_k)} \frac{p!}{\prod_{k=1}^p k^{j_k} j_k!} & \prod_{k \text{ odd}} t_k^{\frac{1}{2}(k-1)j_k} \prod_{k \text{ even}} t_k^{\frac{1}{2}(k-2)j_k} t_{\frac{1}{2}k}^{j_k} \\ & \times \prod_k t^{\frac{1}{2}k j_k(j_k-1)} \prod_{k < l} t_{m(k,l)}^{d(k,l)j_k j_l}. \end{aligned} \quad (2.73)$$

Here $m(k, l)$ = least common multiplier of k, l and $d(k, l)$ greatest common divisor of k, l . The sum is taken as before over all sets of (j_k) satisfying

$$1 \cdot j_1 + 2j_2 + \dots + pj_p = p.$$

In terms of this cycle index we can write

$$\pi_p(y) = Z_2(S_p; 1 + y). \quad (2.74)$$

From this the values of $\pi(p, l)$ can be calculated. The first few terms are

$$\begin{aligned} \pi(x, y) = x + x^2(1 + y) + x^3(1 + y + y^2 + y^3) + x^4(1 + y + 2y^2 + 3y^3 \\ + 2y^4 + y^5 + y^6) + x^5(1 + y + 2y^2 + 4y^3 + 6y^4 + 6y^5 + 6y^6 \\ + 4y^7 + 2y^8 + y^9 + y^{10}) + \dots \end{aligned} \quad (2.75)$$

(vi). *Number of connected graphs (unlabelled)*

In deriving $\gamma(x, y)$ from $\pi(x, y)$ we can proceed as for labelled graphs, decomposing the general free graph into mutually exclusive sets made up of one connected component, two connected components, ... q connected components. We then find, using Polya's Theorem, that

$$\pi(x, y) = \gamma(x, y) + Z[\mathbf{S}_2; \gamma(x, y)] + Z[\mathbf{S}_3; \gamma(x, y)] + \dots \quad (2.76)$$

Hence from (2.63),

$$1 + \pi(x, y) = \exp \left[\gamma(x, y) + \frac{\gamma(x^2, y^2)}{2} + \frac{\gamma(x^3, y^3)}{3} + \dots \right]. \quad (2.77)$$

From this values of $\gamma(p, l)$ can be calculated.

A useful practical method (Robinson, 1970) is to write $\gamma(x, y)$ in the form $\sum_{p=1}^{\infty} x^p \gamma_p(y)$ and calculate $\gamma_{p+1}(y)$ recursively as the coefficient of x^{p+1} in

$$\begin{aligned} & \left[1 + \sum_{k=1}^{p+1} x^k \pi_k(y) \right] \exp - \sum_{k=1}^p x^k \gamma_k(y) \exp - \sum_{k=1}^p \frac{x^{2k} \gamma_k(y^2)}{2} \\ & \exp - \sum_{k=1}^p \frac{x^{3k} \gamma_k(y^3)}{3} \dots . \end{aligned} \quad (2.78)$$

The first few terms are

$$\begin{aligned} \gamma(x, y) = & x + x^2 y + x^3 (y^2 + y^3) + x^4 (2y^3 + 2y^4 + y^5 + y^6) \\ & + x^5 (3y^4 + 5y^5 + 5y^6 + 4y^7 + 2y^8 + y^9 + y^{10}). \end{aligned} \quad (2.79)$$

Tables of $\pi(p, l)$ and $\gamma(p, l)$ up to $p = 7$ are given in Uhlenbeck and Ford (1962, p. 200) and up to $p = 18$ in Stein and Stein (1963) where an efficient computational procedure is described in detail.

(vii). *Rooted star trees (unlabelled)*

Let $\theta(n)$ be the number of rooted pure star trees composed of n stars of a particular type joined by articulation points. Define the generating function

$$\Theta(y) = \sum_{n=0}^{\infty} \theta(n) y^n (\theta(0) = 1). \quad (2.80)$$

We can proceed as for Cayley trees and decompose $\Theta(y)$ into mutually

exclusive sets $\Theta_m(y)$ with exactly m main leaves

$$\Theta(y) = \sum_{m=0}^{\infty} \Theta_m(y).$$

Applying Polya's theorem we find that

$$\Theta_m(y) = Z[S_m, \Theta_1(y)]. \quad (2.81)$$

Now $\Theta_1(y)$ consists of a rooted star with star trees hung at vertices other than the root. If there are d different ways of rooting the unlabelled star, then using Polya's theorem, we deduce that

$$\Theta_1(y) = y \sum_q Z[G^{(d)}, \Theta(y)], \quad (2.82)$$

where $G^{(d)}$ is the group of the rooted star. This is, in fact, the sub-group of G (the group of the star) which consists of permutations leaving the root-point unchanged. It can then be shown that

$$\sum_d Z(G^{(d)}) = \frac{\partial Z(G)}{\partial t_1}, \quad (2.83)$$

which we denote by $Z'(G)$. Combining (2.81) (2.82) and (2.83) and using (2.63) we find that (Ford, Norman and Uhlenbeck, 1956)

$$\Theta(y) = \exp \sum_{k=1}^{\infty} \frac{y^k}{k} Z' [G, \Theta(y^k)]. \quad (2.84)$$

To take a specific example, if the star is a triangle G is the dihedral group D_3 which is identical with S_3 .

$$Z(S_3) = \frac{1}{6}(t_1^3 + 3t_1t_2 + 2t_3) \quad (2.85)$$

$$Z'(S_3) = \frac{1}{2}(t_1^2 + t_2) \quad (2.86)$$

and we obtain the equation satisfied by $\Delta(y)$ for rooted cacti (Harary and Uhlenbeck, 1953)

$$\Delta(y) = \exp \left\{ \sum_{k=1}^{\infty} \frac{y^k}{2k} [\Delta^2(y^k) + \Delta(y^{2k})] \right\}. \quad (2.87)$$

The generalization to mixed star trees with n_1 stars of type 1, n_2 stars of type 2, ... n_σ stars of type σ , ... is quite straightforward. The generating

function $\Theta(y_1, y_2, \dots, y_\sigma \dots)$ now satisfies

$$\Theta(y_1, y_2, \dots, y_\sigma) = \exp \sum_{k=1}^{\infty} \frac{1}{k} \sum_{\sigma} y_\sigma^k Z'[\mathbf{G}_\sigma, \Theta(y_1^k, y_2^k, \dots, y_\sigma^k \dots)]. \quad (2.88)$$

If we now wish to go back to our standard generating function $\Phi(x, y)$ giving the number of mixed star trees with p points and l lines, we replace y_σ by $x^{p_\sigma-1} y^{l_\sigma}$ where p_σ, l_σ are the number of points and lines in the star σ , and we multiply by x to take account of the root:

$$\Phi(x, y) = x \Theta(x^{p_1-1} y^{l_1}, x^{p_2-1} y^{l_2}, \dots, x^{p_\sigma-1} y^{l_\sigma} \dots). \quad (2.89)$$

(This result can easily be derived by cutting off the stars one by one from the tree).

(viii). Unrooted star trees (unlabelled)

The passage from rooted to unrooted graphs is no longer trivial for unlabelled graphs since all points are no longer inequivalent. In fact, when we root a free graph C in all possible ways we obtain p_d rooted graphs, where p_d is the number of inequivalent points of C . This quantity must be summed over all star trees to obtain the total number of rooted star trees corresponding to a given set of free star trees. An argument given in Ford, Norman and Uhlenbeck (1956) enables one to express the generating function $\Theta_f(y)$ for unrooted star trees in the following form:

$$\Theta_f(y) = \Theta(y) - y [\Theta(y) Z'(\mathbf{G}, \Theta(y)) - Z(\mathbf{G}, \Theta(y))]. \quad (2.90)$$

The generalization to mixed star trees is straightforward:

$$\Theta_f(y_1, y_2 \dots) = \Theta(y_1, y_2, \dots) - \sum_{\sigma} y_\sigma [\Theta(y_1, y_2, \dots) \\ Z'(\mathbf{G}_\sigma, \Theta(y_1, y_2 \dots)) - Z(\mathbf{G}_\sigma, \Theta(y_1, y_2 \dots))]. \quad (2.91)$$

As a very simple example of the application of (2.90) we take the case of unrooted Cayley trees. The group \mathbf{G} is S_2 and

$$Z(S_2) = \frac{1}{2}(t_1^2 + t_2). \quad (2.92)$$

We readily derive the formula given by Otter (1948)

$$\tau_f(x) = \tau(x) - \frac{1}{2}x[\tau(x)^2 - \tau(x^2)]. \quad (2.93)$$

(ix). Unlabelled stars

No explicit formula has been derived for the generating function $\sigma(x, y)$ for unlabelled stars in terms of $\gamma(x, y)$ for connected graphs analogous to (2.29)

for labelled graphs. However, for practical computation there has been an important step forward recently by Robinson (1970) who has put forward a method of calculating the total number of stars with p vertices. In reading Robinson's paper one should note the alternative terminology of *non-separable graphs* or *2-connected graphs* to describe stars; a *block* of a graph is a maximal star sub-graph. Thus the blocks of mixed star trees are the basic stars from which the trees are constructed.

Robinson works directly with the cycle indices of graphs. He computes the sum of the cycle indices of all graphs among p points, and relates it to the sum of the cycle indices of all connected graphs. He then relates this latter sum to the sum of the cycle indices of the blocks of these graphs which are the stars.

Let us denote by $\mathbf{Z}(\mathbf{C})$ the sum of the cycle indices of all connected graphs, and $\mathbf{Z}(\mathbf{B})$ the sum of the cycle indices of all blocks of these graphs. Robinson derives the relation

$$\mathbf{Z}'(\mathbf{C}) = \exp \sum_{k=1}^{\infty} \frac{t_k}{k} \mathbf{Z}'(\mathbf{B}) [t_1 \mathbf{Z}'(\mathbf{C})] \quad (2.94)$$

which is closely analogous to (2.84). He then divides \mathbf{B} into components \mathbf{B}_p corresponding to p points, and these give rise to the p th order terms in $\mathbf{Z}(\mathbf{B})$. They can be calculated recursively using a method similar to (2.78). Putting all the t_k equal to 1 in $\mathbf{Z}(\mathbf{B}_p)$ gives the total number of stars with p points. Computations were undertaken up to $p = 10$ and the results are given in Table 4 (p. 36).

We quote the first few terms of the generating function $\sigma(x, y)$ derived by hand (Uhlenbeck and Ford, 1962):

$$\begin{aligned} \sigma(x, y) = & x^2y + x^3y^3 + x^4(y^4 + y^5 + y^6) + x^5(y^5 + 2y^6 + 3y^7 \\ & + 2y^8 + y^9 + y^{10}) + \dots \end{aligned} \quad (2.95)$$

3. Asymptotic behaviour

(a). Labelled graphs

We have already given asymptotic formulae for $N(p, l)$, $C(p, l)$ and $S(p, l)$ in (2.25) and (2.48)

$$N(p, l) \sim C(p, l) \sim S(p, l) \sim \binom{\frac{1}{2}p(p-1)}{l} \quad (2.96)$$

as long as $l > p \ln p$. Thus the total number of labelled graphs with p points is asymptotically equal to $2^{\frac{1}{2}p(p-1)}$. We now consider the asymptotic behaviour of different types of graph.

For Cayley trees we were able to give an exact formula for any p ; see (2.35)

$$t_p = p^{p-2}. \quad (2.97)$$

The exact formula (2.40) for Husimi trees is broken down into individual types with n_2 single lines, n_3 triangles, If we wish to find the *total* number of such trees with p points, we require the coefficient of $x^p/p!$ in $T(x)$ where w_2, w_3, w_4 are all put equal to unity in (2.37). From (2.38) we see that $T(x)$ satisfies the implicit equation

$$F(T, x) = T(x) - x \exp S'(T) = 0 \quad (2.98)$$

where $S(x)$ is given by (2.37). If we were dealing with star trees constructed from a particular set of stars we would replace (2.37) by the corresponding star generating function

$$S(x) = \sum_{\sigma} \frac{x^{q_{\sigma}}}{g_{\sigma}} \quad (2.99)$$

summed over the set.

Ford and Uhlenbeck (1956) used the following procedure to calculate the asymptotic behaviour of the coefficient t_p . $T(x)$ is a power series and hence the asymptotic behaviour of t_p is determined by the nearest singularities on the circle of convergence. One of these singularities must be on the positive real axis since all the terms of $T(x)$ are positive. Consider first the case in which the star collection is finite. Then by the implicit function theorem the only singularities of $T(x)$ in the finite plane correspond to values of x for which

$$\frac{\partial F}{\partial T} = 0 = 1 - x S''(T) \exp S'(T) = 1 - TS''(T), \quad (2.100)$$

using (2.98).

$S(x)$ is a polynomial with positive coefficient, and hence there is exactly one real positive T_0 satisfying (2.100). Let x_0 be the corresponding value of x . Proceeding to the second derivative $\partial^2 F / \partial T^2$, it can readily be established that this is non zero at (x_0, T_0) and hence that $T(x)$ has a branch point of order two at x_0 ,

$$T(x) = T_0 - b(x_0 - x)^{\frac{1}{2}} + \dots \quad (2.101)$$

There may also be other singularities on the circle of convergence. These are given by $T = T_0 \exp i\Theta$ where $\Theta = 2\pi m/d$ ($m = 0, 1, \dots, d-1$) where d is the greatest common division of the set of integers $(q_{\sigma} - 1)$.

Using Cauchy's theorem to express t_p as a contour integral in $T(x)$ and evaluating this by the method of steepest descents, Ford and Uhlenbeck

established the following general result:

$$\frac{t_p}{p!} = \begin{cases} \frac{db}{2\pi^{\frac{1}{4}}} p^{-3/2} x_0^{-p+\frac{1}{2}}, \frac{p-1}{d} \text{ an integer} \\ 0 \quad \frac{p-1}{d} \text{ not an integer.} \end{cases} \quad (2.102)$$

The number of *unrooted* trees $t_p^{(r)}$ is obtained as before by dividing by p .

In a subsequent paper, Ford and Uhlenbeck (1957) showed that the above results remain valid for an infinite set of stars if the stars belong to homeomorphic types (IIA5) with cyclomatic number $\leq c$ (c finite). Hence they are certainly valid for the set of mixed Husimi trees corresponding to (2.37). However, they cannot be valid for the set of *all* stars since the result (2.96) then holds, and the generating function has zero radius of convergence.

For the set of mixed Husimi trees the following numerical values were obtained:

$$T_0 = 0.45631 \quad x_0 = 0.23874 \quad b = 0.87270. \quad (2.102')$$

Table I shows a comparison between exact values and asymptotic estimates of t_p for $p = 1$ to 6.

TABLE I. Comparison of exact values and asymptotic estimates of mixed Husimi trees (labelled) (after Ford and Uhlenbeck, 1956)

| p | 1 | 2 | 3 | 4 | 5 | 6 |
|------------|---|---|---|----|-----|------|
| Exact | 1 | 1 | 4 | 31 | 362 | 5676 |
| Asymptotic | 1 | 1 | 3 | 28 | 332 | 5297 |

(b). Unlabelled graphs

The same method can be used to estimate the asymptotic behaviour of unlabelled graphs of particular types but the detailed calculations are more complicated. The case of Cayley trees is no longer trivial and was discussed in detail by Otter (1948). Instead of (2.98) we now have from (2.54) the implicit equation for $\tau(x)$

$$F(\tau, x) = \tau - x \exp \left[\frac{\tau(x^2)}{2} + \frac{\tau(x^3)}{3} + \dots + \frac{\tau(x^r)}{r} + \dots \right]. \quad (2.103)$$

In this relation the function $\tau(x^r)$ is treated as a function of x for $r > 1$ and it can be shown again that $\tau(x)$ has a singularity at x_0 where $0 < x_0 < 1$. Hence $\partial F / \partial \tau = 0$ combined with (2.103) gives the simple relation

$$\tau(x_0) = 1. \quad (2.104)$$

As before we can show that x_0 is a branch point of order 2, and we can obtain a formula for the second derivative

$$\left(\frac{\partial^2 F}{\partial \tau^2} \right)_{1,x_0}$$

If we now wish to determine the asymptotic behaviour of free trees we must use equation (2.93).

The numerical values τ_p for rooted trees and $\tau_p^{(f)}$ for free trees are as follows (Otter 1948):

$$x_0 = 0.3383219$$

$$\tau_p = \frac{bx_0^{-p}}{p^{3/2}} \quad (2.105)$$

$$\tau_p^{(f)} = \frac{b'x_0^{-p}}{p^{5/2}}$$

$$b = 0.4399237, b' = 0.5349485.$$

With little additional difficulty it is possible to calculate the number of trees with a maximum co-ordination number q at a vertex. The formulae (2.105) remain valid for general q , and x_0, b, b' are insensitive to the value of q ; the value for $q = 4$ is as follows

$$x_0 = 0.3551817, b = 0.5178760, b' = 0.6563190. \quad (2.106)$$

The case $q = 4$ is of particular chemical interest, and tables from $p = 1$ to 20 were prepared by Henze and Blair (1931). The asymptotic formula works well even for small values of p (see Table II).

TABLE II. Comparison between exact values and asymptotic estimates of Cayley trees (unlabelled, after Otter, 1948)

| p | $q = \infty$ | | | | $q = 4$ | | | |
|-----|--------------|-------------|----------|-------------|---------|-------------|----------|-------------|
| | Rooted | | Unrooted | | Rooted | | Unrooted | |
| | Exact | Asymp-totic | Exact | Asymp-totic | Exact | Asymp-totic | Exact | Asymp-totic |
| 1 | 1 | 1 | 1 | 2 | 1 | 1 | 1 | 1 |
| 2 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 3 | 2 | 2 | 1 | 1 | 2 | 2 | 1 | 1 |
| 4 | 4 | 4 | 2 | 2 | 4 | 4 | 2 | 1 |
| 5 | 9 | 9 | 3 | 2 | 8 | 8 | 3 | 2 |
| 10 | 719 | 708 | 106 | 86 | 507 | 513 | 75 | 65 |
| 15 | 87 811 | 86 965 | 7 741 | 7 050 | 48 965 | 49 363 | 4 347 | 4 170 |
| 18 | 1 721 159 | 1 708 440 | 123.867 | 114.875 | 830 219 | 838 099 | 60 523 | 59 008 |

TABLE III. Comparison between exact values and asymptotic estimates of mixed Husimi trees (unlabelled, after Ford and Uhlenbeck 1956)

| <i>p</i> | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|----------------|---|---|---|---|----|-----|-----|------|
| Rooted exact | 1 | 1 | 3 | 8 | 26 | 84 | 297 | 1066 |
| Asymptotic | 1 | 1 | 3 | 9 | 30 | 102 | 365 | 1347 |
| Unrooted exact | 1 | 1 | 2 | 4 | 9 | 23 | 63 | 188 |
| Asymptotic | 1 | 1 | 1 | 2 | 5 | 15 | 45 | 146 |

TABLE IV. Number of connected graphs $\gamma(p)$ and stars $\sigma(p)$ with p vertices (exact $\sigma(p)$ taken from Robinson, 1970)

| <i>p</i> | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|------------------------------------|---|---|----|-----|-----|-------|--------|----------|
| $\gamma(p)$ | 2 | 6 | 21 | 112 | 853 | 11117 | 261080 | 11716571 |
| $\sigma(p)$ | 1 | 3 | 10 | 56 | 468 | 7123 | 194066 | |
| $\frac{2^{\frac{1}{2}p(p-1)}}{p!}$ | 1 | 3 | 8 | 46 | 416 | 6658 | 189372 | 9695870 |

For mixed Husimi trees the relation corresponding to (2.103) is (Ford and Uhlenbeck, 1956)

$$F(\Theta, x) \equiv \Theta - x \exp \left\{ \sum_{k=1}^{\infty} \frac{1}{k} \sum_{m=2}^{\infty} Z' [\mathbf{D}_m, \Theta(x^k)] \right\} = 0. \quad (2.107)$$

Putting

$$\frac{\partial F}{\partial \Theta} = 0,$$

and using the original relation (2.107), we find

$$\left(\frac{\partial F}{\partial \Theta} \right)_{x=x_0, \Theta=\Theta(x_0)} = 1 - \Theta(x_0) \sum_{m=2}^{\infty} Z''[\mathbf{D}_m, \Theta(x_0)] = 0 \quad (2.108)$$

where the differentiation in (2.108) for the cycle index is with respect to t_1 as usual. The asymptotic formulae are of the same form as (2.105) with the following numerical values

$$x_0 = 0.22215, \Theta(x_0) = 0.45381, b = 0.58433, b' = 0.50774. \quad (2.109)$$

Exact values are compared with asymptotic estimates in Table III.

If we now proceed to all connected graphs, Polya has shown that the asymptotic behaviour of $\pi(p, l)$

$$\pi(p, l) \sim \frac{1}{p!} \binom{p(p-1)/2}{l} \quad (2.110)$$

as long as p is large and l not too near the two ends of its range. Polya did not publish this result himself, but a proof is quoted in Riddell (1951) for $|l - \frac{1}{4}(p-1)| < cp$ where c is a positive constant, and this covers the majority of graphs. If we compare (2.110) with the corresponding formula (2.96) for labelled graphs we see that for the majority of graphs $C(p, l)$ is equal to $p! \pi(p, l)$ so that the majority of graphs have no symmetry ($g = 1, v = p!$).

This result does not apply however for sets of star trees. For Cayley trees, for example, from (2.97)

$$\frac{t_p}{p!} \sim e^p \quad (2.111)$$

whereas from (2.105)

$$\tau_p \sim (2.9557)^p. \quad (2.112)$$

Hence the average symmetry number g will be of order

$$\left(\frac{2.9557}{e} \right)^p \quad (2.113)$$

for large p . A similar conclusion follows for mixed Husimi trees on comparing the values of x_0 in (2.102') and (2.109).

Particular interest centres around star graphs since they represent the irreducible minimum of graphs which must be considered in perturbation expansions. Although no closed formula has been derived for the asymptotic number $\sigma(p)$ of unlabelled stars, it has been shown (Domb 1969a) that the expression $2^{\frac{1}{2}p(p-1)}/p!$ provides a close approximation (Table IV). This table illustrates the depressing conclusion drawn by Uhlenbeck and his co-workers that the number of stars increases with extraordinary rapidity, and that there is little gain asymptotically in proceeding from connected graphs to stars.

(c). Line grouping

Extensive perturbation expansions have nevertheless been developed for lattice systems without the need to cope with the large numbers of graphs in Table IV. One reason for this is the finite co-ordination number of a lattice which severely restricts the increase in numbers of graphs. However, a more important reason is that for high temperature series expansions, which are of great importance for lattice models, the l th term of the expansion involves graphs which can be constructed with l lines. The number of l -line graphs increases much more slowly with l than does the number of p -point graphs with p . We can see this by studying $\pi(p, l)$ as a function of p for fixed l from formula (2.110) and we find that it increases steadily with p giving rise to a maximum when $l = p - 1$ (Cayley trees). But formula (2.110) is no longer

valid in this region, (since $l < p \ln p$) and instead we have formulae of type (2.105) which increase exponentially with l . It seems likely therefore that the total number of connected graphs with l lines also increases exponentially with l .

Table V (Domb, 1969a) illustrates two important features of line grouping: (a) the much slower increase in the total number of connected graphs; (b) the increased factor gained in proceeding from connected graphs to stars.

Finally to illustrate the behaviour of the distribution $\sigma(p, l)$ for varying l we quote from Heap (1972) the values of $\sigma(8, l)$ (Table VI).

TABLE V. Number of connected graphs $\gamma(l)$ and stars $\sigma(l)$ with l lines

| p | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|-------------|---|---|----|----|----|-----|-----|------|------|-------|
| $\gamma(l)$ | 3 | 5 | 12 | 30 | 79 | 227 | 710 | 2322 | 8071 | 29503 |
| $\sigma(l)$ | 1 | 1 | 2 | 4 | 7 | 16 | 42 | 111 | 331 | 1094 |

TABLE VI. Number of 8-point stars with l lines

| l | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|----------------|-----|-----|-----|-----|-----|-----|------|------|
| $\sigma(8, l)$ | 1 | 6 | 40 | 161 | 429 | 780 | 1076 | 1197 |
| | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 |
| 1114 | 885 | 622 | 386 | 215 | 112 | 55 | 24 | |
| | 24 | 25 | 26 | 27 | 28 | | | |
| | 11 | 5 | 2 | 1 | 1 | | | |

Mention should be made of methods of enumeration which have been used near the Cayley tree limit $l \sim p$ for *labelled* graphs. For connected graphs we have the relation (2.17)

$$\exp f(x, y) = 1 + \sum_{n=1}^{\infty} x^n (1+y)^{n(n-1)/2} / n! = F(x, y). \quad (2.114)$$

Temperley (1958) noted that $F(x, y)$ satisfies a linear partial differential equation of heat conduction type

$$x^2 \frac{\partial^2 F(x, y)}{\partial x^2} = 2(1+y) \frac{\partial F(x, y)}{\partial x}. \quad (2.115)$$

Equation (2.115) can be transformed into an equation for $f(x, y)$ the lowest term of which (corresponding to Cayley trees) is $l^{l-2} x^l y^{l-1} / l!$. This suggests

introducing a new variable $v = xy$ and attempting to find a series expansion in powers of y starting with y^{-1} . Also the form of the coefficient of y^{-1} suggests a further transformation $v = w \exp - w$. Temperley then derived a solution of the form

$$\frac{1}{y} \left(w - \frac{w^2}{2} \right) - \frac{1}{2} \ln(1-w) - \frac{w}{2} - \frac{w^2}{4} + y \left(\frac{5}{24(1-w)^3} \right) + \dots . \quad (2.116)$$

Retaining only the highest powers of $(1-w)^{-1}$ he obtained for the coefficient of y^t

$$A_t \left(\frac{3}{2} \right)^{t-1} \frac{t!}{3t} (1-w)^{-3t}, \quad (2.117)$$

and hence for the number of labelled connected graphs with p points and $(p+t)$ lines, (cyclomatic number $t+1$)

$$B_t \left(\frac{3}{2} \right)^{t-1} \frac{t!}{(3t!)^{\frac{1}{2}}} p! e^p (p)^{\frac{1}{2}(3t-1)}. \quad (2.118)$$

For *labelled stars*, Ford and Uhlenbeck (1957) have provided an exact formula for the number corresponding to a given homeomorphic type. Suppose the homeomorphic type has symmetry number v , K chains, P principal points, L_1 single chains joining a pair of principal points, L_2 double chains, \dots . Let $s^{(T)}(p)$ be the number of stars with p labelled points. To determine $s^{(T)}(p)$ the following quantities must be multiplied together:

- (a) The number of ways of selecting P principal points from p points.
- (b) The number of ways these P points can be assigned to the principal points.
- (c) The number of ways the remaining $(p-P)$ points can be distributed over the K chains, assigning n_k to the k th chain, taking each $n_k \geq 1$, and taking account of the symmetry of the chains.

The result is

$$s^{(T)}(p) = \binom{p}{P} \frac{p! (p-P)!}{v \prod_{m=1}^K (m!)^{L_m}} \sum n_k \left(\begin{matrix} n_k \geq 1 \\ \sum n_k = p-P \end{matrix} \right). \quad (2.119)$$

Defining a generating function

$$S^{(T)}(x) = \sum_{p=P}^{\infty} \frac{s^{(T)}(p)}{p!} x^p. \quad (2.120)$$

Ford and Uhlenbeck deduce that

$$S^{(T)}(x) = \frac{x^p}{v} \prod_{m=1}^K \left[\frac{x^m + mx^{m-1}(1-x)}{m!(1-x^m)} \right]^{L_m}. \quad (2.121)$$

In the paper by Temperley (1958) referred to above the method of deriving a partial differential equation is extended to $S(x, y)$ using (2.28) and (2.29). For small values of t an exact solution can be obtained which gives the same results as (2.121). For larger t Temperley finds an asymptotic formula similar to (2.118) except that the factor e^p is omitted.

The corresponding results for *unlabelled stars* will be discussed shortly (II.B4).

(d)[†] Ladder and non-ladder graphs

There is a class of perturbation problems in which particles are represented by points ordered around a polygon and the interactions correspond to joining the points in all possible ways (see e.g. Domb and Joyce, 1972). It is then of interest to differentiate between *ladder* graphs which have no-crossing bonds, and *non-ladder* graphs which represent the remainder. For example in Fig. 17 β , γ and δ are ladder graphs and α is non-ladder. Domb and Barrett (1973) have shown how to enumerate the total number of ladder graphs $N_L(p, l)$ and the number of connected ladder graphs $C_L(p, l)$ with p points and l lines. (The former corresponds to a classic problem of dissecting a polygon into sub-polygons.) If we write

$$F_L(x, y) = \sum N_L(p, l) x^p y^l \quad (2.122)$$

$$\text{and } f_L(x, y) = \sum C_L(p, l) x^p y^l$$

then $F_L(x, y)$ satisfies the quadratic equation,

$$yF_L^2 + (1+y)x^2F_L + (1+2y)x + (1+y)x^2 = 0, \quad (2.123)$$

and $f_L(x, y)$ satisfies the cubic equation

$$yf_L^3 + yf_L^2 - x(1+2y)f_L + x^2(2+y) = 0. \quad (2.124)$$

4. Listing of graphs

When we actually concern ourselves with the detailed development of perturbation expansions we require complete graph specifications. For connected graphs with $p \leq 6$ the list of Uhlenbeck and Ford (1962)

[†] The term *ladder graph* is here used in a different and more elementary sense than Essam or Wortis (Chapter 3) and Fisher (1970), and follows Chikahisa (1970).

provides a drawing of each graph, the group Γ of the graph, and the symmetry number v . For stars a more extensive list including $p = 7$ has been given by Hoover and de Rocco (1962). (The suggestion made by Domb and Heap (1967) that this list contains errors is incorrect. To the best of these authors' knowledge the list is free from errors.)

However, when we deal with line groupings these lists are insufficient and it is convenient to make use of the homeomorphic classification introduced in II.A5. The first task is to list systematically all HI stars of given cyclomatic number c . For $c = 1$ to 4 these HI stars are drawn in Fig. 16.

For $c = 5$ and 6 Heap (1966, 1969) adopted the following procedure. All the different HI stars having cyclomatic number c can be obtained from those having cyclomatic number $(c - 1)$ by one of the following procedures

- Joining any two distinct vertices by an edge.
- Inserting a two degree vertex on any edge and then joining it to any other vertex by an edge.
- Inserting 2 two degree vertices on any two (not necessarily distinct) edges and joining them by an edge.

In case (a) l is increased by 1 and p remains unchanged; in case (b) l is increased by 2 and p by 1; in case (c) l is increased by 3 and p by 2. Thus in all cases from equation (2.1) c is increased by 1 and one can easily convince oneself that this exhausts all possibilities of increasing c by 1. The three cases are illustrated in Fig. 23.

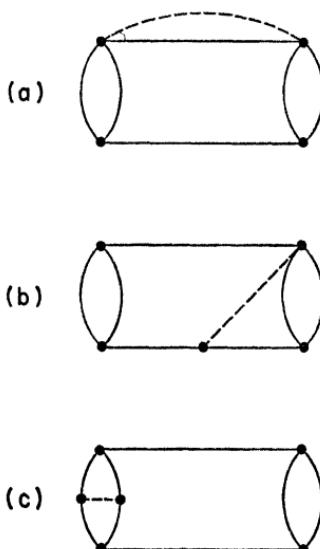


FIG. 23. Increasing the cyclomatic number from $c - 1$ to c (illustrative example).

The major problem is to ensure that no HI star is counted twice, since each HI star can be generated several times, and Heap (1972) describes how this is done most economically by computer with the help of the adjacency matrix.

For some purposes it is useful to list HI stars in accordance with the number of principal points P , and such a classification has been undertaken by Domb and Heap (1967) for $P = 1$ to 5. It is then possible to obtain asymptotic formulae for the total number of HI stars with a given P as a function of l .

Let us now construct all stars of p points which are of a given homeomorphic type. We must first partition p into l parts in all possible ways,

$$\begin{aligned} p &= q_1 + 2q_2 + 3q_3 + \dots kq_k \\ l &= q_1 + q_2 + \dots q_k. \end{aligned} \quad (2.125)$$

For each partition we must determine the number of different colourings of the edges of the HI star with s colours, s being the number of non-zero q_k . Call this number $\sigma_s(l|p)$ (II.B2(c) (iv)). The total number of HI stars is then

$$\sum_{\text{partitions}} m_s(l|p) \sigma_s(l|p) \quad (2.126)$$

where $m_s(l|p)$ is the number of partitions with a given s .

In this manner, exact expressions can be found for the total number of HI stars with a given P in terms of partitions of numbers. Asymptotic behaviour can then be estimated by examining the asymptotic behaviour of the partitions. The same construction can be used to list the stars of a given homeomorphic type, and to estimate their asymptotic behaviour.

For detailed generation of graphs in a computer we refer to Heap (1972).

III. Cluster Integral Theory

The perturbation expansion for an interacting gas, usually known as the cluster integral theory, was initiated by Ursell in 1927, and developed largely by Mayer and his collaborators in 1937-1939 [a parallel development is due to Yvon (1937)]. Although the theory is treated in standard text books on statistical mechanics, its full scope is not always in evidence, and certain aspects of importance for lattice statistics are sometimes omitted; we have therefore thought it worth providing a concise summary of the major results. The theory is in fact an application of the general graph theoretical development which we have already discussed.

A. Cluster integrals

Consider a classical gas in which the interaction potential between molecules 1 at r_1 , 2 at r_2 , ..., N at r_N is $\Phi_N(r_1, r_2, \dots, r_N)$. Standard statistical mechanics (e.g. Rushbrooke, 1949, Ch.16) tells us that the partition function is given by

$$Z_N = \frac{\eta^N}{N!} Q_N = \frac{\eta^N}{N!} \int_V \dots \int_V \exp -\beta \Phi_N dr_1 \dots dr_N \quad (3.1)$$

$$(\eta = (2\pi mkT)^{3/2}/h^3)$$

where Q_N is usually referred to as the configurational integral, and the integrals in each variable are taken over the volume of the container. We first deal with the case of central pair-interaction forces so that

$$\Phi_N(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \sum_{i,j \text{ pairs}} \phi(|\mathbf{r}_i - \mathbf{r}_j|) + \sum_{i=1}^N \psi(\mathbf{r}_i). \quad (3.2)$$

Here $\psi(\mathbf{r})$ is the potential of external forces, and although this is zero in most cases of practical interest, we shall find it useful to retain a non-zero value since a good deal of the formalism remains unchanged.

Writing

$$\left. \begin{aligned} \exp -\beta \phi(|\mathbf{r}_i - \mathbf{r}_j|) &= 1 + f_{ij} \\ \text{and } \exp -\beta \psi(\mathbf{r}_i) &= h_i \end{aligned} \right\} \quad (3.3)$$

we find that Q_N can be written as

$$Q_N = \sum_{(G_N)} w(G_N), \quad (3.4)$$

the sum being taken over all graphs among N labelled points, and the weight of a graph being given by

$$w(G_N) = \int_V \dots \int_V dr_1 dr_2 \dots dr_N \prod_i f_{ij} \prod_{j=1}^N h_i. \quad (3.5)$$

(In the product $\prod_i f_{ij}$ every line of G_N contributes an f_{ij} .)

We easily verify that for any graph G_N consisting of connected parts C_p ,

$$w(G_N) = \prod_{(\text{all } C_p)} w(C_p), \quad (3.6)$$

and the conditions of Theorem I of II.B1 are satisfied. Q_N is the analogue of F_N , and the grand partition function of the system, given by

$$\Xi(\lambda, V, T) = 1 + \sum_{N=1}^{\infty} \frac{(\lambda\eta)^N}{N!} Q_N, (\lambda = \text{fugacity}) \quad (3.7)$$

corresponds to $1 + F(x)$. Hence from Theorem I

$$(M1) \quad \frac{1}{V} \ln \Xi = \sum_{p=1}^{\infty} b_p(V, T) (\lambda\eta)^p = \sum_{p=1}^{\infty} b_p(V, T) \lambda'^p \quad (\lambda' = \lambda\eta)$$

where $b_p(V, T)$ is the analogue of $f_p/p!$. $b_p(V, T)$ termed a *cluster integral* is therefore given by

$$(M1a) \quad b_p(V, T) = \frac{1}{V p!} \sum_{(C_p)} \int_V \dots \int_V d\mathbf{r}_1 \dots d\mathbf{r}_p \prod_i f_{ij} \prod_{i=1}^p h_i.$$

We note that the intermolecular forces have not been restricted in any way, and the volume has been taken to be finite. The factor $1/V$ is introduced so that for short range forces and large volumes $b_p(V, T)$ will tend to a limit independent of volume.

We can now generalize the formula to take account of many body forces. We must first find a generalization of (3.3) and (3.4) and we do this by following the Ursell (1927) construction. Let

$$\begin{aligned} w_{12} &= \exp - \beta\phi(\mathbf{r}_1, \mathbf{r}_2), \\ w_{123} &= \exp - \beta\phi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3), \\ w_{1234} &= \exp - \beta\phi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4). \end{aligned} \quad (3.8)$$

Define $u_{12}, u_{123}, u_{1234}$ ($\equiv u(\mathbf{r}_1, \mathbf{r}_2), u(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3), u(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) \dots$) by the following scheme

$$\begin{aligned} w_{12} &= 1 + u_{12} \\ w_{123} &= 1 + u_{12} + u_{23} + u_{31} + u_{123} \\ w_{1234} &= 1 + \sum_{\text{pairs}} u_{ij} + \sum_{\text{triplets}} u_{ijk} + \sum_{\substack{\text{different} \\ \text{pairs}}} u_{ij} u_{kl} + u_{1234}. \end{aligned} \quad (3.9)$$

At the r th stage we divide the r particles into sub-groups in all possible ways and write 1 for single particles, and the appropriate u_{ijk} for the sub-groups. We have thus constructed the $u_{ij} \dots k$ to correspond to the products of the f_{ij} relating to connected graphs and our method of construction ensures that (3.4) is valid, and that the product property (3.6) holds if we take

$$w(C_p) = \int_V \dots \int_V d\mathbf{r}_1 d\mathbf{r}_2 \dots d\mathbf{r}_p u_{ij \dots k} \prod_{i=1}^p h_i. \quad (3.10)$$

Hence (M1) remains valid with

$$(M1b) \quad b_p(V, T) = \frac{1}{V p!} \sum_{(C_p)} \int_V \dots \int_V d\mathbf{r}_1 \dots d\mathbf{r}_p u_{ij \dots k} \prod_{i=1}^p h_i.$$

From (M1b) we see that it is important to invert the relations (3.9) so that we can express the $u_{ij\dots k}$ in terms of the $w_{ij\dots k}$ which contain the intermolecular forces.

The relations (3.9) can be conveniently thought of as a generalization of the transition from moments to cumulants in statistics. If we take a general $w(\mathbf{r}_1)$ ($= w_1$) and write

$$(M1c) \quad \begin{aligned} w_1 &= u_1 \\ w_{12} &= u_1 u_2 + u_{12} \\ w_{123} &= u_1 u_2 u_3 + u_{12} + u_{23} + u_{31} + u_{123} \end{aligned}$$

we can invert to form

$$(M1d) \quad \begin{aligned} u_1 &= w_1 \\ u_{12} &= w_{12} - w_1 w_2 \\ u_{123} &= w_{123} - w_{12} w_3 - w_{23} w_1 - w_{31} w_2 + 2w_1 w_2 w_3. \end{aligned}$$

The $w_{ij\dots k}$ correspond to moments and the $u_{ij\dots k}$ to cumulants; we shall sometimes use a shorthand notation to denote this

$$u_{123} = [w_{123}]_c.$$

The general rule in (M1d) is that for a term involving k clusters the coefficient is $(-1)^{k-1} (k-1)!$ (see Section IV.B3).

Formulae (M1) are valid for any range of force and since the volume is finite, surface as well as bulk contributions are taken into account. The formulae have been applied to plasmas involving ionic forces (Mayer, 1950) although a rearrangement of diagrams is needed to obtain an expansion of physical significance. The molecular interactions can be replaced by quantum operators, and the partition function is then obtained by taking the trace of the resulting integrals. However, they do *not* take account of *quantum statistics*; for a comprehensive account of this generalization we refer to the review article by C. Bloch (1965). We shall find that the finite volume property has an important application in the finite cluster method for lattice statistics.

The most frequent application of these formulae is to the calculation of the bulk contribution when the intermolecular forces are short-ranged (short compared with the linear dimensions of the container). The integral in (M1a) has the same value for all sets of points \mathbf{r}_i in V except near the surface of the container. When the volume becomes large we can ignore surface effects and write in the thermodynamic limit (see Griffiths Vol. 1 Chapter 2)

$$(M1e) \quad b_p(T) = \lim_{V \rightarrow \infty} \frac{1}{V p!} \sum_{(C_p)} \int_V \dots \int_V d\mathbf{r}_1 \dots d\mathbf{r}_p \prod_i f_{ij} \prod_{i=1}^p h_i$$

as a function of temperature only. We then have by standard thermody-

namics from (M1) that the pressure is given by

$$(M2) \quad \frac{P}{kT} = \sum_{p=1}^{\infty} b_p(T) \lambda'^p$$

$$(M3) \quad \rho = \sum_{p=1}^{\infty} p b_p(T) \lambda'^p.$$

To generalize the result (M1e) to non-central forces we need to show that if the $w_{ij\dots k}$ correspond to short range forces then the $u_{ij\dots k}$ are zero outside the range of the forces. Formally if we divide the particles into a number of groups containing $\alpha_1, \alpha_2 \dots$ particles, then if these groups are sufficiently far apart for the relations

$$w_{ij\dots k} = w_{i_1 j_1 \dots k_1} w_{i_2 j_2 \dots k_2} \text{ (product property)} \quad (3.11)$$

to be satisfied, where $i_1, j_1, \dots k_1 \dots$ are drawn from α_1 , and $i_2, j_2, \dots k_2$ from α_2, \dots then

$$u_{ij\dots k} = 0. \quad (3.12)$$

We can understand this relationship empirically from the way in which the functions $u_{ij\dots k}$ have been constructed. A proof by induction that (3.11) leads to (3.12) was given by Kahn and Uhlenbeck (1938). (See also this Vol. Chapter 5, Section II.B). A more sophisticated general proof was later provided by Sherman (1964). Relation (3.12) ensures that $b_p(V, T)$ as defined by (M1b) tends to a limit independent of volume.

To write down a cluster integral of order p we need to list all connected graphs among p labelled points. But since the value of the integral is independent of the labelling it is convenient to group all integrals of the same type together as unlabelled graphs and multiply by the symmetry number. Thus we can write

$$\begin{aligned} b_1(T) &= \bullet \\ 2!b_2(T) &= \bullet - \bullet \\ 3!b_3(T) &= 3 \quad \begin{array}{c} \bullet \\ | \\ \bullet - \bullet \\ | \\ \bullet \end{array} + \begin{array}{c} \bullet \\ / \backslash \\ \bullet \end{array} \\ 4!b_4(T) &= 12 \quad \begin{array}{c} \bullet \\ | \\ \bullet - \bullet \\ | \\ \bullet \end{array} + 4 \quad \begin{array}{c} \bullet \\ / \backslash \\ \bullet - \bullet \\ | \\ \bullet \end{array} + 12 \quad \begin{array}{c} \bullet \\ | \\ \bullet - \bullet \\ | \\ \bullet \end{array} + 3 \quad \begin{array}{c} \bullet \\ | \\ \bullet - \bullet \\ | \\ \bullet \end{array} \\ &\quad + 6 \quad \begin{array}{c} \bullet \\ | \\ \bullet - \bullet \\ | \\ \bullet \end{array} + \begin{array}{c} \bullet \\ | \\ \bullet - \bullet \\ | \\ \bullet \end{array} \end{aligned} \quad (3.13)$$

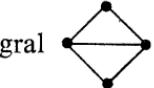
B. Irreducible cluster integrals

The second stage in the reduction of the configurational integral is more restricted and applies only (a) in the thermodynamic limit $V \rightarrow \infty$ (b) for pairwise additive forces (c) taking $h_i = 1$. These restrictions are necessary for Theorem II of II.B1 to apply. If we then define for any connected graph C_p

$$w(C_p) = \lim_{V \rightarrow \infty} \frac{1}{V} \int \dots \int d\mathbf{r}_1 \dots d\mathbf{r}_p \sum_i f_{ij} \quad (3.14)$$

we can show that for a connected graph consisting of stars S_m

$$w(C_p) = \prod_{(S_m)} w(S_m) \quad (3.15)$$

This is illustrated by the example shown in Figure 24. We first integrate over 2, 3 and obtain the cluster integral for a triangle  , which is independent of \mathbf{r}_1 . We then integrate over 4, 5, 6 and obtain the cluster integral  . Finally integration over \mathbf{r}_1 gives V which cancels with the $1/V$ outside the integral.

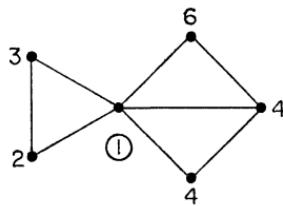


FIG. 24

Applying Theorem II we write for the sum over all stars S_q of q points

$$\beta_{q-1} = \frac{1}{(q-1)!} \sum_{(S_q)} w(S_q) \quad (3.16)$$

so that from (2.27)

$$S'(\lambda') = \sum_{k=1}^{\infty} \beta_k \lambda'^k \quad (3.17)$$

where the β_k are called *irreducible cluster integrals*. The analogue of $R(x)$ in (2.28) is just the density ρ in (M3), and taking logarithms in (2.29) we find that

$$(M4) \quad \ln \lambda' = \ln \rho - \sum_{k=1}^{\infty} \beta_k \rho^k.$$

To obtain P we use the thermodynamic relation

$$\frac{\partial P}{\partial \rho} = \frac{\partial P}{\partial \lambda} \frac{\partial \lambda}{\partial \rho} = \frac{1}{V} \frac{\partial}{\partial \lambda} (kT \ln \Xi) \frac{\partial \lambda}{\partial \rho} = \frac{kT\rho}{\lambda} \frac{\partial \lambda}{\partial \rho} \quad (3.18)$$

But from (M4)

$$\frac{1}{\lambda} \frac{\partial \lambda}{\partial \rho} = \frac{1}{\rho} - \sum_{k=1}^{\infty} k \beta_k \rho^{k-1}. \quad (3.19)$$

Hence we find on integration (the arbitrary function of T being determined by the dilute limit)

$$(M5) \quad \frac{P}{kT} = \rho - \sum_{k=1}^{\infty} \frac{k}{k+1} \beta_k \rho^{k+1} = \frac{1}{V} \ln \Xi$$

To obtain consistency with the generalization to multicomponent systems it is convenient to write this in the following alternative form

$$(M6) \quad P = kT \left[\rho - \sum_{k=2}^{\infty} (k-1) B_k(T) \rho^k \right]$$

where

$$(M6a) \quad \begin{aligned} B_k(T) &= \beta_{k-1}/k \\ &= \frac{1}{k!} \sum_{(S_k)} w(S_k) \end{aligned}$$

From equations (M3) and (M4) we can determine the b_p in terms of the β_k and vice versa. Relation (M4) can be written in the form

$$\rho = \lambda' G(\rho) \quad (3.20)$$

where

$$G(\rho) = \exp \left(\sum_{k=1}^{\infty} \beta_k \rho^k \right) \quad (3.21)$$

Hence following Kahn (1938) we can use the standard Lagrange method of reversion of series (Edwards, 1896, p. 451) to show that

$$\rho = \sum_{p=1}^{\infty} a_p \frac{\lambda'^p}{p!} \quad (3.22)$$

where

$$a_p = \frac{d^{p-1}}{d\rho^{p-1}} [G(\rho)^p]_0 \quad (3.23)$$

Substituting from (3.21) and comparing (3.22) with (M3) we find that

$$(M7) \quad p^2 b_p = \text{coefft of } t^{p-1} \text{ in } \exp p \sum_{k=1}^{\infty} \beta_k t^k.$$

For the first few terms we have

$$\begin{aligned} b_2 &= \frac{1}{2}\beta_1 \\ b_3 &= \frac{1}{3}\beta_2 + \frac{1}{2}\beta_1^2 \\ b_4 &= \frac{1}{4}\beta_3 + \beta_1\beta_2 + \frac{2}{3}\beta_1^3 \end{aligned}$$

It is more difficult to find an explicit expression for the β_k in terms of the b_p . However by direct inversion we find for the first few terms

$$(M8) \quad \begin{aligned} \beta_1 &= 2b_2 \\ \beta_2 &= 3b_3 - 6b_2^2 \\ \beta_3 &= 4b_4 - 24b_2b_3 + \frac{80}{3}b_2^3 \end{aligned}$$

To write down the irreducible cluster integrals of order k in a parallel manner to (3.13) we need to list all *stars* among p labelled points. We group integrals of the same type together as unlabelled graphs and multiply by the symmetry numbers. A useful list going up to $p = 7$ is given by Hoover and de Rocco (1962)

$$1! \beta_1 = \bullet - \bullet$$

$$2! \beta_2 = \triangle \quad (3.24)$$

$$3! \beta_3 = 3 \square + 6 \begin{array}{c} \square \\ \diagdown \diagup \end{array} + \begin{array}{c} \square \\ \times \times \end{array}$$

C. Multicomponent systems

The generalization of the development to multicomponent systems is straightforward, and we shall sketch the theory briefly, and quote the resulting formulae for a two component system; it will be easy to write down the corresponding results for an s component system. In regard to the graph theoretical background we first observe that the points corresponding to each species are labelled independently. By analogy with $F(x)$ in (2.15) we define

$$F(x_1, x_2) = \sum_{n_1, n_2=1}^{\infty} F_{n_1 n_2} x_1^{n_1} x_2^{n_2} / n_1! n_2!, \quad (3.25)$$

and by analogy with $f(x)$ in (2.16)

$$f(x_1, x_2) = \sum_{p_1, p_2=1}^{\infty} f_{p_1 p_2} x_1^{p_1} x_2^{p_2} / p_1! p_2! \quad (3.26)$$

We then establish the first theorem (cf. 2.17)

$$1 + F(x_1, x_2) = \exp f(x_1, x_2). \quad (3.27)$$

Coming to the problem of a condensing gas we need to define the interactions $f_{i_1 j_1}, f_{i_1 j_2}, f_{i_2 j_2}$ for the three possible types of particle interaction. The grand partition function of the system is given by (cf. 3.7)

$$\Xi(\lambda_1, \lambda_2, V, T) = 1 + \sum_{N_1, N_2=1}^{\infty} \frac{(\lambda_1 \eta_1)^{N_1} (\lambda_2 \eta_2)^{N_2}}{N_1! N_2!} Q_{N_1, N_2} \quad (3.28)$$

and applying the first theorem we obtain

$$(M9) \quad \frac{1}{V} \ln \Xi = \sum_{p_1 p_2=1}^{\infty} b_{p_1 p_2}(V, T) \lambda'_1{}^{p_1} \lambda'_2{}^{p_2}$$

where the cluster integral $b_{p_1 p_2}$ is given by (taking all the $h_i = 1$ for simplicity)

$$(M9a) \quad V b_{p_1 p_2} = \frac{1}{p_1! p_2!} \sum_{(c_{p_1 p_2})} \int d\mathbf{r}_1^{(1)} \dots d\mathbf{r}_{p_1}^{(1)} \int d\mathbf{r}_1^{(2)} \dots d\mathbf{r}_{p_2}^{(2)} \prod_f f_{i_r j_s}.$$

Thermodynamics then gives the relations

$$(M10) \quad \frac{P}{kT} = \sum_{p_1, p_2=1}^{\infty} b_{p_1 p_2}(T) \lambda'_1{}^{p_1} \lambda'_2{}^{p_2}$$

$$(M11) \quad \rho_1 = \sum_{p_1 p_2=1}^{\infty} p_1 b_{p_1 p_2} \lambda'_1{}^{p_1} \lambda'_2{}^{p_2}$$

$$(M12) \quad \rho_2 = \sum_{p_1 p_2=1}^{\infty} p_2 b_{p_1 p_2} \lambda'_1{}^{p_1} \lambda'_2{}^{p_2}.$$

For the graphical reduction to stars we need to differentiate between rooted graphs with a point of species 1 as a root, and rooted graphs with a point of species 2 as a root. This is because in our graph reduction procedure we need to join the main leaves together at the same root. We therefore define by analogy with (2.27)

$$S(x_1, x_2) = \sum_{q_1, q_2}^{\infty} s_{q_1 q_2} x_1{}^{q_1} x_2{}^{q_2} / q_1! q_2! \quad (q_1 + q_2 \geq 2), \quad (3.29)$$

and by analogy with (2.28)

$$R_1(x_1, x_2) = x_1 \frac{\partial f}{\partial x_1} = \sum_{p_1, p_2=1}^{\infty} p_1 f_{p_1 p_2} x_1{}^{p_1} x_2{}^{p_2} / p_1! p_2! \quad (3.30)$$

$$R_2(x_1, x_2) = x_2 \frac{\partial f}{\partial x_2} = \sum_{p_1, p_2=1}^{\infty} p_2 f_{p_1 p_2} x_1{}^{p_1} x_2{}^{p_2} / p_1! p_2!. \quad (3.31)$$

We then find by analogy with (2.29),

$$\ln R_1(x_1, x_2) - \ln x_1 = \frac{\partial S}{\partial x_1} (R_1, R_2) \quad (3.32)$$

$$\ln R_2(x_1, x_2) - \ln x_2 = \frac{\partial S}{\partial x_2} (R_1, R_2). \quad (3.33)$$

Applying these formulae to a condensing gas mixture we obtain

$$(M13) \quad \ln \rho_1 - \ln \lambda'_1 = \Sigma k_1 B_{k_1 k_2} \rho_1^{k_1-1} \rho_2^{k_2} \quad (k_1 + k_2 \geq 2)$$

$$(M14) \quad \ln \rho_2 - \ln \lambda'_2 = \Sigma k_2 B_{k_1 k_2} \rho_1^{k_1} \rho_2^{k_2-1}$$

Here $B_{k_1 k_2}$ is defined by

$$(M13a) \quad k_1! k_2! B_{k_1 k_2} = \lim_{V \rightarrow \infty} \frac{1}{V} \sum_{(S_{k_1 k_2})} \int d\mathbf{r}_1^{(1)} \dots d\mathbf{r}_{k_1}^{(1)} \\ \int d\mathbf{r}_1^{(2)} \dots d\mathbf{r}_{k_2}^{(2)} \prod_l f_{l_r j_s}$$

By generalizing the thermodynamic relation (3.18) and integrating we find that

$$(M15) \quad \frac{P}{kT} = \frac{1}{V} \ln \Xi = \rho_1 + \rho_2 - \sum_{k_1, k_2=0}^{\infty} (k_1 + k_2 - 1) B_{k_1 k_2} \rho_1^{k_1} \rho_2^{k_2} \\ (k_1 + k_2 \geq 2).$$

Finally Mayer (1939) has shown how to generalize (M7) to obtain the $b_{p_1 p_2}$ in terms of the $B_{k_1 k_2}$. Writing

$$G_{k_1 k_2} = \sum_{k_1=0}^{\infty} \sum_{k_2=0}^{\infty} k_1^{m_1} k_2^{m_2} B_{k_1 k_2} t_1^{k_1} t_2^{k_2} \quad (3.34)$$

then

$$(M16) \quad p_1 p_2 b_{p_1 p_2} = \text{coefft of } t_1^{p_1} t_2^{p_2} \text{ in } G_{11} \exp\left(\frac{p_1 G_{10}}{t_1} + \frac{p_2 G_{01}}{t_2}\right).$$

The first few terms ($p_1 + p_2 \leq 6$) have been given explicitly by Domb and Hiley (1962). They begin as follows

$$\begin{aligned} b_{20} &= B_{20} \\ b_{11} &= B_{11} \\ b_{30} &= B_{30} + 2B_{20}^2 \\ b_{21} &= B_{21} + 2B_{11}B_{20} + \frac{1}{2}B_{11}^2 \\ b_{40} &= B_{40} + 6B_{30}B_{20} + \frac{1}{3}B_{20}^3 \\ b_{22} &= B_{22} + 2(B_{12}B_{20} + B_{21}B_{02}) + 2B_{11}(B_{12} + B_{21}) \\ &\quad + B_{11}(2B_{20} + B_{12})(2B_{02} + B_{21}) \\ b_{31} &= B_{31} + 4B_{21}B_{20} + B_{21}B_{11} + 3B_{30}B_{11} + \frac{1}{6}B_{11}(6B_{20} + B_{11})^2 \end{aligned} \quad (3.35)$$

D. Correlation functions

The grand partition function provides information about the bulk thermodynamic properties of an N -particle system in equilibrium. If we wish to understand more of the internal structure of the system, we must examine the

correlations between pairs, triplets, ... of molecules, and how they behave as a function of temperature and intermolecular distance. It is a remarkable feature of cluster-integral theory that diagrammatic expansions can be obtained for these correlations which exactly parallel the expansions for the grand partition function.

We first define the canonical molecular distribution functions as follows

$$\begin{aligned} n_1^{(N)}(\mathbf{r}_1) &= \frac{Z_N^{-1}}{(N-1)!} \int_V \dots \int \exp - \beta \Phi_N d\mathbf{r}_2 \dots d\mathbf{r}_N \\ n_2^{(N)}(\mathbf{r}_1, \mathbf{r}_2) &= \frac{Z_N^{-1}}{(N-2)!} \int_V \dots \int \exp - \beta \Phi_N d\mathbf{r}_3 \dots d\mathbf{r}_N \\ n_s^{(N)}(\mathbf{r}_1, \dots, \mathbf{r}_s) &= \frac{Z_N^{-1}}{(N-s)!} \int_V \dots \int \exp - \beta \Phi_N d\mathbf{r}_{s+1} \dots d\mathbf{r}_N \end{aligned} \quad (3.36)$$

They are all functions of T , V , and N . The corresponding grand-canonical molecular distribution functions are defined by

$$\begin{aligned} \rho_1(\mathbf{r}_1) &= (\Xi)^{-1} \sum_{N=1}^{\infty} \lambda'^N Z_N n_1^{(N)}(\mathbf{r}_1) \\ \rho_2(\mathbf{r}_1, \mathbf{r}_2) &= (\Xi)^{-1} \sum_{N=2}^{\infty} \lambda'^N Z_N n_2^{(N)}(\mathbf{r}_1, \mathbf{r}_2) \\ \rho_s(\mathbf{r}_1, \dots, \mathbf{r}_s) &= (\Xi)^{-1} \sum_{N=s}^{\infty} \lambda'^N Z_N n_s^{(N)}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_s) \end{aligned} \quad (3.37)$$

These are functions of T , V and λ .

When we expand the ρ_s in terms of λ we obtain an expansion analogous to that of Theorem I of II.B1 in terms of connected graphs. This can be most simply derived by the method of functional differentiation (Volterra, 1930) and we shall follow the procedure of Stell (1964). A functional derivative is a straightforward generalization of a derivative of a function of many variables

$$dF(x_1, \dots, x_n) = \sum_i \frac{\partial F}{\partial x_i} dx_i \quad (3.38)$$

in which the index i is allowed to take on a continuum of values. x_i thus becomes $x_i(t)$ and instead of (3.38) we have

$$\int \frac{\delta F[x(t)]}{\delta x(t)} dx(t) \quad (3.39)$$

where $\delta F[x(t)]/\delta x(t)$ is used to denote the functional derivative. The derivative is itself a function of $x(t)$, i.e. a functional. If we change $x(t)$ in any functional relation to $x(t) + \delta x(t)$ and obtain a first order term of the form (3.39) we can immediately write down the functional derivative $\delta F[x(t)]/\delta x(t)$.

In the configurational integral (3.1) let us focus attention on $\psi(\mathbf{r}_1)$. If we change this to $\psi(\mathbf{r}_1) + \delta\psi(\mathbf{r}_1)$ and compare the result with (3.39) we deduce that

$$\frac{\delta Q_N}{\delta\psi(\mathbf{r}_1)} = -\frac{\beta}{N!} \int_V \dots \int_V \exp -\beta\Phi_N d\mathbf{r}_2 \dots d\mathbf{r}_N \quad (3.40)$$

and hence that

$$\Xi\rho_1(\mathbf{r}_1) = h_1 \frac{\delta\Xi}{\delta h_1} (h_i = \exp - \beta\psi_i). \quad (3.41)$$

Similarly,

$$\Xi\rho_s(\mathbf{r}_1 \dots \mathbf{r}_s) = \left(h_1 \frac{\delta}{\delta h_1}\right) \left(h_2 \frac{\delta}{\delta h_2}\right) \dots \left(h_s \frac{\delta}{\delta h_s}\right) \Xi \quad (3.42)$$

However if we differentiate $\ln\Xi$ instead of Ξ we find the *cumulants* of the ρ_i (M1d) instead of the *moments*

$$[\rho_2(\mathbf{r}_1, \mathbf{r}_2)]_c = \rho_2(\mathbf{r}_1, \mathbf{r}_2) - \rho_1(\mathbf{r}_1)\rho_1(\mathbf{r}_2) = h_1 h_2 \frac{\delta^2(\ln\Xi)}{\delta h_1 \delta h_2} \quad (3.43)$$

$$\rho_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = h_1 h_2 h_3 \frac{\delta^3 \ln\Xi}{\delta h_1 \delta h_2 \delta h_3}$$

We know that $\ln\Xi$ can be expressed as an expansion in λ' in terms of connected graphs, and each time we operate on an integral in p dimensions corresponding to a connected graph (M1a) with $h_i \delta/\delta h_i$ we obtain the corresponding integral in $(p-1)$ dimensions with the variable r_i fixed. We follow the standard convention of denoting a fixed variable by an open circle, e.g.

$$\begin{array}{ccc} \circ & \text{---} & \bullet \\ | & & 2 \end{array} = \frac{1}{V} \int d\mathbf{r}_2 f_{12} h_1 h_2 \quad (3.44)$$

$$\begin{array}{ccc} & \bullet & \\ & / \diagdown & \\ \circ & & \circ \\ | & & 2 \end{array} = \frac{1}{V} \int d\mathbf{r}_3 f_{13} f_{23} h_1 h_2 h_3$$

We can then easily derive the diagrammatic expansion

$$(M16a) \quad [\rho_2(\mathbf{r}_1, \mathbf{r}_2)]_C =$$

The prescription for obtaining diagrams is to run through each labelled connected graph and root the pair of points 1 and 2. We thus define the cluster integrals analogous to (M1a) as follows

$$(M16b) \quad b_p(\mathbf{r}_1, \mathbf{r}_2, V, T) = \frac{1}{V p!} \sum_{(G_p)} \int \dots \int d\mathbf{r}_3 \dots d\mathbf{r}_{p+2} \prod_i f_{ij} \prod_{i=1}^{p+2} h_i$$

where the sum is taken over all connected graphs of $(p + 2)$ points with two points rooted and the remainder labelled. We then have as the analogue of (M.1)

$$(M16) \quad [\rho_2(\mathbf{r}_1, \mathbf{r}_2)]_C = \lambda'^2 f_{12} h_1 h_2 + \sum_{p=1}^{\infty} b_p(\mathbf{r}_1, \mathbf{r}_2, V, T) \lambda'^{p+2}$$

This formula is valid for finite V and forces of any range, and can be generalized to take account of non-central forces.

For short range forces the $b_p(\mathbf{r}_1, \mathbf{r}_2, V, T)$ tend to a limit $b_p(\mathbf{r}_1, \mathbf{r}_2, T)$ independent of V , and by analogy with (3.13) we write

$$b_1(\mathbf{r}_1, \mathbf{r}_2, T) =$$

$$2! b_2(\mathbf{r}_1, \mathbf{r}_2, T) =$$

| | | | | | | | |
|---|--|-----|--|-----|--|-----|--|
| 2 | | + 2 | | + 2 | | + 2 | |
| + | | + 2 | | + 2 | | | |

$$\begin{array}{ccccccc}
 +2 & \text{Diagram 1} & + & \text{Diagram 2} & + & \text{Diagram 3} & +2 \\
 \text{Diagram 1} & \text{Diagram 2} & \text{Diagram 3} & \text{Diagram 4} & \text{Diagram 5} & \text{Diagram 6} & \text{Diagram 7} \\
 +2 & \text{Diagram 8} & +2 & \text{Diagram 9} & + & \text{Diagram 10} & + \\
 \text{Diagram 8} & \text{Diagram 9} & \text{Diagram 10} & \text{Diagram 11} & & \text{Diagram 12} & \text{Diagram 13}
 \end{array} \quad (3.45)$$

The generalization to $\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_s$ is immediate.

We now change to the density as independent variable using (M3), but remembering that the density corresponds to a sum over all single-rooted connected graphs. Our previous procedure (Theorem II of II.B1) was to decompose the general single-rooted connected graph representing the main leaf $R_1(x)$ into a star “base” and rooted trees hung on its vertices. We must now follow the same procedure for a general two-rooted connected graph to obtain a diagrammatic representation of $[\rho_2(\mathbf{r}_1, \mathbf{r}_2)]_c$. This formula applies only under the restricted conditions outlined previously for a density expansion.

It is clear that our “base” will now consist of all connected graphs rooted at 1 and 2 having no articulation points. Following a similar argument to that used previously we obtain the diagrammatic expansion for the general two rooted connected graphs in the form:

$$\begin{array}{ccccc}
 \text{Diagram 1} & + & \text{Diagram 2} & + & \text{Diagram 3} \\
 \text{Diagram 4} & + & \text{Diagram 5} & + & \text{Diagram 6}
 \end{array} \quad (3.46)$$

We notice that after the first diagram for each term with 1 and 2 unconnected there is a corresponding diagram with 1 and 2 connected, and the two diagrams can be combined into a single diagram with a weight factor $1 + f_{12} = \exp - \beta\phi_{12}$. Hence adding the term ρ^2 , which is equivalent to the diagram



we can conveniently write by analogy with (M6)

$$(M17) \quad \rho_2(\mathbf{r}_1, \mathbf{r}_2) = \rho^2 \exp - \beta\phi_{12} \left[1 + \sum_{k=1}^{\infty} B_k(\mathbf{r}_1, \mathbf{r}_2, T) \rho^k \right]$$

where

$$(M17a) \quad B_k(\mathbf{r}_1, \mathbf{r}_2, T) = \frac{1}{k!} \sum_{(S_k)} w(S_k)$$

the sum being taken over all k -point graphs with no articulation points joining 1 and 2 (1 and 2 are not included in the k and there is no line joining 12). By analogy with (3.45) we write

$$\begin{aligned} B_1(\mathbf{r}_1, \mathbf{r}_2, T) &= \text{Diagram of a single vertex above two vertices labeled 1 and 2.} \\ 2!B_2(\mathbf{r}_1, \mathbf{r}_2, T) &= \begin{array}{c} \text{Diagram of a square with four vertices labeled 1 and 2 at the corners, plus sign,} \\ \text{Diagram of a square with vertices 1 and 2 at the top and right corners, plus sign,} \\ +2 \end{array} + 2 \begin{array}{c} \text{Diagram of a triangle with vertices 1 and 2 at the base, plus sign,} \\ \text{Diagram of a rectangle with vertices 1 and 2 at the bottom, plus sign,} \\ +2 \end{array} \end{aligned} \quad (3.47)$$

The generalization of (M17) to $\rho_s(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_s)$ needs a little care since the irreducible cluster integrals correspond to all non-articulated graphs joining any number from 2 to s of the roots 1, 2 ... s . It is possible to reduce this set of diagrams further, and we refer to Uhlenbeck and Ford (1962, p. 163–6) for details.

IV. Lattice Constants or Embeddings

A. General properties

1. Historical introduction

The first development of series expansions for a lattice model was due to Opechowski (1937) who followed a suggestion of Kramers to derive a high temperature expansion for the Heisenberg model of spin $\frac{1}{2}$, $H(\frac{1}{2})\dagger$. The method was then applied by Kramers and Wannier (1941) to $I(\frac{1}{2})$ both at high and low temperatures, the major aim of the expansions being to test the region of validity of standard closed form approximations (see Burley

[†] We shall follow the notation of Domb (1970) for the Ising and Heisenberg models; $H(s)$ denotes the Heisenberg model of spin s , and $I(s)$ the corresponding Ising model. Unless stated specifically otherwise we consider a model with nearest neighbour interactions; d denotes the dimensions of the lattice and D the dimension of spin (following Stanley in Chapter 7).

in Vol. 2, Chapter 9). The use of extensive series expansions to estimate critical behaviour was first suggested by Domb (1949) for $I(\frac{1}{2})$ ($d = 2$) and was applied by Wakefield (1951) to the specific heat of $I(\frac{1}{2})$ ($d = 3$). A more detailed investigation of $I(\frac{1}{2})$ was then undertaken by Domb and Sykes (1956, 1957a, b). (For an historical survey of the application to the Heisenberg model see Rushbrooke, Baker and Wood, this volume, Chapter 5.)

The calculation of terms in series expansions can be divided into two parts:—(a) One which is independent of lattice structure but which involves weighting of configurations and varies from model to model. (b) One which depends on the particular lattice studied. For example, for the l th term of a high temperature expansion, (b) is related to the number of configurations of different types which can be constructed from l different *bonds* of the lattice; for low temperature expansions for $I(\frac{1}{2})$ it is the number of configurations which can be constructed from v different *vertices* of the lattice.

Since these latter numbers play a fundamental role for all interacting systems on a lattice, Domb and Sykes (1957b) introduced the term *lattice constants* to describe them, and showed how they could be calculated in an elementary way for small l and v . Two systems were introduced corresponding to the above problems, *high temperature* and *low temperature* lattice constants. Each linear graph of l lines gives rise to one lattice constant of each type, and following the graph terminology in II.A1 they defined *connected*, *disconnected*, and *star* lattice constants. A primitive notation was adopted at first in which p_{lx} denotes the high temperature lattice constant of a connected graph of l lines, x being a suffix to distinguish between different types of connected graph; P_{lx} denotes the corresponding low temperature lattice constant. Lattice constants corresponding to disconnected graphs (*separated lattice constants*) are denoted by $[p_{lx}, p_{mx}]$. Lattice constants are defined as the number *per site* for a lattice wrapped on a torus thus avoiding end effects. Hence for a lattice with N sites there are Np_{lx} configurations of type x which can be constructed from l bonds of the lattice. Low temperature lattice constants differ from their high temperature counterparts by the property that all vertices which are nearest neighbours in the lattice must be connected by the nearest neighbour bond.

For most applications a line classification was found to be more convenient than a vertex classification. However if necessary the number of vertices can also be indicated by p_{lx}^v . The above classification is satisfactory if part (a) of the calculation above (which is concerned with the *weighting* of graphs) depends only on their topology and not for example on the angles between bonds. This applies to most calculations concerning the Ising and Heisenberg models and percolation processes; however there are problems in which the topology alone is insufficient, and a sub-classification must be undertaken (e.g. Domb, 1971).

Extensive tables of lattice constants were prepared by Domb and Sykes and were published in the review article by Domb (1960). These tables proved useful for the calculation of the first few terms of series expansions for several different lattice models. The lattice constants in the tables were calculated by elementary means without the use of computers, and a number of different methods of calculation are described in Chapter 5 of the above review. It was shown that *disconnected* lattice constants can be reduced to connected lattice constants, and *connected* lattice constants corresponding to graphs with articulation points can be reduced to *star* lattice constants. Thus in principle star lattice constants represent the basic data from which all other quantities can be derived. However, the process of reduction is often complicated and it is simpler to calculate connected lattice constants directly. It was also shown that the set of low temperature lattice constants can be derived from the set of high temperature lattice constants and *vice versa*.

As an illustration of the early use of lattice constants we quote from Domb and Sykes (1957b) the formula for the high temperature series expansion of the partition function of the Ising model (for notation see Domb 1960).

$$\begin{aligned} \ln Z_N &= N \ln 2 + \frac{q}{2} \cosh K + \Sigma a_r (\tanh K)^r \\ a_3 &= p_3 \\ a_4 &= p_4 \\ a_5 &= p_5 \\ a_6 &= p_6 - p_{5a} - \frac{1}{2} p_3 \\ a_7 &= p_7 - 2p_{7g} - p_{6b} - 2p_{5a}. \end{aligned} \tag{4.1}$$

Here $q = 2p_1$ is the co-ordination number of the lattice. To determine the numerical values of the terms for any lattice it is only necessary to read off the p_{lx} from the tables quoted above and to substitute in (4.1).

When the need arose to extend calculations to higher values of l the above notation proved inadequate. In a definitive paper Sykes *et al.* (1966) introduced a new notation based on the homeomorphic classification of graphs discussed in II.A5 which was more comprehensive and flexible. At the same time they pointed out that lattice constants are identical with what graph theorists usually term *embeddings*, the high temperature set corresponding to *weak embeddings* and the low temperature set to *strong embeddings*. We shall summarize the terminology and results of this paper in the next Sections.

During the early 1960's computers began to be used for calculating lattice constants principally by Eve at the University of Newcastle-upon-Tyne and Martin at the National Physical Laboratory. Subsequently there has been a steady improvement in the speed of computers available and in the design

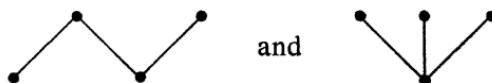
of programmes, and nowadays higher order lattice constants are nearly always calculated by computer (for details see Martin, this volume, Chapter 2). At the same time theoretical developments (to be discussed in Section IV.B2) showed how problems could be formulated to take account only of connected lattice constants. Although this involves a complication in the weighting of the graphs, the result is usually a substantial shortening of the calculation. Hence attention has been confined in recent years to connected and star lattice constants. The most important compilation of connected lattice constants is that of Baker *et al.* (1967) which provides tables for all graphs of up to 8 lines, and for a substantial number of graphs of 9 and 10 lines. For star graphs it is possible to proceed much further (see p. 38, Table V) and Sykes and his collaborators at King's College have derived all star lattice constants of up to 12 lines and a substantial number of lattice constants of 13 and 14 lines. For certain loose packed lattices (e.g. the simple cubic) they have been able to go as far as 20 lines. More details of data available will be given in Section IV.C.

2. Notation and terminology

We shall now add a number of definitions to those in Section II following Sykes *et al.* (1966). It is convenient to assign reference symbols to achieve a systematic arrangement of the various types of linear graph, and we use g_i to denote a graph and order the subscripts i as follows. We denote the number of vertices and lines in g_i by $v(g_i)$, $l(g_i)$, respectively, and abbreviate to v_i , l_i . We order the subscripts so that g_i occurs before g_j if $v_i < v_j$; or if $v_i = v_j$ then if $l_i < l_j$. Thus the sequence begins



If $v_i = v_j$ and $l_i = l_j$ of which the first example is the pair



it is usually sufficient for our present purposes to assign the suffixes arbitrarily. If necessary we could use a method such as was introduced by Nagle (1966) (see Section II.A6) to define a precise order.

In a similar manner we assign symbols c_i , s_i to the various types of connected and star graphs respectively, arranged in the same dictionary order.

We abbreviate $v(c_i)$, $l(c_i)$, $v(s_i)$, $l(s_i)$ whenever it is clear from the context which graph dictionary is being used. For a general arbitrary graph G we abbreviate $v(G)$, $l(G)$ to v_G , l_G and likewise other quantities whenever the meaning is clear.

We denote the number of connected components in g_i by $n(g_i)$ or n_i . We have already defined the *cyclomatic number* $c(g_i)$ in (2.3) by

$$c_i = l_i - v_i + n_i$$

and have noted that it is invariant under the suppression or insertion of vertices of degree 2. We have also defined homeomorphic graphs and have noted that they have the same cyclomatic number.

If g_r and g_s are any two graphs of (4.2) we denote by $g_r \cup g_s$ (union of g_r and g_s) the disconnected graph made up of g_r and g_s . Thus, for example, $g_5 = g_1 \cup g_3$ and $g_4 = g_1 \cup g_2 = g_1 \cup g_1 \cup g_1$.

A graph H is a *subgraph* of G when all its vertices and edges are vertices and edges of G . If A is a subset of the vertices of G , the †*section-graph* $K(A)$ is defined as the subgraph of G consisting of the vertices A and all the edges in G which connect two vertices of A . A *partial* graph P of G is a subgraph of G having the same vertices as G .

Two subgraphs are *vertex-disjoint* if they have no vertices (and hence no edges) in common. Two subgraphs are *edge-disjoint* if they have no edges in common. If H_1 and H_2 are two subgraphs of G we define their *sum graph* $H = H_1 + H_2$ to be the subgraph formed from all the vertices and edges of H_1 and H_2 or both.

Any subgraph G' of a graph G which is isomorphic with a graph g is said to represent an *embedding* of g in G in the *weak* sense (*weak embedding*). Any section graph G^+ of G which is isomorphic with g is said to represent an embedding of g in G in the *strong* sense (*strong embedding*). Evidently a strong embedding is always a weak embedding but the converse statement is not necessarily true. Any weak embedding of g in G defines a subset V' of the vertices of G . We call the section graph with vertices V' the *associated section graph* of the embedding.

The *lattice constant* of a graph g on a graph G is defined as follows:

- (a) Weak (or high temperature) $(g; G) =$ Number of subgraphs of G isomorphic with g = Number of different weak embeddings of g in G .
- (b) Strong (or low temperature) $(g; G) =$ Number of section graphs of G isomorphic with g = Number of different strong embeddings of g in G .

† In French the term corresponding to section graph is *sous-graphe*. Dr. Sykes has pointed out that in the English version of C. Berge (1958) this term has been mistranslated as *sub-graph*. Similarly *sous-graph partial* which corresponds to *sub-graph* has been mistranslated as *partial sub-graph*.

The graph G may be a lattice L of \mathcal{N} sites with a cyclic boundary condition in which case because of the symmetry every lattice constant which does not loop the torus contains a factor \mathcal{N} . It is therefore convenient in this case to redefine the lattice constants *per site* so as to eliminate \mathcal{N} .

It is sometimes convenient for conciseness to revert to the older terminology defined in the previous Section, and we then have

$$(g;L) = p_{lx}, \quad [g;L] = P_{lx} \quad (4.3)$$

where l is the number of lines of g .

For any graph G with v vertices and l lines we have two sets of lattice constants:

- (a) The weak set $(g_i;G)$ for all g_i with $v_i \leq v$ and $l_i \leq l$.
- (b) The strong set $[g_i;G]$ for all g_i with $v_i \leq v$ and $l_i \leq l$.

The set of lattice constants is thus a finite set. For example, the lattice constants of the triangle g_7 are

$$\begin{array}{ll} (g_1;g_7) = 3 & [g_1;g_7] = 3 \\ (g_2;g_7) = 3 & [g_2;g_7] = 0 \\ (g_3;g_7) = 3 & [g_3;g_7] = 3 \\ (g_4;g_7) = 1 & [g_4;g_7] = 0 \\ (g_5;g_7) = 3 & [g_5;g_7] = 0 \\ (g_6;g_7) = 3 & [g_6;g_7] = 0 \\ (g_7;g_7) = 1 & [g_7;g_7] = 1 \end{array} \quad (4.4)$$

It will be noted that many more of the strong lattice constants are zero than of the weak lattice constants, and this is found to be an important characteristic difference.

3. Conversion matrices

We shall now show (following Sykes *et al.*, 1966) that the two sets of strong and weak lattice constants are linearly related, and given any one set for a given graph it is possible to deduce the other set.

Theorem

If $g_i^{(v)}$ is a graph with v vertices and G any graph then

$$(g_i^{(v)}; G) = \sum_j (g_i^{(v)}; g_j^{(v)}) [g_j^{(v)}; G], \quad (4.5)$$

where the summation is taken over all graphs $g_j^{(v)}$ with v vertices.

Proof

Any strong embedding $g_j^{(v)}$ in G will be the associated section graph of $(g_i^{(v)}; g_j^{(v)})$ weak embeddings of $g_i^{(v)}$ in G . By definition the number of these strong embeddings is $[g_j^{(v)}; G]$ and since every embedding of $g_i^{(v)}$ has one, and only one, associated section graph, the result follows.

Corollary

The above result remains valid for connected graphs $c_i^{(v)}$ and stars $s_i^{(v)}$, i.e.

$$(c_i^{(v)}; G) = \sum_j (c_i^{(v)}; c_j^{(v)}) [c_j^{(v)}; G] \quad (4.6)$$

$$(s_i^{(v)}; G) = \sum_j (s_i^{(v)}; s_j^{(v)}) [s_j^{(v)}; G] \quad (4.7)$$

This is because the associated section graph of an embedding of a connected graph must be a connected graph and that of a star must be a star.

The results (4.5) (4.6) and (4.7) are independent of the lattice G , and it is convenient to condense the notation and write

$$(g_i; G) = p_i, \quad [g_i; G] = P_i, \quad (g_i; g_j) = g_{ij}. \quad (4.8)$$

In this notation we have

$$p_i = \sum_j g_{ij} P_j \quad (v_i = v_j) \quad (4.9)$$

or

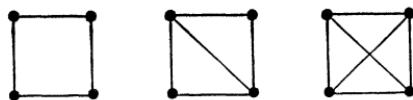
$$\mathbf{p}^{(v)} = \mathbf{g}^{(v)} \mathbf{P}^{(v)} \quad (4.10)$$

where $\mathbf{p}^{(v)}$ and $\mathbf{P}^{(v)}$ are column vectors the elements of which are the weak and strong lattice constants, respectively, of all graphs with v vertices, and $\mathbf{g}^{(v)}$ is a square matrix which we call the v th order conversion matrix for all graphs. We can define similarly $\mathbf{c}^{(v)}$ and $\mathbf{s}^{(v)}$. It is clear by definition that each of these matrices is triangular.

To give a simple numerical illustrative examples $\mathbf{g}^{(3)}$ is a 4×4 matrix (corresponding to g_4, g_5, g_6, g_7)

$$\mathbf{g}^{(3)} = \begin{vmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \\ 0 & 0 & 1 & 3 \\ 0 & 0 & 0 & 1 \end{vmatrix} \quad (4.11)$$

Similarly, $s^{(4)}$ corresponding to



is a 3×3 matrix

$$s^{(4)} = \begin{vmatrix} 1 & 1 & 3 \\ 0 & 1 & 6 \\ 0 & 0 & 1 \end{vmatrix} \quad (4.12)$$

By definition $c^{(v)}$ and $s^{(v)}$ are principal minors of $g^{(v)}$.

The matrix $g^{(v)}$ has certain very simple properties. For example, it can easily be inverted to give a reciprocal $h(v)$ whose elements can be written

$$h_{ij} = (-1)^{l_i - l_j} g_{ij} \quad (4.13)$$

a result originally due to Martin (private communication).

To prove (4.13) Sykes *et al.* (1966) constructed matrices $m^{(v)}(k)$, $k \geq 1$, where

$$m_{ij}^{(v)}(k) = g_{ij}^{(v)} \quad \text{if } l_j = l_i + k \\ 0 \quad \text{otherwise} \quad (4.14)$$

Denote a v -vertex graph g_i with l lines by $g_i(l)$. Now in proceeding from $g_j(l+k)$ to $g_j(l)$ we must drop k lines, and we do this in two stages dropping first one line and then the remaining $(k-1)$ lines. We can drop the first line in k different ways, and if we therefore form the sum over all h (corresponding to graphs with $(l+k-1)$ lines)

$$\sum_h (g_i(l); g_h(l+k-1)) \times (g_h(l+k-1); g_j(l+k)) \quad (4.15)$$

we will form $(g_i(l); g_j(l+k))$ exactly k times. Hence we have the relation

$$(g_i(l); g_j(l+k)) = \frac{1}{k} \sum_h (g_i(l); g_h(l+k-1)) \\ \times (g_h(l+k-1); g_j(l+k)) \quad (4.16)$$

or

$$m_{ij}^{(v)}(k) = \frac{1}{k} \sum_h m_{ih}^{(v)}(k-1) m_{hj}^{(v)}(1) \quad (4.17)$$

In matrix notation (4.17) becomes

$$\mathbf{m}^{(v)}(k) = \frac{1}{k} \mathbf{m}^{(v)}(k-1) \mathbf{m}^{(v)}(1) \quad (4.18)$$

and therefore

$$\mathbf{m}^{(v)}(k) = \frac{1}{k} [\mathbf{m}^{(v)}(1)]^k \quad (4.19)$$

Now

$$\begin{aligned} \mathbf{g}^{(v)} &= \mathbf{1} + \sum_{k=1}^{\frac{1}{2}v(v-1)} \mathbf{m}^{(v)}(k) \\ &= \mathbf{1} + \sum_{k=1}^{\frac{1}{2}v(v-1)} [\mathbf{m}^{(v)}(1)]^k / k! = \exp \mathbf{m}^{(v)}(1) \end{aligned} \quad (4.20)$$

since $[\mathbf{m}^{(v)}(1)]^k$ is zero for $k > \frac{1}{2}v(v-1)$. But

$$\mathbf{h}^{(v)} = [\mathbf{g}^{(v)}]^{-1} = \exp - \mathbf{m}^{(v)}(1) = \mathbf{1} + \sum_{k=1}^{\frac{1}{2}v(v-1)} (-1)^k \mathbf{m}^{(v)}(k) \quad (4.21)$$

from which the result (4.13) follows immediately.

The recurrence relation (4.10) provides a convenient means of computing $\mathbf{g}^{(v)}$ given $\mathbf{m}^{(v)}(1)$. To determine the elements in $m_{ij}^{(v)}(1)$ we need to find the number of ways of removing a single edge from the graph g_j to give the graph g_i . For small values of v ($v \leq 5$) this can readily be determined by hand, but for higher values it is necessary to use a computer. Details of the construction of the matrix of order 1044 for $v = 7$ are given by Heap (1967).

4. Reduction of lattice constants

We now consider following Sykes *et al.* (1966), the reduction of disconnected lattice constants to connected lattice constants, and of articulated lattice constants to star lattice constants.

Suppose that a graph G is the sum graph of two or more of its subgraphs, for example of the three subgraphs H_1, H_2, H_3 isomorphic with some g_i, g_j, g_k of (4.1). Then

$$G = H_1 + H_2 + H_3. \quad (4.22)$$

Now H_1, H_2, H_3 are weak embeddings of g_i, g_j, g_k in G , and we call (4.22) an *overlap partition* of G into g_i, g_j, g_k . In general there will be more than one possible choice of embeddings of g_i, g_j, g_k in G having G as its sum graph, and we define the total number of such choices as the number of

overlap partitions of G into g_i , g_j , g_k and write this number

$$\{g_i + g_j + g_k = G\}. \quad (4.23)$$

For example, there are three overlap partitions of the triangle g_7 into g_3 and g_6 , and three into g_6 and g_6 . Thus

$$\begin{aligned} \{g_3 + g_6 = g_7\} &= 3 \\ \{g_6 + g_6 = g_7\} &= 3. \end{aligned} \quad (4.24)$$

We call these quantities overlap partitions because in general the component graphs do overlap, and have some, or all, of their edges and vertices in common.

We now show that the lattice constant of any disconnected graph on a graph G can be calculated from the connected lattice constants on G .

Theorem

If g_i and g_j are two graphs $g_i \neq g_j$ and G any graph, then

$$(g_i \cup g_j; G) = (g_i; G)(g_j; G) - \sum_k \{g_i + g_j = g_k^{(v)}\} (g_k^{(v)}; G) \quad (4.25)$$

where the summation is taken over all $g_k^{(v)}$ with $v < v_i + v_j$.

Proof

Let us consider the number of pairs of embeddings $(g_i; G)(g_j; G)$. These divide into two disjoint classes.

(a) Pairs for which the embeddings do not overlap and are vertex disjoint. The number of these is by definition $(g_i \cup g_j; G)$.

(b) Pairs for which the respective embeddings have at least one vertex in common. Then if $g_k^{(v)} = g_i + g_j$ is the sum graph of any such pair of embeddings the number of vertices in g_k must be less than $v_i + v_j$. The number of pairs which have any given g_k as sum graph is simply the number of overlap partitions of g_k into g_i and g_j . Further every such pair of embeddings defines some sum graph and therefore the number of pairs in this class is

$$\sum_k \{g_i + g_j = g_k^{(v)}\} (g_k^{(v)}; G) \quad (4.26)$$

where the summation is taken over all $g_k^{(v)}$ with $v < v_i + v_j$.

If $g_i = g_j$ we must take account of symmetry and when we now consider the number of pairs of embeddings we obtain $(g_i \cup g_i; G)$ twice. Some of the configurations of class (b) may also be repeated because of symmetry; it is useful to start by considering the identical configurations as having different colours and then to allow the colours to become the same.

In (4.25) g_i and g_j need not be connected graphs, and by successive applications of the theorem the weak lattice constant of a many component graph can be expressed as a polynomial in the weak lattice constants of connected graphs. It is important to note that this polynomial is independent of G .

As examples we quote the following results (adapted from Domb, 1960); for convenience we have dropped the graph G in the notation.

$$\begin{aligned} \left(\begin{array}{c} \text{triangle} \\ \text{square} \end{array}, \quad \right) &= \left(\begin{array}{c} \text{triangle} \\ \text{square} \end{array} \right) \left(\begin{array}{c} \text{triangle} \\ \text{square} \end{array} \right) - \left(\begin{array}{c} \text{triangle} \\ \text{square} \end{array} \right) \\ &\quad - 3 \left(\begin{array}{c} \text{triangle} \\ \text{square} \end{array} \right) \left(\begin{array}{c} \text{triangle} \\ \text{square} \end{array} \right) - \left(\begin{array}{c} \text{triangle} \\ \text{square} \end{array} \right) - 2 \left(\begin{array}{c} \text{triangle} \\ \text{square} \end{array} \right) \\ \\ \left(\begin{array}{c} \text{triangle} \\ \text{triangle} \end{array}, \quad \right) &= \frac{1}{2} \left(\begin{array}{c} \text{triangle} \\ \text{triangle} \end{array} \right)^2 - \left(\begin{array}{c} \text{triangle} \\ \text{triangle} \end{array} \right) \\ &\quad - \left(\begin{array}{c} \text{triangle} \\ \text{triangle} \end{array} \right) - \frac{1}{2} \left(\begin{array}{c} \text{triangle} \\ \text{triangle} \end{array} \right) \end{aligned} \tag{4.27}$$

From the existence and properties of conversion matrices it is clear that the strong lattice constant of a many component graph can equally well be expressed as a polynomial in the strong lattice constants of connected graphs.

In a similar manner we can express the lattice constants of articulated graphs as polynomials in the lattice constants of star graphs, but this latter reduction can only be carried out for embeddings in *homogeneous* graphs G . (We term a graph *homogeneous* if all its vertices are equivalent.) In this respect the reduction to connected lattice constants parallels the cluster integrals of Section III.A, and the reduction to star lattice constants parallels the irreducible cluster integrals of Section III.B. Let $c_i \circ c_j$ represent an articulated graph with $v_i + v_j - 1$ vertices formed by putting together connected graphs c_i and c_j and identifying one vertex of each as a common vertex \circ . Consider all different weak embeddings of c_i and c_j which pass through \circ where \circ goes over all vertices of G . The total number will consist of $(c_i \circ c_j; G)$ together with embeddings of sum graphs of c_i and c_j having \circ

as common vertex but for which \circ is not an articulation point. Hence we can write down a relation analogous to (4.25) for $(c_i \circ c_j; G)$. As an example we quote (Domb, 1960)

$$\left(\begin{array}{c} \text{Diagram of } c_1 \circ c_2 \\ \text{with 6 vertices and 9 edges} \end{array} \right) = \frac{9}{2} \left(\begin{array}{c} \text{Diagram of } c_1 \\ \text{with 3 vertices and 3 edges} \end{array} \right)^2 - 2 \left(\begin{array}{c} \text{Diagram of } c_2 \\ \text{with 4 vertices and 4 edges} \end{array} \right) - \frac{3}{2} \left(\begin{array}{c} \text{Diagram of } c_1 \circ c_2 \\ \text{with 3 vertices and 3 edges} \end{array} \right) \quad (4.28)$$

As a generalization of an articulation point or *cut-point* an *articulation* or *cut-set* of vertices of a connected graph C is defined as a set whose deletion, together with all incident edges makes the graph disconnected. The above reduction procedure can be applied to connected graphs having cut-sets. For example, for a pair of cut-points by considering all pairs of triangles passing through the pair we can derive the following relation (Domb, 1960)

$$2 \left(\begin{array}{c} \text{Diagram of } c_1 \circ c_2 \\ \text{with 6 vertices and 9 edges} \end{array} \right) = 9 \left(\begin{array}{c} \text{Diagram of } c_1 \\ \text{with 3 vertices and 3 edges} \end{array} \right)^2 / \left(\begin{array}{c} \text{Diagram of } c_2 \\ \text{with 4 vertices and 4 edges} \end{array} \right) - 3 \left(\begin{array}{c} \text{Diagram of } c_1 \circ c_2 \\ \text{with 3 vertices and 3 edges} \end{array} \right) \quad (4.29)$$

However, the validity of (4.29) is restricted to *regular* graphs in which all edges as well as vertices are equivalent.

Although the above reduction procedure is straightforward in principle it rapidly becomes tedious for higher order terms, and nowadays lattice constants of articulated graphs are usually counted directly on a computer by a programme such as that described by Martin (this volume, Chapter 2).

5. Homeomorphic classification

From the previous Section we see that star lattice constants have a particular theoretical significance, and we shall also find that for a number of important problems in lattice statistics only star lattice constants enter directly. In these cases series expansions can be taken much further than when all connected lattice constants are involved, and special attention has therefore been paid to the classification and enumeration of star lattice constants by the research group at King's College.

We have already referred in Section II.A5 to the homeomorphic classification of stars and in fact this classification was introduced by Sykes *et al.* (1966) with the application to lattice constants in mind. We refer back to Fig. 16 for a list of all HI stars of cyclomatic number $c \leq 4$, and for convenience of reference a particular HI star will be described as a *topology*.

Thus the only topology with $c = 1$ is a polygon (p topology). Normal round brackets () are used to denote weak lattice constants, and square brackets [] to denote strong lattice constants; $(l)_p$ denotes the weak lattice constant of an l -gon, and for example for the f.c.c. lattice we have

$$(4)_p = 33, \quad [4]_p = 3. \quad (4.30)$$

For $c = 2$ there is only the θ -topology (Fig. 17) and we denote the lattice constant by $(a, b, c)_\theta$. Thus for the same lattice

$$(1, 2, 3)_\theta = 384, \quad [1, 2, 3]_\theta = 24. \quad (4.31)$$

For $c = 3$ the 4 topologies are denoted by $\alpha, \beta, \gamma, \delta$ with the code shown in Fig. 18, and the following are typical results for eight line graphs on the f.c.c. lattice taken from Sykes *et al.* (1966)

$$\begin{aligned} (1, 1; 1, 1; 2, 2)_\alpha &= 78 & [1, 1; 1, 1; 2, 2]_\alpha &= 24 \\ (1, 2; 1; 2; 1, 1)_\beta &= 564 & [1, 2; 1, 2; 1, 1]_\beta &= 24 \\ (1, 2; 1, 2; 2)_\gamma &= 1056 & [1, 2; 1, 2; 2]_\gamma &= 48 \\ (1, 2, 2, 3)_\delta &= 384 & [1, 2, 2, 3]_\delta &= 12 \end{aligned} \quad (4.32)$$

It will be seen from these examples that the notation is of great help in preparing tables of star lattice constants.

6. Simple chains

The lattice constants of simple chains are of particular interest because they correspond to the total number of steps in a self-avoiding walk. (For a general review of self-avoiding walks and their properties see Domb, 1969b.) They also provide an important contribution to the high temperature expansion for the susceptibility of the Ising and Heisenberg models. However since the total number of chain embeddings is large any direct attempt to count them meets with difficulties.

A key counting theorem enunciated by Sykes in 1961 expresses the lattice constant of a chain in terms of lattice constants of closed graphs (i.e. with no vertices of degree 1) which are much fewer in number, and this has led to great progress in chain enumerations. In accordance with the notation of the previous Section we represent the weak lattice constant of an l -chain by $(l)_c$. We now add another bond to $(l)_c$; this can be done in $2\sigma(l)_c$ ways ($\sigma = q - 1$), one from each end. We form $(l+1)_c$ twice together with tadpoles $(a, b)_t$ (Fig. 15) and polygons. If we take into account the number of times these topologies are formed, we obtain the relation

$$(l+1)_c = \sigma(l)_c - \Sigma(a, b)_t - (l+1)(l+1)_p \quad (4.33)$$

where the sum is taken over all tadpoles of $(l+1)$ lines. If we now add another bond to the free end of a tadpole $(a, b)_t$, we form a tadpole $(a+1, b)_t$, together with dumbbells (d) , figure eights (e) (Fig. 15) and θ topologies (Fig. 17). The tadpoles can then be eliminated from (4.33), and when we take account of the number of different ways in which these new topologies are formed we find that

$$(l+1)_c - 2\sigma(l)_c + \sigma^2(l-1)_c = l(l)_p - (l+1)(l+1)_p \\ + 4\Sigma(a, b, c)_d + 4\Sigma(a, b, c)_e + 6\Sigma(a, b, c)_\theta. \quad (4.34)$$

The sums are taken over all d , e , and θ topologies of $(l+1)$ lines.

In the same paper Sykes (1961) showed how lattice constants of other important topologies with two vertices of degree 1 (Ising susceptibility configurations, see Domb, this volume Chapter 6) could be similarly reduced to lattice constants of closed graphs. His work has subsequently been generalized, particularly by McKenzie (1968) who calculated lattice constants of a large number of topologies which arise when two simple chains overlap. (For a different aspect of the elimination of vertices of degree 1 see Nagle (1968) and in this Volume, Chapter 9.)

The strong lattice constant of a simple chain corresponds to a self-avoiding walk with no near-neighbour contacts. In principle the above counting theorem can be generalized, but many other types of closed configuration enter, and it has therefore been found more efficient to count directly by computer (Hioe, 1967).

B. Weighting of lattice constants

We now return to the part of the calculation referred to in Section IV.A1 which is independent of lattice structure, and is in fact a weighting of the lattice constant to be assigned for each particular model. In developing series expansions for lattice models such as those of ferromagnetism it is helpful to exploit the parallelism with cluster integral developments described in Section III. Instead of the configurational integral of continuum theory we need to evaluate the partition function for a graph G ,

$$Z_{\mathcal{N}} = \langle \exp - \beta \mathcal{H} \rangle \\ \text{where } \mathcal{H} = \sum_{\langle ij \rangle} P_{ij} + \sum_i H_i. \quad (4.35)$$

Here P_{ij} is the interaction operator between molecules connected by bonds of G , and H_i is the field at vertex i . The \mathcal{N} vertices of the graph correspond to the volume V of the container (for this reason we use \mathcal{N} to avoid confusion with the number of molecules N in Section III); for a model of spin $\frac{1}{2}$ the

number of molecules corresponds to the number of spins overturned from the reference configuration of aligned spins. For a model of spin s we use a parallel with a many component gas. The partition function Z_N of a magnet corresponds to the grand partition function $\Xi(\lambda, V, T)$ of the gas.

A cluster integral theorem which applies to a container of any shape is paralleled by a lattice theorem which applies to all graphs G . In lattice problems it is often convenient to make use of the *cyclic boundary condition* and to wrap the lattice on a torus. This makes the lattice homogeneous and eliminates surface effects. But for many applications we are interested only in the thermodynamic limit as V for a gas and N for a magnet tend to infinity.

There are three different approaches to high temperature expansions for Z_N :

- (a) The *primitive method* or *moment expansion* which expands Z_N directly in the form

$$Z_N = \langle 1 \rangle - \beta \langle \mathcal{H} \rangle + \frac{\beta^2}{2!} \langle \mathcal{H}^2 \rangle \dots + \frac{(-1)^l \beta^l}{l!} \langle \mathcal{H}^l \rangle \dots \quad (4.36)$$

This gives rise to disconnected lattice constants and corresponds to the direct expansion of the configurational integral (3.4).

- (b) The *connected lattice constant* or *cumulant expansion* which corresponds to the cluster integral expansion (M1) and its generalization (M9).

- (c) The *star lattice constant* expansion which corresponds to the irreducible cluster integral expansion (M5) or (M6) and its generalization to multi-component systems (M15).

The same methods can be applied to other problems arising on lattices such as percolation and cluster size expansions (see Essam, Volume 2, Chapter 6) and we shall now discuss each of the methods in more detail.

1. The primitive method

This is the method first used by Opechowski (1937) and by Kramers and Wannier (1941), and it is described in detail in Domb (1960). On physical grounds, the assumption was made for large N that

$$Z_N(\beta) \sim [Z(\beta)]^N. \quad (4.37)$$

Now the l th term in (4.36) involves all configurations of l bonds of the lattice, multiple bonds being permitted. From the discussion of Section IV.A4 it is clear that the lattice constant of l separated bonds for a torus will be a polynomial of degree N^l . Other lattice constants will correspond to poly-

nomials of lower degree. The averages of the interactions for particular embeddings are independent of \mathcal{N} . Hence the l th term in (4.36) can be written

$$A^{(l)}(\mathcal{N}) = a_l^{(l)} \mathcal{N}^l + a_{l-1}^{(l)} \mathcal{N}^{l-1} + \dots + a_1^{(l)} \mathcal{N}. \quad (4.38)$$

Assuming an expansion for $Z(\beta)$ of the form

$$Z(\beta) = \sum c_l \beta^l, \quad (4.39)$$

and equating the l th term of $Z(\beta)^{\mathcal{N}}$ to (4.38) we readily find that

$$c_l = A^{(l)}(1). \quad (4.40)$$

If instead of $Z(\beta)$ we expand $\ln Z(\beta)$

$$\ln Z(\beta) = \sum b_l \beta^l \quad (4.41)$$

we find instead that

$$b_l = a_1^{(l)}. \quad (4.42)$$

The above approach was developed heuristically, and it was noted empirically that the relationship (4.37) turned out to be an equality for a sufficiently large torus; if one formally took the logarithm of $Z_{\mathcal{N}}$ one found that all terms except those linear in \mathcal{N} vanished identically. The explanation of this remarkable property will emerge in the next section.

We should make a few remarks about the determination of the averages in (4.36). The l th term involves all weak embeddings of graphs of up to l lines in G . However for an embedding of a graph of $l - m$ lines all possible m -line bondings of the graph embedded must be considered. (An m -line bonding of a graph g consists in the replacement of some of the single edges by multiple edges the total number of added edges being m .) The determination of the number of different m -line bondings of a particular graph is an elementary combinatorial problem.

For each m -line bonding we must now determine the averages of the interactions. For classical interactions like the Ising and classical vector models, this is usually elementary and depends only upon the multiplicity of vertices of the bonded graph. For the Heisenberg model of finite spin s it is a more difficult problem and involves the calculation of averages of spin operators (see Rushbrooke, Baker and Wood, this Volume, Chapter 5). The Ising model of spin $\frac{1}{2}$ has a particular simplifying feature that the above expansion can be rearranged to involve only single-bonded graphs (see Domb, this Volume, Chapter 6).

Low temperature expansions for the Ising model were derived in a similar manner. The l th term in the expansion corresponds to all configurations of l overturned spins and since any two adjacent overturned spins carry their

bond interaction with them, this expansion led naturally to strong lattice constants.

For percolation theory the same procedure could be adopted, the l th term in the expansion corresponding to the probability of a group of l black particles in a background of white particles (see Essam, Volume 2, Chapter 6).

2. Connected lattice constant expansion: finite cluster method

The suggestion that cluster integral theory could be applied to the Ising model first came from Fuchs (1942), but a substantial amplification was made by Rushbrooke and Scoins (1955). A somewhat analogous approach to the problem was initiated independently by Yvon in 1945.

To apply the theory of Section III.A to a finite graph G of \mathcal{N} points we take the following values for the potentials in (3.3):

$$\begin{aligned} h_i &= \sum_r \exp -\beta H_r \delta(\mathbf{r}_i - \mathbf{l}_r) \\ f_{ij} &= -\delta(\mathbf{r}_i - \mathbf{r}_j) + \sum_{r,r'} F_{rr'} \delta(\mathbf{r}_i - \mathbf{l}_r) \delta(\mathbf{r}_j - \mathbf{l}_{r'}) \end{aligned} \quad (4.43)$$

where \mathbf{l}_r and $\mathbf{l}_{r'}$ are vertices of G connected by a bond of G . The bond interaction is thus non zero at only two points. We retain a different field H_r for each vertex and a different interaction $F_{rr'}$ for each bond to retain maximum generality.

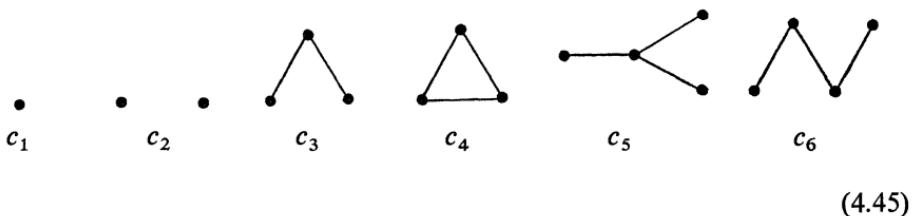
We can therefore use formulae (M1) and (M1a) to evaluate $\ln Z_{\mathcal{N}}$. However each connected graph C_p in (M1a) contains non zero contributions only from bonds and vertices at the ends of the bond. Thus with each C_p we can associate a number of embeddings of connected graphs in G . When we sum over all the C_p to obtain b_p we can group together all the terms corresponding to a particular embedding. We then find that b_p is a linear sum of embeddings each weighted by a function of H_r and $F_{rr'}$ but independent of G . Taking the process a stage further and summing (M1) we find that $\ln Z_{\mathcal{N}}$ is also a linear sum of embeddings each weighted by a function independent of G . If we now put all the H_r equal to H and all the $F_{rr'}$ equal to F , we find for the partition function of any graph G

$$\ln Z_{\mathcal{N}}(G) = \sum_r (c_r; G) \kappa_r(\beta, F, H) \quad (4.44)$$

where the sum is taken over all connected sub-graphs c_r of G , and the weighting functions κ_r depend only on c_r and not on G . We note also that by the method of construction of the functions κ_r , the lowest power of F which can appear in κ_r is F^l where l is the number of bonds of c_r .

Because of the above considerations the formula (4.44) was first put forward by Domb (1960, p. 322, 330), and since this part of the Mayer develop-

ment is valid for an operator interaction, he assumed that the formula would also hold for the Heisenberg model. Domb pointed out that the functions κ_r could be easily calculated from the partition functions of finite clusters. Thus if we denote the first few members of the c_r series as follows,



(4.45)

we derive the following relations:

$$\begin{aligned}\ln Z_1 &= \kappa_1 \\ \ln Z_2 &= \kappa_2 + 2\kappa_1 \\ \ln Z_3 &= \kappa_3 + 2\kappa_2 + 3\kappa_1 \\ \ln Z_4 &= \kappa_4 + 3\kappa_3 + 3\kappa_2 + 3\kappa_1 \\ \ln Z_5 &= \kappa_5 + 3\kappa_4 + 3\kappa_3 + 3\kappa_2 + 4\kappa_1 \\ \ln Z_6 &= \kappa_6 + 2\kappa_5 + 3\kappa_4 + 3\kappa_3 + 4\kappa_2\end{aligned}\quad (4.46)$$

from which the κ_r can be determined as linear functions of the $\ln Z_r$.

A formal proof of relation (4.44) for the Ising and Heisenberg models based on the linked-cluster expansion (see Wortis, this Volume, Chapter 3) was given by Rushbrooke in 1964. He termed the matrix $(c_r; c_s)$ of coefficients in (4.46) which plays a central role in this *finite cluster method* the T matrix. Clearly, it is closely related to the connected lattice constant conversion matrix discussed in Section IV.A3. The method has been of great use for the Heisenberg model of spin $\frac{1}{2}$, and this application is discussed in detail in Chapter 5.

An important generalization of the above result was provided by Sykes *et al.* (1966). They showed that for any weighting of a graph $f(G)$ which has an *extensive property*, i.e. for which

$$f(G \cup G') = f(G) + f(G'), \quad (4.47)$$

a relation of type (4.44) holds, and the above finite cluster theory can be used. Clearly, $\ln Z(G)$ for any type of interaction has an extensive property. But an important new example is the mean number of clusters in a random mixture in percolation theory (Essam, Volume 2, Chapter 6).

The approach of Sykes *et al.* (1966) is independent of the Mayer theory, and uses lattice constant theory above. Let $\pi_i(G)$ denote the set of weak connected lattice constants of a graph G . We know from Section IV.A4

that any function of all the lattice constants of a graph can be reduced to a function of the connected lattice constants. Hence, we can write $f(G)$ in the form

$$f(G) = \psi(G) = \psi[\pi_i(G); t] \quad (4.48)$$

where t is a set of parameters like temperature, magnetic field, or concentration.

It is evident that each connected constant $\pi_i(G)$ satisfies the extensive property since

$$(c_i; G \cup G') = (c_i; G) + (c_i; G'). \quad (4.49)$$

Thus

$$\Psi[\pi_i(G) + \pi_i(G'); t] = \Psi[\pi_i(G); t] + \Psi[\pi_i(G'); t]. \quad (4.50)$$

This relation can then be used to show that $\Psi[\pi_i; t]$ is a *linear* function of the non-negative integers π_i . If the quantities π_i were independently allowed all positive integral values the result would be trivial since by repeated application of (4.50) the unique solution

$$\Psi(\pi_1, \pi_2, \dots; t) = \Psi(0, 0, \dots; t) + \pi_1 \Psi(1, 0, 0, \dots; t) + \pi_2 \Psi(0, 1, 0, \dots; t) + \dots \quad (4.51)$$

would be obtained. However, the quantities π_i are related to one another, and it is necessary to choose a set π_i^* which are linearly related to the π_i and which can independently take all non-negative integral values. Sykes *et al.* (1966) showed how to choose the set π_i^* by subtracting off sub-graphs suitably.

To illustrate the method they took the case of 4 lattice constants corresponding to c_1, c_2, c_3 and c_4 in (4.45). Then

$$\begin{aligned} \pi_4^* &= \pi_4 \\ \pi_3^* &= \pi_3 - (c_3; c_4) \pi_4^* \\ \pi_2^* &= \pi_2 - (c_2; c_3) \pi_3^* - (c_2; c_4) \pi_4^* \\ \pi_1^* &= \pi_1 - (c_1; c_2) \pi_2^* - (c_1; c_3) \pi_3^* - (c_1; c_4) \pi_4^*. \end{aligned} \quad (4.52)$$

The choice of π_3^* ensures that all c_3 which occur *automatically* with c_4 are eliminated; thus π_3^* lists the *independent* occurrences of c_3 . Similarly for π_2^* and π_1^* . Now since $\pi_j^*(G)$ is a linear combination of the set $\pi_i(G)$ it clearly also satisfies the extensive property, and so we may write

$$\Psi(\pi_i; t) = \Psi^*(\pi_i^*; t) \quad (4.53)$$

where

$$\Psi^*[\pi_j^*(G) + \pi_j^*(G'); t] = \Psi^*[\pi_j^*(G); t] + \Psi^*[\pi_j^*(G'); t]. \quad (4.54)$$

Since the π_j^* are independent, this functional relation may be solved to give a solution of the form (4.51), where

$$\begin{aligned}\Psi^*(1, 0, 0, 0; t) &= \Psi(1, 0, 0, 0; t) &= \phi(c_1) \\ \Psi^*(0, 1, 0, 0; t) &= \Psi[(c_1; c_2), 1, 0, 0; t] &= \phi(c_2) \\ \Psi^*(0, 0, 1, 0; t) &= \Psi[(c_1; c_3), (c_2; c_3), 0, 0; t] &= \phi(c_3) \\ \Psi^*(0, 0, 0, 1; t) &= \Psi[(c_1; c_4), (c_2; c_4), (c_3; c_4), 0; t] = \phi(c_4).\end{aligned}\quad (4.55)$$

It thus follows that if $\phi = \Psi(\pi_i(G); t)$ satisfies the extensive property (4.47) then

$$\Psi(\pi_i; t) = \sum_{i=1}^k \pi_i f_i(t) \quad (4.56)$$

where

$$\begin{aligned}f_1(t) &= \phi(c_1) \\ f_2(t) &= \phi(c_2) - (c_1; c_2) f_1(t) \\ f_3(t) &= \phi(c_3) - (c_1; c_3) f_1(t) - (c_2; c_3) f_2(t) \\ f_4(t) &= \phi(c_4) - (c_1; c_4) f_1(t) - (c_2; c_4) f_2(t) - (c_3; c_4) f_3(t).\end{aligned}\quad (4.57)$$

Equations (4.57) follow the same pattern as (4.46). Sykes *et al.* (1966) showed that identical results could be derived for the set of strong lattice constants.

When we apply finite cluster theory to a torus all lattice constants which do not loop the torus are proportional to \mathcal{N} the number of vertices. We now see why in our heuristic construction of $\ln Z_{\mathcal{N}}$ in the previous Section all other powers of \mathcal{N} vanished identically.

Finally, the connection of lattice interacting systems with cluster integrals discussed at the beginning of this Section would lead us to expect that pair correlations $\Gamma(\mathbf{l}_1, \mathbf{l}_2)$ and higher order correlations can also be expressed in terms of connected lattice constants. The most convenient practical way to apply finite cluster theory to this problem for the Ising and Heisenberg models is to construct $\ln Z_{\mathcal{N}}$ for a network in which the points \mathbf{l}_1 and \mathbf{l}_2 are joined by an extra interaction P_{12}' ; and to allow this interaction to tend to zero (see, e.g. Essam, 1970). We then have

$$-\beta \Gamma(\mathbf{l}_1, \mathbf{l}_2) = \frac{\partial}{\partial P_{12}'} (\ln Z_{\mathcal{N}}). \quad (4.58)$$

For percolation theory the correlation is replaced by *pair-connectedness* (see Essam, Volume 2, Chapter 6).

3. Inverse of the T matrix: Moebius inversion†

Equations (4.46) are easy to invert numerically to obtain the κ_r in terms of the $\ln Z_r$; however it is of theoretical interest and importance to derive a general formula for the inverse of the T matrix (or conversion matrix for *connected* lattice constants) in a form analogous to (4.13) (the conversion matrix for *all* lattice constants). Let t_{ij}^* denote the $i-j$ element of \mathbf{T}^{-1} ; Essam (1967) showed that t_{ij}^* could be expressed in terms of *full perimeter lattice constants* which we shall now define.

If G is any graph, G' is said to be a *full perimeter subgraph* of G if all edges of G not in G' (if any) are *incident upon vertices* of G' . The *weak full perimeter lattice constant* $(G'; G)^F$ of G' in G is defined as the number of full perimeter subgraphs of G isomorphic with G' . For example, instead of the matrix (4.46) which gives the values of $(c_r; c_s)$ we have for $(c_r; c_s)^F$ the following values

$$\begin{aligned} (c_1; c_2)^F &= 2, & (c_1; c_3)^F &= 1, & (c_1; c_4)^F &= 0, & (c_1; c_5)^F &= 1 \\ &&&&&& (c_1; c_6)^F &= 0 \\ (c_2; c_3)^F &= 2, & (c_2; c_4)^F &= 3, & (c_2; c_5)^F &= 3, & (c_2; c_6)^F &= 1 \\ (c_3; c_4)^F &= 3, & (c_3; c_5)^F &= 3, & (c_3; c_6)^F &= 2. && \end{aligned} \quad (4.59)$$

Likewise G' is said to be a *full perimeter section graph* of G if all vertices of G not in G' (if any) are *adjacent to vertices* of G' . The *strong full perimeter lattice constant* $[G'; G]^F$ of G' in G is defined as the number of full perimeter section graphs of G isomorphic with G' .

Essam proved the theorem that

$$t_{ij}^* = (-1)^{l_j - l_i} (c_i; c_j)^F, \quad (4.60)$$

where l_i and l_j are the number of lines of graphs i and j , respectively. Thus from (4.59) and (4.60) we can write down the inverse of the matrix (4.46) as follows

$$\left| \begin{array}{cccccc} 1 & 0 & 0 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 3 & -3 & 1 & 0 & 0 \\ -1 & 3 & -3 & 0 & 1 & 0 \\ 0 & 1 & -2 & 0 & 0 & 1 \end{array} \right| \quad (4.61)$$

† I am indebted to Dr. J. W. Essam for introducing me to the topic of Moebius inversion and for supplying the material on which this section is based.

Two interesting particular cases are provided by a linear chain c_n and a polygon p_n :

$$\kappa(c_n) = \ln Z(c_n) - 2 \ln Z(c_{n-1}) + \ln Z(c_{n-2}) \quad (4.62)$$

$$\kappa(p_n) = \ln Z(p_n) - n \ln Z(c_{n-1}) + n \ln Z(c_{n-2}) \quad (4.63)$$

For the matrix of strong embeddings of which the $i - j$ element τ_{ij} is $[c_i; c_j]$, Essam proved that the matrix element of the inverse, τ_{ij}^* , is given by

$$\tau_{ij}^* = (-1)^{v_j - v_i} [c_i; c_j]^F \quad (4.64)$$

where v_i and v_j are the number of vertices of graphs i and j , respectively.

The above results (and a number of similar results in combinatorial analysis) are most readily derived by *Moebius inversion* which we shall now briefly discuss. It is more convenient to deal with *labelled* graphs so that each embedded sub-graph is treated separately. We subsequently treat all graphs which are isomorphic as identical in order to derive results relating to lattice constants.

Let S be the set of all connected sub-graphs of a labelled graph G , and let f be a function defined on S . A new function ϕ may be obtained from f using the relation

$$\phi(g) = \sum_{g' \subseteq g} f(g') \quad \text{for } g, g' \in S. \dagger \quad (4.65)$$

We shall consider the problem of expressing f in terms of ϕ . Defining a zeta function by

$$\zeta(g', g) = \begin{cases} 1 & \text{for } g' \subseteq g \\ 0 & \text{otherwise,} \end{cases} \quad (4.66)$$

relation (4.65) may be rewritten

$$\phi(g) = \sum_{g' \in S} f(g') \zeta(g', g). \quad (4.67)$$

This is a matrix relation, and in order to solve the problem we must find the matrix inverse of ζ .

For our current example $\phi(g)$ corresponds to $\ln Z(g)$ and $f(g')$ corresponds to the functions $\kappa(g')$ on the right-hand side of (4.66). We have encountered another example previously in (4.5) in connection with the conversion matrix for *all* graphs with v vertices; here S is the set of all partial

[†] We write " $g \leq g'$ " if g' is contained in g ; if in addition $g' \neq g$ we write $g' \subset g$. " $g' \in S$ " means g' belongs to S .

graphs (see Section IV.A2) of G , $\phi(g)$ is given by $(g^{(v)}; G)$, and $f(g')$ by $[g'^{(v)}; G]$.

The theory of Moebius inversion relates to *partially ordered sets*. A set S is said to be partially ordered if there is an ordering relation $A \subseteq B$ between pairs of elements in S . (This relation does not usually hold between every pair of elements; if it does the set is *completely ordered*.) Clearly the connected and partial graphs above form a partially ordered set. The ordering relation in these cases is illustrated by means of branching diagrams in Figs 25, 26. Another example which we have encountered in equation (M1c)

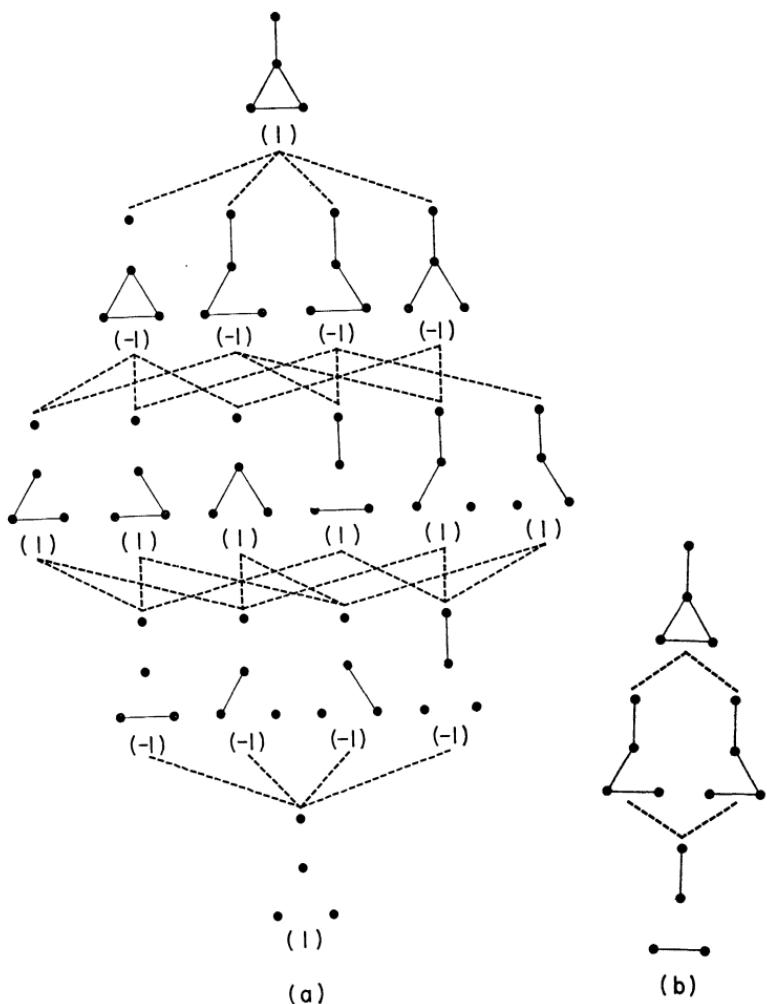


FIG. 25. (a). The partial ordering of the subgraphs of a graph. (b). A segment of a partially ordered set (a).

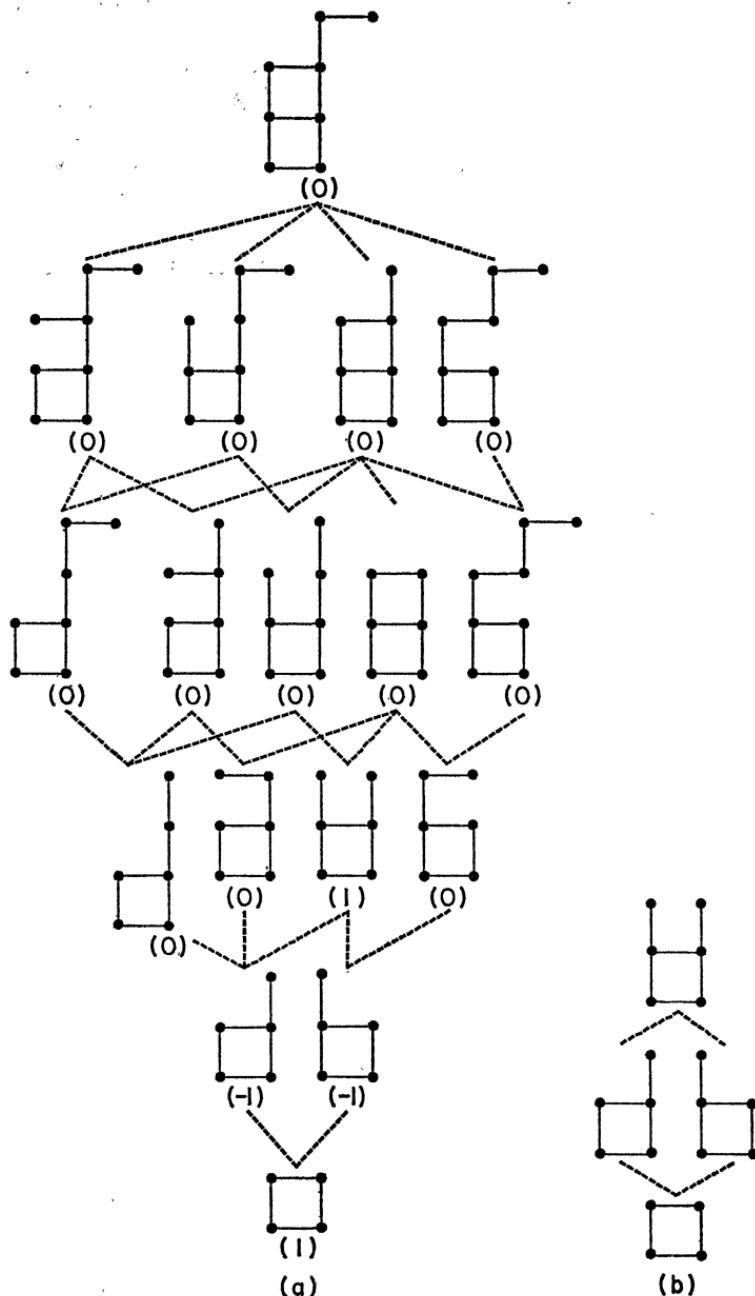


FIG. 26. Partial ordering of the connected subgraphs of a graph. (a). The figure shows a segment terminating on the square (b). The subset Γ_p of the square.

of Section III.A is the set of partitions (or clusters) of r labelled points. We define a partition P_i as contained in a partition P_j if every cluster of P_i is contained in a cluster of P_j . Equation (M1c) is then the analogue of (4.65) which we wish to invert to give (M1d). Finally the most common example in elementary combinatorial analysis is the principle of inclusion and exclusion (e.g. Marshall Hall, 1967, p. 8). Suppose we have N objects and a number of properties $P(1), P(2), \dots, P(n)$. Let N_i be the number of objects with property $P(i)$ and more generally $N_{i_1 \dots i_r}$ the number of objects with properties $P(i_1) P(i_2) \dots P(i_r)$. The N_i and $N_{i_1 \dots i_r}$ are not mutually exclusive. However if \mathcal{N}_i is the number of objects with property i and no others, and $\mathcal{N}_{i_1 \dots i_r}$ the number with properties $i_1, i_2 \dots i_r$ and no others the $\mathcal{N}_{i_1 \dots i_r}$ are mutually exclusive. The set S of properties $P(i_1) P(i_2) \dots P(i_r)$ ($r = 1, 2, \dots, n$) is partially ordered, and we have relations like

$$\begin{aligned} N_i &= \mathcal{N}_i + \sum_{j \neq i} \mathcal{N}_{ij} + \sum_{j,k \neq i} \mathcal{N}_{ijk} \dots \\ N_{ij} &= \mathcal{N}_{ij} + \sum_{k \neq i,j} \mathcal{N}_{ijk} + \sum_{k,l \neq i,j} \mathcal{N}_{ijkl} + \dots \end{aligned} \quad (4.68)$$

which correspond to (4.65). We wish to invert (4.68) and determine the $\mathcal{N}_{i_1 \dots i_r}$ in terms of the $N_{i_1 \dots i_r}$.

We refer the reader to the definitive paper by Rota (1964) for an historical survey of Moebius inversion and for many additional examples of its application. The technique of solution which we now use also follows the discussion in this paper.

A segment $[g, g']$ of S is defined as the set of all elements $g'' \in S$ such that $g \subseteq g'' \subseteq g'$ (see Fig. 25b for an illustration). Define the Moebius function $\mu(g, g')$ by induction over the number of elements g'' of the segment $[g, g']$ as follows:

$$\begin{aligned} \mu(g, g) &= 1 \\ \mu(g, g') &= - \sum_{g \subseteq g'' \subseteq g'} \mu(g, g'') (g \neq g'). \end{aligned} \quad (4.69)$$

Note that the summation in the second line does not include g' , so that the definition implies the relation

$$\sum_{g \subseteq g'' \subseteq g'} \mu(g, g'') = 0 \quad (g \neq g'). \quad (4.70)$$

We also have that if $g \not\subseteq g'$ there are no elements g'' and

$$\mu(g, g') = 0. \quad (4.71)$$

From the definition (4.69), we can calculate $\mu(g, g')$ numerically, and the values are shown in brackets in Figs 25, 26.

From (4.70) we see that μ is the inverse of ζ since

$$\sum_{g'' \in S} \mu(g, g'') \zeta(g'', g') = \sum_{g \subseteq g'' \subseteq g'} \mu(g, g'') = \begin{cases} 1 & g = g' \\ 0 & g \neq g' \end{cases} \quad (4.72)$$

Using the equality of left and right inverses, we may write

$$\sum_{g'' \in S} \mu(g, g'') \zeta(g'', g') = \sum_{g'' \in S} \zeta(g, g'') \mu(g'', g') = \delta(g, g') \quad (4.73)$$

where $\delta(g, g')$ is the unit matrix. Multiplying (4.67) by $\mu(g, g')$, summing over g , and using (4.73) we find for the solution

$$f(g') = \sum_{g \in S} \phi(g) \mu(g, g'). \quad (4.74)$$

We notice from Fig. 25(a) that the values of μ alternate in successive lines from +1 to -1 and this suggests the general solution when S is the set of *all* partial graphs

$$\begin{aligned} \mu(g, g') = (-1)^{l'-l} & \quad g \subseteq g' \\ 0 & \quad g \not\subseteq g' \end{aligned} \quad (4.75)$$

where l and l' are the numbers of lines in g and g' , respectively. Formula (4.75) can be established by induction. Assume that it is true for $l' - l \leq n - 1$; using (4.69) we may write when $l' - l = n$,

$$\begin{aligned} \mu(g, g') &= - \sum_{g \subseteq g'' \subset g'} (-1)^{l''-l} = - \sum_{r=0}^{n-1} \binom{n}{r} (-1)^r \\ &= -(1-1)^n + (-1)^n. \end{aligned} \quad (4.76)$$

In fact, it is easy to see that this problem is equivalent to the principle of inclusion and exclusion. Result (4.75) agrees with that derived previously in (4.13) when we treat all isomorphic graphs as identical.

The derivation of μ_Γ the Moebius function for the set Γ of connected subgraphs of a connected graph C needs more care. Let $\mu_\Gamma(g, g')$ be the Moebius function for all $g' \in \Gamma$ with g a fixed element of Γ . Define the *edge perimeter* P of g as the set of edges of C which are not in g but are incident on vertices in g . Denote by Γ_p the set of graphs which are formed from g together with any subset of edges from P . (See Fig. 26(b).) Clearly Γ_p is a subset of Γ . If g_p is the subgraph of C consisting of g together with all the edges in P , then the segment $[g, g_p]$ is the set Γ_p . Since this set is isomorphic with the set of all subsets of P ,

$$\mu_\Gamma(g, g') = (-1)^{l'-l} (g' \in \Gamma_p). \quad (4.77)$$

We shall now show that

$$\mu_{\Gamma}(g, g') = 0 \quad (g' \notin \Gamma_p), \quad (4.78)$$

again using induction over $l' - l$. If $g' \notin \Gamma_p$ then $l' - l \geq 2$; the elements of Γ with $l' - l = 2$ which do not belong to Γ_p are formed from g together with a chain of two edges just one of which belongs to P . Direct calculation from (4.69) shows that (4.78) is valid for all such graphs. If we examine the values of $\mu_{\Gamma}(g, g')$ in Fig. 26(a) [derived from (4.69)] we find the property that when $\mu_{\Gamma}(g, g')$ becomes zero for a graph $g' \notin \Gamma_p$, then $\mu(g, g'^*)$ remains zero for any graph g'^* formed by the addition of further lines to g' .

Formally let $l' - l = n \geq 3$ and assume that (4.78) is true for $l' - l \leq (n-1)$. Taking a graph $g^* \notin \Gamma_p$ with $l^* - l = n$, we have from (4.69) that $\mu(g, g^*)$ is given by a sum of $\mu(g, g'')$ for $g \subseteq g'' \subseteq g^*$. For $g'' \notin \Gamma_p$, $\mu(g, g'') = 0$ by our assumption. The remaining terms are the g'' which do belong to Γ_p ; if \hat{g} is the graph obtained from g^* by deleting the edges which do not belong to g or Γ_p then these terms are $[g, \hat{g}]$. Hence,

$$\mu(g, g^*) = - \sum_{g \subseteq g'' \subseteq \hat{g}} \mu(g, g'') = 0. \quad (4.79)$$

This completes the proof of (4.78).

If $g' \in \Gamma_p$, g is said to have *full edge perimeter* in g' . We have thus shown that $\mu(g, g') = 0$ unless g has full edge perimeter in g' in which case $\mu(g, g') = (-1)^{l'-l}$. When we treat isomorphic graphs as identical we obtain (4.60).

The above results can be extended to section graphs. Instead of (4.75) we have

$$\mu(g, g') = \begin{cases} (-1)^{v' - v} & (g \subseteq g') \\ 0 & (g \not\subseteq g') \end{cases} \quad (4.80)$$

where now $g, g' \in S$ the set of *all* section graphs of G . Instead of (4.77) and (4.78) we have

$$\mu_{\Gamma}(g, g') = \begin{cases} (-1)^{v' - v} & (g \in \Gamma_p) \\ 0 & (g \notin \Gamma_p), \end{cases} \quad (4.81)$$

i.e. μ_{Γ} is zero unless g has *full vertex perimeter* in g' .

It should be noted that $\mu(g, g')$ depends only on the type of subgraph allowed (e.g. partial graph, connected graph, section graph) and not on the graphs G and C from which the sets were derived. This is clear since only the segment $[g, g']$ is involved in the definition.

4. Star lattice constant expansions

The connected lattice constant expansion of Section IV.B2 parallels the cluster integral expansion (M1) of the Mayer development. It is natural to proceed a stage further and obtain a parallel to the irreducible cluster integral expansion (M5) by changing to the density as independent variable. Rushbrooke and Scoins (1955) derived the important result that for a lattice gas model this change of variable leads to an expansion for $\ln Z_{\mathcal{N}}$ involving only star lattice constants. To prove this result Rushbrooke and Scoins considered all irreducible diagrams which use the vertices of an articulated lattice constant; these can be divided exactly into pairs which do or do not have a line joining two molecules at the articulation point, and each such pair cancels to give zero.

In applying the above result, we must remember that the Mayer expansion (M5) applies only in the thermodynamic limit. Actually we need not be so restrictive the requirement for validity being that all lattice points are equivalent, i.e. that the graph G whose partition function we are evaluating is homogeneous (see Section IV.A4). It will certainly apply to a torus. For such a graph G_h we have instead of (4.44)

$$\ln Z_{\mathcal{N}}(G_h) = \sum_r (s_r; G_h) \kappa_r(\rho, F), \quad (4.82)$$

where the sum is taken over all star sub-graphs of G_h .

For lattice systems the reduction from connected to star lattice constants is of much greater benefit than for a continuum. For high temperature expansions we are usually concerned with line grouping rather than point grouping, and we have already noted in Section II.B3 how much fewer is the number of stars for given l than connected graphs for the same l .

Unfortunately there is no simple prescription for calculating the $\kappa_r(\rho, F)$ for general ρ analogous to the finite cluster equations (4.46). This is because equation (4.82) cannot be applied to any star subgraphs s_r which are not homogeneous. The only method so far devised of tackling this problem has been to use a multi-component expansion of type (M15), the number of components being equal to the number of inequivalent points in s_r (Yvon, 1948; Domb and Hiley, 1962) and the procedure in this case rapidly becomes cumbersome.

Fortunately there is a particularly density $\rho = \frac{1}{2}$ corresponding to $H = 0$ for which the multicomponent expansion reduces to a single-component expansion and for which all the weight functions $\kappa_r(\frac{1}{2}, F)$ can readily be determined. We shall establish this result for the Ising model from first principles, since we shall then find that it applies equally to a number of other models.

Consider the partition function for the Ising model in zero field of an articulated graph $c_1 \circ c_2$ formed by connecting two graphs c_1 and c_2 at an articulation point 0. Since the partition functions of c_1 and c_2 are independent of the orientation of the spin at 0, it is easy to see that

$$Z(c_1 \circ c_2) = \frac{1}{2} Z(c_1) Z(c_2). \quad (4.83)$$

Hence, if we define a weighting function for a connected graph c with v vertices,

$$w(c) = \ln Z(c) - v \ln 2, \quad (4.84)$$

we find that for any articulated graph $c_1 \circ c_2$

$$w(c_1 \circ c_2) = w(c_1) + w(c_2). \quad (4.85)$$

Clearly w satisfies (4.47) for disjoint graphs, and we can apply equations (4.46) taking w instead of $\ln Z$ in the left-hand side. When we make use of (4.85) in these equations we find that all weights κ for articulated graphs are zero.

The same result applies to the classical vector model (Domb and Wood, 1965; Joyce and Bowers, 1966; for further details see Stanley, this Volume, Chapter 7) for which the partition functions of c_1 and c_2 are again independent of the orientation of the spin at 0; it is also valid for the Ashkin-Teller (1943) and Potts (1952) models which have the same property.

Essam and Sykes (1966) showed that it applies to the mean number of clusters in a site percolation process (see Essam, Volume 2, Chapter 6); we shall now demonstrate this by an alternative argument. We can divide the configurations of c_1 into two classes (i) those in which 0 is occupied (ii) those in which 0 is unoccupied. Denote the mean number of clusters subject to (i) by $\kappa_1^{(1)}$ and subject to (ii) by $\kappa_1^{(2)}$; the mean number of clusters in c_1 is then

$$\kappa(c_1) = p\kappa_1^{(1)} + (1-p)\kappa_1^{(2)}. \quad (4.86)$$

If we define similarly $\kappa_2^{(1)}$ and $\kappa_2^{(2)}$ for c_2 an analogous relation holds. We now join the configurations of c_1 and c_2 at 0, which must be either unoccupied or occupied in both c_1 and c_2 for this union to be possible. When 0 is unoccupied the mean number of clusters is $\kappa_1^{(2)} + \kappa_2^{(2)}$; when it is occupied the mean number is $\kappa_1^{(1)} + \kappa_2^{(1)} - 1$. Thus

$$\begin{aligned} \kappa(c_1 \circ c_2) &= (1-p)(\kappa_1^{(2)} + \kappa_2^{(2)}) + p(\kappa_1^{(1)} + \kappa_2^{(1)} - 1) \\ &= \kappa(c_1) + \kappa(c_2) - p. \end{aligned} \quad (4.87)$$

Thus if we define

$$w(c_1) = \kappa(c_1) - vp \quad (4.88)$$

relation (4.85) holds.

An analogous result can be derived for bond percolation processes, but one must be careful to include null-clusters (Essam and Sykes, 1966; a null-cluster is an isolated site which is the meeting point of two or more occupied bonds). Baker (1971) has shown that the same result can be established for the logarithm of the chromatic polynomial (the number of ways of colouring the vertices of a graph under the restriction that no two vertices joined by an edge may be given the same colour). For the relation of these problems to the Whitney rank function (Whitney, 1932) see Essam (1971).

When only star lattice constants enter we can use the cyclomatic number classification (Section IV.A5, Figs 16–18) and instead of (4.46) we write

$$\begin{aligned}
 w(a)_p &= \kappa(a)_p \\
 w(a, b, c)_\theta &= \kappa(a, b, c)_\theta + \kappa(a + b)_p + \kappa(b + c)_p + \kappa(c + a)_p \\
 w(a, b; c, d; e, f)_\alpha &= \kappa(a, b; c, d, e, f)_\alpha + \kappa(b, c + e, d + f)_\theta \\
 &\quad + \kappa(a, d + e, c + f)_\theta + \kappa(d, a + e, b + f)_\theta \\
 &\quad + \kappa(c, b + e, a + f)_\theta + \kappa(f, a + c, b + d)_\theta \\
 &\quad + \kappa(e, a + d, b + c)_\theta + \kappa(d + e + c + f)_p \\
 &\quad + \kappa(a + f + b + e)_p + \kappa(a + d + b + c)_p \\
 &\quad + \kappa(a + f + c)_p + \kappa(f + d + b)_p \\
 &\quad + \kappa(b + e + c)_p + \kappa(a + d + e)_p \\
 w(a; b; c, d; e, f)_\beta &= \kappa(a, b; c, d; e, f)_\beta + \kappa(c, d, b + e + f)_\theta \\
 &\quad + \kappa(c, d, a + e + f)_\theta + \kappa(a, b, d + e + f)_\theta \\
 &\quad + \kappa(a, b, c + e + f)_\theta + \kappa(a + b)_p \\
 &\quad + \kappa(c + d)_p + \kappa(a + e + c + f)_p \\
 &\quad + \kappa(b + e + c + f)_p + \kappa(a + e + d + f)_p \\
 &\quad + \kappa(b + e + d + f)_p \\
 w(a, b; c, d; e)_\gamma &= \kappa(a, b; c, d; e)_\gamma + \kappa(c, d, b + e)_\theta + \kappa(c, d, a + e)_\theta \\
 &\quad + \kappa(a, b, d + e)_\theta + \kappa(a, b, c + e)_\theta + \kappa(a + b)_p \\
 &\quad + \kappa(c + d)_p + \kappa(a + e + c)_p + \kappa(b + e + c)_p \\
 &\quad + \kappa(a + e + d)_p + \kappa(b + e + d)_p \\
 w(a, b, c, d)_\delta &= \kappa(a, b, c, d)_\delta + \kappa(a, b, c)_\theta + \kappa(a, b, d)_\theta \\
 &\quad + \kappa(a, c, d)_\theta + \kappa(b, c, d)_\theta + \kappa(a + b)_p + \kappa(a + c)_p \\
 &\quad + \kappa(a + d)_p + \kappa(b + c)_p + \kappa(b + d)_p + \kappa(c + d)_p
 \end{aligned} \tag{4.89}$$

Although the equations are simple to solve in principle, it will be seen that the sub-graph subtractions rapidly become cumbersome. Fortunately for applications to series expansions a technique has been introduced for each of the above problems which avoids the subgraph subtraction of equations (4.89).

For the Ising and classical vector models the whole of the theory applies when the interactions along the edges of the net are all different. Let us therefore consider an Ising model for a star graph with a different interaction along each edge. We know from the above general development (Section IV.B2) that if we expand the κ derived from (4.89) for such a graph every term in the expansion must contain at least one term coming from each edge*. None of the subtracted subgraph κ 's can contain such terms. Thus if we expand $\ln Z$ for the above star and take account *only of terms containing all the interactions* we will obtain the correct expansion. The role of the subgraphs is simply to eliminate all terms which do not contain all the interactions, and *they can therefore be ignored*.

The above method was proposed independently by Domb (1967) and Jasnow and Wortis (1967). It has been used extensively for high temperature specific heat series by the research group at King's College under the direction of Dr. M. F. Sykes. We illustrate its use by considering the expansion of $\ln Z$ for the θ -graph. The partition function for the Ising model in zero field for any graph G can be put in the form (see Domb, this Volume, Chapter 6)

$$Z(G) = 2^v \prod_{i=1}^l (\cosh \beta J_i) \left[1 + \sum_{(g_i)} w_i w_j \dots w_k \right] \quad (4.90)$$

$(w_i = \tanh \beta J_i).$

Here the sum is taken over *all* subgraphs g_i (connected or disconnected) of G which have even vertices. For each subgraph a bond of strength J_i contributes w_i . When we form $w(G)$ in (4.84) the term in v disappears, and the term in $(\cosh \beta J_i)$ contributes only to the lowest star ; it does not enter into the closed circuit graphs in (4.89). Therefore we can confine attention to the portion in square brackets.

For the θ graph we find

$$\ln Z_\theta = \ln(1 + w_a w_b + w_b w_c + w_c w_a) \quad (w_a = \tanh \beta J_a, \text{etc.}) \quad (4.91)$$

which we denote in an obvious short hand notation by $\ln(1 + ab + bc + ca)$.

* It is worth pointing out that this result can be obtained directly from the primitive method if the disconnected lattice constants are reduced by means of overlap partitions. It therefore applies equally to the other problems (percolation, chromatic polynomial) mentioned above.

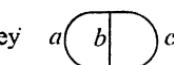
If we expand and retain only terms containing abc we find

$$\begin{aligned} -a^2bc - b^2ca - c^2ab + (a^3b^2c + a^2b^3c + ab^2c^3 + ab^3c^2 \\ + a^3bc^2 + a^2bc^3) + 2a^2b^2c^2. \end{aligned} \quad (4.92)$$

Each of these terms can be described as a *bonding* of the θ -topology and we can construct a table giving the weights corresponding to each bonding (Table VII). It will be seen that the method lends itself readily to computerization.

TABLE VII

| Weight | Bonding |
|--------|---|
| -1 |  |
| -1 |  |
| -1 |  |
| +1 |  |
| +1 |  |
| +1 |  |
| +1 |  |
| +1 |  |
| +2 |  |

Key 

To deal with the case of usual interest, i.e. a θ -topology with all interactions equal but with r, s, t lines on the respective bonds, we merely replace w_a, w_b and w_c by w^r, w^s , and w^t and so on. It will be seen that the numerical weights listed in Table VII depend only on the topology and the particular

bonding considered, but are independent of the number of two-degree vertices. They may therefore be described as *invariants* of the topology. We may note that because of the prescription (4.90) for the Ising model all bondings with non-zero weight must satisfy the following conditions:

- (i) all vertices of the bonded topology must have even degree;
- (ii) the bonding must correspond to a superposition of cycles. This can most readily be shown by forming $\ln Z(G)$ in (4.90) and reducing the disconnected lattice constants by using overlap partitions. It is easy to see that all the terms in (4.92) satisfy these conditions. However, a term like a^4bc satisfies condition (i) but not condition (ii) and therefore has zero weight.

Similar results can be obtained for the classical vector model with a number of important modifications. Instead of one variable $w = \tanh \beta J$ we have an infinite set of variables, which in D dimensions are (Stanley, 1969)

$$w_t = I_{\frac{1}{2}D-1+t}(\beta J)/I_{\frac{1}{2}D-1}(\beta J). \quad (4.93)$$

The partition function for a graph G is much more complicated and general formulae when $D = 2, 3$ have been given by Joyce (1967) in terms of $3 - j$ and $6 - j$ symbols. However the pattern of behaviour is preserved, and we can define D -dimensional weights corresponding to particular bondings of a topology which are invariants. Also, the conditions (i) and (ii) of the previous paragraph must be satisfied for a bonding to have non-zero weight.

Recently the present author (Domb 1972) has suggested a new method by which these weights can be calculated directly. The method is particularly simple for topologies which are *ladder graphs* (see Section II.B3(d)); these weights can be calculated by replacing a single interaction J by a parallel pair of interactions J', J'' and determining the appropriate transformation function for w in terms of w', w'' . In this way a number of general theorems can be formulated for such ladder topologies. For non-ladder topologies an alternative method reduces the cyclomatic number by allowing a suitably chosen interaction to become infinite.

For the percolation problem Essam and Sykes (1966) found likewise that certain numbers can be defined for each star graph which depend only on the topology and are therefore invariant. For the site percolation problem they showed that the weight function (4.88) for any star graph S with v -vertices is of the form $k(S)p^v$. The invariants k they termed k -weights. Since the expansion can be undertaken equally well for weak or strong lattice constants, it is possible to define weak or strong k -weights. Similar results hold for the bond-percolation problem provided that care is taken with null-clusters (for further details see Essam, Volume 2, Chapter 6). Finally in the

paper referred to previously Baker (1971) has derived an analogous set of invariants for the chromatic polynomial.

C. Tabulation of lattice constants

The first tables of lattice constants were calculated by Domb and Sykes and are reproduced in Domb (1960). Since these tables were prepared with the primitive method (Section IV.B1) in mind, lattice constants of disconnected graphs are also listed. Weak lattice constants are listed of *all* graphs with up to five lines, and strong lattice constants of *all* graphs with up to five vertices. These data are sometimes useful even nowadays. In addition a number of general overlap partition formulae of type (4.27) are given. The lattices considered are the s.q. and p.t. (plane triangular) in two dimensions and the s.c., b.c.c. and f.c.c. in three dimensions.

We note two misprints in these tables; p. 356, Table C, line 5, column 2, should read -6567840 instead of -6267840 ; and on p. 356, 5 lines from the bottom, in the formula for $[p_3, p_6]$, the last term should read $2p_{6c}$ instead of $2p_{8c}$.

For *connected* lattice constants the most extensive tables currently available are in the compendium of Baker *et al.* (1967) who deal with the same lattices quoted above. The following connected graphs are considered:

- (a) all those with $l \leq 8$;
- (b) all those with $l \leq 10$ and $v \leq 7$;
- (c) for $l = 9$ all those with even vertices and all those with no more than two vertices of order one;
- (d) for $l = 10$ all those with even vertices;
- (e) for $l = 10$ a number of particular graphs with odd vertices.

For the s.q. and s.c. lattices, the tables are complete. For the other lattices there are a number of gaps in the higher order graphs. The elements of the T-matrix (Section IV.B3) are also listed.

One error has been noted by Dr. J. W. Essam; on p. 239 the lattice constant of graph 865 for the s.q. lattice should read 6856 instead of 17664.

For *star* lattice constants a comprehensive set of data has been built up by Dr. Sykes and his collaborators at King's College, and in addition to the above mentioned lattices the h.c. (honeycomb) lattice in two dimensions, and the diamond lattice in three dimensions have been considered. Sykes *et al.* (1966) provide tables of all non-zero weak lattice constants with $l \leq 9$ for the f.c.c. lattice and with $l \leq 16$ for the diamond lattice; they also list all non-zero strong lattice constants with $v \leq 7$ for the f.c.c. lattice.

Subsequent work has extended these tables considerably. The values of l reached depend on the co-ordination of the lattice. For close-packed lattices

TABLE VIII. Lattice Constants of β Graphs of l Lines for the Triangular and f.c.c. Lattices

| Beta Graphs | | T | f.c.c. | Beta graphs | | T | f.c.c. |
|-------------|---|--|--|---|---|--|--|
| $l = 8$ | 1.2.1.2.1.1 | 6 | 564 | $l = 12$ | 1.2.1.2.1.5 1.2.1.2.2.4 1.2.1.2.3.3 1.2.1.3.1.4 1.2.1.3.2.3 1.2.1.4.1.3 1.2.1.4.2.2 | 1164 1170 588 1104 1104 816 408 | 2707 560 2718 480 1362 060 3201 888 3232 176 2521 968 1271 856 |
| $l = 9$ | 1.2.1.2.1.2 1.2.1.3.1.1 1.2.2.2.1.1 | 30 24 0 | 6 696 5 472 1 656 | 1.2.1.5.1.2 1.2.1.6.1.1 1.2.2.2.1.4 1.2.2.2.2.3 1.2.2.3.1.3 1.2.2.3.2.2 1.2.2.4.1.2 1.2.2.5.1.1 1.2.3.3.1.2 1.2.3.4.1.1 1.3.1.3.1.3 | 756 516 288 300 276 138 264 126 0 0 312 | 2511 408 1587 288 1258 848 1269 312 1671 120 841 392 1452 576 802 128 567 648 1 025 220 | |
| $l = 10$ | 1.2.1.2.1.3 1.2.1.2.2.2 1.2.1.3.1.2 1.2.1.4.1.1 1.2.2.2.1.2 1.2.2.3.1.1 1.3.1.3.1.1 1.3.2.2.1.1 2.2.2.2.1.1 | 102 51 120 60 12 6 24 0 0 | 46 128 23 052 64 560 32 760 21 264 16 992 13 470 7 968 1 224 | 1.3.1.3.2.2 1.3.1.4.1.2 1.3.1.5.1.1 1.3.2.2.1.3 1.3.2.2.2.2 1.3.2.3.1.2 1.3.2.4.1.1 1.3.2.5.1.1 1.3.3.3.1.2 1.3.3.4.1.1 1.3.1.3.1.3 | 156 552 336 120 60 0 120 60 0 0 | 520 554 1 820 544 1 067 364 744 336 376 872 1 060 944 523 536 196 536 474 180 593 520 478 656 312 816 141 948 72 786 372 672 163 440 61 200 129 360 | |
| $l = 11$ | 1.2.1.2.1.4 1.2.1.2.2.3 1.2.1.2.1.3 1.2.1.3.2.2 1.2.1.4.1.2 1.2.1.5.1.1 1.2.2.2.1.3 1.2.2.2.2.2 1.2.2.3.1.2 1.2.2.4.1.1 1.2.3.3.1.1 1.3.1.3.1.2 1.3.1.4.1.1 1.3.2.2.1.2 1.3.2.3.1.1 1.4.2.2.1.1 2.2.2.2.1.2 2.2.2.3.1.1 2.3.2.3.1.1 | 330 330 360 180 276 168 60 30 60 30 0 120 120 120 24 12 0 0 0 0 | 345 192 346 392 436 224 219 312 380 784 219 216 159 264 79 992 224 016 110 208 41 376 155 256 160 320 101 808 81 576 47 256 17 616 25 152 | 1.4.1.4.1.1 1.4.2.2.1.2 1.4.2.3.1.1 1.5.2.2.1.1 2.2.2.2.1.3 2.2.2.2.2.2 2.2.2.3.1.2 2.2.2.4.1.1 2.2.3.3.1.1 2.3.2.3.1.1 | 150 60 60 0 150 60 0 24 9 30 0 12 12 9 6 0 6 | 478 656 593 520 478 656 312 816 141 948 72 786 372 672 163 440 61 200 129 360 | |

p.t. and f.c.c., all star lattice constants have been derived with $l \leq 12$, and a substantial number of lattice constants (needed for Ising specific heat expansions) for $l = 13, 14$. For loose-packed lattices, data for larger l are available, for the s.c. up to $l = 20$, for the diamond up to $l = 24$, and for the h.c. up to $l = 32$.

Most of these data have not yet been published; indeed for the higher values of l it is questionable whether tabulation serves a useful purpose since the data becomes very extensive and it is more efficient to store them on magnetic tape for subsequent use in specific applications. However for lower values of l tables could be useful, and efforts are currently in hand to publish the data in a suitable form. Typical data for β -graphs on the f.c.c. lattice ($l \leq 12$) are reproduced in Table VIII.

Particular attention has been paid to lattice constants of chains (l_c) and polygons (l_p , because of their significance for self-avoiding walks. Martin, Sykes and Hioe (1967) give tables of chains for the p.t. lattice ($l \leq 17$) and the f.c.c. lattice ($l \leq 12$); for loose-packed lattices Sykes, Guttman, Watts and Roberts (1972) give the following data: h.c. ($l \leq 34$), s.q. ($l \leq 24$), s.c. ($l \leq 19$), b.c.c. ($l \leq 15$). For polygons Sykes, McKenzie, Watts & Martin (1972) give the following data: s.q. ($l \leq 26$), p.t. ($l \leq 18$), s.c. ($l \leq 20$), b.c.c. ($l \leq 16$), f.c.c. ($l \leq 14$). For the diamond lattice chains with $l \leq 16$ are given by Essam and Sykes (1963) (the figure for $l = 16$ should read 42922452 instead of 42922308). In regard to *strong* lattice constants for chains and polygons, data are given by Hioe (1967) for the s.q., p.t., s.c. and f.c.c. lattices, and by Kumbar and Windwer (1971) for the diamond lattice. We may also mention that weak lattice constant data corresponding to overlap partitions for a pair of chains have been tabulated by McKenzie (1968).

Finally, mention should be made of the hydrogen peroxide lattice having co-ordination number 3 in three dimensions for which lattice constant data have been assembled by Betts and his collaborators (1969).

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2. Computer Techniques for Evaluating Lattice Constants

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I. Introduction

It has long been recognised that certain problems in statistical mechanics and elsewhere can be transformed to problems of combinatorial type. This crucial fact is fully considered in other articles in this series and elsewhere (see particularly the preceding article), where it is shown that in many cases, provided that complete information on relevant embeddings of networks in other networks is available, the original problem is thereby completely solved. However, counting the number of ways that one network may be embedded in another is in itself a problem of classic difficulty, and no general analytic approach has ever been devised.

Originally, the counting of embeddings had to be done "by hand", at first by direct methods and later, when the required counts became prohibitively large, by indirect methods. However subtle and ingenious the techniques employed, there always remained a hard core of tedious counting which had to be done, and towards the end of the 1950's the use of a computer began to be seriously considered.

Access to a computer solves few problems, and often creates several.

The main obstacle to progress in the counting of embeddings has always been that the relevant numbers grow roughly exponentially with the size of the network to be embedded; a law of sharply diminishing returns thus operates. There is no doubt that with present methods, where fast computer programs are used in close conjunction with ingenious indirect approaches, the ultimate barrier of computer time (or lack of it) has been nearly met. A fresh theoretical approach to embedding counting will be needed for anything more than marginal advances.

This article is devoted entirely to the general questions to be considered in the design of counting programs which approach the limits of efficiency. The basic principles of such programs are very similar, and are best illustrated by examples. Here we offer two: cluster-counting on a crystal lattice, and the embedding of networks in a crystal lattice. The account reflects my own experience in problems of this kind; however, where details of others' work are available, it is apparent that, overall, the various approaches generally have much in common.

II. Nature of the Problem

The overwhelming majority of applications is to systems with the symmetry of one or other of the usual crystal lattices, and we shall consider embeddings only in such lattices. It is not difficult to extend the methods to more general networks.

For our purposes, a **crystal lattice** is a network of **sites** connected by **bonds**, the whole arrangement having the translational and rotational symmetry of one of the "usual" lattices. In most cases, only nearest-neighbour bonds are of interest, but the methods described here do not require any such restriction.

A **configuration** is a network of **points** connected by **lines** and a configuration is said to be **embedded** in a lattice when the points of the configuration fall on a selection of the sites of the lattice in such a way that:

- (i) no two points of the configuration fall on the same site of the lattice (self-exclusion);
- (ii) any two points which are joined by a line must fall on two sites joined by a bond.

A **count** is an enumeration of all possible ways in which a given **class** of configurations may be embedded in the lattice.

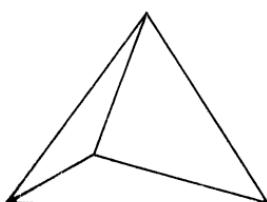
Strictly, a count is infinite (unless it happens to be zero) since the lattice is an infinite network. However, we always agree that a count will mean a *count per site*:

$$\text{count per site} = \lim_{N \rightarrow \infty} \frac{1}{N} (\text{count for a region of the lattice with } N \text{ sites}).$$

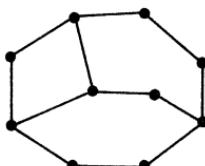
(Clearly the *shape* of the region as $N \rightarrow \infty$ must be properly chosen.) The existence of the count per site is an extensive property of the lattice, not necessarily shared by other infinite networks.

One of the simplest types of configuration is the *cluster* (called by some authors *animal* or *polyomino*). Imagine a collection of n sites chosen from the lattice and consider the configuration formed by taking along with the n sites the set of all bonds joining pairs of them. If the resulting configuration is *connected*, we call it an n -**cluster**. The count of n -clusters is an important combinatorial property of a lattice. A variant which is useful in the low-temperature theory of the Ising model is the (n, m) -cluster: this is an n -cluster whose bonds are exactly m in number.

Topology



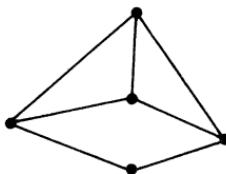
Realisations



$\propto (1, 3; 1, 3; 2, 2)$
10 points, 12 lines

 α -graph

4 vertices
6 bridges



$\propto (1, 1; 1, 1; 1, 2)$
5 points, 7 lines

and so on

FIG. 1.

A **topology**—as the name suggests—is a class of configurations whose points and lines are connected in a prescribed topological manner; sometimes we refer to a topology as a **graph**. As illustrated in Fig. 1, a configuration is not uniquely specified by its topology, and there are generally many different **realisations** of the same topology, specified by the lengths of the **bridges** joining the **vertices** of the topology. A very common counting problem is, given a topology, to obtain the count of each of its realisations with a prescribed number of lines.

The count of a specified realisation of a given topology is a *high-*

temperature lattice constant; the name is derived from the application to statistical mechanics. There is a different kind of embedding problem—the low-temperature count; this is subject to a restriction additional to those given above, namely

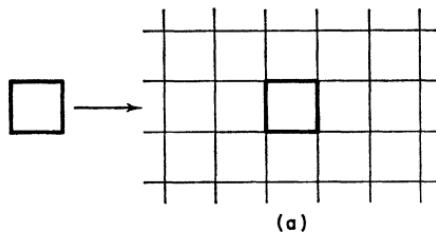
- (iii) any two points *not* joined by a line must fall on two sites *not* joined by a bond.

Once the algorithms for obtaining high-temperature lattice constants have been developed, incorporating the extra restriction for low-temperature counting presents little difficulty, and we shall not consider it at all.

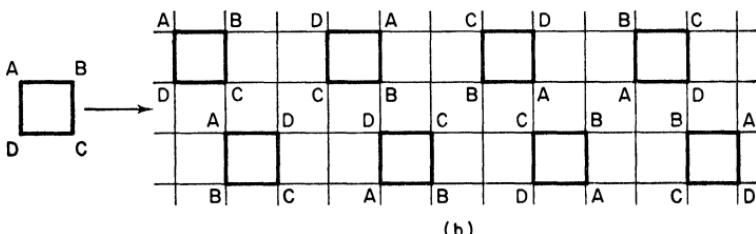
In this article we outline the computer approach to evaluating topology counts and cluster counts. However, there are some features which are common to all problems of this kind, and we shall begin by making some general remarks aimed at clarifying one difficulty in particular which always arises but which has not always been fully appreciated in the past.

III. Canonical Labellings

The difficulty is that a computer algorithm for obtaining a count never answers the question that we would like to ask; the best it can do is to answer a closely related question. The reason for this resides in the fact that the configurations appropriate to statistical mechanics are invariably *unlabelled*, in the sense that points are indistinguishable, and so are lines.



(a)



(b)

FIG. 2 (a) Unlabelled square; lattice constant=1.

(b) Labelled square; lattice constant=8.

Generally, if we impose a further structure on a configuration by attaching a different *label* to each point, the count of the **labelled configuration** will be greater than the count for the unlabelled configuration. Figure 2 illustrates this phenomenon for the case of the lattice constant for a square embedded in the square lattice.

The point is that whatever algorithm we design to perform a count, it will inevitably build up the configurations point by point and line by line. Any complete configuration generated by the algorithm must therefore carry an implied labelling, namely the order in which the elements have been added. Thus, there is a sense in which any algorithm (and any computer, by implication) can count only *labelled* configurations, and, if we are not careful, we may have to correct the result by a combinatorial factor which may be as large as $n!$ for an n -point configuration.

There is another way of expressing the basic difficulty, one which highlights the more practical aspects of the problem. A "good" algorithm is one which considers each embedding of interest once and just once; at an early stage, the architect of a good algorithm must ask how he is to guarantee that any generated configuration has not already appeared by virtue of being constructed in a different order. An obvious, if intolerably inefficient, way would be to store details of every generated configuration, to be scanned for repetitions. We must do much better than this, and the most desirable goal is an algorithm which will generate each configuration exactly once, without needing to refer to what has appeared previously.

It pays to recognise that there must be an implied labelling, and to make it explicit. This may be done by formulating a set of **canonical rules** which will, for any given n -point configuration already embedded in the lattice, label the points with $1, 2, \dots, n$; whatever these rules may be, they must satisfy the crucial requirements:

- (i) for any n -point configuration embedded in the lattice, the labelling must be *unique*;
- (ii) if the point labelled n is removed from the configuration, there must remain an allowable $(n - 1)$ -point configuration, properly labelled according to the rules.

There are no other necessary requirements, though we shall naturally adopt rules which are easily incorporated in a computer program. Any such set of rules will be said to provide a **canonical labelling**.

From the requirement of uniqueness, the count of canonically labelled configurations is the *same* as that of unlabelled configurations.

Once we have chosen a scheme of canonical labelling, we may associate with any canonically labelled n -point configuration a *unique* sequence of canonically labelled j -point configurations ($j = n - 1, n - 2, \dots, 2, 1$) such

that the j -point configuration is obtained by removing the point labelled $(j+1)$ from the $(j+1)$ -point configuration. On reversing this sequence, we immediately see the relevance to the computing problem: the program must be so written that any n -point configuration is built up through its canonical sequence and in no other way. This ensures that no configuration

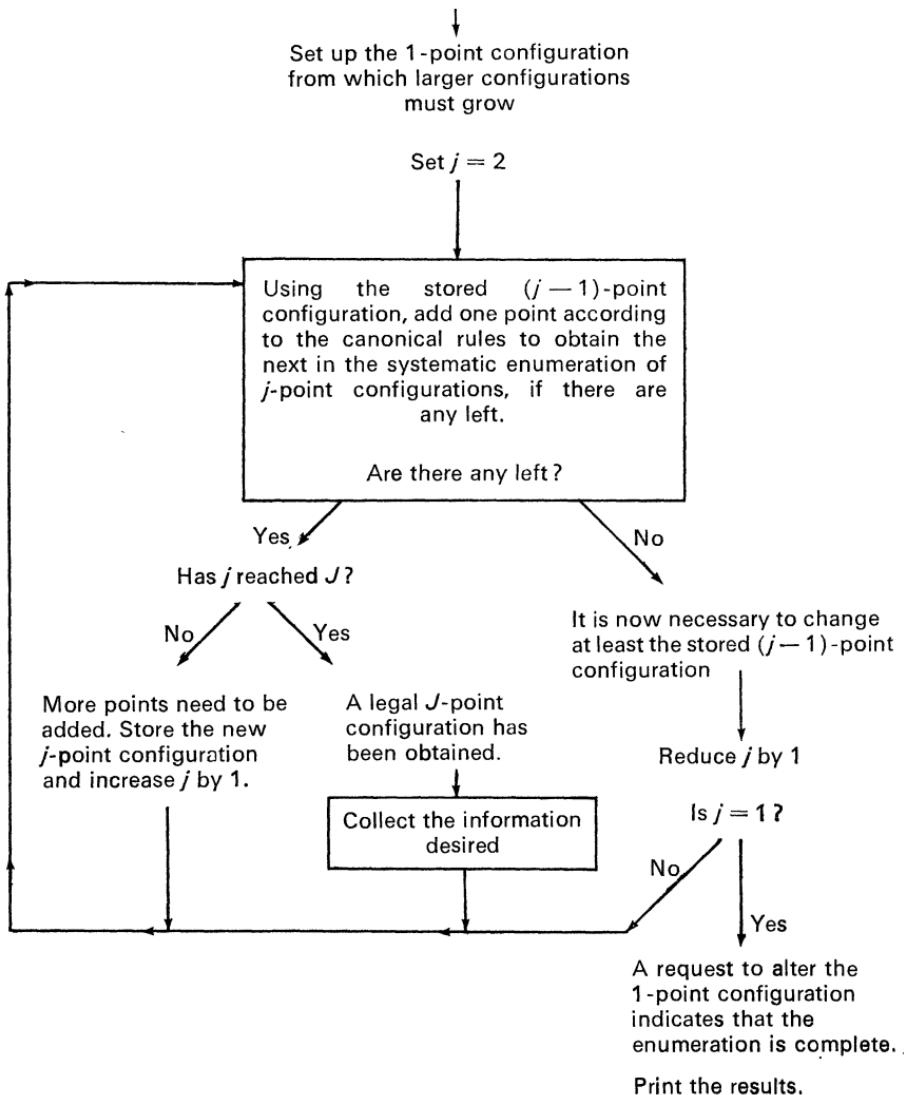


FIG. 3. The general form of the flowchart for the systematic generation of a class of J -point configurations. The parts which depend on the type of count to be performed have been boxed in.

can appear more than once in any count, and it would be difficult to find a more efficient way of doing this.

Of course, it is necessary to ensure that each relevant configuration appears *exactly* once in the course of the count; we therefore must formulate a scheme for generating all canonical sequences systematically. The obvious inductive method is the following: suppose we are able to generate all $(j - 1)$ -point configurations just once in a systematic way. For each configuration let us generate in turn each canonically labelled j -point configuration whose canonical sequence contains the $(j - 1)$ -point configuration. Then we will have generated each j -point configuration just once.

The flowchart for such a process has a characteristic appearance (Fig. 3), whatever the details of the count are, whether of clusters, topologies, or anything else.

The actual choice of a canonical labelling will depend on the nature of the problem. Sometimes a natural labelling suggests itself; for example, in the very important instance of the self-avoiding walk, we label the first point of the walk 1, the second 2, and so on. [As it happens, this labelling is not quite canonical, since we may use the same labelling scheme from the other end of the walk, and we find

$$\text{count of labelled walks} = 2 \times (\text{count of unlabelled walks}).$$

Sometimes we are prepared to accept a labelling which is not quite canonical in this sense, for the sake of convenience.]

Usually there is no natural choice of labelling, and an arbitrary prescription has to be made. The only criteria are then the convenience of the programmer and the efficiency of the program.

IV. Computer Representation of a Network

There are several different ways of setting up a computer representation of any given network, and what is appropriate in one context may be quite inappropriate in another. Perhaps the most obvious and usual method of describing a network is to use the adjacency matrix

$$\eta_{AB} = \begin{cases} 1 & \text{if the points A and B of the} \\ & \text{network are linked by a line;} \\ 0 & \text{otherwise.} \end{cases}$$

An obviously equivalent description is by a list of all linked pairs (A, B) for which $\eta_{AB} = 1$. The adjacency matrix naturally lends itself to computer use in many graph-theoretical fields; on the other hand, for the applications we have in mind here a minor generalisation is more appropriate.

As the computer description of a *realisation of a topology* we have adopted a natural analogue of the adjacency matrix

$$\beta_{AB} = \begin{cases} n & \text{if the vertices A and B of the topology are} \\ & \text{linked by a bridge of length } n; \\ 0 & \text{otherwise.} \end{cases}$$

An equivalent description which has been used—especially for program input—is a list of all the bridges, with their lengths, which appear in the realisation.

A crystal lattice, considered as a network of sites and bonds, is in a class by itself, since an adjacency matrix or any equivalent description would be altogether too unwieldy. We rely on the fact that a regular lattice has a natural vector structure and that therefore lists of the adjacency vectors carrying any site to its nearest neighbours are enough to describe the lattice completely. For lattices like the s.q., p.t., s.c., b.c.c. and f.c.c. all sites are exactly equivalent and one list of vectors is sufficient. For other lattices, the diamond and kagomé lattices for example, there are several distinct types of site, and more lists become necessary. In illustration, the description of the *diamond* lattice requires two lists, each containing four adjacency vectors:

| | <i>Adjacency Vectors</i> | <i>Type of Neighbour</i> |
|--|--|------------------------------|
| Vectors starting from <i>even</i> sites | $\begin{cases} (1, 1, 1) \\ (1, -1, -1) \\ (-1, 1, -1) \\ (-1, -1, 1) \end{cases}$ | Odd Odd Odd Odd |
| Vectors starting from <i>odd</i> sites | $\begin{cases} (-1, -1, -1) \\ (-1, 1, 1) \\ (1, -1, 1) \\ (1, 1, -1) \end{cases}$ | Even Even Even Even |

Clearly this almost provides the most compact description of the lattice and, apart from two minor differences now to be described, is the way in which regular lattices are presented to the computer programs.

The first difference is trivial: the *type* of a site is not specified by words such as “even” or “odd”, but is given an integer value $0, 1, 2, \dots$; this makes programming somewhat more convenient. Much more important is the difference that *single* integers (rather than two or three components) are used to represent the vectors of the lattice, resulting in significant economies in vector arithmetic and thus in computer time. It follows that a region of the physical lattice must be linearly mapped (*f*) on the integers

of the computer lattice in such a way that (if v is the vector position of a general point of the physical lattice)

$$v_1 + v_2 = v_3 \quad \text{implies} \quad f(v_1) + f(v_2) = f(v_3).$$

The region must be chosen to be large enough to avoid "wrap-around" interference.

The computer representation of a (complete or partial) embedding requires consideration. Obviously, a list of the coordinates of occupied sites in the order of their canonical labelling contains complete information on the embedding; but to retain information *only* in this form would lead to unacceptable loss in efficiency. An impressive improvement is gained by storing the same information in other ways; in particular, part of the computer memory is set aside for an array of binary digits (or, equivalently, logical variables) representing the sites of a region of the lattice. If a site is occupied by the current configuration the corresponding digit is a "1"; otherwise it is a "0".

When a site comes to be occupied by a point, the coordinate of the site is added to the coordinate list, and the appropriate digit is set to "1". When it needs to be known whether a site has been already occupied and is therefore not available for further occupation, it is much quicker to refer to the appropriate digit than to search the coordinate list. On the other hand, when a site comes to be released once again (as must happen when the algorithm backtracks to change an "earlier" part of the embedding), the last entry of the coordinate list is used to set the appropriate digit to "0", before being itself erased.

Information redundancy of this kind is a not untypical feature of non-numerical computing of a combinatorial character.

V. Counting n -clusters on a Crystal Lattice

Let us now turn to the first of two specific problems, the enumeration of n -clusters on a regular lattice. As shown in Section III, the first task must be to define a scheme of canonical labelling. There are many possibilities, and we have chosen one which is particularly convenient for computer programming.

Consider an n -cluster on the lattice, and label it according to the following canonical rules:

- (i) Once and for all, choose an arbitrary fixed order for the adjacency vectors of the lattice;
- (ii) Once and for all, choose any arbitrary fixed order for the sites of the lattice (a convenient choice is to order according to the value of $f(v)$, where v is the vector position of the site, and f is the linear map of IV);

(iii) the point of the cluster which falls on the site which is *earliest in the above ordering* is to be labelled 1;

(iv) points adjacent to point 1 are to be labelled 2, 3, ... and will be said to be **attached** to point 1; when more than one point is adjacent to point 1, the fixed order of the adjacency vectors defines the sequence of labelling;

(v) when all points adjacent to point 1 have been labelled, the labelling sequence continues with any still unlabelled points adjacent to point 2 (which are then said to be *attached* to point 2); when such points have been labelled, we move to point 3, and so on.

As an example, Fig. 4 shows the eleven distinct 3-clusters in the triangular lattice, with the canonical labelling which results from the choice of orderings:

- the adjacency vectors are ordered clockwise from the "9-o'clock" position;
- the "earliest" point of the cluster, labelled 1, is the bottom left-hand site.

Evidently this kind of canonical labelling induces a tree structure on the cluster.

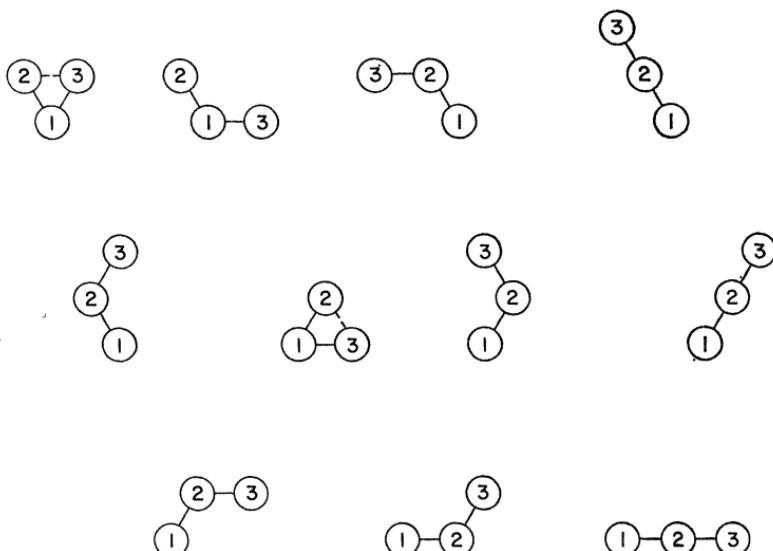


FIG. 4. The eleven distinct 3-clusters on the triangular lattice, canonically labelled in accordance with the scheme of Section V. Note that in the two cases where site 3 is a neighbour of both the other sites, it is *attached* (in the sense of Section V) to site 1 only.

These rules are used as the basis of a computer algorithm for obtaining systematically all canonically labelled j -clusters from $(j - 1)$ -clusters, for inclusion at the appropriate point in the flow-chart of Fig. 3. To start with, the point with label 1 is placed on some fixed site of the lattice, say the origin. In adding a further point to a $(j - 1)$ -cluster, we have an obvious requirement that:

(a) the point j must be *attached* to a point of the $(j - 1)$ -cluster in the sense of rule (iv) above. In order that rule (iii) should continue to be satisfied we require that:

(b) the point j must occupy a site "later" than the site occupied by point 1. Not all such points need to be considered; if the point $(j - 1)$ is attached to point k , then j cannot be attached to any point $k' < k$, and it may be attached to point k itself only by an adjacency vector "later" than that of point $(j - 1)$ (in the sense of rule (i)). Thus the first new point j to be considered is attached to point k by the next adjacency vector (if any), and the last point j is attached to point $(j - 1)$ by the last adjacency vector.

Even so, it is still possible to generate j -clusters which are not canonically labelled, unless we regard certain sites as prohibited from time to time. As soon as a site is occupied by point j , it becomes j -prohibited until further notice; as soon as all possible sites for point j have been tried (that is, when

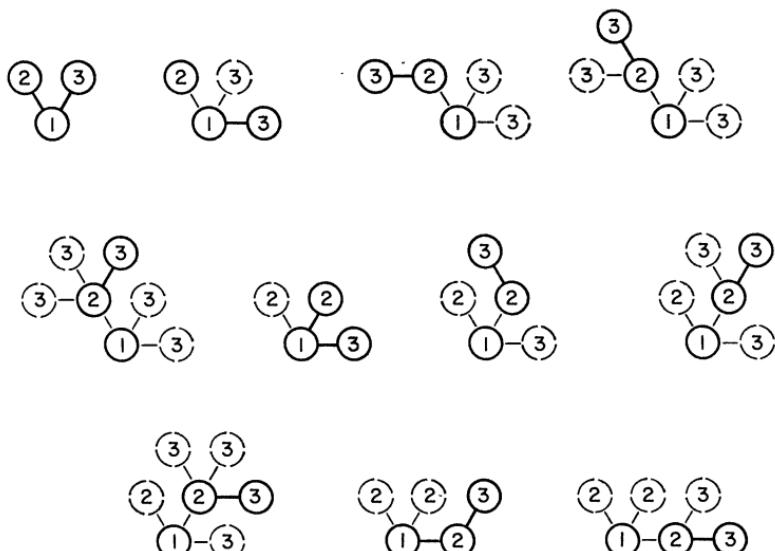


FIG. 5. The clusters of Fig. 4 are shown along with the sites which become j -prohibited (broken circles) as the algorithm of Section 5 is executed. In stepping from one diagram to the next it usually happens that just one new point has to be attached without any other change; in consequence, the algorithm provides an economical route to cluster enumeration.

the current ($j-1$)-cluster is about to be changed) all j -prohibited sites are freed. The requirement which now guarantees canonical labelling at every stage is:

- (c) the point j must not be already prohibited at any level.

The computer algorithm designed on these lines is a "good" one in two senses; first, it is compact and simple to program (characteristically, it is simpler to write the program than to describe it); second, changes in moving from one complete cluster to the next are minimised. The second point is of paramount importance for computer speed, and it is most easily grasped from Fig. 5, which shows the entire sequence of prohibited points from a small but typical computation: each diagram has in general a very large part in common with its predecessor.

Counting rates of about 10,000 per second have been achieved with a FORTRAN program executed by a CDC 6600 computer. This is certainly not the best possible, but has been found to be entirely satisfactory for our applications.

VI. Counting Lattice Constants on a Crystal Lattice

A realisation of a topology has much more structure than an n -cluster, and we therefore expect that the enumeration of their embeddings will be a more complex matter. In order to break down topologies into constituent parts, it is convenient to introduce a few further definitions before turning to the problem of the canonical labelling.

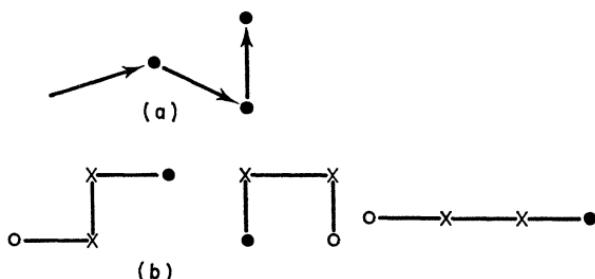


FIG. 6. Three examples of segments arising from embedding a 3-step bridge in the s.q. lattice. (a) Bridge of three steps. (b) Examples of segments arising from embedding the bridge in the s.q. lattice.

- : origin (in this example not a site of any segment)
- × : ordinary sites (two in number)
- : destination sites (as always, one in number)

As already indicated in Section II, a topology may be regarded as a set of vertices linked by bridges in a specified way. When a topology is embedded in the crystal lattice, the self-exclusion requirement implies that each bridge must be embedded as a self-excluding walk on the lattice, from one vertex (the *origin*) to another (the *destination*). Such an embedded bridge provides the simplest instance of the concept of a *segment* (Fig. 6).

A **segment** is a pattern of distinct lattice sites consisting of an **origin**, a **destination site** and (possibly) a set of **ordinary sites**. The origin need not be one of the sites of the pattern. It is rather a reference datum; a segment is placed on the lattice by decreeing on which site the origin is to fall, and all sites of the segment are then fixed by their given vector distance from the origin of the segment. Thus the segment should be regarded as a *rigid* pattern of sites which may however fall anywhere on the lattice.

Clearly an embedding of a topology in the lattice may be regarded as a network of segments whose origins or destinations are at the vertices of the topology and whose ordinary points fall along the bridges. Consequently, a natural approach to enumerating such embeddings is to construct each as a network of segments S_1, S_2, \dots . The rules for such a construction are:

- (i) The origin of each segment S_q must be placed on either
 - (a) the origin of the lattice, or
 - (b) the destination site of an earlier segment $S_{q'} (q' < q)$.
- (ii) The destination site of each segment may be required to fall either
 - (c) on the lattice origin, or
 - (d) on the destination site of an earlier segment, or
 - (e) on neither of the above.

Which of the possibilities (a), ..., (e), apply to each segment is dictated by the topology under consideration.

As an example we may take the tetrahedral topology (Fig. 7) with four vertices O, A, B and C, and six segments S_1, S_2, \dots, S_6 . A possible synthesis which illustrates all five of the possibilities is:

| <i>Segment</i> | <i>Origin</i> | <i>Destination site</i> | <i>Possibilities realised</i> |
|----------------|---------------|-------------------------|-------------------------------|
| S_1 | O | A | a, e |
| S_2 | A | B | b, e |
| S_3 | B | O | b, c |
| S_4 | O | C | a, e |
| S_5 | C | A | b, d |
| S_6 | B | C | b, d |

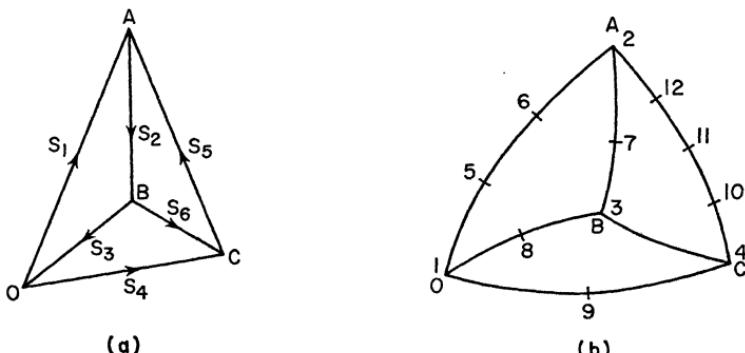


FIG. 7. Example of the segment network of Section VI. For each segment, the arrow points from the segment origin to the destination site. O is the origin of the lattice: (a) topology (b) canonically labelled realisation.

It can be seen from this example that the embedding remains connected throughout its construction.

We are now in a position to specify a canonical labelling for the embedding. There are many ways of doing this; some methods lead to extremely inefficient programs. From the point of view of computing efficiency it is difficult to improve on the labelling now to be described. This is:

- (i) the first point is the lattice origin, followed by
- (ii) the new vertices in the order in which they appear for the first time as segments are added in the construction process, followed by
- (iii) the ordinary sites in the order in which they appear in the construction process.

Observe that in this ordering the *ordinary* sites of the first segment come after the *last destination* site to appear; in other words, the computer algorithm (which adds new sites in the order of the canonical labelling) stakes out the destination sites before filling in the bridges with ordinary sites. The important consequence is that ordinary sites do not begin to be chosen until there is a reasonable likelihood that all the vertices may be linked with bridges of appropriate length. Avoiding blind alleys in this way is an important part of this type of computing, and may on occasions result in savings of many orders of magnitude in computer time.

Other savings are achieved by avoiding repetition as far as possible. On embedding, the bridges of a topology become self-avoiding walks on the lattice, and in all but the very simplest cases the same self-avoiding walk may be laid down a very large number of times in the course of an

Begin to stake out the topology
vertices on the lattice: set segment no. $j_1 = 1$

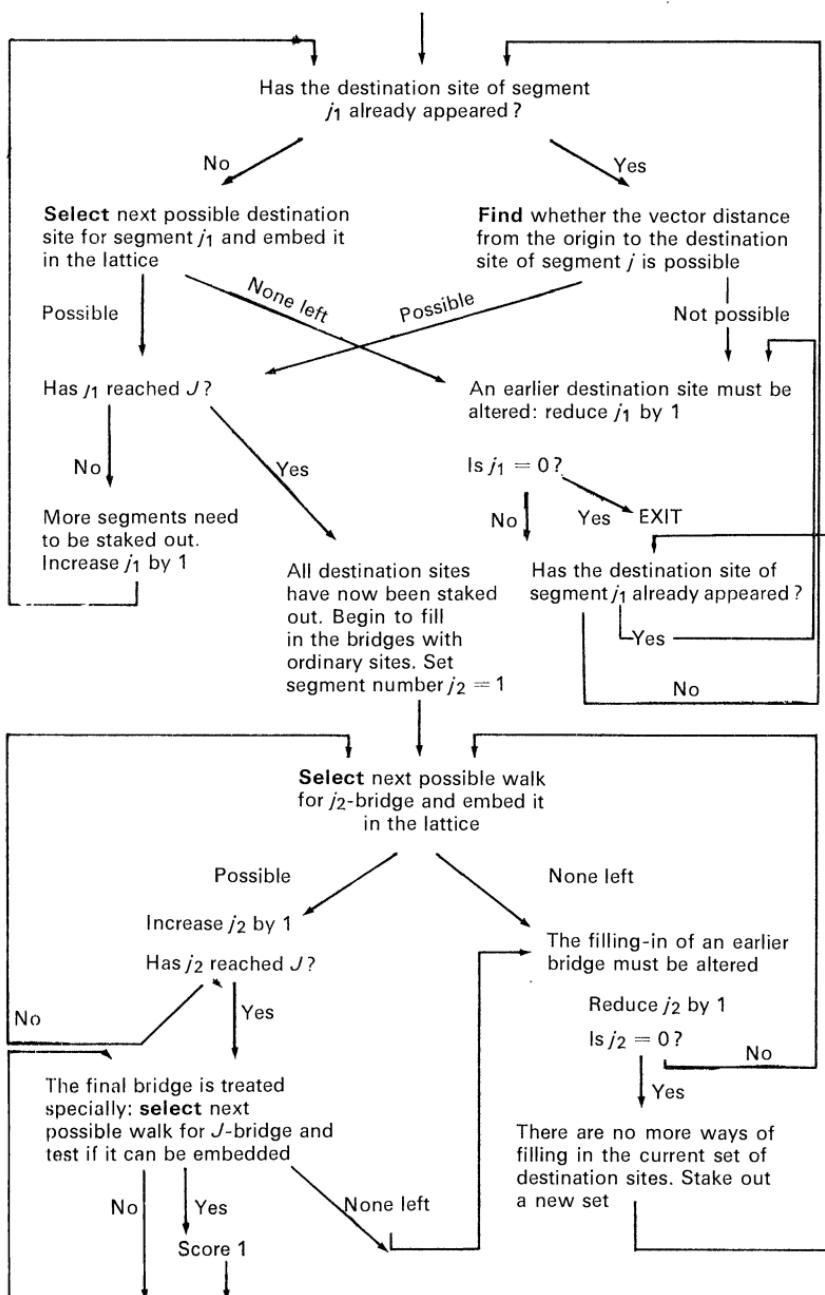


FIG. 8. Summarised algorithm for the enumeration of the embeddings of a given topology in a given crystal lattice.

enumeration (not necessarily as the same segment). Thus, it is wasteful to generate such walks repeatedly; our technique has been to generate walks of moderate length beforehand, and to keep their details readily available in a major area of computer memory.

This in itself would already make the program very fast in execution. A further substantial increase in speed (of a factor of 2 or 3) is obtained by noticing that it is now never necessary to lay the ordinary sites of the *final* segment on the lattice (and, by implication, to remove them later); such sites are already mutually self-avoiding as a result of their generation at the preliminary stage. All that is needed for the final segment is to check that the ordinary sites *can* be laid on the lattice without interfering with the earlier segments of the configuration. Provided that the program information is properly organised, such a test is very simple to carry out. In our version of the program the test is coded as a loop of only seventeen computer instructions for the IBM360. This program fragment has been designed with great care, as it is estimated that in some enumerations (in particular on the f.c.c. lattice) it may be executed for 90% or 95% of the total running time.

A condensed flowchart for the process is shown in Fig. 8, the upper part of which shows how the topology vertices are staked out, while the lower part describes the procedure for filling in the bridges. Each part has the basic structure of Fig. 3, though it should be noted that the parameters j_1 and j_2 here label segments and not points. Where the words *select* and *find* appear in heavy type, they refer to the body of information about self-avoiding walks which is assumed to be already available in the store.

Programs embodying these principles have been written for the National Physical Laboratory ACE (now obsolete), the English Electric KDF9 and the IBM360 computers. In favourable cases, topology embeddings have been counted at speeds of about 10^6 successes per minute (on the IBM360).

References

There is much published work in statistical physics which relies heavily on configuration-counting by computer. Not many publications give details of computing procedures, however, and it seems inappropriate to list them here; in any case, they are almost certainly to be found in the bibliographies of the other articles in this volume. An exception is W. F. Lunnon, (1971), "Counting Polyominoes": article in "Computers in Number Theory" (A. O. L. Atkin and B. J. Birch, eds.). Academic Press, London and New York.

3. Linked Cluster Expansion

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I. Introduction

A. Motivation

The study by the method of perturbative series expansions of the thermodynamic properties of models described by lattice Hamiltonians has historically been of great value in the understanding of critical phenomena. Onsager's brilliant solution of the two-dimensional nearest-neighbour zero-field spin $\frac{1}{2}$ Ising model (Onsager, 1944) proved beyond question that mean-field, Landau-like descriptions of the critical region were qualitatively, quantitatively, and fundamentally false. On the other hand, Onsager's methods and those used by subsequent workers in obtaining rigorous solutions for particular one- and two-dimensional models were quite specialised and have done little to suggest viable techniques for first-principle calculations—even approximate—of the critical properties of more complicated systems, particularly in three dimensions. Ideally a general technique is required, embodying a physically correct understanding of the large fluctuations dominating the singular, critical behaviour and from which all relevant quantities could be calculated qualitatively accurately and to any desired degree of precision, given only the requisite labour. Such a general technique is not currently available, though recent Russian work (Gribov and Migdal, 1969; Migdal,

1969, 1970; Polyakov, 1969, 1970) may point in the right direction. Series expansions, although they provide little physical understanding of the critical processes, have made possible precise and reliable estimates of a variety of critical properties for a wide class of model systems. Critical exponents derived from series were important data in the formation of the scaling hypothesis (Essam and Fisher, 1963; Fisher, 1965; Kadanoff, 1966; Kadanoff *et al.*, 1967; Widom, 1965a, b; Domb and Hunter, 1965). Similarly, series-derived model information is often compared quantitatively with measurements in the analysis of experimental data. This chapter will attempt neither a review of important results derived by series methods nor a detailed assessment of the contribution of these results to the understanding of critical phenomena. The interested reader is referred to several useful review articles (Domb, 1960; Fisher, 1963, 1965, 1967; Helfand, 1963). Our present focus is methodology rather than results.

Domb and Sykes (Domb, 1949, 1960; Domb and Sykes, 1956, 1957, 1961) were the first to develop series methods for the study of critical phenomena. The volume of subsequent work, following this initial exploration, has been considerable. Many refinements of techniques and extensions to other model systems are discussed elsewhere in this volume; however, the main lines of the original work remain clear. There are three stages in the argument:

- (i) a parameter x is selected in terms of which the desired thermodynamic or correlation function of the chosen model system may perturbatively be expanded;
- (ii) a finite number of coefficients in the perturbation series expansion are computed;
- (iii) extrapolative analysis of the computed coefficients *in the light of the expected form of the critical behaviour* locates the critical point and gives estimates of singular behaviour.

The parameter x selected at stage (i) is often a typical interaction energy (such as the exchange energy J) divided by the thermal energy $kT = \beta^{-1}$, $\beta = \beta J$. For certain special cases such as the Ising model the low-temperature parameter $x = \exp(-\beta J)$ may also be used. The quantity Q whose critical behaviour as a function of x is to be studied must have an expansion about $x = 0$,

$$Q(x) = \sum_{n=0}^{\infty} a_n x^n,$$

with a finite radius of convergence. At stage (ii) a finite number of the coefficients a_n are determined, $a_0, a_1, \dots, a_{n_{\max}}$. Typically the calculation is in principle straightforward; however, the increased labour necessary for calculating each succeeding coefficient is large. A rule of thumb is that the

computation of a_{n+1} involves at least as much labour as the cumulative calculation of a_0, \dots, a_n . Thus, while there is in principle no limit to the number of calculable coefficients, there is in practice a rather sharp upper bound n_{\max} (which depends on the details of the model being considered) determined by such practical considerations as time and patience and, at the next level, electronic computer capacity and funding. Finally at stage (iii) critical properties are extracted from the available coefficients by methods described in this volume (Gaunt and Guttman, Chapter 4) and elsewhere (Baker, 1965; Domb and Sykes, 1961; Fisher, 1967).

The limiting link in the above schema is stage (ii), determination of the expansion coefficients. Typically the first few coefficients are trivial and no special methodology is necessary. However, in higher orders the bookkeeping is extremely involved; and, scrupulous accuracy is necessary in determining the coefficients, since (in stage (iii)) extrapolation makes apparent critical-point behaviour exceedingly sensitive to tiny fractional changes in the last few available coefficients. For these reasons, it becomes of paramount importance to have a well-defined, systematic procedure for computing coefficients, which incorporates as many short cuts as possible and minimises the opportunity for careless error. It is to this systematisation which we now turn.

B. Derivation of series expansions

All systematic methods for the determination of series coefficients are at some level graphical or diagrammatic.[†] With each coefficient is associated a set of graphs of some given topological type. To each graph corresponds a numerical contribution according to a well-defined rule. To calculate the required coefficient, one simply sums all contributions. There are, thus, three steps in the calculation:

- (i) enumerate the contributing graphs;
- (ii) calculate the contribution of each;
- (iii) add.

Accordingly, graphical methods differ in (a) which diagrams contribute and (b) what rules determine the contributions.

The rule for calculating the contribution (ii) of each graph generally consists of two parts:

(a) a factor, *the weight of the graph*, which depends only on its topology, and

[†] We shall use the terminology "graph" rather than "linear graph" or "diagram." Although an extensive mathematical literature on graph theory exists (Berge, 1958; Harary, 1969; Ore, 1962), physicists have been far from universal in adopting its terminology. We shall introduce terminology in detail as we proceed, conforming in general to the recent compilation of Essam and Fisher (1970). (See also Domb, this volume, Chapter 1).

(b) the configurational multiplicity of the graph, determined by the number of different ways it can be *embedded* in the underlying lattice subject to certain constraints.

Different graphical expansions differ with respect to both weights and embedding constraints. The three main embedding systems are *strong*, *weak*, and *free* (Domb, 1960; Sykes *et al.*, 1966; Jasnow, 1969; Jasnow and Wortis, 1968) in order of decreasingly stringent constraints. The strong and weak systems are discussed elsewhere in this volume (Chapter 1), and the relation between them has been investigated by Sykes *et al.* (1966). The free embedding system and its relation to the weak system is considered in the appendix to this article.

In high-order calculations the number of graphs which potentially contribute in (i) above is enormous. Many of these may have no possible embeddings once the constraints (b) have been applied. Broadly speaking, the more restrictive the constraints, the fewer the possible embeddings. This very significant simplification favours restrictive expansions.

An alternative and in many ways complementary method of cutting down the number of contributing graphs is to perform a selective resummation or *renormalisation* in which classes of graphs with related topologies are lumped together. The calculation of the weights (a) of the remaining graphs is then more complicated, and the net effect is a trade-off of algebraic complexity for topological complexity. The special simplicity of the configurational factors (b) for the free or unrestricted embeddings makes the renormalisation method most appropriate. As a rule the restrictive embeddings are best in low dimensionality and for rather open lattice structures. For close-packed lattices and in higher dimensionality the renormalisation method seems preferable. In any given study, there may be additional considerations favouring one method or another. For example, for the high-temperature Ising model the weak-embedding method (Section II.D) becomes increasingly complex for higher spin, while for the free-embedding linked-cluster expansion the spin enters merely as a parameter.

This article will deal exclusively with the free-embedding expansions and their renormalisation. Connection with the weak-embedding expansion is discussed in Section II.D for the $s = \frac{1}{2}$ Ising model.

C. The linked-cluster expansion: historical

The prototypical free-embedding expansion is the linked-cluster expansion for the classical fluid, dating from the work of Ursell (1927), Yvon (1935), and Mayer (1937). Good reviews of more recent work are given by Uhlenbeck and Ford (1962) and by Stell (1964) (see also Chapter 1). The original expansion is in terms of the non-interacting single particle density n_0 , with the pair-potential in the combination $[\exp(-\beta v(\mathbf{r}_1 - \mathbf{r}_2)) - 1]$ as expansion

parameter. The simplest (one-point) renormalisation produces the familiar virial expansion (Huang, 1963), in which n_0 is replaced by the fully interacting particle density n . This renormalisation can be interpreted as a Legendre transformation in which the (inhomogeneous) particle density replaces the (non-uniform) one-particle potential as fundamental variables. De Dominicis (1962) showed that a second renormalisation can be done in which two-point correlations replace the pair potentials in a Legendre transformation generated by the entropy. A truncation of this two-point renormalisation yields the hypernetted chain approximation (Van Leuwen *et al.*, 1959; Meeron, 1960).

The linked-cluster expansion for the *quantum* fluid has been studied by many authors (Martin and Schwinger, 1959; Kadanoff and Baym, 1962; Abrikosov *et al.*, 1965). Because of the non-commutativity of operators, the extra complexity of time-dependence enters the calculation even for thermodynamic quantities. The expansion is in powers of the pair-potential; however, there are a number of energy variables, so there is no single dimensionless expansion parameter. The one-point renormalization, first done by Luttinger and Ward (1960) for the thermodynamic properties, replaces the non-interacting one-particle propagator by the fully interacting one-particle propagator. The two-point renormalisation was carried through by De Dominicis and Martin (1964a, b), again in terms of a generalised entropy functional.

The early expansions for magnetic systems, especially the Ising and Heisenberg models which have been important in the study of critical phenomena, were all of the weak (high-temperature) and strong (low-temperature) embedding types. Horwitz and Callen (1961) showed how an earlier expansion due to Brout (1959, 1960, 1961) could be rearranged to eliminate excluded volume restrictions. A direct derivation of the free, linked-cluster expansion for the Ising model in terms of the expansion parameter βJ was first given by Englert (1963). Because of the non-particle-like kinematics, the class of graphs contributing to this expansion contains multiple bonds and is considerably larger than the class which contributes to the classical fluid expansion. The reason for this is explained in Section II.G. Englert (1963) also performed the one-point renormalisation of the Ising linked-cluster expansion, though it was not until the work of Bloch and Langer (1965) that the connection with a Legendre transformation was understood. The parallel development for the classical Heisenberg model was done by Jasnow and Wortis (1968) and used for the first time to generate high-temperature series expansions (Jasnow and Wortis, 1968; Jasnow and Moore, 1968). The two-point renormalisation was originally carried through by Wortis *et al.* (1969) and has proved very useful in obtaining high-temperature series (Ferer *et al.*, 1969; Moore, 1969, 1970; Moore *et al.*, 1969).

The generalisation of the Englert formalism to the spin s quantum mechanical Heisenberg model was first done by Stinchcombe *et al.* (1963). It was not until the work of Vaks *et al.* (1968a, b), who employed a partial one-particle renormalisation, that the expansion was used systematically in calculations. The full renormalisations are carried out in Section III.D, where strong parallels with the quantum fluid are pointed out. However, in the calculation of those high-temperature series of relevance to the study of critical phenomena, no form of the linked-cluster expansion has yet been made competitive with the weak-embedding method of Baker *et al.* (1967) for the $s = \frac{1}{2}$ Heisenberg model (see also this Volume, Chapter 5).

In studying the properties of an assembly of electrons on a lattice, interacting via a zero-range interaction, Hubbard (1963, 1964a, b, 1965, 1966) has developed a linked-cluster expansion in powers of the kinetic energy, structurally identical to the unrenormalised expansion for the quantum Heisenberg model, only with the added complication of Fermi statistics.

D. Format and aim of this article

The intent of this article is frankly pedagogical. We hope to make the linked-cluster expansion for systems like the Ising and Heisenberg models available to the reader *as a working tool*. To this end we have included a considerable number of simple, worked examples. While these may strike the initiate as superfluous, it is hoped that the non-expert may find them useful. The central results of the theory are the rules (in the sense of I.B (i)–(iii)) for writing down the original graphical expansions and their renormalisations. From a practical point of view, the important thing is to be able to apply the rules in actual calculation. Characteristically, the detailed derivation of the rules, while logically necessary, is often not very illuminating. Such derivations tend to involve cumbersome combinatorial arguments with little obvious physical meaning. Without pretending to rigor, we have attempted to sketch all important steps and to point out—often by a simple example—what the essential topological content of the general proof must be. References are given to more detailed proofs, when they are available in the literature.

The usefulness of the linked-cluster expansion is by no means restricted to the derivation of series expansions for critical properties. Many approximate closed-form solutions for thermodynamic and correlation functions can be derived by graphical methods by selective truncation of graphical sums. Despite much effort, no such approach has yet yielded correct properties in the critical region; however, qualitatively correct phase diagrams and quantitative non-critical results can be obtained for a variety of systems. While our primary orientation is towards the derivation of series expansions for problems in critical phenomena, we have attempted to develop the theory in

such a way that it applies immediately to a variety of non-critical calculations as well.

The methods illustrated are sufficiently general to apply to any system which is spatially local in the absence of the perturbing interaction. For the sake of clarity it seemed wise, however, to couch the discussion in terms of specific examples. Directions of possible generalisation are remarked.

Section II develops the linked-cluster expansion and its various renormalisations for the spin s Ising model. This development, which illustrates all the topological content of the renormalisation method in the simplest possible context, is carried through in full detail. Section II.D explores the relation between the linked-cluster and weak-embedding expansions for the $s = \frac{1}{2}$ Ising model. Section II.G shows how the magnetic expansion reduces for the classical fluid to the Ursell-Yvon-Mayer expansion.

In Section III linked-cluster expansions for a variety of other more complicated systems are sketched. The topological content of these expansions and their renormalisations are identical to those of the Ising model. Omitting redundant derivations, we have attempted to bring out the parallels with the Ising development. Once these are understood, all results may be written down by inspection.

II. The Linked-Cluster Expansion with Commuting Variables: The Ising Model

A. Notation and preliminaries

The Hamiltonian for the spin s Ising model is usually written,

$$\mathcal{H} = -\frac{1}{s^2} \sum_{\langle ij \rangle} J_{ij} s_{zi} s_{zj} - \frac{m}{s} \sum_i H_i s_{zi}, \quad (1)$$

where $\sum_{\langle ij \rangle}$ denotes the sum over distinct pairs. Each spin \mathbf{s}_i ($i = \mathbf{R}_1, \dots, \mathbf{R}_N$) is situated at one of the N sites of a regular lattice and interacts via its z -component magnetic moment $m s_{zi}$ ($s_z = -s, -s+1, \dots, s$) with an inhomogeneous external magnetic field $(1/s)H_i$. Each spin pair is coupled by the spin-dependent energy $(-J_{ij}/s^2)s_{zi}s_{zj}$, where the exchange coupling J_{ij} , which may in principle be different for each pair, is normally a function only of the difference variable $(\mathbf{R}_i - \mathbf{R}_j)$. Note that $J_{ii} = 0$. The factors of $1/s$ are chosen so as to normalise the maximum interaction between parallel spins. The classical limit, in which the spins become classical unit vectors, is achieved by taking $s \rightarrow \infty$.

It will be convenient to introduce as variables the operators $\mu = s_z/s$, which range in the interval $[-1, 1]$. We then rewrite (1) in terms of dimensionless variables,

$$-\beta \mathcal{H} = \frac{1}{2} \sum_{1,2} v(12) \mu(1) \mu(2) + \sum_1 h(1) \mu(1), \quad (2)$$

where $\beta \equiv 1/kT$ and the numerical arguments, which will henceforth stand for lattice sites, run over the points $\mathbf{R}_1, \dots, \mathbf{R}_N$. The dimensionless exchange coupling is $v(ij) \equiv \beta J_{ij}$; the reduced magnetic field is $h(i) \equiv \beta mH_i$. The partition function and free energy of the Ising model are given by

$$\text{Tr exp}(-\beta \mathcal{H}) = Z[h, v] = \exp W[h, v]$$

and (3)

$$F = -kT W[h, v],$$

where the functional dependence of the thermodynamics on the fields and exchange couplings has been emphasised by the use of square brackets.

The advantage of maintaining the fields and couplings variable *independently* for each site and pair is that all correlation functions may be found by differentiation directly from the dimensionless free energy W . For example,

$$\mathcal{M}_1(1) \equiv \langle \mu(1) \rangle \equiv \frac{\langle s_{z1} \rangle}{s} = \frac{1}{Z} \frac{\delta Z}{\delta h(1)} = \frac{\delta W}{\delta h(1)} = \frac{dW}{d(\beta mH_1)}. \quad (4)$$

We use the standard notation $\langle X \rangle = (1/Z)\text{Tr } X \exp(-\beta \mathcal{H})$. By using the functional notation for the derivative $\delta/\delta h$, we stress that it is the *local field at the site 1* which is being varied. Similarly, the two-point (cumulant) correlations are available as second derivatives:

$$\mathcal{M}_2(12) \equiv \langle \mu(1)\mu(2) \rangle - \langle \mu(1) \rangle \langle \mu(2) \rangle = \frac{\delta^2 W}{\delta h(1)\delta h(2)}. \quad (5)$$

The n -point (cumulant) correlations are defined by

$$\mathcal{M}_n(1 2 \dots n) \equiv \frac{\delta^n W}{\delta h(1) \dots \delta h(n)}, \quad n = 1, 2, \dots. \quad (6)$$

Derivatives of W with respect to the pairwise exchange couplings also generate correlations:

$$\frac{\delta W}{\delta v(12)} = \langle \mu(1)\mu(2) \rangle, \quad (7)$$

which can be rewritten using (4) and (5) in the general form,

$$\frac{\delta W}{\delta v(12)} = \frac{\delta^2 W}{\delta h(1)\delta h(2)} + \frac{\delta W}{\delta h(1)} \frac{\delta W}{\delta h(2)}. \quad (8)$$

Equation (8) constitutes a non-linear functional differential equation for the free energy. The appropriate initial condition is

$$W[h, v = 0] \equiv W_0[h] = \ln \text{Tr} \exp \left(\sum_1 h(1) \mu(1) \right) = \sum_1 M_0^0(1), \quad (9)$$

with

$$M_0^0[1; h(1)] \equiv \ln \left[\sum_{\mu=-1}^1 e^{h(1)\mu} \right] = \ln \left[\frac{\sinh \left(\frac{h(1)}{2s} (2s + 1) \right)}{\sinh \left(\frac{h(1)}{2s} \right)} \right], \quad (10)$$

which is even in h . While the system (8)–(10) cannot in general be solved, it can be used to develop W in powers of v . This development, interpreted graphically, is just the linked-cluster expansion for the Ising model free energy W . Once W is known, eqn (6) yields the corresponding linked-cluster expansions for all correlation functions. In actual calculation—i.e. once the graphical rules are known—it is often most convenient (Stanley and Kaplan, 1966; Stanley, 1967) to find the correlations directly and evaluate physical quantities from them. For example, the susceptibility per site and the total energy are respectively (in dimensionless variables),

$$\chi = \sum_2 \mathcal{M}_2(12),$$

$$-E = \frac{1}{2} \sum_{1,2} v(12)[\mathcal{M}_2(12) + \mathcal{M}_1(1)\mathcal{M}_1(2)] + \sum_1 h(1)\mathcal{M}_1(1).$$

B. Unrenormalised linked-cluster expansion

The linked-cluster expansion for $W[h, v]$ is nothing more than the many-variable Taylor development,

$$W[h, v] = \left[\exp \left(\sum_{\text{pairs}} v(12) \frac{\delta}{\delta \tilde{v}(12)} \right) \right] W[h, \tilde{v}] \Big|_{\tilde{v}=0}. \quad (11)$$

The first few terms read,

$$W[h, v] = W_0[h] + \sum_{\langle 12 \rangle} v(12) \frac{\delta}{\delta \tilde{v}(12)} W[h, \tilde{v}] \Big|_{\tilde{v}=0}$$

$$+ \frac{1}{2} \sum_{\langle 12 \rangle} \sum_{\langle 34 \rangle} v(12)v(34) \frac{\delta}{\delta \tilde{v}(12)} \frac{\delta}{\delta \tilde{v}(34)} W[h, \tilde{v}] \Big|_{\tilde{v}=0} + \dots. \quad (12)$$

In each order the coefficient of v^n has the form of $\frac{\delta^n W}{\delta v^n} \Big|_{v=0}$, which by successive use of (8) can always be expressed in terms of products of the correlation functions \mathcal{M} evaluated in the non-interacting limit $v = 0$. At $v = 0$, all the lattice sites are entirely uncorrelated with one another, so the correlations are spatially local,

$$\mathcal{M}_n(1 \dots n)|_{v=0} = \delta(1 \dots n) M_n^0(1), \quad (13)$$

where $\delta(1 \dots n) = 1$ when all lattice points, $1, \dots, n$, are identical and vanishes otherwise. The quantities $M_n^0(1)$ are called *bare* or *unrenormalised semi-invariants* (Englert, 1963). Note that $M_n^0(1)$ depends only on the field $h(1)$ at the site 1. It follows from (9) and (6) that

$$M_n^0(h) = \frac{d^n}{dh^n} M_0^0(h), \quad (14)$$

or

$$W_0[h] = \sum_1 \sum_{n=0}^{\infty} \frac{(h(1))^n}{n!} M_n^0(h=0). \quad (15)$$

This locality is directly responsible for the *linked-cluster* property, which in turn underlies the extensivity of the thermodynamic functions as $N \rightarrow \infty$ for appropriately regular and short-ranged potentials (Ruelle, 1969).

The above will become clearer as we work out the first few contributions in detail. Using (8), we evaluate,

$$\frac{\delta W}{\delta v(12)} \Big|_{v=0} = [\mathcal{M}_2(12) + \mathcal{M}_1(1)\mathcal{M}_1(2)]_{v=0} = M_1^0(1)M_1^0(2), \quad (16)$$

where in the final equality we have used (13) and explicitly noted that $1 \neq 2$. Thus, the first order term in W is just

$$\sum_{\langle 12 \rangle} M_1^0(1)v(12)M_1^0(2) = \frac{1}{2} \sum_{1,2} M_1^0(1)v(12)M_1^0(2). \quad (17)$$

Evaluation of the third term in (12) necessitates using eqn (8) twice:

$$\begin{aligned} \frac{\delta^2 W}{\delta v(12)\delta v(34)} &= \frac{\delta}{\delta v(34)} \frac{\delta W}{\delta v(12)} = \frac{\delta^2}{\delta h(1)\delta h(2)} \frac{\delta W}{\delta v(34)} \\ &+ \left[\frac{\delta}{\delta h(1)} \frac{\delta W}{\delta v(34)} \right] \frac{\delta W}{\delta h(2)} + \frac{\delta W}{\delta h(1)} \left[\frac{\delta}{\delta h(2)} \frac{\delta W}{\delta v(34)} \right], \end{aligned}$$

$$\left. \frac{\delta^2 W}{\delta v(12)\delta v(34)} \right|_{v=0} = (\delta(13)\delta(24) + \delta(14)\delta(23))M_2^0(1)M_2^0(2) \\ + M_1^0(1)M_1^0(3)\delta(24)M_2^0(2) \\ + M_1^0(1)M_1^0(4)\delta(23)M_2^0(2) \\ + M_1^0(2)M_1^0(3)\delta(14)M_2^0(1) \\ + M_1^0(2)M_1^0(4)\delta(13)M_2^0(1). \quad (18)$$

Thus,

$$W[h, v] = \sum_1 M_0^0(1) + \frac{1}{2} \sum_{1,2} M_1^0(1)v(12)M_1^0(2) \\ + \frac{1}{4} \sum_{1,2} M_2^0(1)v^2(12)M_2^0(2) \\ + \frac{1}{2} \sum_{1,2,3} M_1^0(1)v(12)M_2^0(2)v(23)M_1^0(3) \\ + \text{order } v^3 \text{ and higher.} \quad (19)$$

It should be apparent at this point that finding the coefficient of v^n is a trivial but tedious task.

Luckily there is a general method for writing down immediately all terms in the expansion (11) (or (19)) for $W[h, v]$. The rule associates the terms of the expansion in a one-to-one manner with a set of linear graphs. After stating the rule and discussing its application, we shall return in Section II.C to its derivation. Before setting down the rule, we must introduce some terminology from graph theory (Essam and Fisher, 1970, see also Domb this Volume, Chapter 1):

Graphical definitions I:

A graph is a set of vertices (points) and edges (lines). Each edge is incident at two distinct vertices.[†] An n -rooted graph, $n = 0, 1, 2, \dots$, has n fixed, distinguishable, external or rooted vertices. All remaining internal vertices are free.

The valence of a vertex is the number of edges incident at that vertex. A vertex of valence n is called n -valent.

A connected graph is a graph with the property that any pair of its vertices is joined by a continuous sequence of edges. A graph which is not connected is disconnected.

Two n -rooted graphs are isomorphic if, when their external vertices are put in one-to-one correspondence, there exists at least one way in which their internal vertices and edges may be placed in one-to-one correspondence in such a way that all connectivity is maintained. The number of distinct ways in which a

[†] “Loops,” in which a single edge is incident with both ends at the same vertex, are prohibited.

graph can be made isomorphic to itself is called the symmetry factor† g of the graph. A set of graphs are topologically distinct if no two of them are isomorphic.

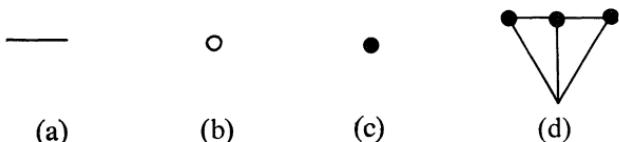


FIG. 1. The fundamental graphical elements: (a) an edge, (b) an external vertex, (c) an internal vertex, (d) a graph in which the external vertex carries no vertex factor.

When picturing graphs (see Fig. 1), we draw the edges as lines and the external and internal vertices as open and filled circles, respectively. The only exception to this comes in Section II.E and after, where, in the process of

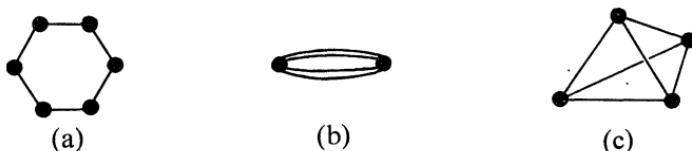


FIG. 2. Symmetry factors for the unrooted graphs (a), (b), and (c) are 12, 48, and 24 respectively. The general n -gon has a symmetry factor $2n$. The n -fold multiedge has a symmetry factor $2n!$. The complete n -vertex graph (all pairs connected by a single edge) has a symmetry factor $n!$.

renormalisation, we shall need a vertex with which no algebraic factor is associated. For such a vertex the circle will be omitted. Some unrooted graphs and their symmetry factors are shown in Fig. 2.

In order to calculate $W[h, v]$ one takes the set of all topologically distinct 0-rooted connected graphs. One associates with each graph a contribution according to Rule 1 below, and one sums all such contributions:

Rule 1: Free Energy W , Unrenormalised Form

- Assign a dummy label to each internal vertex.
- For each edge joining vertices i and j write a factor $v(ij)$.
- For each l -valent internal vertex i write a factor $M_l^0(i)$ (eqn (10), (14)).
- Sum each internal vertex label freely over the entire lattice.
- Divide by the symmetry factor of the unrooted graph.

† This is termed "symmetry number" in Chapter 1. The graphs in the present chapter may contain multiple bonds between vertices which are treated as non-identical.

In this spirit we write,

$$\begin{aligned}
 W[h, v] = & \left\{ \begin{array}{l} \text{sum of all topologically} \\ \text{distinct unrooted connected} \\ \text{graphs according to Rule 1} \end{array} \right\} \\
 = & \bullet + \frac{1}{2} \text{ (graph)} + \frac{1}{4} \text{ (graph)} + \frac{1}{2} \text{ (graph)} + \frac{1}{12} \text{ (graph)} + \frac{1}{6} \text{ (graph)} \\
 & + \frac{1}{2} \text{ (graph)} + \frac{1}{6} \text{ (graph)} + \frac{1}{2} \text{ (graph)} + \text{order } v^4 \text{ and higher.}
 \end{aligned} \tag{20}$$

The symmetry factor for each graph is given in the form $1/g$. The reader will verify that the first four terms of (20) correspond in sequence to the first four terms of (19), according to Rule 1. The remaining terms in (20) give all contributions to W which are third order in the interaction, i.e., which come from graphs with exactly three edges. Figure 3 gives the contribution to W of a more complicated graph.

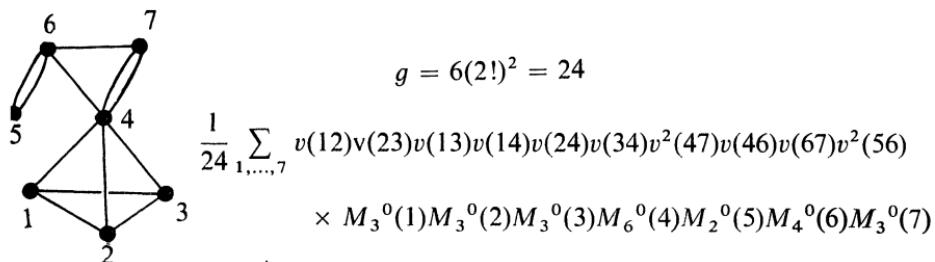


FIG. 3. A twelfth order contribution to the Ising free energy according to Rule 1.

Equation (20) gives $W[h, v]$ for arbitrary inhomogeneous fields and interactions. Although this freedom will be useful in what follows, it is worth pointing out that, if the free energy is all we wish to calculate, considerable simplification is gained by immediately specialising to the translationally invariant case,

$$h(1) = h, \quad v(12) = V(\mathbf{R}_1 - \mathbf{R}_2). \tag{21}$$

The bare semi-invariants $M_n^0(h)$ are independent of position, and the formal extensivity of W is realised,

$$\begin{aligned}
 \frac{W}{N} = & M_0^0(h) + \frac{1}{2}(M_1^0(h))^2 \sum_{\mathbf{R}} V(\mathbf{R}) \\
 & + \frac{1}{4}(M_2^0(h))^2 \sum_{\mathbf{R}} V^2(\mathbf{R}) + \frac{1}{2}(M_1^0(h))^2 M_2^0(h) \left[\sum_{\mathbf{R}} V(\mathbf{R}) \right]^2 \\
 & + \text{order } v^3 \text{ and higher,}
 \end{aligned} \tag{22}$$

where \mathbf{R} runs over the entire lattice and boundary effects have been neglected (periodic boundary conditions). It is easy to see from (10) and (14) that $M_n^0(h)$ has parity $(-1)^n$, so that, when $h = 0$, all odd semi-invariants vanish and, of the explicit terms in (22), only the first and third survive.

The most studied example of (22) is when, in addition to (21), the potential acts between nearest-neighbour sites only,

$$v(12) = \begin{cases} v, & \text{when 1 and 2 are nearest neighbours,} \\ 0, & \text{otherwise.} \end{cases} \quad (23)$$

In this case (22) simplifies to

$$\frac{W}{N} = M_0^0(h) + \frac{q}{2} (M_1^0(h))^2 v + \left[\frac{q}{4} (M_2^0(h))^2 + \frac{q^2}{2} (M_1^0(h))^2 M_2^0(h) \right] v^2 \\ + \text{order } v^3 \text{ and higher,} \quad (24)$$

where q , the *coordination number* of the lattice, is just the number of nearest neighbours of any site. Let us in this case consider a given n -edged graph G_n and examine its contribution $W(G_n)$ to the full free energy. Because of the nearest-neighbour restriction, all terms in the sum required by Rule 1(d) are identical. The number of such terms we write as $Nm(G_n)$, where $m(G_n)$ is the *free multiplicity of the graph* G_n . $m(G_n)$ measures the number of distinct ways per site of the underlying lattice† in which the *vertex-labelled graph* G_n can be embedded in the lattice with each vertex assigned to a site of the lattice and each edge lying along a nearest-neighbour bond. In the appendix to this article the free multiplicity is discussed, some of its simple properties are given, and it is related to the weak lattice constants. Jasnow (1969) has tabulated the free multiplicities of 2-rooted graphs for a variety of lattices. It is important to notice that, because the sum in Rule 1(d) is unrestricted, *it is quite permissible for graphically distinct vertices to occupy the same lattice site*. This is in contrast to the weak and strong lattice constant systems used in other types of expansions and discussed for example by Domb (1960) and by Sykes *et al.* (1966). (See Domb this Volume, Chapter 1.) The contribution $W(G_n)$ now is

$$W(G_n) = \frac{N}{g(G_n)} m(G_n) v^n \left(\prod_{G_n} M^0 \right), \quad (25)$$

where, by the notation $\prod_{G_n} M^0$, we intend to evoke the product of semi-invariants required for the graph G_n by Rule 1(c). To find the coefficient of v^n in the

† For a finite lattice with free surfaces $m(G_n)$ is not strictly intensive. This remark is not entirely pedantic, since it shows where in the expansion the boundary contribution to W may be found. (See Watson, Vol. 1, Chapter 4.) We shall in the text continue to assume periodic boundary conditions, thus guaranteeing intensivity of the multiplicity.

expansion for W we have only to sum up the contributions of all n -edged graphs. If one is given a list of graphs G_n along with corresponding symmetry factors and multiplicities, the labour, which is entirely clerical, might be organized as shown in Fig. 4.

| G | $g(G)$ | $m(G)$ | $W(G)/N$ |
|---|--------|--------------|---------------------------------------|
|  | 12 | q | $\frac{1}{2}qv^3(M_3^0)^2$ |
|  | 6 | q^3 | $\frac{1}{6}q^3v^3(M_1^0)^3M_3^0$ |
|  | 2 | q^2 | $\frac{1}{2}q^2v^3M_1^0M_2^0M_3^0$ |
|  | 6 | $6p(\Delta)$ | $p(\Delta)v^3(M_2^0)^3$ |
|  | 2 | q^3 | $\frac{1}{2}q^3v^3(M_1^0)^2(M_2^0)^2$ |

FIG. 4. Bookkeeping for the evaluation of the v^3 term in the nearest-neighbour Ising model free energy. The total v^3 contribution is the sum of the five terms in the right hand column. q is the coordination number of the lattice and $p(\Delta)$ is its weak lattice constant for the triangle graph. For loose-packed lattices $p(\Delta) = 0$. $p(\Delta) = 2, 8$ on the triangle and f.c.c. lattices, respectively.

So far we have discussed only the free energy expansion. Equations (4)–(6) allow corresponding linked-cluster expansions to be written down for all Ising model cumulant correlations \mathcal{M}_n simply by term-by-term differentiation of the free energy. Note that (i) the fields appear in W only through the semi-invariants M_n^0 and (ii) differentiation of an $M_n^0(h)$ has by (14) the very simple effect,

$$\left(\frac{d}{dh}\right)^l M_n^0(h) = M_{n+l}^0(h). \quad (26)$$

Consider, for example, differentiation of the first few terms (19) of W :

$$\begin{aligned} \frac{\langle s_{z1} \rangle}{s} &= \langle \mu(1) \rangle \equiv \mathcal{M}_1(1) \equiv \frac{\delta W}{\delta h(1)} \equiv M_1(1) \\ &= M_1^0(1) + \sum_2 M_2^0(1)v(12)M_1^0(2) \\ &\quad + \frac{1}{2} \sum_2 M_3^0(1)v^2(12)M_2^0(2) \end{aligned}$$

$$\begin{aligned}
 & + \sum_{2,3} M_2^0(1)v(12)M_2^0(2)v(23)M_1^0(3) \\
 & + \frac{1}{2} \sum_{2,3} M_3^0(1)v(12)M_1^0(2)v(13)M_1^0(3) \\
 & + \text{order } v^3 \text{ and higher.}
 \end{aligned} \tag{27}$$

The effect of differentiation is to fix by turn each graphical vertex and to increase by one the order of its bare semi-invariant. When two vertices of the same graph are topologically equivalent, their contributions are, of course, identical.

The result of the above procedure is easily expressed in terms of a graphical rule; however, while we are at it, it will be useful to define a somewhat more general quantity, the full significance of which will only appear in Section II.E. In this spirit we define $M_n(1)$ the *n*th order renormalised semi-invariant,

$$M_n(1) = \left\{ \begin{array}{l} \text{sum of all topologically} \\ \text{distinct 1-rooted connected} \\ \text{graphs according to Rule 2.} \end{array} \right\} \tag{28a}$$

Rule 2: Renormalised Semi-Invariants, Unrenormalised Form

- Assign the label 1 to the external (root) vertex and a dummy label to each internal vertex.
- For each edge joining vertices i and j write a factor $v(ij)$.
- For each l -valent internal vertex i write a factor $M_l^0(i)$. For each l -valent external vertex write a factor $M_{n+l}^0(1)$.
- Sum each internal vertex label freely over the entire lattice.
- Divide by the symmetry factor of the 1-rooted graph.

The graphical representation (cf. (20)) starts,

$$\begin{aligned}
 M_n(1) = & \circ + \bullet + \frac{1}{2} \bullet + \circ + \frac{1}{2} \bullet + \frac{1}{2} \bullet + \frac{1}{2} \bullet \\
 & + \frac{1}{2} \bullet + \frac{1}{6} \bullet + \frac{1}{2} \bullet + \frac{1}{2} \bullet + \frac{1}{2} \bullet \\
 & + \frac{1}{2} \bullet + \frac{1}{2} \bullet + \circ + \bullet + \bullet \\
 & + \text{order } v^4 \text{ and higher.}
 \end{aligned} \tag{28b}$$

The open circle represents the external vertex 1. Notice that the symmetry factors for the rooted graphs differ from those of their unrooted analogs. When $n = 1$, Rule 2 gives the magnetisation (27) of the Ising model.

An additional derivative of (27) gives the pair correlations (5). Note that there are two types of terms, those in which the $\delta/\delta h(2)$ derivative hits the

already rooted external vertex 1 and those in which it fixes a second internal vertex. The former terms are summed by Rule 2 with $n = 2$. Thus,

$$\mathcal{M}_2(12) = \delta(12)M_2(1) + \left\{ \begin{array}{l} \text{sum of all topologically distinct} \\ \text{2-rooted connected graphs} \\ \text{according to Rule 3.} \end{array} \right\} \quad (29)$$

Rule 3: Pair Correlations, Unrenormalised Form

- (a) Assign the labels 1 and 2 to the external vertices and dummy labels to the internal vertices.
- (b) For each edge joining vertices i and j write a factor $v(ij)$.
- (c) For each l -valent internal vertex i write a factor $M_l^0(i)$. For each l -valent external vertex $j = 1, 2$ write a factor $M^0_{l+1}(j)$.
- (d) Sum each internal vertex label freely over the entire lattice.
- (e) Divide by the symmetry factor of the 2-rooted graph.

Thus,

$$\begin{aligned} \mathcal{M}_2(12) - \delta(12)M_2(1) = & \frac{1}{2} \circ_1 \circ_2 + \frac{1}{2} \circ_1 \circ_2 \text{ (double loop)} + \circ_1 \text{ (triangle)} + \circ_1 \circ_2 + \circ_1 \circ_2 \\ & + \frac{1}{6} \circ_1 \circ_2 \text{ (double loop)} + \circ_1 \circ_2 \text{ (bridge)} + \frac{1}{2} \circ_1 \circ_2 + \frac{1}{2} \circ_1 \circ_2 + \circ_1 \circ_2 \\ & + \frac{1}{2} \circ_1 \circ_2 + \circ_1 \circ_2 \\ & + \circ_1 \circ_2 \\ & + \text{order } v^4 \text{ and higher.} \end{aligned} \quad (30)$$

Note that graphs which have the labels of their external vertices interchanged are considered distinct.

Higher order correlations go similarly. In each case multiply differentiated vertices must be counted separately. Thus, for example,

$$\begin{aligned} \mathcal{M}_3(123) = & \delta(123)M_3(1) + \delta(12)M_{21}(13) + \delta(13)M_{21}(32) \\ & + \delta(23)M_{21}(21) + \left\{ \begin{array}{l} \text{sum of all topologically} \\ \text{distinct 3-rooted connected graphs,} \end{array} \right\} \end{aligned} \quad (31)$$

where $M_{21}(ij)$ stands for the sum of all topologically distinct 2-rooted connected graphs by Rule 3 modified for double differentiation at the i vertex.

Equations (20), (28), (30), (31) and their higher order analogs give a recipe for calculating all terms in the Taylor expansions of thermodynamic and correlation functions for the Ising model. Unfortunately the number of contributing graphs in higher orders proliferates very rapidly, so that the unrenormalised linked-cluster expansion is seldom a practical tool. The renormalisations necessary to render it practical will be taken up in Section II.E. Before going on, however, we present (II.C) a proof of the unrenormalised expansions and discuss (II.D) the relation of the unrenormalised linked-cluster expansion to the more conventional weak-embedding expansion for the $s = \frac{1}{2}$ Ising model. Both these sections may be skipped without destroying the continuity of the development.

C. Proof of the unrenormalised linked-cluster expansion

Proofs of Rule 1 for the unrenormalised linked-cluster expansion for the Ising model free energy have been given by Englert (1963), Bloch and Langer (1965), and Jasnow (1969). Jasnow's proof is in essence simply a systematisation of the procedure we have used in (16)–(19) to generate the first few orders of the expansion from eqn (8). In what follows we prefer to use the approach of Bloch and Langer, since it is particularly direct and follows the same line as the conventional proofs of the classical-fluid linked-cluster theorem (Huang, 1963; Mayer, 1937; Uhlenbeck and Ford, 1963; Domb, this Volume, Chapter 1).

Direct expansion of the partition function (3) yields:

$$\begin{aligned} \exp W[h, v] &= Z[h, v] = \text{Tr} \exp \left(\sum_1 h(1)\mu(1) \right) \sum_{n=0}^{\infty} \frac{1}{2^n n!} \left(\sum_{1,2} v(12)\mu(1)\mu(2) \right)^n \\ &= Z_0(h) \sum_{n=0}^{\infty} \frac{1}{2^n n!} \left[\sum_{1,2,\dots,2n} v(12) \dots v(2n-1, 2n) \langle \mu(1) \dots \mu(2n) \rangle_0 \right], \end{aligned} \quad (32)$$

where $\langle \rangle_0$ refers to an expectation value in the $v = 0$ ensemble. Expectation values of products such as occur in (32) can always be written in terms of cumulants, e.g.

$$\begin{aligned} \langle \mu(1)\mu(2) \rangle &= \mathcal{M}_2(12) + \mathcal{M}_1(1)\mathcal{M}_1(2) \\ \langle \mu(1)\mu(2)\mu(3) \rangle &= \mathcal{M}_3(123) + \mathcal{M}_2(12)\mathcal{M}_1(3) + \mathcal{M}_2(13)\mathcal{M}_1(2) \\ &\quad + \mathcal{M}_2(23)\mathcal{M}_1(1) + \mathcal{M}_1(1)\mathcal{M}_1(2)\mathcal{M}_1(3). \end{aligned} \quad (33)$$

The general rule is that $\langle \mu(1) \dots \mu(2n) \rangle$ is a sum of products of cumulant correlations in which each term corresponds to a partition of the arguments $(1 \dots 2n)$ and every possible partition appears once and only once.

The bracketed sum in (32) requires evaluation of $\langle \mu(1) \dots \mu(2n) \rangle$ in the $v = 0$ ensemble, for which the cumulant correlations \mathcal{M}^0 contain spatial

δ -functions and bare semi-invariants (13). Because $v(ij) = 0$ when $i = j$, the locality property eliminates from (32) any term in $\langle \mu(1) \dots \mu(2n) \rangle_0$ in which both ends of the same bond $v(ij)$ have been assigned to the same \mathcal{M}^0 , i.e., $v(12)\mathcal{M}^0(12\dots) = 0$. The remaining bracketed quantities can be expressed graphically in the sense of Rule 1 (a)-(d) if we include both *connected and disconnected graphs*. The $n = 1$ and $n = 2$ brackets are, for example, respectively,

$$\left[\begin{array}{c} \bullet \\ | \\ \bullet \end{array} \right] \text{ and } \left[\begin{array}{c} \bullet & \bullet \\ | & | \\ \bullet & \bullet \end{array} \right] + 4 \left[\begin{array}{c} \bullet & \bullet \\ & \backslash \\ & \bullet \end{array} \right] + 2 \left[\begin{array}{c} \bullet \\ \parallel \\ \bullet \end{array} \right], \quad (34)$$

where the numerical factors come from different permutations of the dummy labels. Disconnected contributions are products of *connected components*. Let us label all topologically distinct connected components by some index $\alpha = 1, 2, \dots$ and the corresponding contributions according to Rule 1 (a)-(d) by w_α . Figure 5 shows how the first few lines of such a listing might look.

| α | G_α | w_α |
|----------|------------|---|
| 1 | | $\sum_{1,2} M_1^0(1)v(12)M_1^0(2)$ |
| 2 | | $\sum_{1,2,3} M_1^0(1)v(12)M_2^0(2)V(23)M_1^0(3)$ |
| 3 | | $\sum_{1,2} M_2^0(1)(v(12))^2 M_2^0(2)$ |

FIG. 5. A partial listing of the contributions of the various connected components in the bracket of eqn (32).

Any term in the bracket is simply a product of one or more w_α , $\prod_{\alpha=1}^{\infty} w_\alpha^{n_\alpha}$, where $n_\alpha = 0, 1 \dots$ is the number of times each G_α appears. For example, the terms in (34) are just $[w_1]$ and $[w_1^2 + 4w_2 + 2w_3]$. Note that each term may appear a number of times. This is because the arguments $1, 2, \dots, 2n$ are summed, so contributions in which these arguments have been *permuted in such a way as to leave the topology unchanged* are identical. The number of such permutations for a graph specified by a given set of $\{n_\alpha\}$ is just

$$2^n n! \prod_{\alpha=1}^{\infty} \frac{1}{n_\alpha! g_\alpha^{n_\alpha}},$$

where g_α is the symmetry factor referred to in Rule 1(e). The total contribution to the bracket in (32) of each topology $\{n_\alpha\}$ is just

$$2^n n! \prod_\alpha \frac{1}{n_\alpha!} \left(\frac{w_\alpha}{g_\alpha} \right)^{n_\alpha}. \quad (35)$$

Substitution of (35) into (32) gives

$$W[h, v] = W_0[h] + \sum_{\alpha=1}^{\infty} \frac{w_\alpha}{g_\alpha}, \quad (36)$$

which is identical to Rule 1.

The graphical rules for correlation functions may be derived by arguments essentially similar to the above (Englert, 1963). In the evaluation of $\langle X \rangle = \text{Tr } X \exp(-\beta \mathcal{H}) / Z[h, v]$, the denominator divides out all unrooted graphs. The whole procedure is entirely analogous to our treatment of W , and we prefer the method of term-by-term differentiation described in II.B.

D. Relation of the linked-cluster and weak-embedding expansions for the free energy

The relation between the linked-cluster and weak-embedding expansions is simple in principle, although, as will be seen in what follows, the enumeration of those terms in one which correspond to a given term in the other can be quite involved. The relation is most easily studied by means of an example. We choose for this purpose the $s = \frac{1}{2}$ Ising model free energy W .

The standard weak-embedding expansion (Newell and Montroll, 1953; Domb, 1960) uses the operator identity $\exp(\alpha A) = \cosh \alpha + A \sinh \alpha$, valid for any operator A such that $A^2 = 1$, to rewrite the $s = \frac{1}{2}$ Ising partition function (3). Thus,

$$\begin{aligned} W[h, v] &= \sum_1 \ln (2 \cosh h(1)) + \frac{1}{2} \sum_{1,2} \ln \cosh v(12) \\ &\quad + \ln 2^{-N} \text{Tr} \left[\prod_1 (1 + \mu(1) \tanh h(1)) \prod_{\langle 12 \rangle} (1 + \mu(1)\mu(2) \tanh v(12)) \right], \end{aligned} \quad (37)$$

where $\prod_{\langle 12 \rangle}$ denotes the product over all pairs of sites. Development of the trace in powers of $\tanh v$ yields the weak-embedding expansion. We maintain ~~us~~ individually variable the local fields and bond strengths in order to facilitate detailed comparison with the linked-cluster form of the development. Terms which survive the trace must have an even number of factors $\mu(i)$ at each site i and, thus, can be designated uniquely by listing the contributing bonds $\tanh v(ij)$. The topology of the contributing bonds constitutes a graph. Both connected and disconnected graphs appear. When the logarithm is taken, all those parts of the disconnected contributions which go as N^n , $n > 1$,

cancel against iterations of lower orders, thus guaranteeing extensivity in the thermodynamic limit.

The first few terms in the resulting expression are shown in equation (38):

$$\begin{aligned}
 W[h, v] - W_0[h] &= \frac{1}{2} \sum_{1,2} \ln \cosh v(12) \\
 &= \frac{1}{2} \sum_{1,2} \tanh h(1) \tanh v(12) \tanh h(2) \\
 &\quad + \frac{1}{2} \sum_{\substack{2 \\ 1 \neq 3}} \tanh h(1) \tanh v(12) \tanh v(23) \tanh h(3) \\
 &\quad - \left[\frac{1}{4} \sum_{1,2} \tanh^2 h(1) \tanh^2 v(12) \tanh^2 h(2) \right. \\
 &\quad \left. + \frac{1}{2} \sum_{\substack{2 \\ 1 \neq 3}} \tanh h(1) \tanh v(12) \tanh^2 h(2) \tanh v(23) \tanh h(3) \right] + \dots \\
 &= \text{graph} + \text{graph} + \text{graph} + \dots, \tag{38}
 \end{aligned}$$

where we have indicated the graph corresponding to each term in the weak-embedding sense. Each edge i, j carries a factor $\tanh v(ij)$. Each vertex i with odd valence carries a factor $\tanh h(i)$. The disconnected graphs come from the expansion of the logarithm.

On the other hand, the bare semi-invariants (14) for the linked-cluster expansion are for $s = 1/2$,

$$\begin{aligned}
 M_n^0(h) &= \frac{d^n}{dh^n} \ln(2 \cosh h), \\
 M_1^0 &= \tanh h, \quad M_2^0 = 1 - \tanh^2 h, \dots, \tag{39}
 \end{aligned}$$

Substitution into (19) gives,

$$\begin{aligned}
 W[h, v] - W_0[h] &= \frac{1}{2} \sum_{1,2} \tanh h(1) v(12) \tanh h(2) \\
 &\quad + \frac{1}{4} \sum_{1,2} (1 - \tanh^2 h(1)) v^2(12) (1 - \tanh^2 h(2)) \\
 &\quad + \frac{1}{2} \sum_{1,2,3} \tanh h(1) v(12) (1 - \tanh^2 h(2)) v(23) \tanh h(3) + \dots \\
 &= \frac{1}{2} \text{graph} + \frac{1}{4} \text{graph} + \frac{1}{2} \text{graph} + \dots \tag{40}
 \end{aligned}$$

To compare (38) and (40), it is necessary (i) to expand $\ln \cosh v$ and $\tanh v$ in powers of v and (ii) to dissect out of the free linked-cluster sums those contributions from each set of distinct bonds. The connections in Fig. 6 show which set of graphs in one expansion contribute to a given term of the other.

Note that each weak graph will, in a complete tabulation, contribute to an infinite number of linked-cluster graphs (since $\tanh v$ has all odd powers of v), while each linked-cluster graph contributes only to a finite number of weak graphs (with the same number of lines or fewer).

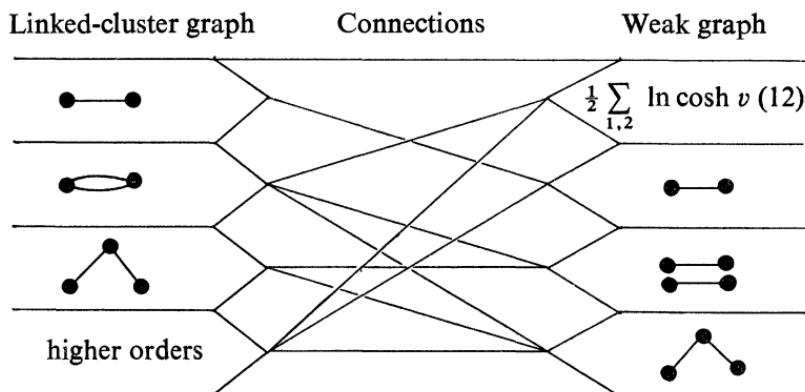


FIG. 6. Graphical correspondences between the linked-cluster and weak-embedding expansions for the $s = \frac{1}{2}$ Ising free energy. Connections show which graphs in one expansion contribute to a given term in the other.

To clarify this relation it is useful to sort the terms of both expansions according to which connected set of bonds $\{v(ij)\}$ is used. This sorting according to a *physical cluster* of bonds has been discussed by Rushbrooke and Morgan (Rushbrooke and Morgan, 1961; Morgan and Rushbrooke, 1961; Rushbrooke, 1964), Elliott and Heap (Elliott and Heap, 1962; Heap, 1963), Jasnow and Wortis (1967), and others. Such a physical cluster receives on the one hand contributions from all *linked-cluster* graphs which can be embedded in it using every physical bond *at least once* (note that the free sums allow multiple usage of each site and bond—quite complicated graphs can be “collapsed” to fit into simple physical clusters) and on the other hand contributions from all weak graphs which can be embedded in it using every bond *once and only once*. A further sorting of these correspondences by powers of $v(ij)$ for each bond extends Fig. 6 as far as patience permits.

The complexity of the interrelation between the two types of expansion rests—in a language restricted to the nearest-neighbour case (23)—on the connection between the free multiplicities $m(G)$ defined after (24) and the weak lattice constants. This connection, which is touched upon in the appendix, has not yet been seriously explored.

E. Vertex renormalisation: the correlations

To make the linked-cluster expansion practical from a calculational point of view, one must find a way of reducing the number of contributing graphs.

This is done by selective resummation of classes of graphs. The effect is to introduce a degree of implicitness into the procedure and thus to exchange topological complexity for algebraic complexity.

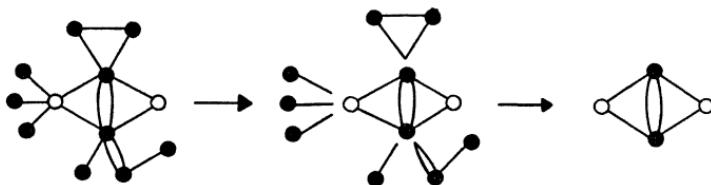


FIG. 7. The graph at the left is 1-reducible at several of its vertices. When all 1-insertions at the reducible vertices have been clipped away, the resulting 1-skeleton shown at the right is 1-irreducible.

We motivate the development by considering a rooted graph such as that shown in Fig. 7. Every such graph can be regarded as composed of a basic *skeleton graph* decorated by additions or *insertions*. There are an infinite number of insertions, which can be made singly or in combinations at each vertex of such a skeleton. The contributions to each graph corresponding to the insertions at a given vertex enter multiplicatively and are independent of the rest of the graph, since the sum in part (d) of the Rules is always free. The summed contributions of a fixed bare skeletal vertex with all its possible decorations defines a factor we shall call the *renormalised semi-invariant* M_n , where n gives the number of incident skeletal lines. See Fig. 8. Calculation of a skeleton with renormalised semi-invariants at the vertices sums the infinite number of bare-perturbation-theory graphs having that skeleton.

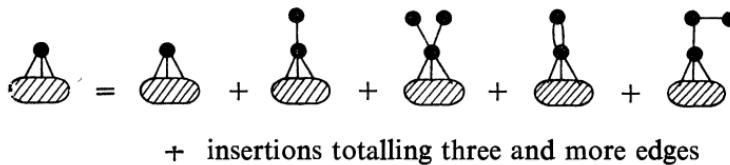


FIG. 8. Vertex renormalisation sums graphs differing only by insertions at a given vertex. The black circle in the graph at the left represents the renormalised vertex factor M_3 . The cross-hatched oval, which stands for the remainder of the graph contains one or more rooted vertices. The vertex undergoing renormalisation may itself be a root.

Before continuing, it will be useful to supplement the graphical terminology introduced after eqn (19). In the discussion below all graphs will be assumed *connected* unless explicitly stated to the contrary.

Disassembly of a Vertex†

A vertex V of a graph G is disassembled by the following procedure:

- (i) Clip away all edges from V (thereby dividing G into a number of disconnected parts).
- (ii) Reattach to V all clipped edges belonging to disconnected parts containing external vertices.
- (iii) Join to one another the clipped edge ends belonging to each additional connected part (if any).

This process is pictured for several graphs in Fig. 9.

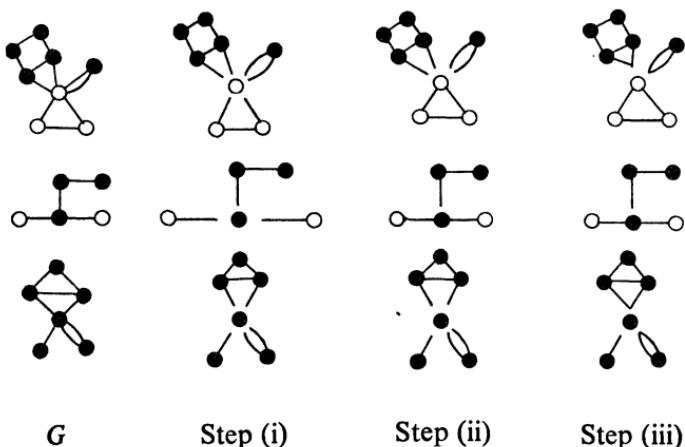


FIG. 9. Disassembly of various graphical vertices.

Graphical Definitions II

The unrooted parts formed in the process of disassembly are called 1-insertions. The clipped vertex of a 1-insertion will be regarded as the external vertex of the 1-insertion and will be drawn without a circle.‡

An articulation point of a rooted graph is a vertex the disassembly of which produces at least one 1-insertion. An articulation point of an unrooted graph is a vertex the disassembly of which produces at least two 1-insertions.

A graph which contains no articulation points is 1-irreducible. A graph which contains one or more articulation points is 1-reducible.

The 1-skeleton of a rooted graph is the graph produced by disassembling in turn all vertices of the graph and discarding all 1-insertions thereby produced.

† This operation differs, for example, from *deletion of a vertex*, which removes all incident edges (Essam and Fisher, 1970), in that no graphical elements are gained or lost. From the algebraic point of view, we are simply *regrouping* the factors in each perturbation theoretic term. This is the origin of the slight differences which will appear between our terminology and that of Essam and Fisher.

‡ This notation is intended to suggest that such a vertex carries no semi-invariant factor.

Any rooted graph has a *unique 1-irreducible 1-skeleton*, as illustrated in Fig. 7, to which it can be reduced by clipping away all 1-insertions. (Note that the open circle is the 1-skeleton of every 1-rooted graph.) Conversely any rooted graph can be constructed from a 1-irreducible 1-skeleton in a unique way by appending appropriate combinations of 1-insertions at each skeletal vertex.[†]

Because of the free sums in parts (d) of Rules 1–3, each 1-insertion enters as a factor in the overall graphical contribution. To keep track of the appropriate subscript on the bare semi-invariant, it is necessary to classify 1-insertions according to the *valence of the external vertex*. We therefore define the *self-field* $G_n(1)$ as,

$$G_n(1) = \left\{ \begin{array}{l} \text{sum of all topologically} \\ \text{distinct } n\text{-valent 1-insertions} \\ \text{according to Rule 4} \end{array} \right\} \quad (41a)$$

Rule 4: Self-Field, Unrenormalised Form

- (a) Assign the label 1 to the external vertex and a dummy label to each internal vertex.
- (b) For each edge joining vertices i and j write a factor $v(ij)$.
- (c) For each l -valent internal vertex i write a factor $M_l^0(i)$. For the external vertex write a factor 1.
- (d) Sum each internal vertex label freely over the entire lattice.
- (e) Divide by the symmetry factor of the 1-insertion.

In this form G_n depends on v and h (via the M_l^0 's). The graphical representation of the first few G_n 's looks like:

$$\begin{aligned} G_1(1) &= \begin{array}{c} \bullet \\ | \end{array} + \begin{array}{c} \bullet \\ | \\ \backslash \end{array} + \frac{1}{2} \begin{array}{c} \bullet \\ | \\ / \end{array} + \begin{array}{c} \bullet \\ | \\ \backslash \\ | \end{array} + \begin{array}{c} \bullet \\ | \\ / \\ | \end{array} + \text{order } v^4 \text{ and higher.} \\ G_2(2) &= \frac{1}{2} \begin{array}{c} \bullet \\ | \\ \backslash \end{array} + \frac{1}{2} \begin{array}{c} \bullet \\ | \\ / \end{array} + \frac{1}{2} \begin{array}{c} \bullet \\ | \\ \backslash \\ | \end{array} + \text{order } v^4 \text{ and higher} \\ G_3(1) &= \frac{1}{6} \begin{array}{c} \bullet \\ | \\ \backslash \\ | \\ \backslash \end{array} + \text{order } v^4 \text{ and higher.} \end{aligned} \quad (41b)$$

The factors G_n play the physical role of a generalized 1-body effective field. They have a parallel in the classical-fluid expansion (see II.F), and are closely analogous to the quantum-mechanical self-energy operator Σ (Kadanoff and Baym, 1962).

We are now in a position to calculate the net contribution of all possible

[†] Note that an *unrooted* graph does not possess a unique construction from an underlying 1-skeleton. It can, for example, be constructed by decorating *any* isolated vertex. Because of this ambiguity the free energy must be handled separately from the correlations (see Section II.F).

decorations of a single given skeletal vertex, as pictured for example in Fig. 8. The presence of k identical 1-insertions at the same vertex makes a multiplicative contribution of $k!$ to the overall symmetry factor for the decoration of an n -valent skeletal vertex:

$$\begin{aligned} M_n(1) &= M_n^0(1) + \sum_{l=1}^{\infty} G_l(1) M_{n+l}^0(1) + \frac{1}{2} \sum_{l,m=1}^{\infty} G_l(1) G_m(1) M_{n+l+m}^0(1) + \dots \\ &= \left[\exp \sum_{l=1}^{\infty} G_l(1) \frac{\delta^l}{\delta \tilde{h}^l} \right] M_n^0[1; \tilde{h}] \Big|_{\tilde{h}=h(1)}, \end{aligned} \quad (42)$$

with $n = 1, 2, 3, \dots$, which is a re-expression of (28) and includes the magnetisation $\mathcal{M}_1(1) = M_1(1)$ as a special case.[†]

Summation of all rooted graphs having the same 1-skeleton is now accomplished by the replacement $M_n^0 \rightarrow M_n$ at the skeletal vertices. The only difficulty in passing from (42) to the above statement is the question of symmetry factors. Suppose a given rooted graph G is composed of a 1-skeleton, G_s , decorated by a series of 1-insertions G_{I1}, G_{I2}, \dots . The symmetry factor $g(G)$ is composed of several factors,

$$\frac{1}{g(G)} = \frac{1}{g(G_s)} \frac{1}{\Pi g(G_I)} \frac{F_{EV}}{F_{SV}}. \quad (43)$$

F_{SV} (SV = single vertex) stands for the combinatorial factors arising from the presence of identical 1-insertions at a single vertex. F_{EV} (EV = equivalent vertex) stands for the combinatorial factors by which the skeletal symmetry factor $g(G_s)$ is reduced due to distinct decoration of previously equivalent skeletal vertices. For example, for the graph of Fig. 7, $g(G_s) = 4$, $\Pi g(G_I) = 2^2 = 4$, $F_{SV} = 3! = 6$, $F_{EV} = 2$, and $g(G) = 48$. In the renormalised form only the factor $1/g(G_s)$ is explicit. The $g(G_I)$ are absorbed in the self-fields; the F_{SV} are incorporated in the exponential form of (42); and, the F_{EV} are supplied by equivalent cross-terms in the expansion of the product of renormalised semi-invariants.

The procedure for finding the vertex renormalised form of a bare expansion is to group all contributing graphs with the same 1-skeleton and to sum them by putting $M_n^0 \rightarrow M_n$. For example, the two-point part of the pair correlations given by (29), (30), and Rule 3 may be re-expressed as,

$$\mathcal{M}_2(12) = \delta(12) M_2(1) + \left\{ \begin{array}{l} \text{sum of all topologically distinct} \\ \text{2-rooted 1-irreducible connected} \\ \text{graphs according to Rule 5.} \end{array} \right\}. \quad (44)$$

[†] Equation (42) is the classical analog of the quantum many-body Dyson equation (Kadanoff and Baym, 1962). M_n^0 corresponds to the bare propagator G_0 , and M_n corresponds to the renormalised propagator G . The fact that M_n^0 and M_n are spatially local reflects the locality of the Hamiltonian (1) in the absence of interaction.

Rule 5: Pair Correlations, Vertex Renormalised Form

- Assign labels 1 and 2 to the external vertices and dummy labels to the internal vertices.
- For each edge joining vertices i and j write a factor $v(ij)$.
- For each l -valent internal vertex i write a factor $M_l(i)$. For each l -valent external vertex $j = 1, 2$ write a factor $M_{l+1}(j)$.
- Sum each internal vertex label freely over the entire lattice.
- Divide by the symmetry factor of the 2-rooted graph.

Graphically,

$$\mathcal{M}_2(12) - \delta(12)M_2(1) = \begin{array}{c} \text{Diagram 1} \\ \text{Diagram 2} \\ \vdots \\ \text{Diagram n} \end{array} + \frac{1}{2} \begin{array}{c} \text{Diagram 1} \\ \text{Diagram 2} \\ \vdots \\ \text{Diagram n} \end{array} + \frac{1}{2} \begin{array}{c} \text{Diagram 1} \\ \text{Diagram 2} \\ \vdots \\ \text{Diagram n} \end{array} + \frac{1}{6} \begin{array}{c} \text{Diagram 1} \\ \text{Diagram 2} \\ \vdots \\ \text{Diagram n} \end{array} + \text{order } v^4 \text{ and higher.} \quad (45)$$

Equation (45) sums an infinite number of terms in the unrenormalised expansion and is exact through order v^3 with fewer graphs than the corresponding bare expression (30). The simplification is even more impressive in higher orders.

In contrast to the bare expansion, for which the vertex factors M_n^0 are known directly (see (10) and (14)), the renormalised expansion is only useful after the semi-invariants M_n have been calculated (e.g. from (41) and (42)). This is facilitated by using a renormalised expression for the self-fields G_n :

$$G_n(1) = \left\{ \begin{array}{l} \text{sum of all topologically distinct 1-irreducible} \\ \text{1-insertions which are } n\text{-valent at the external} \\ \text{vertex according to Rule 6.} \end{array} \right\}. \quad (46)$$

Rule 6: Self-Field, Vertex Renormalised Form

Same as Rule 4 except:

- For each l -valent internal vertex i write a factor $M_l(i)$. For the external vertex write a factor 1.

$$\begin{aligned} G_1(1) &= \text{Diagram 1} \quad (\text{exact!}), \\ G_2(1) &= \frac{1}{2} \text{Diagram 1} + \frac{1}{2} \text{Diagram 2} + \frac{1}{4} \text{Diagram 3} + \frac{1}{2} \text{Diagram 4} + \text{order } v^5 \text{ and higher,} \\ G_3(1) &= \frac{1}{6} \text{Diagram 1} + \frac{1}{2} \text{Diagram 2} + \text{order } v^5 \text{ and higher.} \end{aligned} \quad (47)$$

In this form the self-field depends functionally on v and the set M_n , $n = 1, 2, \dots$. Thus, $G(1) = G[1; M, v]$, and (42) becomes a non-linear equation, schematically,

$$M = \exp(G[M, v])M^0 \text{ or, more symmetrically, } M^0 = \exp(-G[M, v])M, \quad (48)$$

which can in principle be inverted to give $M[M^0, v]$. Once the M 's are known as functions of the variables h and v , then eqns (44) and (45) and their higher-order analogs evaluate the cumulant correlations.

In the derivation of high-temperature series expansions (Jasnow, 1969; Jasnow and Wortis, 1968) eqns (47) and (48) are solved iteratively in powers of v . To zeroth order $M_n = M_n^0$, which are given by (10) and (14). Note that $G_n \sim v^n$. Once the M_n 's are known to order v^l , (47) gives the G 's to order $l + 1$. These new G 's in (48) give the M_n 's to order $l + 1$, and so on. Stanley (1967) lists all $h = 0$ \mathcal{M}_2 graphs necessary through order v^8 (close-packed lattices) and v^9 (loose-packed lattices).

To go beyond iteration, it is necessary to use other methods (such as those discussed in Section II.H) to find $G[M, v]$. Inverting (48) may be facilitated by forming the Fourier transforms of the bare semi-invariants,

$$M_n^0(h) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikh} (ik)^n M_0^0(k), \quad (49)$$

where some care must be taken for $n = 0, 1$. Then, from (42),

$$M_n(h) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \left(\exp \sum_{l=1}^{\infty} (ik)^l G_l[M, v] \right) e^{ikh} (ik)^n M_0^0(k). \quad (50)$$

In the translationally invariant situation (21), (50) is a set of coupled algebraic equations for the numbers M_n , $n = 1, 2, \dots$.

F. Vertex renormalisation: the free energy

Free energy graphs are unrooted and hence have no unique 1-skeleton. The direct regrouping described in Section II.E is therefore inapplicable. This obstacle can be circumvented by two routes. De Dominicis (1962), Englert (1963), and Bloch and Langer (1965) use a topological method. Following an earlier publication (Wortis, *et al.*, 1969), we prefer simply to integrate eqn (4),

$$M_1(1) = \frac{\delta W[h, v]}{\delta h(1)}, \quad (51)$$

subject to the boundary condition that, as $h(1) \rightarrow \infty$, the only contributing state is $\mu(1) = 1$ for all sites 1. Thus, $M_1^0(1) = 1$, $M_n^0(1) = 0$, $n > 1$, and only the first two terms in (20) are non-vanishing, with analogous simpli-

fications for other quantities: as $h(1) \rightarrow \infty$ for all sites 1,

$$\begin{aligned} W &= \sum_1 h(1) + \frac{1}{2} \sum_{1,2} v(12), \\ M_1(1) &= 1, \quad G_1(1) = \sum_1 v(12), \\ M_n(1) &= G_n(1) = 0 \text{ for } n > 1. \end{aligned} \quad (52)$$

Equation (42) with $n = 1$ provides a vertex renormalised expression for $M_1(1)$. Our task is to construct a functional W which satisfies (51) subject to (52).

Naively, it might seem that a good candidate for W would be $\Sigma_1 M_0(1)$, with $M_0(1)$ defined by (42) with $n = 0$. On closer inspection we note that G_n depends on h through the renormalised semi-invariants $G[M(h), v]$. Thus, direct differentiation of (42) gives

$$\frac{\delta}{\delta h(1)} \sum_2 M_0(2) = M_1(1) + \sum_2 \sum_{n=1}^{\infty} \frac{\delta G_n(2)}{\delta h(1)} M_n(2). \quad (53)$$

Another appealing candidate is the symmetrical quantity,

$$\Phi[M, v] = \left\{ \begin{array}{l} \text{sum of all topologically distinct 1-irreducible} \\ \text{0-rooted graphs† according to Rule 7.} \end{array} \right\}. \quad (54)$$

Rule 7: The Functional Φ , Vertex Renormalised Form

Same as Rule 1 except:

(c) *For each l -valent internal vertex i write a factor $M_l(i)$.*

$$\begin{aligned} \Phi[M, v] = \frac{1}{2} &\bullet + \frac{1}{4} \bullet + \frac{1}{12} \bullet + \frac{1}{6} \bullet \triangle \bullet + \frac{1}{48} \bullet \square + \frac{1}{4} \bullet \square \bullet + \frac{1}{8} \bullet \square \square \\ &+ \text{order } v^5 \text{ and higher.} \end{aligned} \quad (55)$$

Φ , which is like a thermodynamic potential, has as its natural variables v and the renormalised semi-invariants. It is easy to verify that

$$\frac{\delta \Phi[M, v]}{\delta M_n(1)} = G_n(1). \quad (56)$$

For example, consider the first term of (55):

$$\frac{1}{2} \bullet = \frac{1}{2} \sum_{2,3} M_1(2)v(23)M_1(3). \quad (57)$$

Differentiation of (57) with respect to $M_1(1)$ yields $G_1(1) = \sum_2 v(12)M_1(2)$. (Note that (57) is the only 1-irreducible graph containing a 1-valent vertex.) In general, term-by-term differentiation of (55) leads directly to (47). The

† The single vertex is specifically omitted from this sum.

only point requiring comment is the symmetry factors. It suffices to note that, in the differentiation (56), vertices in (55) equivalent under symmetry operations of the graph contribute additively. The factor thus produced serves to lower the symmetry factor of the unrooted graph to that of the 1-rooted graph as required by Rule 6(e).

What is the field derivative of Φ ? Use of (56) and the chain rule gives,

$$\frac{\delta \Phi}{\delta h(1)} = \sum_2 \sum_{n=1}^{\infty} \frac{\delta \Phi}{\delta M_n(2)} \frac{\delta M_n(2)}{\delta h(1)} = \sum_2 \sum_{n=1}^{\infty} G_n(2) \frac{\delta M_n(2)}{\delta h(1)}. \quad (58)$$

The sum of (53) and (58) yields,

$$\frac{\delta}{\delta h(1)} \left[\sum_2 M_0(2) + \Phi \right] = M_1(1) + \frac{\delta}{\delta h(1)} \left[\sum_2 \sum_{n=1}^{\infty} G_n(2) M_n(2) \right]. \quad (59)$$

Thus,

$$W = \sum_2 M_0(2) + \Phi - \sum_2 \sum_{n=1}^{\infty} G_n(2) M_n(2), \quad (60)$$

which can easily be shown to satisfy (52). When once the renormalised semi-invariants have been computed (as discussed in II.E), then (60) evaluates the free energy.

If properly interpreted, (60) has an interesting stationarity property. Consider the functional

$$\begin{aligned} \mathcal{W}_1[M, v; h] \equiv & \sum_2 \left[\left(\exp \sum_{n=1}^{\infty} G_n[2; M, v] \frac{d^n}{dh^n} \right) M_0^0(\tilde{h}) \Big|_{\tilde{h}=h(2)} \right] \\ & + \Phi[M, v] - \sum_2 \sum_{n=1}^{\infty} G_n[2; M, v] M_n(2), \end{aligned} \quad (61)$$

which is equal to W provided the M_n , $n \geq 1$, are related to the fields h via (42). We choose to regard \mathcal{W}_1 as depending separately on the M_n 's, $n \geq 1$, (via $\Phi[M, v]$ and $G[M, v]$) and the fields h which appear explicitly in the M_n^0 's of first term on the right. Direct differentiation of (61) using (56) gives,

$$\begin{aligned} \frac{\delta \mathcal{W}_1}{\delta M_1(1)} \Big|_{h \text{ fixed}} = & \sum_2 \sum_{n=1}^{\infty} \frac{\delta^2 \Phi}{\delta M_1(1) \delta M_n(2)} \\ & \times \left[\left(\exp \sum_{k=1}^{\infty} G_k(2) \frac{d^k}{d\tilde{h}^k} \right) M_n^0(\tilde{h}) \Big|_{\tilde{h}=h(2)} - M_n(2) \right], \end{aligned} \quad (62)$$

so that the physical free energy W is a stationary point of \mathcal{W}_1 . An additional derivative of (62) shows that the stationary point is not necessarily an extremum.

There is another related variational principle (Bloch and Langer, 1965) which can be proved to be a maximum principle. The free energy $W[h, v]$ is

ultimately a functional of the inhomogeneous applied magnetic field h . We are free, equivalently, to regard W as functional of the inhomogeneous magnetisation M_1 via the dependence $W[h[M_1, v], v]$ provided that the magnetisation $M_1 = M_1[h, v]$ is invertable. This will be so, provided that the Jacobian connecting M_1 and h is non-vanishing, which in turn is proved by the observation that the real symmetrical fluctuation matrix,

$$\frac{\delta M_1(1)}{\delta h(2)} \equiv \frac{\delta^2 W}{\delta h(1)\delta h(2)} = \langle (\mu(1) - \langle \mu(1) \rangle)(\mu(2) - \langle \mu(2) \rangle) \rangle, \quad (63)$$

is positive definite. The generator of the Legendre transformation to the variables $[M_1, v]$ is,

$$\Psi[M_1, v] \equiv W[h[M_1, v], v] - \sum_2 h[2; M_1, v] M_1(2),$$

with

$$\frac{\delta \Psi}{\delta M_1(1)} = \sum_2 \frac{\delta W}{\delta h(2)} \frac{\delta h(2)}{\delta M_1(1)} - \sum_2 \frac{\delta h(2)}{\delta M_1(1)} M_1(2) - h_1(1) = -h[1; M_1, v]. \quad (64)$$

Notice that

$$-\frac{\delta^2 \Psi}{\delta M_1(1)\delta M_1(2)} = \frac{\delta h[1; M_1, v]}{\delta M_1(2)}$$

is the inverse of (63) and, therefore, positive definite. The functional,

$$\mathcal{W}_2[M_1, v; h] \equiv \Psi[M_1, v] + \sum_1 h(1) M_1(1), \quad (65)$$

(as in (61) the field h is to be regarded as a parameter) has the property that it is a maximum and equal to the physical free energy W when M_1 is put equal to the physical magnetisation distribution corresponding to the field h .

The functional \mathcal{W}_2 is asymmetrical in the renormalised semi-invariants because of the special relationship (4) between h and M_1 . By defining a set of fictitious fields (Bloch and Langer, 1965; Wortis *et al.*, 1969) related to the higher-order semi-invariants as h is to M_1 , it is possible to define an entirely symmetrical generalisation of \mathcal{W}_2 , which is stationary under variations of all M_n 's, $n \geq 1$, but, unfortunately, not maximal.

G. The classical-fluid linked-cluster expansion as a special case

It is not our purpose in this section to review the extensive literature on the classical fluid (De Dominicis, 1962; Stell, 1964). Rather, we wish to sketch the classical-fluid linked-cluster development only sufficiently so that the reader familiar with the classical situation will appreciate the very close parallel with the present development. Skipping this section will not destroy the continuity of the text.

It is convenient to introduce a single-particle potential field $u(\mathbf{r})$, which plays a role analogous to that of the magnetic field h . The Hamiltonian for N particles can then be written,

$$-\beta \mathcal{H}_N = \sum_{i=1}^N \left(-\frac{\mathbf{p}_i^2}{2m} + u(\mathbf{r}_i) \right) + \sum_{\langle ij \rangle}^N v(\mathbf{r}_i - \mathbf{r}_j), \quad (66)$$

where all energies are in units of kT and we have chosen u and v positive when they tend to bind. All momentum integrals are trivial and the grand partition function is written (Huang, 1963),

$$\Xi[u, v] = \sum_{N=0}^{\infty} \frac{z^N}{N!} \int (\mathrm{d}\mathbf{r}_1) \dots (\mathrm{d}\mathbf{r}_N) \exp \left(\sum_{i=1}^N u(\mathbf{r}_i) + \sum_{\langle ij \rangle}^N v(\mathbf{r}_i - \mathbf{r}_j) \right), \quad (67)$$

where z is the fugacity $e^{\beta\mu}/\lambda^d$ (μ = chemical potential, λ = thermal wavelength, d = dimensionality). In analogy to (3) we write

$$W[u, v] = \ln \Xi. \quad (68)$$

The connection with thermodynamics is $\beta PV = \ln \Xi$, where P is the pressure and V , the volume. The usual n -particle distribution functions are,[†]

$$\rho_n(\mathbf{r}_1, \dots, \mathbf{r}_n) \equiv \rho_n(1 \dots n)$$

$$= \frac{1}{\Xi} \sum_{l=n}^{\infty} \frac{z^l}{(l-n)!} \int (\mathrm{d}\mathbf{r}_{n+1}) \dots (\mathrm{d}\mathbf{r}_l) \exp \left[\sum_{i=1}^l u(\mathbf{r}_i) + \sum_{\langle ij \rangle}^l v(\mathbf{r}_i - \mathbf{r}_j) \right] \quad (69)$$

which may be generated by differentiation,

$$\frac{1}{\Xi} \frac{\delta \Xi}{\delta u(1)} = \rho_1(1), \quad \frac{1}{\Xi} \frac{\delta^2 \Xi}{\delta u(1) \delta u(2)} = \rho_2(12) + \delta(12)\rho_1(1), \text{ etc.}$$

Cluster functions \bar{U} may be derived by direct differentiation of W ,

$$\bar{U}_n(1 \dots n) \equiv \frac{\delta^n W}{\delta u(1) \dots \delta u(n)}, \quad (70)$$

which are the analogs of our $\mathcal{M}_n(1 \dots n)$ of (6) and differ from the usual Ursell functions U_n (Stell, 1964) by the presence of δ -functions, e.g.,

$$\begin{aligned} \bar{U}_2(12) &\equiv \frac{\delta^2 W}{\delta u(1) \delta u(2)} = \rho_2(12) - \rho_1(1)\rho_1(2) + \delta(12)\rho_1(1) \\ &= U_2(12) + \delta(12)\rho_1(1). \end{aligned}$$

[†] Functional differentiation with respect to a continuous function at a point requires a little discussion (Morita and Hiroike, 1961a, b; Volterra, 1959; Berezin, 1966). Since this discussion is entirely irrelevant to our main purposes, we simply remark that the concerned reader may henceforth imagine himself to be dealing with a gas confined to a lattice.

The non-interacting free energy is (cf. (9)):

$$W_0[u] \equiv W[u, v = 0] = \int (\mathrm{d}\mathbf{r}) M_0^0(\mathbf{r}) = z \int (\mathrm{d}\mathbf{r}) e^{u(\mathbf{r})}, \quad (71)$$

from which it follows that (cf. 14),

$$M_n^0(\mathbf{r}) = z e^{u(\mathbf{r})} \text{ for all } n = 0, 1, 2, \dots \quad (72)$$

By choosing $n = 1$ and comparing with (69), $z e^{u(\mathbf{r})}$ may be identified with $\rho_1^0(\mathbf{r})$, the non-interacting particle density. The unrenormalised rule for the free energy may now be derived just as in Sections II.B or II.C. Everything is exactly the same except that the unrenormalised semi-invariants are given by (72) in place of (10) and (14). To compute the difference $(W[u, v] - W_0[u])$, one sums all topologically distinct unrooted connected graphs according to (cf. Rule 1):

Rule 8A: Classical-Fluid Free Energy W, Unrenormalised v-form

- (a) Assign a dummy label to each internal vertex.
- (b) For each edge joining vertices i and j write a factor $v(ij)$.
- (c) For each vertex i write a factor $z e^{u(i)} = \rho_1^0(i)$.
- (d) Integrate each internal vertex label freely over the volume of the container.
- (e) Divide by the symmetry factor of the unrooted graph.

Equation (20) gives the first few terms of the sum.

The important difference between Rule 8A and Rule 1 is in part (c), where Rule 8A requires a vertex factor $\rho_1^0(i)$ independent of valence. This valence-independence, which follows directly from the exponential form of M_0^0 (eqn (72)), is the only important respect in which the magnetic expansion differs from the classical-fluid expansion. This difference produces a number of simplifications.

The reader will have noticed that the expansion given by Rule 8A is in terms directly of the pair potential rather than of the Mayer f -function, $f(12) \equiv (e^{v(12)} - 1)$. To obtain the traditional form we sum over multiedges:

$$f(12) = | + \frac{1}{2} \langle \rangle + \frac{1}{6} \langle \langle \rangle \rangle + \dots + \frac{1}{n!} \left[\bigcirc \bigcirc \right]_n + \dots \quad (73)$$

Note that each edge of multiplicity n contributes to the symmetry factor g a factor $n!$. By omitting the vertex circles in (73), we wish to emphasise that f contains none of the vertex factors 8A(c). We now group together in a class all graphs contributing to 8A which differ only in the degree of multiplicity of corresponding edges. The replacement $v(12) \rightarrow f(12)$ sums each such class, producing the familiar result that to calculate $(W[u, v] - W_0[u])$ one may

sum all topologically distinct unrooted connected graphs *with no multiedges* according to:

Rule 8B: Classical-Fluid Free Energy W , Unrenormalised f -form

Same as Rule 8A except:

- (b) For each joining vertices i and j write a factor $f(ij) = (e^{v(ij)} - 1)$.

The first few terms in this form of the expansion are (cf. (20)),

$$\begin{aligned} W[u, f] - W_0[u] &= \frac{1}{2} \text{ (single vertex)} + \frac{1}{2} \text{ (two vertices connected by one edge)} + \frac{1}{6} \text{ (three vertices forming a triangle)} + \frac{1}{2} \text{ (four vertices forming a square)} + \frac{1}{6} \text{ (five vertices forming a pentagon)} \\ &\quad + \text{order } f^4 \text{ and higher.} \\ &= \frac{1}{2} \int (dr_1)(dr_2) \rho_1^0(1) f(12) \rho_1^0(2) + \dots \end{aligned} \quad (74)$$

Note that the summation over graphs differing only with respect to edge multiplicity *cannot* be done in the magnetic case, since each level of multiplicity requires a different vertex factor M_n^0 due to the changed valence.

Vertex renormalization goes through just as before. Because the vertex factors M_n^0 are valence-independent, there is no need to classify the self-fields G_n according to their external valence. The renormalised vertex is just the local density $\rho_1(r)$ (cf. the identification $M_1(1) = M_1(1)$, the local magnetisation, after (42)). The self-field $G(1)$ is therefore (cf. Rule 6 and eqn (46)),

$$G(1) = \left\{ \begin{array}{l} \text{sum of all topologically distinct} \\ \text{1-irreducible 1-insertions with} \\ \text{no multiedges according to Rule 9.} \end{array} \right\} \quad (75)$$

Rule 9: Classical-Fluid Self-field, Vertex Renormalized f -form

- (a) Assign the label 1 to the external vertex and a dummy label to each internal vertex.
- (b) For each edge joining vertices i and j write a factor $f(ij) = (e^{v(ij)} - 1)$.
- (c) For each internal vertex i write a factor $\rho_1(i)$. For the external vertex write a factor 1.
- (d) Integrate each internal vertex label freely over the volume of the container.
- (e) Divide by the symmetry factor of the 1-insertion.

The first few terms are:

$$G(1) = \text{ (single vertex)} + \frac{1}{2} \text{ (two vertices connected by one edge)} + \frac{1}{2} \text{ (four vertices forming a square)} + \text{order } f^5 \text{ and higher.} \quad (76)$$

Of course, corresponding expressions in terms of v rather than f or in terms of the unrenormalised vertex ρ_1^0 (cf. Rule 4) could also be written down.

The analog of (42), expressing the decoration of an unrenormalised vertex is simply,

$$\rho_1(1) = e^{G(1)} \rho_1^0(1). \quad (77)$$

Note the absence of derivatives. The vertex renormalised free energy is given by (cf. (60)),

$$W = \int (d\mathbf{r}_1) \rho_1(1) + \Phi - \int (d\mathbf{r}_1) G(1) \rho_1(1), \quad (78)$$

where, in terms of the Mayer f -function, Φ is given by the sum of all topologically distinct connected 1-irreducible unrooted graphs with *no multiedges* according to *Rule 10* (cf. Rule 7):

Rule 10: Classical-Fluid Functional Φ , Vertex Renormalised f -form.

Same as Rule 9 except:

(e) *Divide by the symmetry of the unrooted graph.*

Rules 9 and 10 give Φ and G as functions of the particle density ρ_1 . In the translationally invariant situation $u(1) = 0$, $v(12) = v(\mathbf{r}_1 - \mathbf{r}_2)$, (78) may be expanded in powers of the density. Graphs with exactly n vertices contribute to ρ_1^n . Thus,

$$\begin{aligned} \beta P &= \frac{W}{V} = \rho_1 + \frac{\Phi}{V} - \rho_1 G \\ &= \rho_1 - \frac{\rho_1^2}{2} \int (d\mathbf{r}) f(\mathbf{r}) - \frac{\rho_1^3}{3} \int (d\mathbf{r}_1)(d\mathbf{r}_2) f(\mathbf{r}_1)f(\mathbf{r}_2)f(\mathbf{r}_1 - \mathbf{r}_2) \\ &\quad + \text{order } \rho_1^4 \text{ and higher.} \end{aligned} \quad (79)$$

which is just the ordinary virial expansion.

H. Φ -Derivable approximations

Despite renormalisation, the series expansions always involve an infinite number of terms. When there is a small expansion parameter (e.g. v or ρ_1), then it may be that only a finite number of terms contribute appreciably. On the other hand, there are situations where it is convenient to have an analytic solution for the free energy, correlations, etc., which is at least qualitatively valid over a wide range of parameters. Such solutions must sum an infinite subset of perturbation theory graphs. Which subset to choose is dictated by an understanding of the physics. So far it has not been possible to pick out an analytically summable subset of graphs which gives proper critical behaviour; however, these closed-form approximations are of sufficient historical interest and sufficient practical importance in *non-critical* regions that they deserve mention.

We shall not attempt to review the history of approximate solutions to the Ising model (Newell and Montroll, 1953; Brush, 1967; see also Burley Volume 2, Chapter 9). Rather we limit ourselves to the presentation of a certain class of those solutions which are closely related to the development of Sections II.E and II.F and which are complete and internally consistent in a sense which will be made clear below.

The basic philosophy of the Φ -derivable approximations (Baym, 1962; Bloch and Langer, 1965) is that they involve direct approximation for the free energy functional in the presence of arbitrary inhomogeneous fields h . Thus, corresponding approximations to all correlation functions may be obtained from

$$\mathcal{M}_n(1 \dots n)_{\text{approx}} = \frac{\delta^n W_{\text{approx}}}{\delta h(1) \dots \delta h(n)}, \quad (80)$$

with the guarantee that, being related to the same underlying free energy, they will all have singular behaviour at the same points and obey certain self-consistency conditions such as the well-known susceptibility sum rule,

$$N\chi = \frac{d^2 W}{dh^2} = \sum_{1,2} \mathcal{M}_2(12). \quad (81)$$

The procedure is as follows:

Step (a): Choose an approximate $\bar{\Phi}[\bar{M}, v]$ consisting of a subset of the terms of (55) (Rule 7). The approximate free energy $\bar{W}[\bar{M}, v]$ is given by (60):

$$\bar{W}[\bar{M}, v] = \sum_2 \bar{M}_0(2) + \bar{\Phi} - \sum_2 \sum_{n=1}^{\infty} \bar{G}_n(2) \bar{M}_n(2), \quad (82)$$

where the bar denotes “approximate.” The expression (82) is highly implicit and incomplete until a rule is given for computing \bar{G} and \bar{M} . We now show how to choose \bar{G} and \bar{M} in such a way as to achieve consistency.

Step (b): Take

$$\bar{G}_n[1; \bar{M}, v] = \bar{G}_n(1) = \frac{\delta \bar{\Phi}}{\delta \bar{M}_n(1)}, \quad (83)$$

which is still a functional of the unknown \bar{M} ’s.

Step (c): Define \bar{M} ’s as solutions of (42),

$$\bar{M}_n(1) = \left[\exp \sum_{l=1}^{\infty} G_l(1) \frac{\delta^l}{\delta \tilde{h}^l} \right] M_n^0[1; \tilde{h}]_{\tilde{h}=h(1)}. \quad (84)$$

This finally makes (82) and (83) explicit.

It is now easy to show by direct differentiation of (82) that

$$\frac{\delta \bar{W}}{\delta h(1)} \equiv \bar{\mathcal{M}}_1(1) = \bar{M}_1(1). \quad (85)$$

In effect and for the *approximate* \bar{W} , this simply reverses the steps which lead from (51) to (60). To get the pair correlations, one need only take another field derivative of (85). It is advantageous to perform the calculation a little more generally. From (84)

$$\frac{\delta \bar{M}_n(1)}{\delta h(2)} = \delta(12)\bar{M}_{n+1}(1) + \sum_{l=1}^{\infty} \bar{M}_{n+l}(1) \frac{\delta \bar{G}_l(1)}{\delta h(2)}. \quad (86)$$

Now, \bar{G} depends on h only through the semi-invariants \bar{M} , so, using the chain rule,

$$\frac{\delta \bar{M}_n(1)}{\delta h(2)} = \delta(12)\bar{M}_{n+1}(1) + \sum_{l,k,3} \bar{M}_{n+l}(1) \bar{I}_{l,k}(13) \frac{\delta \bar{M}_k(3)}{\delta h(2)}, \quad (87)$$

where I is the symmetric matrix,

$$\bar{I}_{lk}(13) = \frac{\delta^2 \bar{\Phi}}{\delta \bar{M}_l(1) \delta \bar{M}_k(3)} \equiv \langle 1l | \bar{I} | 3k \rangle. \quad (88)$$

Finally, solution of (87) with $n = 1$ gives,

$$\bar{\mathcal{M}}_2(12) = \sum_{l=1}^{\infty} \langle 11 | (1 - \bar{M}\bar{I})^{-1} | 2l \rangle \bar{M}_{l+1}(2). \quad (89)$$

A few examples will serve to make the above more concrete:

1. The Effective-field Approximation

This well known approximation (Smart, 1966), the analog of the Hartree approximation in quantum statistics, follows from the choice at Step (a) of (see eqn (55)) $\bar{\Phi}[\bar{M}, v] = \frac{1}{2} \bullet \bullet$ and corresponds to the sum of all bare free energy graphs ((20) and Rule 1) having no closed loops. Physically the effective-field approximation is expected to be best for systems with long-range interactions, although it is worth emphasising that effective-field *critical behaviour* has no relation to reality for any physical system with finite range interactions.

Continuing to Step (b) we find,

$$\bar{G}_1(1) = \sum_2 v(12)\bar{M}_1(2) \quad \text{and} \quad \bar{G}_n = 0, \quad n > 1. \quad (90)$$

Thus (Step (c)),

$$\begin{aligned}\bar{M}_n(1) &= \left[\exp \bar{G}_1(1) \frac{\delta}{\delta \tilde{h}} \right] M_n^0[1; \tilde{h}]|_{\tilde{h}=h(1)} \\ &= M_n^0 \left(h(1) + \sum_2 v(12) \bar{M}_1(2) \right).\end{aligned}\quad (91)$$

For $n = 1$ and in the translationally invariant situation (21) this reduces for $s = \frac{1}{2}$ to the well-known self-consistency condition,

$$M_1 = \tanh(h + V(0)M_1), \quad (92)$$

where $V(0) \equiv V(\mathbf{k} = 0)$. The free energy in this approximation is

$$\frac{W}{N} = \ln [\exp(h + V(0)\bar{M}_1) + \exp(-h - V(0)\bar{M}_1)] - \frac{1}{2}V(0)\bar{M}_1^2. \quad (93)$$

Finally, from (88)

$$\bar{I}_{ln}(12) = \begin{cases} v(12), & \text{when } l = n = 1 \\ 0, & \text{otherwise} \end{cases} \quad (94)$$

and

$$\mathcal{M}_2(k) = \sum_{\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}} \mathcal{M}_2(\mathbf{r}) = \frac{\bar{M}_2}{1 - \bar{M}_2 V(\mathbf{k})}. \quad (95)$$

2. Ring graphs:

The first correction to the effective-field approximation in powers of the inverse range of the potential is usually taken to be† the inclusion in Φ of graphs with ring topologies.‡ Here, therefore, we choose (Bloch and Langer, 1965; Horwitz and Callen, 1961),

$$\bar{\Phi}[\bar{M}, v] = \frac{1}{2} \text{ (loop)} + \frac{1}{4} \text{ (square)} + \frac{1}{6} \text{ (triangle)} + \dots + \frac{1}{2n} \left[\text{ (ring)} \right]_n + \dots \quad (96)$$

with

$$\bar{G}_1(1) = \sum_2 v(12) \bar{M}_1(2),$$

$$\bar{G}_2(1) = \frac{1}{2} \left[\text{ (loop)} + \text{ (square)} + \text{ (triangle)} + \dots \right], \quad (97)$$

$$\bar{G}_n = 0 \text{ for } n > 2.$$

† The inverse-range expansion loses its meaning in the critical region and the above language is intended to be suggestive only (Horwitz and Callen, 1961; Englert, 1963).

‡ The quantum analog of the ring approximation is the self-consistent dielectric, bubble, or K -approximation. Propagator lines become points and correspond to our vertex functions.

In the translationally invariant limit,

$$\bar{G}_1 = V(0)\bar{M}_1, \quad \bar{G}_2 = \frac{1}{2}C(\mathbf{r} = 0),$$

where

$$C(\mathbf{r}) = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}} \frac{V(\mathbf{k})}{1 - \bar{M}_2 V(\mathbf{k})}, \quad (98)$$

so that the two fundamental semi-invariants are determined (Step (c)) by the non-linear coupled equations:

$$\begin{aligned} \bar{M}_1 &= \left[\exp G_2 \frac{\delta^2}{\delta \tilde{h}^2} \right] M_1^0 (\tilde{h} + V(0)\bar{M}_1) |_{\tilde{h}=h} \\ \bar{M}_2 &= \left[\exp G_2 \frac{\delta^2}{\delta \tilde{h}^2} \right] M_2^0 (\tilde{h} + V(0)\bar{M}_1) |_{\tilde{h}=h}, \end{aligned} \quad (99)$$

which can, for example, be recast along the lines of (50).

The matrix \bar{I} now has (in its valence indices) two non-vanishing components

$$\begin{aligned} \bar{I}_{11}(12) &= v(12) \\ \bar{I}_{22}(12) &= \frac{1}{2}[C(12)]^2. \end{aligned} \quad (100)$$

I. Analysis of the two-point function

Before proceeding to the two-point or *bond* renormalisation, we must analyse the structure of the 2-rooted graphs and their contributions to the correlations M_2 more carefully than heretofore (De Dominicis, 1962; Stell, 1964).

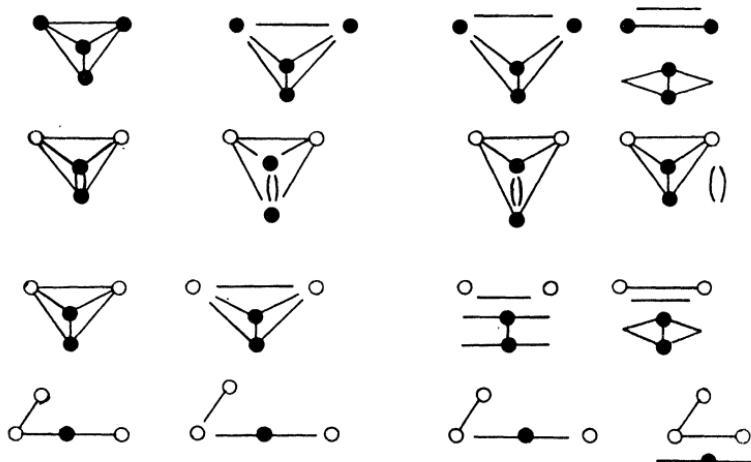


FIG. 10. Disassembly of various vertex pairs.

Disassembly of a vertex pair

A vertex pair V_1 and V_2 of a (1-irreducible) graph G is *disassembled* by the following procedure:

- (i) Clip away all edges from both V_1 and V_2 (thereby dividing G into a number of disjoint parts).
- (ii) Reattach to V_1 and V_2 all clipped edges belonging to disconnected parts containing external vertices.
- (iii) If there are any additional disconnected parts,
 - (a) rejoin the clipped ends of each (V_1 ends and V_2 ends separately)
 - (b) insert in the rooted part a single edge joining V_1 and V_2 .

This process is pictured for several graphs in Fig. 10. The definitions which follow refer to 1-irreducible graphs.

Graphical definitions III

The unrooted parts formed in the process of disassembly are called 2-insertions. A 2-insertion which is not simply a bond is complex.

An articulation pair of a rooted graph is a pair of vertices the disassembly of which produces either one complex 2-insertion or any two or more 2-insertions. An articulation pair of an unrooted graph is a pair of vertices the disassembly of which produces either two complex 2-insertions or any three or more 2-insertions.

A graph is 2-irreducible if it contains no articulation pairs.

The 2-skeleton of a rooted graph is the graph produced by disassembling all pairs of vertices and discarding all 2-insertions thereby produced.

The following definitions classify important types of 2-rooted graphs:

The 2-rooted graph consisting of a single edge joining the external vertices is called the bond graph.

An internal vertex of a 2-rooted graph is said to be a nodal point if all paths between the two external vertices pass through it. A graph is nodal if it contains one or more nodal points; otherwise it is non-nodal.

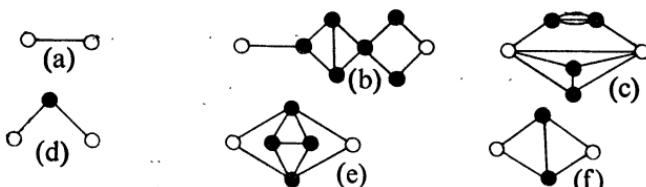


FIG. 11. Various 1-irreducible 2-rooted graphs: (a) the bond graph; (b) a simple nodal graph (two nodal points); (c) a ladder graph; (d) a simple, nodal graph; (e) an elementary graph (contains one internal articulation pair); (f) the lowest order elementary graph.

A 2-rooted graph is simple if it is not the bond graph and if disassembly of its external vertices produces exactly one 2-insertion. A 2-rooted graph is a ladder graph if it is neither a bond graph nor a simple graph, i.e. if disassembly of its external vertices produces two or more 2-insertions.

A 2-rooted graph is elementary if it is both simple and non-nodal.

Examples of these definitions are given in Fig. 11.

Let us now consider the contributions of these various types of graph to the two-point cumulant correlations $\mathcal{M}_2(12) - \delta(12)M_2(1)$ (eqn (29) or (44)) or the related two-point parts of the higher correlations, e.g. (31). We use the vertex renormalised form of the expansions. It is convenient to sort the contributing graphs according to their valence at the external vertices and to supply by hand appropriate vertex factors at the external vertices. We therefore define as fundamental quantities the l, n -valent correlation factors,

$$C_{ln}(12) = \left\{ \begin{array}{l} \text{sum of all topologically distinct 1-irreducible} \\ \text{2-rooted connected graphs, which are } l\text{-valent at} \\ \text{the external vertex 1 and } n\text{-valent at the external} \\ \text{vertex 2, according to Rule 11.} \end{array} \right\} \quad (101)$$

Rule 11: l, n -valent Correlation Factors C_{ln} , Vertex Renormalised Form

- Assign labels 1 and 2 to the external vertices and dummy labels to all internal vertices.
- For each edge joining vertices i and j write a factor $v(ij)$.
- For each k -valent internal vertex i write a factor $M_k(i)$. For each external vertex write a factor 1.
- Sum each internal vertex label freely over the entire lattice.
- Divide by the symmetry factor of the 2-rooted graph.

For example,

$$C_{11}(12) = \frac{1}{1} \frac{2}{2} + \text{order } v^5 \text{ and higher,}$$

$$C_{21}(12) = \frac{1}{1} \frac{2}{2} + \frac{1}{1} \frac{2}{2} + \frac{1}{1} \frac{2}{2} + \text{order } v^5 \text{ and higher.}$$

$$C_{22}(12) = \frac{1}{1} \frac{2}{2} + \text{order } v^5 \text{ and higher.} \quad (102)$$

The graphs contributing to (44) by Rule 5 may be classified according to valence at the external vertices, so (44) may be re-expressed, in terms of the correlation factors,

$$\mathcal{M}_2(12) = M_2(1)\delta(12) + \sum_{l,n=1}^{\infty} M_{l+1}(1)C_{ln}(12)M_{n+1}(2). \quad (103)$$

We now proceed to analyse C into its constituent graphical parts. The motivation for this analysis is that it will allow us to invert the relation (101) $C[M, v]$ to provide $v[M, C]$. This expression plays a role in the bond renormalisation of Section II.J equivalent to that of eqn (48) in the vertex renormalisation of Section II.E: C is determined as the solution of a complicated integral equation, thus buying enormous graphical simplification at the expense of increased algebraic complexity.

All contributions to C may now be classified according as they are nodal (N) or non-nodal (I),

$$C_{ln} = I_{ln} + N_{ln}, \quad (104)$$

where, for example,

$$I_{11} = \text{——— (exact),}$$

$$I_{21} = I_{12} = 0 \text{ (exact),}$$

$$I_{22}(12) = \frac{1}{2} \text{———} + \text{———} + \text{———} + \frac{1}{2} \text{———} + \text{order } v^5 \text{ and higher.} \quad (105)$$

The non-nodal part I is derivable from the functional $\Phi[M, v]$, eqn (54), Rule 7, (see also eqn (88)),

$$I_{ln}(12) = \frac{\delta^2 \Phi[M, v]}{\delta M_l(1) \delta M_n(2)}, \quad (106)$$

so that (105) can be checked by direct differentiation of the first few terms of (55). The non-nodal property of I follows from the fact that Φ is 1-irreducible. As in the expression (56) for G_n , the essential point is that the presence of identical contributions from vertex pairs in Φ which are topologically equivalent lowers the symmetry of the unrooted graph to that of the corresponding 2-rooted graph. Nodal contributions may be classified according to the number of nodal points:

$$N_{ln}(12) = \sum_{3,k,m} I_{lk}(13)M_{k+m}(3)I_{mn}(32) + \sum_{\substack{3,4 \\ k,m \\ s,t}} I_{lk}(13)M_{k+m}(3)I_{ms}(34)M_{s+t}(4)I_{tn}(42) + \dots. \quad (107)$$

Again, the essential observation is that the symmetry factor of a nodal graph is just the product of the symmetry factors of its non-nodal components. A matrix notation is useful:

$$\begin{aligned}\langle l1|I|n2 \rangle &\equiv I_{ln}(12), \\ \langle l1|M|n2 \rangle &\equiv \delta(12)M_{l+n}(1), \\ \langle l1|C|n2 \rangle &\equiv C_{ln}(12),\end{aligned}\tag{108}$$

where matrix multiplication involves a sum over valences and lattice points. It is easy formally to write C in terms of I ,

$$C = I(1 - MI)^{-1},\tag{109}$$

or inverting,

$$I = (1 + CM)^{-1}C, \quad N = C - (1 + CM)^{-1}C,\tag{110}$$

which will be useful below.

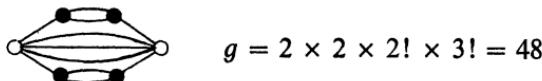


FIG. 12. A ladder graph and its symmetry factor. The symmetry factor is composed multiplicatively of the symmetry factors of the simple or bond insertions ($2 \times 2 \times 1 \times 1 \times 1$) and factorials due to the presence of identical insertions ($2! \times 3!$).

The general 2-rooted graph is either a bond graph, a simple graph (S), or a ladder graph (L),

$$C_{ln} = v_{ln} + S_{ln} + L_{ln},\tag{111}$$

where

$$v_{ln}(12) = \begin{cases} v(12), & l = n = 1 \\ 0, & \text{otherwise.} \end{cases}\tag{112}$$

Each ladder graph L is composed of two or more simple or bond graphs glued together at the external vertices (see e.g. Fig. 11(b) and (f)). The symmetry factor for the ladder graph is just the product of the symmetry factors for the individual insertions times a product of factorials due to the presence of identical 2-insertions, as illustrated in Fig. 12. Therefore, C can be written entirely in terms of $(v + S)$,

$$C_{ln} = (v + S)_{ln} + \frac{1}{2} \sum_{km} \delta(l - k - s)(v + S)_{km}(v + S)_{st} \delta(n - m - t) + \dots,\tag{113}$$

or in matrix notation,

$$C = (e^{v+S} - 1),\tag{114}$$

where the δ -functions, which guarantee proper valence at the external vertices, have been left implicit. Equation (114) can, of course, be inverted to give $(v + S)$ in terms of C . Substitution in (111) evaluates,

$$L = C - \ln(1 + C), \quad (115)$$

or, more explicitly expanding the logarithm,

$$\begin{aligned} L_{ln}(12) &= \frac{1}{2} \sum_{\substack{k,m \\ s,t}} \delta(l-k-s)C_{km}(12)C_{st}(12)\delta(n-m-t) \\ &\quad - \frac{1}{3} \sum_{\substack{k,m \\ s,t \\ u,v}} \delta(l-k-s-u)C_{km}(12)C_{st}(12)C_{uv}(12) \\ &\quad \times \delta(n-m-t-v) + \dots. \end{aligned} \quad (116)$$

Having succeeded in expressing $L[C]$ and $N[M, C]$, we now make the crucial observations that all non-nodal graphs are bond, ladder, or elementary,

$$I_{ln} = v_{ln} + L_{ln} + E_{ln}, \quad (117)$$

or, alternatively, that all simple graphs are either nodal or elementary,

$$S_{ln} = N_{ln} + E_{ln}. \quad (118)$$

When combined with (104) or (111), respectively, these give

$$C_{ln} = v_{ln} + N_{ln} + L_{ln} + E_{ln}. \quad (119)$$

Now, solve for v and substitute (110) and (115),

$$v = (1 + CM)^{-1}C - C + \ln(1 + C) - E. \quad (120)$$

This constitutes $v[M, C]$ provided we can express $E[M, C]$, which will be done in Section II.J. The lowest order elementary graph is shown as Fig. 11(f).

The approximation $E = 0$ in (120) provides an integral equation for C , which in the context of the classical fluid is called the hypernetted chain equation (Van Leuwen *et al.*, 1959; Meeron, 1960; Stell, 1964). The corresponding equation in the magnetic case was first derived by Englert (1963) and has been studied by Orlans (1963).

J. Renormalisation of the interaction

Bond or interaction renormalisation is the name given to the next (two-point) level of selective resummation. The development is closely parallel to Section II.E. There M^0 was replaced by M as the graphical vertex element with a consequent restriction to 1-irreducible graphs. Here we will replace the potential v by the general two-point correlation factor C introduced in (101).

Consider a general 1-irreducible n -rooted connected graph, $n \geq 3$. Such a graph has a unique 2-irreducible 2-skeleton defined (in Section II.I) by

successive disassembly of all vertex pairs, a process which for each pair of vertices cuts away all 2-insertions and replaces them by a single edge. Conversely, every such graph can be constructed in a unique way by decorating its underlying 2-skeleton, i.e., replacing each edge in turn by an appropriate 1-irreducible 2-rooted graph. This process is illustrated in Figure 13. It produces every 1-irreducible n -rooted graph once and only once.

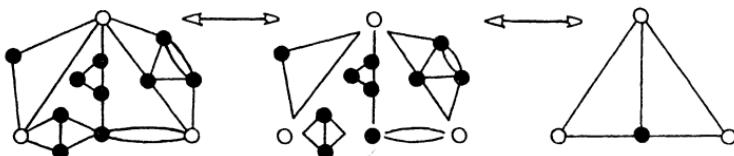


FIG. 13. A 3-rooted graph reduced to (built up from) its 2-skeleton.

Summation of all graphs having the same 2-skeleton is now accomplished simply by reinterpreting skeletal lines as the correlation factor C (instead of v). As in the case of vertex renormalization,[†] the only subtle point is that the symmetry factors work out. In building each 1-irreducible (but *not* 2- irreducible) graph by decoration of its 2-skeleton, the symmetry factor of each 2-rooted decoration enters multiplicatively. The lowering of skeletal symmetry due to distinct decorations of previously equivalent skeletal edges is taken care of by the cross-terms in the product of C 's for the bond-renormalised graph.

We illustrate by treating the 3-point correlations \mathcal{M}_3 , eqn (31), explicitly. Note first that the two-point parts $M_{21}(12)$, etc., may, by a trivial extension of the reasoning leading to (103), be written as,

$$M_{21}(12) = \sum_{l,n=1}^{\infty} M_{l+2}(1)C_{ln}(12)M_{n+1}(2). \quad (121)$$

The full expression then is,

$$\begin{aligned} \mathcal{M}_3(123) &= \delta(123)M_3(1) - \delta(12)M_{21}(13) - \delta(13)M_{21}(32) - \delta(23)M_{21}(21) \\ &= \left\{ \text{sum of all topologically distinct 3-rooted 2-irreducible connected graphs according to Rule 12.} \right\} \end{aligned} \quad (122)$$

Rule 12: Three-point Correlations, Vertex and Bond Renormalised Form

- (a) Assign labels 1, 2, 3 to the external vertices and dummy labels to all internal vertices.
- (b) For each edge joining vertices i and j write a factor $C_{ij}(ij)$.

[†] There is a close parallel here with the discussion surrounding eqn (43), particularly if one chooses (as we shall not) to discuss the decoration in terms of constituent 2-insertions.

To write the proper vertex factors it is convenient to define the *generalised valence* (*g-valence*) n_i of a vertex i as,

$$n_i = \sum_{\text{incident edges}} l_i,$$

i.e., the *g-valence* is obtained by summing the valence labels l_i of all correlation factors incident at i .

- (c) For each internal vertex i of *g-valence* n_i write a factor $M_n(i)$. For each external vertex i of *g-valence* n_i write a factor $M_{n_i+1}(i)$.
- (d) Sum each internal vertex label freely over the entire lattice. Sum all valence labels $l_i = 1, 2 \dots$.
- (e) Divide by the symmetry factor of the 3-rooted graph.

The first few graphs in the sum (122) are,

$$+ \text{order } C^4 \text{ and higher.} \quad (123)$$

As an application of Rule 12, the fifth term in (123) is,

$$= \sum_{\substack{i_1 \dots i_6 \\ l_1 \dots l_6}} C_{l_1 l_4}(14) C_{l_2 l_5}(24) C_{l_3 l_6}(34) M_{l_4 + l_5 + l_6}(4) M_{l_1 + 1}(1) M_{l_2 + 1}(2) M_{l_3 + 1}(3). \quad (124)$$

Formulations such as (122) are only useful if correlation factors C are known, so we must return to the problem raised in Section II.I of finding the relation $v[M, C]$, whose inversion $C[M, v]$ evaluates the correlations. Expression (120) lacks only $E[M, C]$. All elementary 2-rooted graphs may be obtained by decoration of 2-rooted graphs which are elementary and contain no articulation pair *except the pair consisting of the two external vertices*.† Such graphs will be called *elementary 2-rooted 2-skeletons*.

To express E_{ln} , then, one calculates the contributions of all l, n -valent elementary 2-rooted 2-skeletons according to Rule 13.

Rule 13: Elementary Correlation Factors, Vertex and Bond Renormalised Form

- (a) Assign the labels 1 and 2 to the external vertices and dummy labels to all internal vertices.

† The two external vertices of a 2-rooted graph are always an articulation pair. Disassembly at the external vertices leaves the bond graph.

- (b) For each edge joining vertices i and j write a factor $C_{l_i l_j}(ij)$.
- (c) For each internal vertex i of g -valence n_i (see Rule 12) write a factor $M_{n_i}(i)$. For each external vertex write a factor 1.
- (d) Sum each internal vertex label freely over the entire lattice. Sum all valence labels $l_i = 1, 2, \dots$.
- (e) Divide by the symmetry factor of the 2-rooted graph.

The first few terms are:

$$\begin{aligned}
 E_{ln}(12) = & \frac{1}{2} \begin{array}{c} \text{graph} \\ \text{with 2 internal} \\ \text{and 2 external vertices} \end{array} + \frac{1}{2} \begin{array}{c} \text{graph} \\ \text{with 3 internal} \\ \text{and 1 external vertex} \end{array} + \frac{1}{2} \begin{array}{c} \text{graph} \\ \text{with 2 internal} \\ \text{and 3 external vertices} \end{array} + \frac{1}{2} \begin{array}{c} \text{graph} \\ \text{with 4 internal} \\ \text{and 2 external vertices} \end{array} \\
 & + \begin{array}{c} \text{graph} \\ \text{with 5 internal} \\ \text{and 1 external vertex} \end{array} + \frac{1}{2} \begin{array}{c} \text{graph} \\ \text{with 3 internal} \\ \text{and 3 external vertices} \end{array} + \frac{1}{2} \begin{array}{c} \text{graph} \\ \text{with 4 internal} \\ \text{and 2 external vertices} \end{array} + \frac{1}{6} \begin{array}{c} \text{graph} \\ \text{with 6 internal} \\ \text{and 1 external vertex} \end{array} \\
 & + \text{graphs with at least four internal vertices.}
 \end{aligned} \tag{125}$$

There are 56 distinct elementary 2-rooted 2-skeletons with four internal points, not counting as distinct graphs which differ only through interchange of external vertices (such as the third and fourth or seventh and eighth graphs in (125)).

$$\frac{1}{2} \begin{array}{c} \text{graph} \\ \text{with 4 internal} \\ \text{and 2 external vertices} \end{array} = \frac{1! 2!}{3!} \left[\frac{1}{4} \begin{array}{c} \text{graph} \\ \text{with 4 internal} \\ \text{and 1 external vertex} \end{array} + \frac{1}{2} \begin{array}{c} \text{graph} \\ \text{with 3 internal} \\ \text{and 2 external vertices} \end{array} \right]$$

FIG. 14. A self-field graph (1-insertion) can be formed by superposing the external vertices of the corresponding 2-rooted simple graphs. See eqn (126).

The self-fields G_n may be expressed in terms of the correlation factors C_{ln} . The general relation is,

$$G_{l+n}(1) = \frac{l! n!}{(l+n)!} S_{ln}(11). \tag{126}$$

The presence only of simple graphs on the right of (126) guarantees that the result of superposing root points will be a 1-insertion. The factorials compensate for the difference in symmetry factors between the 1-rooted and 2-rooted graphs and the fact that a given 1-insertion may be obtained from several distinct simple graphs, as illustrated in Fig. 14. Equation (126) can be expressed directly in terms of C by using (114) and noting $v(11) = 0$,

$$G_{l+n}(1) = \frac{l! n!}{(l+n)!} \langle l1 | \ln(1+C) | n1 \rangle. \tag{127}$$

The full renormalisation $[M^0, v] \rightarrow [M, C]$ is then expressed by equation (48) and (120),

$$\begin{aligned} M^0 &= e^{-G[M]} M, \\ v &= (1 + CM)^{-1} C - C + \ln(1 + C) - E[M, C], \end{aligned} \quad (128)$$

which invert the bare perturbation-theoretic relations $M[M^0, v]$ (28) and $C[M^0, v]$. The only graphical part of (128) is $E[M, C]$, eqn (125), which (although it is still an infinite graphical sum) requires *enormously fewer graphs* to any given order in v than analogous bare expansions such as (30). On the other hand, regarded as an integral equation for C in terms of v , eqn (128) is highly non-linear. Even the simplest approximation $E = 0$ (Orlans, 1963) cannot be solved exactly.

Iterative solution in powers of v (Ferer *et al.*, 1969; Moore *et al.*, 1969) is simple in principle though still time-consuming. To find all terms in M and C up to a given power of v , one needs only a finite number of graphs in E . In zero field, for example, E first enters in order v^7 and the single graph Fig. 11(f) suffices through order v^8 (v^9 with nearest-neighbour interactions only on loose-packed lattices). It is convenient to iterate simultaneously both of eqns (128). Once the M 's and C 's are known from (128) or some approximation thereto, then (103) gives the pair correlations $\mathcal{M}_2(12)$ and (122) (and higher order analogs) give \mathcal{M}_n , $n > 2$.

To complete the story we need an expression for $W[M, C]$, the fully renormalised generalisation of the vertex renormalised (60). This derivation can be done topologically in analogy to De Dominicis' work on the classical fluid (De Dominicis, 1962). The algebraic derivation (Wortis, *et al.*, 1969) simply integrates eqn (7). To carry out this integration efficiently it is necessary to introduce a slight generalisation of our present development. We merely quote the result (Wortis *et al.*, 1969),

$$W = \sum_1 M_0(1) - \sum_1 \sum_{l=1}^{\infty} G_l(1) M_l(1) + \frac{1}{2} \sum_{1,2} v(12) [\mathcal{M}_2(12) + \mathcal{M}_1(1)\mathcal{M}_1(2)] + \Omega[M, C], \quad (129)$$

where

$$\begin{aligned} \Omega[M, C] &= \frac{1}{2} \sum_{1,2} \sum_{l,n=1}^{\infty} M_l(1) \langle l1 | [C - (1 + C) \ln(1 + C)] | 2n \rangle M_n(2) \\ &\quad + \frac{1}{2} \text{Tr}[\ln(1 + MC) - MC + \frac{1}{2} MCMC] \\ &\quad + \left\{ \begin{array}{l} \text{sum of all topologically distinct 2-irreducible} \\ \text{unrooted graphs} \dagger \text{ according to Rule 14.} \end{array} \right\} \end{aligned} \quad (130)$$

[†]The graphs  ,  , and  are specifically excluded.

Rule 14: The Functional $\Omega[M, C]$, Vertex and Bond Renormalised Form

- Assign dummy labels to all internal vertices.
- For each edge joining vertices i and j write a factor $C_{l_i l_j}(ij)$.
- For each internal vertex of g -valence n_i (see Rule 12) write a factor $M_{n_i}(i)$.
- Sum each internal vertex label freely over the entire lattice. Sum all valence labels $l_i = 1, 2 \dots$.
- Divide by the symmetry factor of the unrooted graph.

The trace in (130) refers to the matrix representation (108), e.g.

$$\frac{1}{2} \text{Tr} [\ln(1 + MC)] = \frac{1}{2} \sum_1 \sum_{n=1}^{\infty} \langle n1 | \ln(1 + MC) | n1 \rangle. \quad (131)$$

The first four terms in the graphical sum are,

$$\begin{aligned} \frac{1}{4!} \text{Diagram} &+ \frac{1}{8} \text{Diagram} + \frac{1}{12} \text{Diagram} + \frac{1}{5!} \text{Diagram} \\ &+ \text{graphs with six or more vertices.} \end{aligned} \quad (132)$$

The evaluation (130) is, of course, not necessary in series calculations, since, once \mathcal{M}_1 and \mathcal{M}_2 are known explicitly to a given order in v , eqn (7) can be integrated term-by-term.

K. Further renormalisation: comments

Vertex (1-point) and interaction (2-point) renormalisations have now been carried out explicitly. De Dominicis (1962) has given a very brief discussion of 3-point renormalisation for the classical fluid. We shall not develop higher order renormalisations, but the lines which such a development would follow should now be apparent: l -vertex disassembly defines l -insertions and an l -skeleton. All order n correlations $n > l$ can be summed by decorating l -skeletons with combinations of l -insertions. The only point requiring finesse is the derivation of the higher order analogs of eqns (128), expressing the l -order potentials (identically zero for the Ising model) in terms of the l -correlation factors.

III. Further Applications and Extensions of the Linked-Cluster Expansion

A. Orientation

The linked-cluster expansion was developed in detail in Section II for the specific example of the spin s Ising model. This is the simplest and most studied application. The bare graphical expansions of Section II.B were

renormalised with respect to vertices in Sections II.E and II.F and then with respect to edges in Sections II.I and II.J. The renormalisation process depended on two quite general properties, (i) graph topology and (ii) the freedom of the lattice sums in part (d) of all graphical rules.

Linked-cluster expansions closely analogous to the Ising expansion exist for a wide variety of other systems, both quantum and classical. The criterion is simply that the system be *spatially local in the absence of interactions*. Once a bare (unrenormalised) expansion is known to exist which is graphical and contains free lattice sums, its renormalisation is immediate. The presence of extra variables, non-commutativity of operators, etc., present only clerical problems and have no influence on the arguments leading to renormalisation.

In this section we shall briefly sketch some of these extensions and generalisations. Our purpose will be to reduce the analysis to a stage where the Ising development is clearly applicable. Generalisation of results from Section II can then be written down by inspection. The subsections which follow are intended to be independent of one another, although they will draw extensively on the material of Section II.

B. Inclusion of additional local fields

Inclusion in the Hamiltonian (1) or (2) of additional spatially local fields is a useful if trivial generalisation. Consider, for example, the dimensionless Hamiltonian,

$$-\beta\mathcal{H} = \frac{1}{2} \sum_{1,2} v(12)\mu(1)\mu(2) + \sum_1 h(1)\mu(1) + \sum_1 \Delta(1)X(1), \quad (133)$$

where $X(1)$ is a local operator belonging to the dynamical subsystem at site 1 and Δ is an external field which couples locally to X . For example, a single-ion magnetic anisotropy would be written with $X(1) = \mu^2(1)$ and $\Delta(1)$ the local anisotropy field.[†]

The free energy W is now a functional of Δ in addition to h and v , $W[h, \Delta, v]$. The Ising derivative relations (4)–(8) continue to hold; however, in addition,

$$\frac{\delta W}{\delta \Delta(1)} = \langle X(1) \rangle, \quad \frac{\delta^2 W}{\delta \Delta(1) \delta \Delta(2)} = \langle X(1)X(2) \rangle - \langle X(1) \rangle \langle X(2) \rangle, \text{ etc.} \quad (134)$$

[†] This model, which has been studied for $s = 1$ by Griffiths (1970), Blume *et al.* (1971), and Oitmaa (1970), is interesting in that (at least in the effective-field approximation) it exhibits either a second order transition, a first order transition, or no transition at all depending on the value of Δ ,

The initial condition (9) and (10) is modified by Δ ,

$$W_0[h, \Delta] = \sum_1 M_0^0(1) = \sum_1 \left[\ln \sum_{\mu=-1}^1 \exp [h(1)\mu + \Delta(1)X] \right]. \quad (135)$$

For example, in the Griffiths-Blume model referred to above,

$$M_0^0(1) = M_0^0[1; h, \Delta] = \ln (1 + 2 e^\Delta \cosh h). \quad (136)$$

The bare semi-invariants continue to be defined by (14),

$$M_n^0(h, \Delta) = \frac{\partial^n}{\partial h^n} M_0^0(h, \Delta), \quad (137)$$

but now depend parametrically on Δ at each site.

In the development of unrenormalised perturbation theory, the semi-invariants appeared as derivatives of W_0 , i.e. directly in the form (137). Thus, Rules 1 through 4 (eqns (20), (28), (30), and (31)) are unchanged except that they are now to be carried out in terms of the bare semi-invariants (135), (137), instead of (10), (14). The subsequent renormalisation, which simply replaces the bare semi-invariants M_n^0 by their renormalised analogs, goes through unchanged.

Once having incorporated Δ as a parameter into the semi-invariants, it is extremely easy to generate correlations involving the operators X . The procedure mimics the discussion preceding eqns (27)-(31). For example, to find $\langle X \rangle$ using (134), we note that Δ appears in the unrenormalised expansion for W only through the semi-invariants, so, schematically,

$$\frac{\delta W}{\delta \Delta(1)} = \sum_{n=0}^{\infty} \frac{\delta W[M^0, v]}{\delta M_n^0(1)} \frac{\delta M_n^0(1)}{\delta \Delta(1)}. \quad (138)$$

In graphical terms, $\delta W / \delta M_n^0$ roots one l -valent vertex of a previously unrooted graph and $\delta M_n^0(1) / \delta \Delta(1)$ replaces the semi-invariant at that vertex by a new type of mixed semi-invariant generated from $M_0^0(h, \Delta)$ by both h and Δ derivatives. Denote

$$M_{l,n}^0(h, \Delta) \equiv \frac{\partial^l \partial^n}{\partial h^l \partial \Delta^n} M_0^0(h, \Delta). \quad (139)$$

Then (cf. (28)),

$$\langle X(1) \rangle = \left\{ \begin{array}{l} \text{sum of all topologically distinct} \\ \text{1-rooted connected graphs according} \\ \text{to Rule 2'}. \end{array} \right\} \quad (140)$$

Rule 2':

Same as Rule 2 for $n = 1$ except:

- (c) *For each l -valent internal vertex i write a factor $M_l^0(i)$. For each l -valent external vertex write a factor $M_{l,1}^0(1)$.*

Since the operator X is not coupled to the interaction, it appears only at external vertices, and the generalised semi-invariants (139) $n \neq 0$ do not enter self-fields. Thus, vertex renormalisation of the generalised semi-invariants follows (42),

$$M_{l,n}(1) = \left[\exp \sum_{k=1}^{\infty} G_k[1; M, v] \frac{\delta^k}{\delta \tilde{h}^k} \right] M_{l,n}^0[1; \tilde{h}, A]|_{\tilde{h}=h(1)}. \quad (141)$$

The analog of (45) is

$$\langle X(1)X(2) \rangle - \langle X(1) \rangle \langle X(2) \rangle = \delta(12)M_{0,2}(1) + \left\{ \begin{array}{l} \text{sum of all topologically distinct} \\ \text{2-rooted 1-irreducible connected} \\ \text{graphs according to Rule 5'.} \end{array} \right\} \quad (142)$$

Rule 5':

Same as Rule 5 except:

- (c) *For each l -valent internal vertex i write a factor $M_l(i)$. For each l -valent external vertex i write a factor $M_{l,1}(i)$.*

Correspondingly, the analogue of (103) is,

$$\langle X(1)X(2) \rangle - \langle X(1) \rangle \langle X(2) \rangle = \delta(12)M_{0,2}(1) + \sum_{l,n=1}^{\infty} M_{l,1}(1)C_{ln}(12)M_{n,1}(2), \quad (143)$$

so that, if the correlation factors C have been found in the calculation of $\mathcal{M}_2(12)$, the extra work required to complete the $X-X$ correlations is minimal.

C. Several commuting variables: the classical Heisenberg model

The first application of the linked-cluster method to the derivation of the high-temperature expansions useful in the study of critical phenomena was in connection with the anisotropic classical Heisenberg model. Joyce (1967) developed the unrenormalised form of the expansion by generalising the work of Horwitz and Callen (1961) and generated the first few terms in perturbation theory. Jasnow and Wortis (1968) and Jasnow (1969) applied the vertex renormalisation to go to higher orders. The Hamiltonian is,

$$\mathcal{H} = - \sum_{\langle ij \rangle} J^\alpha(ij) t_{\alpha i} t_{\alpha j} - m \sum_i \mathbf{H}(i) \cdot \mathbf{t}_i, \quad (144)$$

$\alpha = x, y, z$

where the sum is over distinct pairs $i \neq j$, $J(ij)$ is the exchange coupling between sites i and j , m is the magnetic moment, and $\mathbf{H}(i)$ is the magnetic field at site i . \mathbf{t}_i is a classical unit vector associated with site i . Rewriting (144) in dimensionless units,

$$-\beta\mathcal{H} = \frac{1}{2} \sum_{\substack{i, j \\ \alpha=x, y, z}} v^\alpha(12) t_\alpha(1) t_\alpha(2) + \sum_{\substack{\alpha \\ \alpha=x, y, z}} h^\alpha(1) t_\alpha(1), \quad (145)$$

where $v = \beta J$, $h = \beta m H$, and numerical arguments stand for lattice sites. We define as usual,

$$W[\mathbf{h}, v] = \ln \text{Tr} \exp(-\beta\mathcal{H}), \quad (146)$$

where the trace indicates integration of each unit vector \mathbf{t} over its unit sphere. Cumulant correlations are generated via the second term on the right of (145),

$$\frac{\delta W}{\delta h^\alpha(1)} = \langle t_\alpha(1) \rangle = \mathcal{M}_\alpha(1),$$

$$\frac{\delta^2 W}{\delta h^\alpha(1) \delta h^\beta(2)} = \langle t_\alpha(1) t_\beta(2) \rangle - \langle t_\alpha(1) \rangle \langle t_\beta(2) \rangle = \mathcal{M}_{\alpha\beta}(12), \quad (147)$$

and so forth, where the Greek subscripts stand for Cartesian coordinates and are paired with the space indices.

The differential equation which (in analogy to (8)) generates the linked-cluster expansion is

$$\frac{\delta W}{\delta v^\alpha(12)} = \frac{\delta^2 W}{\delta h^\alpha(1) \delta h^\alpha(2)} + \frac{\delta W}{\delta h^\alpha(1)} \frac{\delta W}{\delta h^\alpha(2)}. \quad (148)$$

The non-interacting free energy W_0 is

$$W_0[\mathbf{h}] = \sum_1 M_0^0(1),$$

$$M_0^0(1) = M_0^0[1; \mathbf{h}(1)] = \ln \int d\Omega \exp [\mathbf{h}(1) \cdot \mathbf{t}] = \ln \left[\frac{4\pi \sinh|h(1)|}{|h(1)|} \right]. \quad (149)$$

The bare semi-invariants, which enter the Taylor series coefficients as the cumulant correlations associated with an isolated site, now carry an extra set of Cartesian subscripts,

$$M_n^0(1, \alpha_1 \dots \alpha_n) \equiv \frac{\delta^n M_0^0(1)}{\delta h^{\alpha_1}(1) \dots \delta h^{\alpha_n}(1)}, \quad (150)$$

which is totally symmetrical in the α 's.

In constructing the Taylor development of the free energy W along the lines of (11), there is an extra Cartesian index α which goes with each poten-

tial factor $v^x(12)$ and must be summed† $\alpha = x, y, z$. The two $(\delta/\delta h^\alpha)$'s which go with v^x by (148) tie each edge v^x to bare semi-invariants containing α at its two ends. The *topology of the graphs* on the other hand depends only on spatial structure and goes through exactly as for the Ising model. The rule for the unrenormalised free energy, which could also be derived along the lines of Section II.C, is (cf. Rule 1, eqn (20)),

$$W[\mathbf{h}, v] = \left\{ \begin{array}{l} \text{sum of all topologically distinct unrooted} \\ \text{connected graphs according to Rule 15.} \end{array} \right\}$$

Rule 15: Classical Heisenberg Model Free Energy W, Unrenormalised Form

- (a) Assign a dummy label to each internal vertex and a Cartesian index to each edge.
- (b) For each edge indexed γ and joining vertices i and j write a factor $v^\gamma(ij)$.
- (c) For each l -valent vertex i write a factor $M_l^0(i, \gamma_1 \dots \gamma_l)$, where $\gamma_1 \dots \gamma_l$ are the Cartesian indices of the edges incident at i .
- (d) Sum each internal vertex label freely over the entire lattice. Sum the Cartesian index of each edge $\gamma = x, y, z$.
- (e) Divide by the symmetry factor of the unrooted graph.

Since topology is unchanged from the Ising case, the first few contributing graphs are given by (20). For example,

$$\frac{1}{2} \text{Diagram} = \frac{1}{2} \sum_{1,2,3} \sum_{\gamma_1, \gamma_2} v^{\gamma_1}(12) v^{\gamma_2}(23) M_1^0(1, \gamma_1) M_2^0(2, \gamma_1 \gamma_2) M_1^0(3, \gamma_2). \quad (151)$$

Linked-cluster rules for the cumulant correlations are derived via (147). $W[M^0, v]$ depends on the fields \mathbf{h} only through the semi-invariants M^0 . Differentiation fixes a vertex, increases its order by one, and attaches a Cartesian label. The reduction of the unrooted symmetry factor to that appropriate to the rooted graph depends on topology alone and does not differ from the Ising case. As an example, we give the expression for the pair correlations (cf. Rule 3, eqn (30)), which are the easiest route to the susceptibility matrix:

$$\mathcal{M}_{\alpha\beta}(12) - \delta(12)M_2(1, \alpha\beta) = \left\{ \begin{array}{l} \text{sum of all topologically distinct} \\ \text{2-rooted connected graphs according} \\ \text{to Rule 16.} \end{array} \right\} \quad (152)$$

† For an interacting system of classical plane rotors (Bowers and Joyce, 1967; Stanley, 1968), the unit vector \mathbf{t} is restricted to a plane. The trace operation is an angular integral from 0 to 2π , thus changing the evaluation (149)–(150) of the semi-invariants. The sum over α is only $\alpha = x, y$. Otherwise, everything is exactly as here sketched.

Rule 16: Classical Heisenberg Model Pair Correlations, Unrenormalised Form

- Assign a dummy label to each internal vertex and a Cartesian index γ to each edge. Assign the pair $(\alpha, 1)$ to one of the two external vertices and $(\beta, 2)$ to the other.
- For each edge indexed γ and joining vertices i and j write a factor $v^\gamma(ij)$.
- For each l -valent internal vertex i write a factor $M_l^0(i, \gamma_1 \dots \gamma_l)$. For each l -valent external vertex $i = 1, 2$ write a factor $M_{l+1}^0(i, \gamma, \gamma_1 \dots \gamma_l)$ with $\gamma = \alpha(\beta)$ for vertex 1(2). The indices $\gamma_1 \dots \gamma_l$ are the Cartesian labels of incident edges.
- Sum each internal vertex label freely over the entire lattice. Sum the Cartesian index of each edge $\gamma = x, y, z$.
- Divide by the symmetry factor of the 2-rooted graph.

Contributing graphs are given by (30).

Renormalisations go through exactly as for the Ising model. The extra complexity introduced by the Cartesian sums is entirely clerical. The renormalisation of the semi-invariants will serve to illustrate this point. The self-field $G_n(1)$ at the point 1 must now carry the n Cartesian indices of the edges incident at the external vertex. In the process of decoration, by which the renormalised semi-invariant is formed, each of these edges must be matched to the bare semi-invariant. Thus, the self-field (cf. Rule 6, eqn (47)),

$$G_n(1, \alpha_1 \dots \alpha_n) = \left\{ \begin{array}{l} \text{sum of all topologically distinct 1-} \\ \text{irreducible 1-insertions which are} \\ \text{\textit{n}-valent at the external vertex} \\ \text{according to Rule 17.} \end{array} \right\} \quad (153)$$

Rule 17: Classical Heisenberg Model Self-Field, Vertex Renormalised Form

- Assign the Cartesian indices $\alpha_1, \dots, \alpha_n$ to the n edges incident at the external vertex 1. Assign a Cartesian index γ to each additional edge. Assign a dummy label to each internal vertex.
- For each edge indexed γ and joining vertices i and j write a factor $v^\gamma(ij)$.
- For each l -valent internal vertex i write a factor $M_l(i, \gamma_1 \dots \gamma_l)$ (the renormalised semi-invariant to be defined below). For the external vertex write a factor of 1.
- Sum each internal vertex label freely over the entire lattice. Sum the Cartesian indices of all edges not incident at the external vertex $\gamma = x, y, z$.
- Divide by the symmetry factor of the 1-rooted graph.

Contributing graphs and symmetry factors are as given by eqn (47). One representative term in the evaluation of G_3 is shown in Fig. 15. Unlike the semi-invariants, $G_n(1, \alpha_1 \dots \alpha_n)$ is not in general symmetric under permutations of its Cartesian indices,[†] though it will, of course, reflect any symmetries of the Hamiltonian (144), (145). The renormalised semi-invariant is (cf. (42)),

$$M_n(1, \alpha_1 \dots \alpha_n) = \left[\exp \sum_{l=1}^{\infty} \sum_{\gamma_1 \dots \gamma_l} G_l(1, \gamma_1 \dots \gamma_l) \frac{\delta^l}{\delta \tilde{h}^{\gamma_1} \dots \delta \tilde{h}^{\gamma_l}} \right] M_n^0[1, \alpha_1 \dots \alpha_n; \tilde{h}]|_{\tilde{h}=\mathbf{h}(1)}. \quad (154)$$

The vertex renormalised form of (152) sums 1-irreducible 2-rooted graphs by a rule identical to Rule 16 except for the replacement $M^0 \rightarrow M$.

$$\frac{1}{2} = \frac{1}{2} \sum_{\substack{2,3 \\ y=x,y,z}} v^{\alpha_1}(12)v^{\alpha_2}(13)v^{\alpha_3}(13)v^y(23) \times M_2(2, \alpha_1 \gamma)M_3(3, \alpha_2 \alpha_3 \gamma)$$

FIG. 15. A contribution to G_3 .

Like G , the correlation factors C must now carry Cartesian indices labelling lines incident at external vertices. Thus,

$$\begin{aligned} & \mathcal{M}_{\alpha\beta}(12) - \delta(12)M_2(1, \alpha\beta) \\ &= \sum_{l,n=1}^{\infty} \sum_{\substack{\alpha_1 \dots \alpha_l \\ \beta_1 \dots \beta_n}} M_{l+1}(1, \alpha\alpha_1 \dots \alpha_l)C_{ln}(1, \alpha_1 \dots \alpha_l; 2, \beta_1 \dots \beta_n)M_{n+1}(2, \beta\beta_1 \dots \beta_n). \end{aligned} \quad (155)$$

D. Non-commuting variables: the quantum Heisenberg model

In treating the quantum many-particle problem (Martin and Schwinger, 1959; Kadanoff and Baym, 1962; Abrikosov *et al.*, 1965), it is customary to focus attention not on the operator $\exp(-\beta\mathcal{H})$, whose trace gives the thermodynamics, but rather on the time-ordered unitary operator,

$$U(t_1, t_2) = \left[\exp \left(-i \int_{t_2}^{t_1} dt \mathcal{H}(t) \right) \right]_+, \quad (156)$$

which generates the time translations of the state vector of the system from time t_2 to time t_1 . Time-dependence is therefore introduced *ab initio* into the

[†] In the renormalisation, G is contracted with the symmetrical semi-invariant, thus picking out its symmetrical part, so it is possible to define G to be symmetrised without changing what follows.

formalism, making all calculation significantly more involved than is the case classically. This time-dependence also seems inescapable when dealing with *magnetic* systems, and it appreciably enhances the difficulty of practical algebraic calculation. However, it is important to emphasise at the outset that, once all definitions have been properly generalised, the topological properties of the theory are identical to those of the Ising model, discussed in Section II.

The Hamiltonian of the spin s anisotropic Heisenberg Model is

$$\mathcal{H} = -\frac{1}{s^2} \sum_{\substack{\langle ij \rangle \\ \alpha=x,y,z}} J^\alpha(ij) s_{\alpha i} s_{\alpha j} - \frac{m}{s} \sum_i \mathbf{H}(i) \cdot \mathbf{s}_i. \quad (157)$$

It is convenient to introduce the normalised operators $\mathbf{t}(1) = [\mathbf{s}(\mathbf{r}_1, t_1)]/s$, where in dealing with quantum systems the numerical label 1 refers to both the lattice site \mathbf{r}_1 and the time t_1 . In units such that $\hbar = 1$,

$$\mathbf{t}(1) \cdot \mathbf{t}(1) = \left(1 + \frac{1}{s}\right), \quad \mathbf{t}(1) \times \mathbf{t}(2)|_{t_1=t_2} = i\delta(\mathbf{r}_1 \mathbf{r}_2) \frac{\mathbf{t}(1)}{s}. \quad (158)$$

In terms of the variables $J \equiv v$, $m\mathbf{H} \equiv \mathbf{h}$, then,

$$-\mathcal{H}(t) = \frac{1}{2} \sum_{\substack{\mathbf{r}_1, \mathbf{r}_2 \\ \alpha}} v^\alpha(\mathbf{r}_1 \mathbf{r}_2 t) t_\alpha(\mathbf{r}_1, t) t_\alpha(\mathbf{r}_2, t) + \sum_{\mathbf{r}_1, \alpha} h^\alpha(\mathbf{r}_1, t) t_\alpha(\mathbf{r}_1, t). \quad (159)$$

It is important in the development which follows formally to maintain \mathbf{h} and v as functions of time *independently variable* for each point and bond.

Now, in the physical limit, in which \mathcal{H} is time-independent, $U(t_1, t_2) = \exp(-i\mathcal{H}t)$ and $U(-i\beta, 0) = \exp(-\beta\mathcal{H})$. This observation motivates the restriction of all time variables to the pure imaginary interval $[0, -i\beta]$, where for purposes of time-ordering "larger" times are those lying nearer $-i\beta$. Note that for a finite system with a bounded Hamiltonian (like (159)) there is certainly no difficulty in analytically continuing the time variables in (156). We shall not attempt to discuss the more formidable problem of the $N \rightarrow \infty$ limit. The proper definition of the generalised free energy W in the presence of time-variation is

$$W[\mathbf{h}, v] = \ln \text{Tr } U(-i\beta, 0). \quad (160)$$

Functional differentiation† generates time-ordered correlation functions in

† See footnote on p. 145. Functional differentiation with respect to a continuous function $f(t)$ may be defined by approximating f by a sequence of functions which are piecewise constant, $f = f_i$ for t in the internal Δt_i . Then t in Δt_i ,

$$\frac{\delta}{\delta f(t)} \equiv \lim_{\Delta t_i \rightarrow 0} \frac{1}{\Delta t_i} \frac{\delta}{\delta f_i}.$$

which all times are restricted to $[0, -i\beta]$,

$$(-i) \frac{\delta W[\mathbf{h}, v]}{\delta h^\alpha(1)} = \langle t_\alpha(1) \rangle = \mathcal{M}_\alpha(1),$$

$$(-i)^2 \frac{\delta^2 W[\mathbf{h}, v]}{\delta h^\alpha(1) \delta h^\beta(2)} = \langle (t_\alpha(1) t_\beta(2))_+ \rangle - \langle t_\alpha(1) \rangle \langle t_\beta(2) \rangle = \mathcal{M}_{\alpha\beta}(12), \quad (161)$$

which should be compared with (147). In (161) all operators have Heisenberg time-dependence $X(t) = U^{-1}(t, 0)X(0)U(t, 0)$ and the expectation value is defined with respect to $U(-i\beta, 0)$,

$$\langle X \rangle = \frac{\text{Tr } U(-i\beta, 0)X}{\text{Tr } U(-i\beta, 0)}. \quad (162)$$

The notation $()_+$ indicates an ordering of all operators right to left by increasing times. The physical correlation functions (for real times) may be obtained from (161) and higher order analogs by analytic continuation in the time variables. Of course, W requires no analytic continuation and, when \mathbf{h} and v are time-independent, $\mathcal{M}_\alpha(1)$ is, too. The procedure for continuation is discussed at length in the many-particle literature and is not of immediate relevance to our present concerns, which are mainly topological. The analog of the functional differential equation (8) is

$$\begin{aligned} (-i) \frac{\delta W}{\delta v^\alpha(12)} &= \langle t_\alpha(1) t_\alpha(2) \rangle|_{t_1=t_2+} \\ &= (-i)^2 \left[\frac{\delta^2 W}{\delta h^\alpha(1) \delta h^\beta(2)} + \frac{\delta W}{\delta h^\alpha(1)} \frac{\delta W}{\delta h^\beta(2)} \right] \Big|_{t_1=t_2+}. \end{aligned} \quad (163)$$

In the absence of interaction (cf. (9) and (10)),

$$W[\mathbf{h}, v=0] = W_0[\mathbf{h}] = \sum_1 M_0^0(1),$$

where,

$$M_0^0(1) = \ln \text{Tr} \left(\exp i \int_0^{-i\beta} dt \sum_\alpha h^\alpha(1) t_\alpha(1) \right)_+. \quad (164)$$

The unrenormalised semi-invariants are now time-dependent,

$$M_n^0(\mathbf{r}, t_1 \dots t_n) = \frac{(-i)^n \delta^n M_0^0(\mathbf{r})}{\delta h^{\alpha_1}(\mathbf{r}, t_1) \dots \delta h^{\alpha_n}(\mathbf{r}, t_n)}. \quad (165)$$

Unlike (10) or (149), (164) cannot in general (i.e. for time-dependent \mathbf{h}) be evaluated in closed form, so (165) cannot be used in a practical way to

evaluate the semi-invariants. This need not cause difficulty in practice, since \mathbf{h} is normally time-independent in the physical limit, and each M_n^0 can then be evaluated directly. For example, when $\mathbf{h}(\mathbf{r}) = 0$,

$$M_1^0\left(\mathbf{r}, \frac{\alpha}{t}\right) = \langle t_\alpha(\mathbf{r}, t) \rangle = 0,$$

$$M_2^0\left(\mathbf{r}, \frac{\alpha_1 \alpha_2}{t_1 t_2}\right) = \langle (t_{\alpha_1}(\mathbf{r}, t_1) t_{\alpha_2}(\mathbf{r}, t_2))_+ \rangle - \langle t_{\alpha_1}(\mathbf{r}, t_1) \rangle \langle t_{\alpha_2}(\mathbf{r}, t_2) \rangle$$

$$= \frac{\delta(\alpha_1 \alpha_2)}{3} \left(1 + \frac{1}{s}\right),$$

$$M_3^0\left(\mathbf{r}, \frac{\alpha_1 \alpha_2 \alpha_3}{t_1 t_2 t_3}\right) = \begin{cases} 0, & \text{unless } (\alpha_1 \alpha_2 \alpha_3) \text{ are some permutation of } (xyz), \\ \frac{(+i)}{6s} \left(1 + \frac{1}{s}\right), & \text{for time orderings giving } (xyz) \text{ and} \\ & \text{cyclic permutations,} \\ \frac{(-i)}{6s} \left(1 + \frac{1}{s}\right), & \text{for time orderings giving } (yxz) \text{ and} \\ & \text{cyclic permutations.} \end{cases} \quad (166)$$

When $\mathbf{h} = 0$, M_n^0 is constant for any given time ordering and the evaluation reduces to finding traces of spin-operator products. The presence of a time-independent non-zero field makes things only marginally more complicated. Relevant traces have been evaluated to high order by Dalton and Rimmer (1968).

It is sometimes convenient to have equations of motion for the M_n^0 's. When $v = 0$,

$$i \frac{\partial}{\partial t} t_\alpha = [t_\alpha, \mathcal{H}] = (-i) \sum_\beta \epsilon^{\alpha\beta\gamma} \frac{h^\beta}{s} t_\gamma, \quad (167)$$

where $\epsilon^{\alpha\beta\gamma}$ is the completely antisymmetric matrix,

$$\epsilon^{\alpha\beta\gamma} = \begin{cases} 1, & \text{when } \alpha\beta\gamma \text{ is a cyclic permutation of } xyz, \\ -1, & \text{when } \alpha\beta\gamma \text{ is a cyclic permutation of } yxz, \\ 0, & \text{otherwise.} \end{cases}$$

Thus, for example,

$$\sum_\gamma (\mathcal{G}_0^{-1}(t_1))^{\alpha\gamma} M_2^0\left(\mathbf{r}, \frac{\gamma\beta}{t_1 t_2}\right) = - \frac{\delta(t_1 t_2)}{s} \sum_\gamma \epsilon^{\alpha\beta\gamma} M_1^0\left(\mathbf{r}, \frac{\gamma}{t_1}\right),$$

where

$$(\mathcal{G}_0^{-1}(t))^{\alpha\gamma} \equiv \delta^{\alpha\gamma} i \frac{\partial}{\partial t} + i \sum_{\beta} \varepsilon^{\alpha\beta\gamma} \frac{h^{\beta}}{s}. \quad (168)$$

The general form is, schematically,

$$\mathcal{G}_0^{-1} M_n^0 = \frac{1}{s} \sum M_{n-1}^0 \delta, \quad (169)$$

which can help to evaluate those parts of the semi-invariants that are not time-independent. In the classical limit $s \rightarrow \infty$, the semi-invariants become entirely time-independent and go over into their classical forms (149), (150).

Unrenormalised perturbation theory for the Heisenberg model has been developed by Stinchcombe *et al.* (1963) and by Vaks *et al.* (1968a, b). To develop W in powers of v , there are as usual two routes. Either we directly expand the time-ordered exponential U (Englert, 1963) (cf. Section II.C) or we use (163) to generate the coefficients in the Taylor expansion (cf. (11) and (12)). It is clear from either point of view that each potential line v carries a factor i and requires a time integral over the interval $[0, -i\beta]$. Otherwise, the topology of the development parallels exactly Sections II.B, II.C, and III.C. The result is

$$W = \left\{ \begin{array}{l} \text{sum of all topologically distinct unrooted} \\ \text{connected graphs according to Rule 18.} \end{array} \right\} \quad (170)$$

Rule 18: Heisenberg Model Free Energy W , Unrenormalised Form

- (a) Assign to each vertex a dummy spatial label \bar{r} . Assign to each edge a Cartesian index γ and a time variable \bar{t} .
- (b) For each edge labeled γ, \bar{t} and joining vertices \bar{r}_i and \bar{r}_j write a factor $iv^{\gamma}(\bar{r}_i \bar{r}_j \bar{t})$.
- (c) For each l -valent vertex \bar{r} with incident edges $\gamma_1 \bar{t}_1, \dots, \gamma_l \bar{t}_l$ write a factor

$$M_l^0 \left(\bar{r}, \frac{\gamma_1 \dots \gamma_n}{\bar{t}_1 \dots \bar{t}_n} \right).$$

- (d) Sum each internal vertex label freely over the entire lattice. Integrate each time variable $\int_0^{-i\beta} dt$. Sum each Cartesian index $\gamma = x, y, z$.
- (e) Divide by the symmetry factor of the unrooted graph.

The first few contributing graphs are given by (20). Note that in the classical limit each time integral provides a factor $(-i\beta)$ which combines with (iv) to form βv which was called v in III.C. It is also possible (and convenient when v is isotropic) to use a spherical representation, t_z, t_+, t_- .

The correlation functions (161) are derived by differentiation. For example,

$$\mathcal{M}_{\alpha\beta}(12) - \delta(\mathbf{r}_1\mathbf{r}_2)M_2\left(\mathbf{r}_1, \frac{\alpha\beta}{t_1 t_2}\right) = \left\{ \begin{array}{l} \text{sum of all topologically distinct} \\ \text{2-rooted connected graphs} \\ \text{according to Rule 19.} \end{array} \right\} \quad (171)$$

Rule 19: Heisenberg Model Pair Correlations, Unrenormalised Form

- (a) Assign to each internal vertex a dummy spatial label \bar{r} . Assign to each edge a Cartesian index γ and a time variable \bar{t} . Assign to the external vertices 1 and 2 the labels $(\mathbf{r}_1 t_1 \alpha)$ and $(\mathbf{r}_2 t_2 \beta)$.
- (b) For each edge labeled γ, \bar{t} and joining vertices \bar{r}_i and \bar{r}_j write a factor $i v^\gamma(\mathbf{r}_i \mathbf{r}_j \bar{t})$.
- (c) For each l -valent internal vertex \bar{r} with incident edges $\gamma_1 \bar{t}_1, \dots, \gamma_l \bar{t}_l$ write a factor

$$M_l^0\left(\bar{r}, \frac{\gamma_1}{\bar{t}_1} \dots \frac{\gamma_l}{\bar{t}_l}\right).$$

For each l -valent external vertex $i = 1, 2$ write a factor

$$M_{l+1}^0\left(\mathbf{r}_i, \frac{\gamma \gamma_1}{t_i \bar{t}_1} \dots \frac{\gamma_l}{\bar{t}_l}\right),$$

where $\gamma = \alpha(\beta)$ if $i = 1(2)$.

- (d) Sum each internal vertex label freely over the entire lattice. Integrate each internal time $[0, -i\beta]$. Sum the Cartesian index of each edge $\gamma = x, y, z$.
- (e) Divide by the symmetry factor of the 2-rooted graph.

Graphs are given by (30). For example,

$$\begin{aligned} \frac{1}{2} \text{O} \bullet \text{O} = & \frac{(i)^2}{2} \sum_{\gamma_1, \gamma_2} \int_0^{-i\beta} d\bar{t}_1 d\bar{t}_2 v^{\gamma_1}(\mathbf{r}_1 \bar{r} \bar{t}_1) v^{\gamma_2}(\bar{r} \mathbf{r}_2 \bar{t}_2) M_2^0\left(\mathbf{r}_1, \frac{\alpha}{t_1} \frac{\gamma_1}{\bar{t}_1}\right) \\ & \times M_2^0\left(\mathbf{r}_2, \frac{\gamma_1 \gamma_2}{\bar{t}_1} \frac{\beta}{\bar{t}_2}\right) M_2^0\left(\mathbf{r}_2, \frac{\gamma_2 \beta}{\bar{t}_2} \frac{\beta}{t_2}\right). \end{aligned} \quad (172)$$

The first few terms of the Heisenberg model correlations have been evaluated by another method by Tahir-Kheli and McFadden (1969) and McFadden and Tahir-Kheli (1970a, b).

Renormalisation is straightforward. In calculating insertions such as the self-fields G the external vertex takes a factor 1 and the γ, t labels of all

edges incident at it remain unsummed. Renormalisation proceeds as previously (cf. (42), (154)),

$$M_n(\mathbf{r}, \frac{\alpha\beta}{tt'}, \dots) = \left\{ \exp \sum_{l=1}^{\infty} (-i)^l \int_0^{-i\beta} d\bar{t}_1 \dots d\bar{t}_l \sum_{\gamma_1 \dots \gamma_l} G_l(\mathbf{r}, \frac{\gamma_1 \dots \gamma_l}{\bar{t}_1 \dots \bar{t}_l}) \right. \\ \times \left. \frac{\delta^l}{\delta h^{\gamma_1}(\mathbf{r}, \bar{t}_1) \dots \delta h^{\gamma_l}(\mathbf{r}, \bar{t}_l)} \right\} M_n^0(\mathbf{r}, \frac{\alpha\beta}{tt'}, \dots). \quad (173)$$

The analog of the many-particle Dyson equation is made most evident by applying \mathcal{G}_0^{-1} to (173). The result in rather schematic form is (cf. (169)),

$$\mathcal{G}_0^{-1} M_n = \frac{1}{s} \sum M_{n-1} \delta + \frac{1}{s} \sum_l G_l M_{n+l-1}. \quad (174)$$

Renormalisation has not been carried out systematically in the literature beyond the molecular field approximation, $\Phi = \frac{1}{2} \frac{1}{V} \sum_i \delta(\mathbf{r}_i)$. Better approximations based on (174) seem to give high-temperature results similar to Résibois and De Leener (1966, 1969) and De Leener and Résibois (1966, 1969).

E. Fermion variables

The only complications produced by the introduction of fermion variables are sign factors. In the fourth of his papers on what is now known as the Hubbard model, Hubbard (1965) has developed the unrenormalised perturbation theory for the fermion Hamiltonian,

$$\mathcal{H} = \sum_{\mathbf{r}_1, \mathbf{r}_2, \sigma} t^\sigma(\mathbf{r}_1, \mathbf{r}_2) a_\sigma^+(\mathbf{r}_1) a_\sigma(\mathbf{r}_2) + I \sum_{\mathbf{r}_1} n_\uparrow(\mathbf{r}_1) n_\downarrow(\mathbf{r}_1), \quad (175)$$

($n_\sigma = a_\sigma^+ a_\sigma$) where I represents an intratomic coulomb repulsion and $t(\mathbf{r}_1, \mathbf{r}_2)$ is an interatomic hopping integral. To use the methods we have developed, one regards the second term in (175) as the (spatially local) non-interacting Hamiltonian and expands in powers of the kinetic energy. In order to have the freedom of functional methods it is necessary to introduce anticommuting fields (Schwinger, 1951) which couple directly to the fermion creation and destruction operators,

$$\mathcal{H}'(t) = \sum_{\mathbf{r}, \sigma} \xi_\sigma(\mathbf{r}, t) a_\sigma(\mathbf{r}, t) + \eta_\sigma(\mathbf{r}t) a_\sigma^+(\mathbf{r}, t). \quad (176)$$

The reader is referred to Hubbard's work for further details. Renormalisation has not yet been used.

Appendix: The Relation of the Free Multiplicities to the Weak Lattice Constants

Part (d) of all linked-cluster-expansion rules requires for a given graph the summation of a number of terms, each one associated with a specific realisation of that graph on the underlying lattice, i.e. with a specific assignment of each graphical vertex to a given lattice site. When interactions are uniform, isotropic in the lattice, and restricted to nearest neighbors (e.g. (21), (23)), all terms in such a summation are identical. In such a situation the total contribution of the graph is the value of any one term times the number of terms. The number of terms is called the *free multiplicity*.

We confine our main discussion to unrooted graphs for the sake of simplicity. For specificity we shall always take the underlying lattice to be large and toroidally connected. An *embedding of a graph G in a lattice* is an assignment of the graph vertices to the sites of the lattice in such a way that all graph edges lie along nearest-neighbour bonds of the lattice. *Free* embedding allows several distinct graph vertices to be assigned to the same lattice site. *Weak* embedding allows no more than one vertex to be assigned to each site. The *free multiplicity* $m(G)$ of an unrooted graph G on a given lattice is the number of distinct *free* embeddings of the *labelled* graph G (i.e. the vertices are regarded as distinguishable) in the lattice *per site of the lattice*. The *weak lattice constant* $p(G)$ of the unrooted graph G in the lattice is the number of distinct *weak* embeddings of the *unlabelled* graph G in the lattice *per site of the lattice*. We show below that $m(G)$ and $p(G)$ are closely related.†

We assert that for a given lattice:

- (i) For a properly chosen set of graphs $G \in S$, $m(G)$ is related to $p(G)$ by a conversion matrix A (Sykes *et al.*, 1966),

$$m(G) = \sum_{G' \in S} A(G|G')p(G'), \quad A(G|G') \geq 0.$$

- (ii) A is a non-singular matrix and can therefore be inverted, giving the weak lattice constants p in terms of the m 's.

Note first of all that any graph with multiple edges has the same embeddings as the corresponding *reduced* graph in which all multiple edges have been replaced by single edges. We therefore restrict attention to graphs having only single edges.

Define a *collapse of a graph G* as a graph formed from G by (a) identifying (figuratively, “gluing together”) previously distinct vertices of G ‡ and (b)

† The weak lattice constants are closely related to the strong lattice constants and derivable from them, as shown by Sykes *et al.* (1966). See Domb this volume, Chapter 1, Section IV.

‡ No “loops” (i.e. edges with both ends at the same vertex) may be formed in this process.

reducing all multiple edges thus formed. The graph G and all its collapses form the *collapse chain* of G . The members of the collapse chain of G can be ordered (in general, in a variety of ways), $G = G_1, G_2 \dots$, so that no graph G_n collapses into any graph to its left ($l < n$). Such an ordering is a *standard ordering*. The collapse chain of the graph  is shown in Fig. 16. The *collapse matrix* $C(G|G') \geq 0$ is the number of distinct ways in which the *labelled graph* G collapses into the *unlabelled graph* G' .

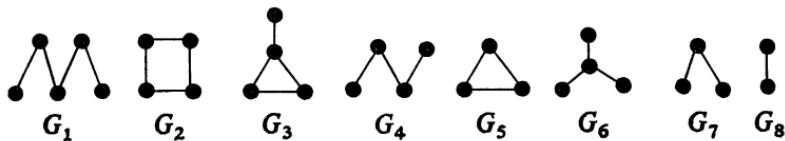


FIG. 16. A collapse chain arranged in standard order.

In the process of counting the free multiplicity of G , all collapses G' are included. Each collapse G' has $g(G')p(G')$ labelled weak embeddings per site of the lattice. Thus,

$$m(G) = \sum_{G'} C(G|G') g(G') p(G'),$$

where the sum is over the graphs in the collapse chain of G . This proves (i). The matrices C and A for the collapse chain shown in Fig. 16 are given below.

$$A = \begin{bmatrix} 1 & 1 & 2 & 2 & 3 & 1 & 4 & 1 \\ 1 & 0 & 0 & 0 & 0 & 2 & 1 \\ 1 & 0 & 2 & 0 & 0 & 0 \\ 1 & 1 & 0 & 2 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 3 & 1 \\ 1 & 1 \\ 1 \end{bmatrix} \quad C = \begin{bmatrix} 2 & 8 & 4 & 4 & 18 & 6 & 8 & 2 \\ 8 & 0 & 0 & 0 & 0 & 4 & 2 \\ 2 & 0 & 12 & 0 & 0 & 0 \\ 2 & 6 & 0 & 4 & 2 \\ 6 & 0 & 0 & 0 & 0 \\ 6 & 4 & 2 \\ 2 & 2 \\ 2 \end{bmatrix} \quad (\text{A.2})$$

To prove part (ii) of the original assertion note that, when the collapse chain of G is arranged in standard order, both C and A are triangular. All diagonal elements are positive, so $\det A \neq 0$ and A^{-1} exists.

There is no difficulty in extending the above to sets of graphs formed by taking the union of two or more collapse chains.

The free multiplicity of an n -rooted graph G on a given lattice is the number of free embeddings of the labelled graph G in the lattice *subject to the condition that the external vertices are fixed on the lattice sites r_1, \dots, r_n* .

The simplifying feature of the free multiplicities (relative, for example, to the weak or strong lattice constants) is that different parts of the graph do not interfere with one another, since they can interpenetrate on the lattice. Thus, the free multiplicities are larger than the weak or strong lattice constants but often far easier to evaluate. For example, the free multiplicity of the unrooted chain of n links is just q^n (q = coordination number). Similarly the free multiplicity of a 1-rooted graph whose external vertex is an articulation point is just the product of the free multiplicities of the associated 1-insertions. These and other related observations are discussed by Jasnow (1969). They are incorporated in a natural way into the renormalisations we have performed in the text.

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4. Asymptotic Analysis of Coefficients

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I. Introduction

A. General problem

It can be seen in other chapters of this volume how power series expansions may be developed for various lattice models in any dimension. The expansions are exact as far as they go, and clearly represent a good deal of

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configurational information. For example, the zero-field reduced susceptibility of the spin $\frac{1}{2}$ Ising model, $I(\frac{1}{2})$, on a triangular lattice has the high temperature expansion (Sykes, 1961; Sykes *et al.*, 1972a; Domb this volume, Chapter 6)

$$\begin{aligned}\chi(w) = & 1 + 6w + 30w^2 + 138w^3 + 606w^4 + 2,586w^5 \\ & + 10,818w^6 + 44,574w^7 + 181,542w^8 + 732,678w^9 \\ & + 2,935,218w^{10} + 11,687,202w^{11} + 46,296,210w^{12} \\ & + 182,588,850w^{13} + 717,395,262w^{14} \\ & + 2,809,372,302w^{15} + 10,969,820,358w^{16} + \dots\end{aligned}\quad (1.1)$$

In this article, the use of power series expansions in calculating the properties of the model, particularly in the critical region, will be considered.† “The misuse of power series” has been discussed by Fisher (1965).

An important assumption is that at the critical point z_c the functions $F(z)$ of interest have power law singularities of the form

$$F(z) \approx A \left(1 - \frac{z}{z_c}\right)^{-\lambda}, \quad (z \rightarrow z_c^-), \quad (1.2)$$

where λ is the critical exponent and A is usually called the amplitude of the singularity. The special case $\lambda = 0$ could mean that $F(z)$ is finite at $z = z_c$, or that $F(z)$ diverges logarithmically, namely

$$F(z) \approx A_0 \left| \ln \left(1 - \frac{z}{z_c}\right) \right|, \quad (z \rightarrow z_c^-). \quad (1.3)$$

Actually, (1.2) and (1.3) represent only the dominant asymptotic behaviour, and in general one should always expect higher-order correction terms. These may be additive as in

$$F(z) \approx A \left(1 - \frac{z}{z_c}\right)^{-\lambda} \left[1 + B \left(1 - \frac{z}{z_c}\right)^\varepsilon + \dots \right], \quad (\varepsilon > 0), \quad (1.4)$$

for example; they may be multiplicative like

$$F(z) \approx A \left(1 - \frac{z}{z_c}\right)^{-\lambda} \left| \ln \left(1 - \frac{z}{z_c}\right) \right|^v, \quad (v \gtrless 0), \quad (1.5)$$

or they may be more complicated still, such as

$$F(z) \approx A \left(1 - \frac{z}{z_c}\right)^{-\lambda} \left| \ln \left(1 - \frac{z}{z_c}\right) \right|^v \left[1 + B \left(1 - \frac{z}{z_c}\right)^\varepsilon + \dots \right]. \quad (1.6)$$

† Note added in proof: For a recent alternative review, see D. L. Hunter and G. A. Baker, Jr., *Phys. Rev. B* 7, 3346 (1973).

Although there is no proof that (1.2) is generally correct, it is in the cases where exact solutions are available (see Domb, 1960; Joyce, Vol. 2, Chapter 10). Approximate theories (see Domb, 1960) provide further support, and much of the experimental data on real fluids and ferromagnets can be fitted using singularities of this form (see Heller, 1967). For a detailed discussion of the power law assumption, and an explanation of the critical exponent notation (α' , α , β , γ' , γ , ...) the reader is referred to the review article by Fisher (1967).

We will focus our attention only on those methods for which the inclusion of more and more coefficients leads to successive approximation schemes which appear to converge with reasonable regularity and speed. Extrapolation enables one to draw conclusions about the critical point behaviour and to estimate the 'errors' involved. However, we stress that the error estimates are, unfortunately, in no sense rigorous and only represent a subjective assessment of the rate of convergence of the available numerical data. In principle, one could easily be quite misled by the initial coefficients for there is no mathematical reason why the apparent asymptotic behaviour of the first ten to twenty terms, say, should continue to infinity. Fortunately, there is often a good deal of additional information to guide one. Several general results [e.g. Yang and Lee (1952); Rushbrooke (1963); Griffiths (1965); Gallavotti *et al.* (1967); Lebowitz and Penrose (1968); Griffiths Vol. 1, Chapter 2] have been proved rigorously and these are of assistance in putting some of the conjectures on a firm foundation. In addition, a number of exact solutions are known [e.g. the two-dimensional Ising model (see Domb, 1960), the ice, ferroelectric and antiferroelectric models (Lieb, 1967a, b, c; Vol. 1 Chapter 8), and the three-dimensional spherical and Gaussian models (Berlin and Kac, 1952; Joyce, Vol. 2, Chapter 10)] and these provide an excellent testing ground for any extrapolation scheme which seems promising. Physical arguments also play a role in suggesting the type of behaviour to be expected of the model. If, in addition, several independent methods of analysis all give similar or at least consistent results, then numerical estimates and conjectures can usually be put forward with a moderate degree of confidence. However, we do not mean to imply that for a given function, all methods of analysis work equally well. The final error estimates are often referred to as 'confidence limits'. Thus, series analysis as developed and extended by Domb and Sykes and their co-workers, and by Baker, Rushbrooke and others, has led to remarkably accurate estimates of critical points, exponents, and amplitudes for the Ising model. For example, the exponent $\gamma = 1\frac{1}{4}$ characterizing the high temperature susceptibility of the two-dimensional Ising model close to the Curie temperature, was suggested (Domb and Sykes, 1957) on the basis of up to nine terms of the exact series expansions, some time before its theoretical justification was known (Fisher, 1959a). Similar techniques have also been

applied to the Heisenberg model [e.g. Rushbrooke and Wood (1958); Baker *et al.* (1967); Rushbrooke *et al.*, this volume, Chapter 5], to the $X - Y$ model [e.g. Betts *et al.* (1970); Betts, this volume, Chapter 8], and to various other model systems [e.g. Sykes and Essam (1964); Gaunt and Fisher (1965); Domb (1969)] with considerable success. The coherent pattern of critical behaviour which is beginning to emerge from these studies is further indirect evidence of the essential correctness of the series approach. However, even if the numerical estimates are slightly in error, they should, nevertheless, yield excellent representations of the various functions over most of the physical region, breaking-down only in the immediate vicinity of the critical point.

B. Basic properties of power series

Let us begin by summarizing some of the fundamental properties of power series (see Dienes, 1957). Suppose the function $F(z)$ has the power series expansion

$$F(z) = \sum_{n=0}^{\infty} a_n z^n \quad (1.7)$$

about the origin $z = 0$. If

$$\lim_{n \rightarrow \infty} |a_n|^{-1/n} = z_0, \quad (1.8)$$

then the series converges for $|z| < z_0$ and diverges for $|z| > z_0$. Correspondingly, there must be at least one singularity (non-analytic point) on the circle of convergence $|z| = z_0$. Unfortunately, the sequence $|a_n|^{-1/n}$ is often slowly convergent so that its practical value in estimating z_0 from the leading coefficients is rather limited (Rushbrooke and Wood, 1958; Stanley and Kaplan, 1967).

If all the coefficients a_n are known exactly one can, in principle, analytically continue the function across the z -plane as far as a natural boundary of the function, beyond which it remains undefined. The nature of the coefficients is determined by the singularities of $F(z)$. The singularities nearest the origin will dominate the behaviour for large n . If the dominant singularity is on the positive real axis, the coefficients will eventually all have the same sign. Conversely, if the dominant singularity is on the negative real axis, the coefficients must eventually alternate in sign. More irregular behaviour of the signs for large n indicates that the dominant singularities are in the complex plane. Since the coefficients are assumed real, the singularities must then occur in complex conjugate pairs.

Of course, if the dominant singularity is sufficiently strong and/or well-separated from the competing singularities, it may determine the sign of *all* the coefficients, even for small n . Consider, for example, the spontaneous magnetization of the Ising model for the plane square and triangular lattices. The exact results (Onsager, 1949; Yang, 1952; Potts, 1952) are

$$I(u) = (1+u)^{1/4} (1-u)^{-1/2} (1-6u+u^2)^{1/8} \quad (1.9)$$

and

$$I(u) = (1+u)^{3/8} (1-u)^{-3/8} (1+3u)^{-1/8} (1-3u)^{1/8}, \quad (1.10)$$

respectively. Since $u = \exp(-4J/kT)$, the ‘physical domain’ or region of the complex plane of physical interest, is the positive real axis from $u = 0$ to 1, since this corresponds to $0 \leq T \leq \infty$. Expanding (1.9) about $u = 0$ one finds

$$I(u) = 1 - 2u^2 - 8u^3 - 34u^4 - 152u^5 - 714u^6 - 3,472u^7 - \dots \quad (1.11)$$

so that the singularities at $u = \pm 1$ and $(3 + 2\sqrt{2})$ are dominated by the closest singularity at $u = u_c = 3 - 2\sqrt{2} = 0.171572 \dots$. This is also the ‘physical’ singularity and corresponds to the Curie point. For the triangular lattice, there are two competing singularities equidistant from the origin at $u = \pm \frac{1}{3}$. The ‘non-physical’ singularity at $u = -\frac{1}{3}$ must ultimately dominate the expansion of the spontaneous magnetization, since it has a negative exponent. On expansion, (1.10) yields

$$\begin{aligned} I(u) = & 1 - 2u^3 + 0u^4 - 12u^5 + 2u^6 \\ & - 78u^7 + 24u^8 - 548u^9 + 228u^{10} - \dots \end{aligned} \quad (1.12)$$

so that once again the dominant singularity in fact determines the signs of all the coefficients. Finally, let us consider the corresponding expansion for the body-centred cubic lattice (Sykes *et al.*, 1965, and further unpublished work; Domb, this volume, Chapter 6), namely

$$\begin{aligned} I(u) = & 1 - 2u^4 - 16u^7 + 18u^8 - 168u^{10} + 384u^{11} - 314u^{12} - 1,632u^{13} \\ & + 6,264u^{14} - 9,744u^{15} - 10,014u^{16} + 86,976u^{17} - 205,344u^{18} \\ & + 80,176u^{19} + 1,009,338u^{20} - 3,579,568u^{21} + 4,575,296u^{22} \\ & + 8,301,024u^{23} - \dots, \end{aligned} \quad (1.13)$$

which is known through u^{28} . No exact solution is available in this case, but it seems reasonable to suppose that such erratic behaviour of the coefficients arises because the dominant singularities lie in the complex plane. As we show in Section III.D, numerical analysis of (1.13) confirms that its radius of con-

vergence is determined by a pair of non-physical singularities at

$$u_1, u_2 = (-0.234 \pm 0.305i) \pm (0.001 \pm 0.001i) \quad (1.14)$$

with moduli

$$|u_1| = |u_2| = 0.384 \pm 0.002, \quad (1.15)$$

while the Curie point singularity lies at $u_c \approx 0.53281$.

On the other hand, it is important to realize that the initial coefficients may be considerably influenced by contributions from singularities other than that which ultimately dominates. Note, for example, how the magnitudes of the coefficients in (1.12) fall into two sequences. This behaviour is due to the singularity at $u = \frac{1}{2}$. A more spectacular example is provided by the spin $\frac{1}{2}$ Heisenberg model, $H(\frac{1}{2})$, for the simple cubic lattice. The first ten terms of the high temperature zero-field susceptibility expansion $\chi(K)$ have been calculated by Baker *et al.* (1967) and are all positive. On analysis, they indicate a strong ferromagnetic singularity at $K = K_c > 0$ of the form

$$\chi(K) \approx C / \left(1 - \frac{K}{K_c}\right)^\gamma$$

where $\gamma = 1.43 \pm 0.01$ and C is the amplitude. However, physical considerations lead one to expect a weak antiferromagnetic singularity at $K = -K'_c < 0$ with $K'_c \neq K_c$. By studying the staggered susceptibility, Rushbrooke and Wood (1963) found the Néel temperature is roughly 13% higher than the corresponding Curie temperature so that $K'_c < K_c$. It follows that the antiferromagnetic singularity will eventually dominate the ferromagnetic one and that the series coefficients must ultimately alternate in sign. However, one can show (Domb *et al.*, 1964) by making reasonable assumptions about the nature of the antiferromagnetic singularity that the first alternation in sign occurs only after the order of a hundred terms! Thus, we can understand how it is possible to derive from only ten coefficients quite accurate information about the ferromagnetic singularity of the Heisenberg model even though $K'_c < K_c$. Similar behaviour can be expected for all 'loose-packed' lattices (i.e. those which can be decomposed into two equivalent sublattices and, therefore, admit simple antiferromagnetic ordering) and for all spin values except $s = \infty$ when $K'_c = K_c$ again (Rushbrooke and Wood, 1963; Fisher, 1967).

C. Comment on content

We have discussed the general problem of series analysis, and made some comment on the basic properties of power series. In the following sections we will discuss, and illustrate with examples, the various methods of analysing the power series expansions which frequently arise in statistical mechanics.

To illustrate the various methods of analysis, we will use, in the main, series expansions which arise in the study of the Ising model of ferromagnetism. These series have been derived by M. F. Sykes and co-workers at King's College, who have generously made available for this article a number of previously unpublished series. We will restrict ourselves to those methods of series analysis which are in frequent use. For this reason we have not discussed a number of other schemes for extracting information from power series expansions, for example those proposed by Alexanian and Wortman (1966), Suzuki (1967) and Gordon (1968). There probably exist other methods of analysis which should be mentioned of which we are quite unaware. If so, we wish to extend our apologies to the authors concerned.[†]

In the next section, we commence with a description of the ratio method, one of the oldest and most successful methods of series analysis. Other methods of analysis are then discussed.

II. Ratio Method

A. Preliminary estimates

The ratio method is usually used to determine the location and nature of a singularity which lies on the real axis and is dominant. Let us suppose that the dominant singularity of some function $F(z)$ is, in fact, on the positive real axis at $z = z_0 = z_c$, and that all the coefficients are of one sign. (If the coefficients of $F(z)$ alternate in sign, first replace z by $-z$.) For the ferromagnetic Ising model, high temperature series like (1.1) are the best known examples of this kind of expansion, but the in-field magnetization series along the critical isotherm (Gaunt *et al.*, 1964; Gaunt, 1967) and certain low temperature series such as (1.11) provide further examples. In all these cases, the physical domain is the positive real axis between $z = 0$ and 1 , so that z_c is also the physical singularity.

It follows from (1.8) that

$$a_n \approx f(n) \mu^n, \quad (2.1)$$

or more precisely

$$\lim_{n \rightarrow \infty} [a_n / f(n) \mu^n] = 1, \quad (2.2)$$

where the unknown function $f(n)$ satisfies

$$\lim_{n \rightarrow \infty} [f(n)]^{1/n} = 1 \quad (2.3)$$

and $\mu = 1/z_c$. For $f(n)$ let us consider the form

$$f(n) = A \binom{g+n}{n} = A \frac{(g+1)(g+2)\dots(g+n)}{n!} \quad (2.4)$$

[†] Mention should be made of the recent recurrence relation method (Guttmann and Joyce, 1972 and 1973) and the work of Baker and Hunter (1973).

which behaves asymptotically like

$$f(n) \approx An^g/\Gamma(g+1) \quad (2.5)$$

where $\Gamma(x)$ is the gamma function. By Appell's comparison theorem (Dienes, 1957), this form for $f(n)$ implies for $g > -1$ and real z that

$$F(z) \approx A(1-\mu z)^{-(1+g)} [1 + O(1-\mu z)], \quad (z \rightarrow z_c^-). \quad (2.6)$$

Evidently, the parameters g and A directly determine the critical exponent and amplitude, respectively, at the singularity $z = z_c = 1/\mu$. For $g \leq -1$, (2.6) correctly represents the *singular* part of $F(z)$ although a multiplicative factor, for example $\ln(1-\mu z)$, must arise if $g = -1, -2, -3, \dots$. In view of our basic assumption that the various singularities are power laws, (2.6) justifies (2.4) or (2.5) as the natural first choice for $f(n)$ (Domb and Sykes, 1956, 1957). The exact solutions for the two-dimensional Ising model (see Domb, 1960) provide further support, as do some weaker asymptotic results which have been rigorously proved (see Hammersley and Welsh, 1962; Kesten, 1963, 1964) for a related class of problems in lattice statistics, namely the problem of self-avoiding walks (see Domb, 1969).

Given the practical problem of estimating z_c , g and A , one may, following Domb and Sykes (1956, 1957), consider the ratios of successive coefficients

$$\mu_n = a_n/a_{n-1}. \quad (2.7)$$

From (2.1) and (2.4), we expect

$$\mu_n \approx \mu \left[1 + \frac{g}{n} + O\left(\frac{1}{n^2}\right) \right], \quad (n \rightarrow \infty), \quad (2.8)$$

so that the ratios should vary linearly with $1/n$ as $n \rightarrow \infty$. The intercept on $1/n = 0$ will give z_c , and from the slope μg , g may be determined.

If only a limited number of terms are known, we must hope that the initial ratios will be sufficiently well-behaved to enable an accurate extrapolation to be made. This depends, amongst other things, upon the proximity and nature of any other singularities. It is easily seen that more distant singularities z_j will contribute to $f(n)$ factors like $[1 + O(z_c/z_j)^n]$, which decay to zero exponentially fast. However, other weaker singularities on the circle of convergence at $z = z_0 e^{\pm i\theta}$, say, lead to more slowly decaying oscillatory factors like

$$1 + Bn^{-h} \exp(\pm in\theta), \quad (h > 0). \quad (2.9)$$

Singularities coincident with, but weaker than (2.6), can also occur. These may considerably affect the rate of convergence and lead to misleading

estimates, particularly of the critical exponent. The above problems will be discussed in more detail as they arise.

Let us test (2.8) by applying it to the high temperature Ising susceptibility series (1.1) for the triangular lattice. The ratios μ_n normalized by dividing by the lattice coordination number q are plotted versus $1/n$ in Fig. 1. The plot is

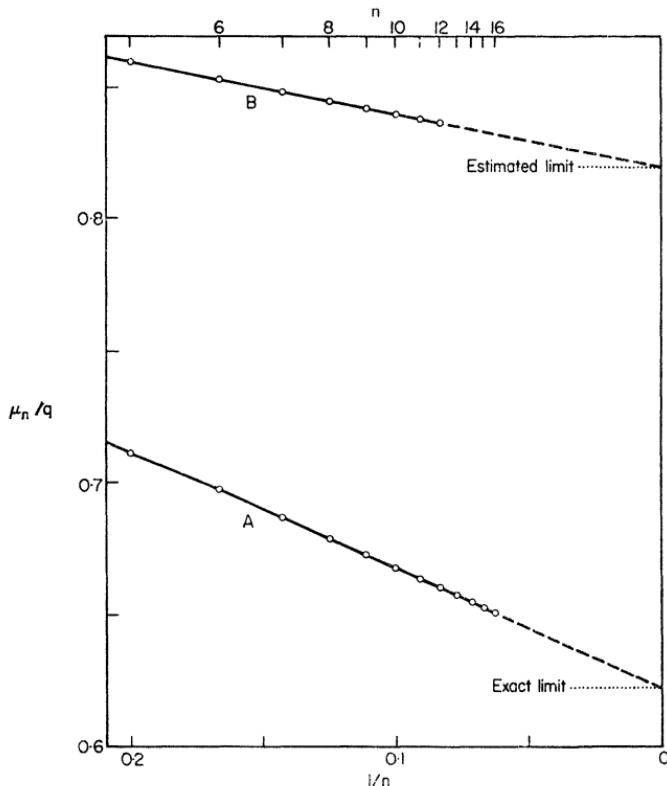


FIG. 1. Successive ratios μ_n of the coefficients of the $I(\frac{1}{2})$ susceptibility expansions of the triangular (A) and face-centred cubic (B) lattices plotted versus $1/n$. (q = lattice coordination number.)

very linear and a rough extrapolation to $1/n = 0$ yields an estimate close to the exactly known limit (e.g. Houtappel, 1950)

$$\mu = 1/w_c = (2 + \sqrt{3}) = 3.73205 \dots \quad (2.10)$$

Thus, the ratios appear to settle down to their asymptotic behaviour even for quite small n .

If the exact value of the critical point is unknown, a preliminary estimate is often obtained from the sequence (Domb and Sykes, 1957, 1961)

$$\mu(n, m) = \frac{1}{n - m} [n\mu_n - m\mu_m] \quad (2.11)$$

by estimating its limiting value as $n \rightarrow \infty$. Taking $m = n - 1$ corresponds to calculating the linear intercepts from adjacent points. However, the use of alternate points ($m = n - 2$) is more usual, since they often lead to more regular sequences. As we shall see, this is particularly true for the loose-packed lattices because of the characteristic odd/even oscillation which occurs. Instead of (2.11) one sometimes uses

$$\mu(n, m; \varepsilon) = \frac{1}{n - m} [(n + \varepsilon)\mu_n - (m + \varepsilon)\mu_m], \quad (2.12)$$

which corresponds to linear intercepts as calculated from plots of μ_n versus $1/(n + \varepsilon)$. The small 'shift' ε gives a range of sequences and allows to some extent for the higher order terms in (2.8).

Similarly, to obtain a preliminary estimate of g , the sequence of slopes

$$g(n, m; \varepsilon) = (n + \varepsilon) \left[\frac{\mu_n}{\mu(n, m; \varepsilon)} - 1 \right] \quad (2.13)$$

corresponding to the linear intercepts $\mu(n, m; \varepsilon)$ can be tried (Stanley, 1967, 1968a). Values of (2.12) and (2.13) when $m = n - 2$ and $\varepsilon = 0, \frac{1}{2}$ for the series (1.1) are presented in Table 1. From the last few mean values, we estimate

$$\mu = 1/w_c = 3.732 \pm 0.003, \quad (2.14)$$

$$\gamma = 1 + g = 1.75 \pm 0.03. \quad (2.15)$$

As explained in Section I.A, the uncertainties are obtained by a subjective assessment of the convergence rate. A comparison of (2.14) with the exact result (2.10) shows that our estimate of the critical point is rather accurate, and that the error estimates are on the conservative side. Similarly, (2.15) fits in well with the rigorous result $\gamma = 1\frac{1}{4}$ (Fisher 1959a; Kadanoff, 1966; Wu, 1966; Cheng and Wu, 1967).

In view of the above success, one has more confidence in applying the method to the three-dimensional lattices. Certainly in the case of the high temperature susceptibility expansion for the three-dimensional spherical model, for which up to 100 coefficients are known, predictions based upon the above procedures are in good agreement with the exact results (Stanley,

1968b). For the Ising model, the normalized ratios, μ_n/q , of the high temperature susceptibility expansion for the face-centred cubic lattice are plotted versus $1/n$ in Fig. 1 for $n \leq 12$ (Domb and Sykes, 1961; Sykes *et al.*, 1972b). As first demonstrated by Domb and Sykes (1957), the ratios appear to settle down just as fast as those for the triangular lattice. Indeed, working with only the first 8 coefficients, Domb and Sykes were able to make an accurate estimate of w_c , and also suggested $\gamma \approx 1.250$.

TABLE I

Estimation of the critical point $\mu = 1/w_c$ and critical exponent $\gamma = 1 + g$ for the triangular lattice from the Ising susceptibility series, $\chi(w)$.†

| n | $\mu(n, n-2; 0)$ | $\mu(n, n-2; \frac{1}{2})$ | $g(n, n-2; 0)$ | $g(n, n-2; \frac{1}{2})$ | $g_n(0)$ | μ_n^* |
|-----|------------------|----------------------------|----------------|--------------------------|----------|-----------|
| 3 | 3.90000 | 3.55000 | 0.5385 | 1.0352 | 0.6977 | 3.68000 |
| 4 | 3.78261 | 3.63043 | 0.6437 | 0.9431 | 0.7066 | 3.69794 |
| 5 | 3.76832 | 3.68515 | 0.6621 | 0.8689 | 0.7171 | 3.71072 |
| 6 | 3.76728 | 3.71528 | 0.6626 | 0.8188 | 0.7255 | 3.71848 |
| 7 | 3.75293 | 3.71618 | 0.6853 | 0.8157 | 0.7283 | 3.72161 |
| 8 | 3.74141 | 3.71379 | 0.7086 | 0.8217 | 0.7305 | 3.72372 |
| 9 | 3.74013 | 3.71900 | 0.7116 | 0.8094 | 0.7326 | 3.72541 |
| 10 | 3.73946 | 3.72279 | 0.7132 | 0.7992 | 0.7344 | 3.72665 |
| 11 | 3.73807 | 3.72453 | 0.7170 | 0.7941 | 0.7359 | 3.72756 |
| 12 | 3.73689 | 3.72568 | 0.7205 | 0.7905 | 0.7370 | 3.72826 |
| 13 | 3.73609 | 3.72665 | 0.7232 | 0.7871 | 0.7380 | 3.72880 |
| 14 | 3.73550 | 3.72743 | 0.7253 | 0.7842 | 0.7389 | 3.72924 |
| 15 | 3.73502 | 3.72806 | 0.7271 | 0.7817 | 0.7396 | 3.72959 |
| 16 | 3.73464 | 3.72857 | 0.7287 | 0.7795 | 0.7403 | 3.72989 |

† See equations (2.12), (2.13), (2.20) and (2.22).

B. Neville tables

We have been led to consider sequences of one sort or another, and in estimating their limits as $n \rightarrow \infty$ it is sometimes useful to construct a Neville table (Hartree, 1952). A Neville table for an arbitrary sequence $\{e_n^0\}$ is a triangular array of elements e_n^r , where n labels the rows and $r = 0, 1, 2, \dots, n$, the columns. The elements of the r th column are generated from the $(r-1)$ th by

$$e_n^r = [ne_n^{r-1} - (n-r)e_{n-1}^{r-1}]/r. \quad (2.16)$$

If the sequence $\{e_n^0\}$ is considered as a function of $1/n$, the element e_n^r is simply the intercept on the $1/n = 0$ axis of the r th degree curve through the

$(r + 1)$ successive points $e_n^0, e_{n-1}^0, \dots, e_{n-r}^0$. Hence, $r = 1$ corresponds to the linear intercepts, $r = 2$ to the quadratic intercepts, $r = 3$ to the cubic intercepts, and so on. Neville tables are particularly useful when the $1/n$ plot of the initial sequence has a steady curvature, since the various sequences allow for curvature of successively higher degree. For example (Jasnow and Wortis, 1968), if

$$e_n^0 = e \left(1 + \frac{a}{n} + \frac{b}{n^2} \right)$$

for all n , then the sequences $\{e_n^2\}, \{e_n^3\}, \dots$ would all be constant and equal to e , while the sequences $\{e_n^1\}$ would monotonically approach the limit e . More generally, however, care is required, since the later columns of a Neville table tend to magnify any small irregularities in the initial sequence.

In a typical example, the initial sequence $\{e_n^0\}$ might be the slopes $g(n, m; \epsilon)$ given by (2.13), or it might be the ratios of coefficients, μ_n . In the latter case, the first column ($r = 1$) would then coincide with the sequence $\mu(n, n - 1)$ given by (2.11). For loose-packed lattices, Bowers and Woolf (1969) have replaced (2.16) by

$$e_n^r = [ne_n^{r-1} - (n - 2r)e_{n-2}^{r-1}]/2r \quad (2.17)$$

which for $r = 1$ is identical to $\mu(n, n - 2)$. Although it is usually unnecessary to resort to complete Neville tables for the simple Ising model, they have proved of great utility in the study of the Heisenberg model (Rushbrooke and Wood, 1958; Baker *et al.*, 1967; Jasnow and Wortis, 1968; Bowers and Woolf, 1969; Rushbrooke *et al.*, this volume, Chapter 5).

C. Refined estimates

Given the exact value of μ , or an estimated value μ' , one may form the sequence of approximations (Domb and Sykes, 1957)

$$g_n \equiv n \left(\frac{\mu_n}{\mu'} - 1 \right). \quad (2.18)$$

According to (2.8),

$$g_n \approx g \left[1 + O\left(\frac{1}{n}\right) \right], \quad (n \rightarrow \infty), \quad (2.19)$$

so that g_n should approach g linearly against $1/n$, provided μ' is sufficiently accurate. In analogy with (2.13), a modified version of (2.18), namely

$$g_n(\epsilon) = (n + \epsilon) \left(\frac{\mu_n}{\mu'} - 1 \right), \quad (2.20)$$

is sometimes used (e.g. Gaunt *et al.*, 1964).

Values of $g_n(0)$ for the series (1.1), calculated using the exact critical point (2.10), will be found in Table I. For $n \geq 5$ they increase quite linearly with $1/n$; from the last six linear intercepts from adjacent points, all of which round to 0.750, we conclude that

$$\gamma = 1 + g = 1.750 \pm 0.001. \quad (2.21)$$

This represents a tremendous improvement in accuracy over the preliminary estimate (2.15).

If one has the exact value of g , or a good estimate g' , one may usually obtain a more rapidly convergent sequence of estimates for μ from the sequence (Domb and Sykes, 1961)

$$\mu_n^* \equiv \frac{n\mu_n}{n + g'} \approx \mu \left[1 + O\left(\frac{1}{n^2}\right) \right], \quad (n \rightarrow \infty). \quad (2.22)$$

Since the leading correction term is of $O(1/n^2)$, the limit μ should be

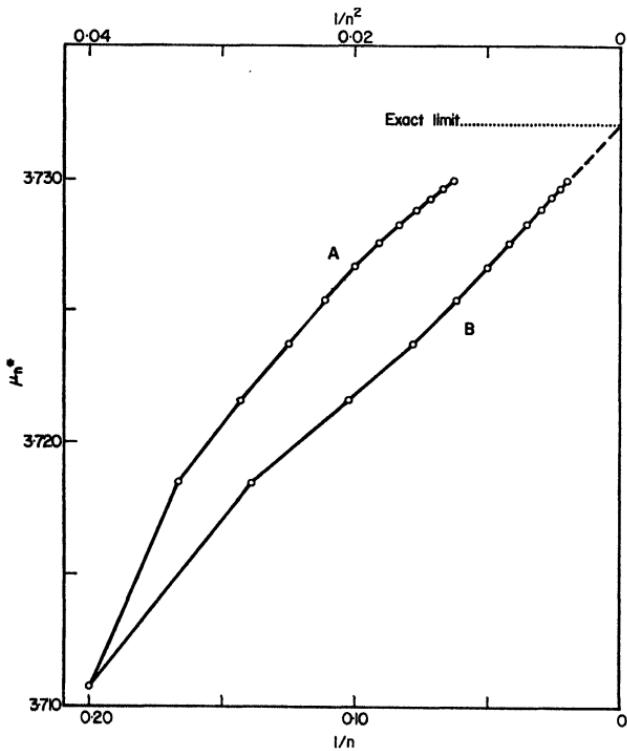


FIG. 2. Refined critical point estimates $\mu_n^* \equiv n\mu_n/(n + \frac{1}{4})$ for the triangular $I(\frac{3}{4})$ lattice plotted versus $1/n$ (A) and $1/n^2$ (B).

approached horizontally versus $1/n$. Even if g' differs somewhat from g this will only affect the convergence through a term $(g - g')/n$.

The sequence μ_n^* is tabulated in Table 1 for the series (1.1) using $g' = 0.75$. A plot versus $1/n$ is shown in Fig. 2 and is consistent with a horizontal approach (as $n \rightarrow \infty$) to the exactly known limit.

If μ and g are known accurately, the amplitude of the singularity may be estimated [see (2.1) and (2.4)] from the sequence (e.g. Sykes and Fisher, 1962; Sykes *et al.*, 1967)

$$A_n = \frac{a_n}{\binom{g+n}{n} \mu^n}. \quad (2.23)$$

Equations (2.1) and (2.5) suggest the alternative sequence

$$A'_n = \frac{a_n \Gamma(g+1)}{n^g \mu^n}, \quad (2.24)$$

but this is not usually very satisfactory. For example, values of A_n and A'_n for the series (1.1), calculated using $g = \frac{3}{4}$ and the exact critical point (2.10), are as follows:

| n | A_n | A'_n |
|-----|--------|--------|
| 10 | 0.8593 | 0.9152 |
| 11 | 0.8583 | 0.9091 |
| 12 | 0.8574 | 0.9039 |
| 13 | 0.8566 | 0.8996 |
| 14 | 0.8560 | 0.8959 |
| 15 | 0.8554 | 0.8926 |
| 16 | 0.8549 | 0.8898 |

The sequence A_n appears to be converging much more rapidly than the sequence A'_n , and extrapolation versus $1/n$ yields

$$A = 0.8472 \pm 0.0002 \quad (2.25)$$

in excellent agreement with other estimates (Sykes and Fisher, 1962; Sykes *et al.*, 1972a). More generally, however, small errors in μ and g are magnified in estimating the amplitude A , so that rather lower accuracy is obtained than in the above case.

D. Loose-packed lattices

The triangular and face-centred cubic lattices are examples of "close-packed" lattices, i.e. they cannot be decomposed into two equivalent sublattices. A new feature arises when the procedure we have just outlined is applied to the loose-packed Ising lattices in either two or three dimensions. For example, the ratios μ_n for the $\chi(w)$ expansion of the plane square and simple cubic lattices (Sykes and Fisher, 1962; Fisher and Sykes, 1962; Sykes *et al.*, 1972a, b) are plotted versus $1/n$ in Fig. 3. The variation is again quite linear *but with a*

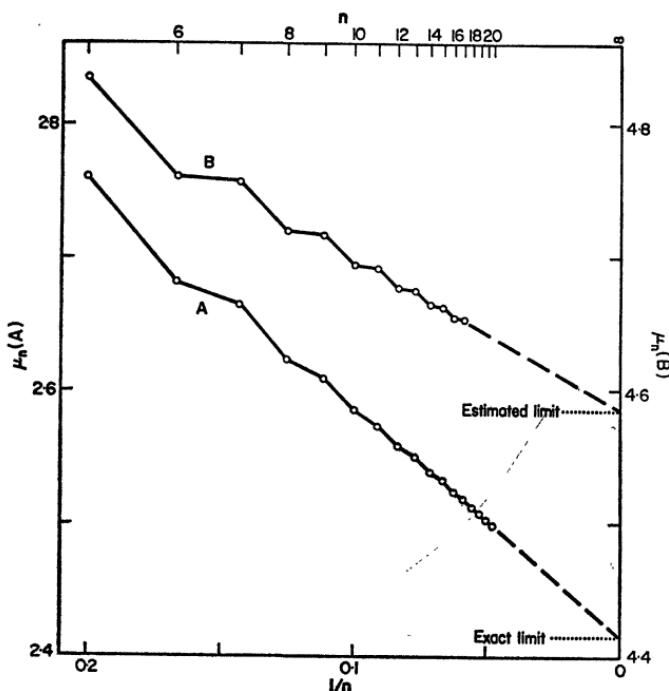


FIG. 3. Successive ratios μ_n of the coefficients of the $I(\frac{1}{2})$ susceptibility expansions of the square (A) and simple cubic (B) lattices plotted versus $1/n$.

superimposed oscillation, characteristic of loose-packed lattices (Domb and Sykes, 1957), and caused by the presence of an antiferromagnetic singularity at $v = -v_c$. [This may be seen by setting $\theta = \pi$ in (2.9).]

The oscillations can be reduced, but not eliminated, by plotting the quantities

$$\rho_n = (a_n/a_{n-2})^{\frac{1}{2}} \approx \mu \left(1 + \frac{g}{n} \right), \quad (n \rightarrow \infty), \quad (2.26)$$

rather than μ_n . (The reason for this will become clear in Section VI.C.) Thus, the approach and formulae used for the close-packed lattices can be tried, but with ρ_n replacing μ_n (Stanley, 1967):

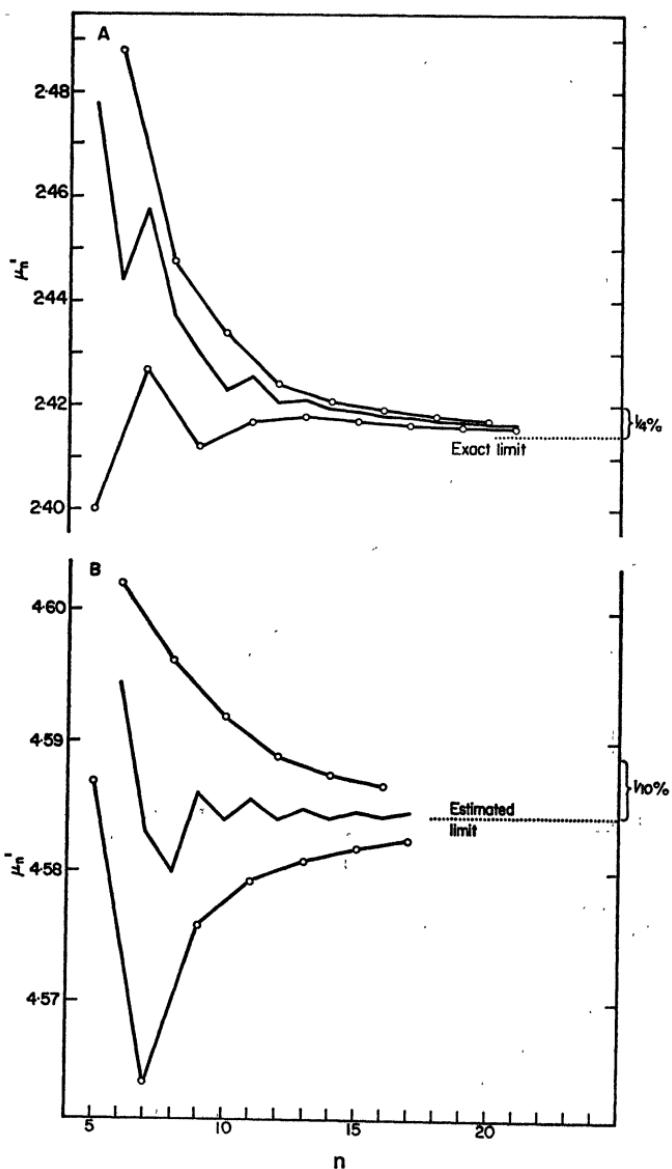


FIG. 4. Preliminary critical point estimates $\mu'_n \equiv \mu(n, n - 2; 0)$ and their successive arithmetic means $\bar{\mu}_n = \frac{1}{2}(\mu'_n + \mu'_{n-1})$ for the square (A) and simple cubic (B) $I(1)$ lattices plotted versus n .

Alternatively, and more usually, one extrapolates either the even and odd ratios separately, or their successive arithmetic means (Domb and Sykes, 1961). It then transpires that despite the odd/even oscillations, the accuracy of the final critical point parameters are comparable to those achieved for the close-packed lattices. In summary, then, estimates of μ derived from expansions of $\chi(w)$ by using the ratio method are believed to be in error by

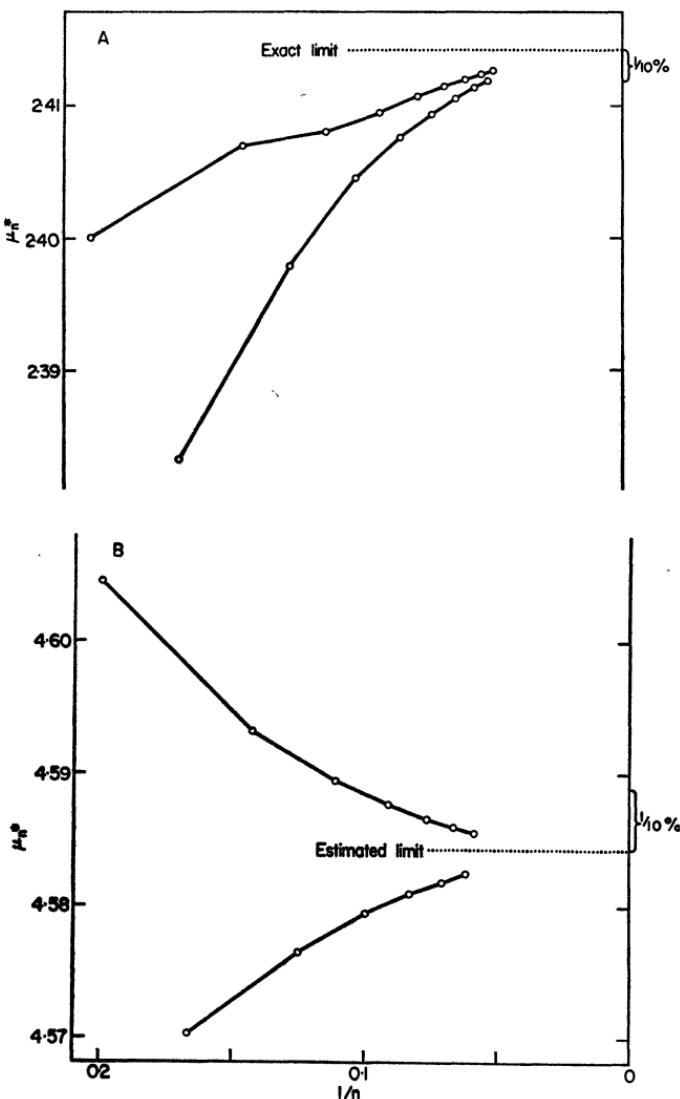


FIG. 5. Refined critical point estimates $\mu_n^* = n\mu_n/(n + g)$ for the square (A) and simple cubic (B) $I(\frac{1}{2})$ lattices plotted versus $1/n$. (Square, $g = \frac{1}{4}$; simple cubic, $g = \frac{1}{3}$.)

no more than a few parts in 10^4 for *all* lattices, and this expectation is confirmed explicitly in two dimensions by the exact results (see Domb, 1960). Similarly, estimates of γ appear to be accurate to within a few parts in 10^3 , and suggest the conjectures $\gamma = 1\frac{3}{4}$ in two dimensions and $\gamma = 1\frac{1}{4}$ in three dimensions, *irrespective of lattice structure*. The former conjecture is strongly supported by arguments at first semi-rigorous but later made rigorous (Fisher, 1959a; Kadanoff, 1966; Wu, 1966; Cheng and Wu, 1967; Abraham, 1973), while the latter conjecture, even if it should turn out not to be quite correct, is obviously an excellent representation for most practical purposes. These striking results for the lattice-independence of the exponent γ also seem very reasonable from a physical view-point, especially when one remembers the exact results $\alpha' = \alpha = 0$ (logarithm) and $\beta = \frac{1}{8}$ for *all* two-dimensional Ising lattices (e.g. Domb, 1960). They might be considered, therefore, as further indirect evidence in support of our extrapolation procedures.

To substantiate the above claims for the loose-packed lattices, we present a few examples. Thus, following Domb and Sykes (1961), the two branches of $\mu'_n \equiv \mu(n, n - 2; 0)$ corresponding to odd and even values of n are plotted versus n in Figs 4A and 4B for the square and simple cubic lattices, respectively. Their successive arithmetic means $\overline{\mu'_n} \equiv \frac{1}{2}(\mu'_n + \mu'_{n-1})$ are also shown. For the square lattice, one sees that the exact limit $\mu = 1 + \sqrt{2}$ (Onsager, 1944) is approached quite regularly for $n \geq 9$. The extrapolated limit for the simple cubic lattice also appears to be rather accurate. However, as before, the most accurate estimates of μ are based upon (2.22), with $g' = \frac{3}{4}$ or $\frac{1}{4}$ for two or three dimensions, respectively. Accordingly, values of μ_n^* are plotted versus $1/n$ in Figs 5A and 5B for the square and simple cubic lattices, respectively, whilst values of $\overline{\mu_n^*} \equiv \frac{1}{2}(\mu_n^* + \mu_{n-1}^*)$ are listed in Table II. The behaviour is apparently more regular for the simple cubic lattice than it is for the square lattice, and enables us to estimate

$$\mu = 4.5842 \pm 0.0002, (w_c = \mu^{-1} = 0.21814 \pm 0.00001). \quad (2.27)$$

Alternatively, given a good estimate μ' of μ , the exponent γ may be estimated from the sequence $\gamma_n(\varepsilon) \equiv 1 + g_n(\varepsilon)$, defined by (2.20), or from their successive means $\overline{\gamma_n(\varepsilon)} \equiv \frac{1}{2}[\gamma_n(\varepsilon) + \gamma_{n-1}(\varepsilon)]$. These sequences have been calculated for the simple cubic lattice using $\varepsilon = 0$ and the central value in (2.27), and are presented in Table II. For comparison, corresponding results for the square lattice, calculated using $\varepsilon = \frac{1}{2}$ and the exact critical point, are also given. From these sequences alone one might estimate

$$\gamma = 1.751 \pm 0.002 \quad (2.28)$$

for the square lattice and

$$\gamma = 1.250 \pm 0.001 \quad (2.29)$$

for the simple cubic lattice. In the latter case, however, the error limits in the final estimate of γ would have to be increased slightly owing to uncertainties in the value of μ .

TABLE II

Estimation of the critical point $\mu = 1/w_c$ and critical exponent γ for the square and simple cubic lattices from the Ising susceptibility series, $\chi(w)$.†

| Square | | | | Simple Cubic | | |
|--------|----------------------|-------------------------|------------------------------------|----------------------|---------------|--------------------------|
| n | $\overline{\mu_n}^*$ | $\gamma_n(\frac{1}{2})$ | $\overline{\gamma_n(\frac{1}{2})}$ | $\overline{\mu_n}^*$ | $\gamma_n(0)$ | $\overline{\gamma_n(0)}$ |
| 3 | 2.29091 | 1.8492 | 1.7279 | 4.52992 | 1.2721 | 1.2268 |
| 4 | 2.36959 | 1.6777 | 1.7635 | 4.58534 | 1.2232 | 1.2477 |
| 5 | 2.36959 | 1.7878 | 1.7327 | 4.57989 | 1.2732 | 1.2482 |
| 6 | 2.39163 | 1.7187 | 1.7532 | 4.58737 | 1.2310 | 1.2521 |
| 7 | 2.39511 | 1.7787 | 1.7487 | 4.58174 | 1.2643 | 1.2476 |
| 8 | 2.40245 | 1.7341 | 1.7564 | 4.58487 | 1.2362 | 1.2502 |
| 9 | 2.40296 | 1.7652 | 1.7496 | 4.58300 | 1.2607 | 1.2484 |
| 10 | 2.40630 | 1.7425 | 1.7538 | 4.58449 | 1.2395 | 1.2501 |
| 11 | 2.40706 | 1.7602 | 1.7514 | 4.58358 | 1.2585 | 1.2490 |
| 12 | 2.40859 | 1.7452 | 1.7527 | 4.58434 | 1.2415 | 1.2500 |
| 13 | 2.40919 | 1.7582 | 1.7517 | 4.58382 | 1.2570 | 1.2493 |
| 14 | 2.41007 | 1.7464 | 1.7523 | 4.58427 | 1.2428 | 1.2499 |
| 15 | 2.41046 | 1.7568 | 1.7516 | 4.58395 | 1.2560 | 1.2494 |
| 16 | 2.41105 | 1.7474 | 1.7521 | 4.58425 | 1.2439 | 1.2500 |
| 17 | 2.41131 | 1.7556 | 1.7515 | 4.58404 | 1.2553 | 1.2496 |
| 18 | 2.41171 | 1.7482 | 1.7519 | | | |
| 19 | 2.41190 | 1.7548 | 1.7515 | | | |
| 20 | 2.41218 | 1.7486 | 1.7517 | | | |
| 21 | 2.41233 | 1.7541 | 1.7514 | | | |

† See equations (2.20) and (2.22). Note that $\overline{\theta_n} \equiv \frac{1}{2}(\theta_n + \theta_{n-1})$.

E. Extrapolation formulae

Once estimates for μ , g and A are available, it is possible to construct a "representation" or "mimic" function for the numerical evaluation of $F(z)$. When the first N coefficients are known exactly, one writes (Domb and Sykes, 1957)

$$F(z) \simeq A/(1 - \mu z)^{1+g} + R_N(z), \quad (2.30)$$

with

$$R_N(z) = \sum_{n=0}^N \left[a_n - A \binom{g+n}{n} \mu^n \right] z^n. \quad (2.31)$$

The remainder $R_N(z)$ is usually regarded as a "correction polynomial", but could equally well be considered as a truncated series and then approximated

by a Padé approximant (see Section III). In either case, the expansion of the right-hand side of (2.30) will agree with the exact expansion of $F(z)$ through order z^N . Although the extrapolation formula (2.30) may be evaluated for all values of z , it will only be accurate when z is on or close to the positive real axis between $z = 0$ and $z = z_c$.

For some functions, the singularity is so weakly divergent that the correction polynomial makes a significant contribution to the total, even quite close to the singularity. Usually, this implies that sequences of estimates for the critical exponent converge rather slowly. For example, a convincing ratio analysis of the high temperature specific heat of the three-dimensional Ising model was only achieved (Sykes *et al.*, 1967) after the series for the face-centred cubic lattice had been extended through order K^{12} . It was then found that the singular behaviour can be closely represented by

$$C_H/k \approx 1.091 \left(1 - \frac{T_c}{T}\right)^{-\alpha} - 1.244, \quad (T \rightarrow T_c +), \quad (2.32)$$

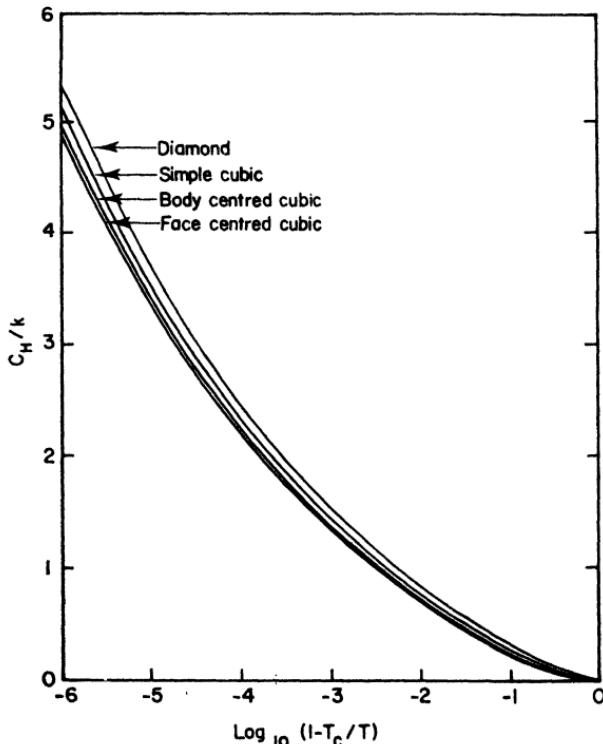


FIG. 6. Specific heat ($T > T_c$) of $I(\frac{1}{2})$ for various three-dimensional lattices as calculated from appropriate mimic functions. (From Hunter, 1967.)

with $\alpha = \frac{1}{8}$. (The series for other three-dimensional lattices are consistent with the hypothesis that α is independent of lattice structure.) The constant term in (2.32) is obtained by evaluating the appropriate correction polynomial at T_c . Notice that even when

$$\left(1 - \frac{T_c}{T}\right) = 10^{-4},$$

the divergent term is less than three times the size of the constant term. [In two dimensions, the specific heat singularity is even weaker ($\alpha = 0$, corresponding to a logarithm) and convergence is again very slow (Domb, 1965).] Finally, evaluation of the complete mimic functions for temperatures T between $T = \infty$ and $(1 - T_c/T) = 10^{-6}$, reveals [see Fig. 6, after Hunter (1967)] the relative insensitivity of the specific heat to changes in lattice structure for a given dimension.

Sometimes, more complicated forms for the remainder seem desirable. For example, for the zero-field specific heat of the Ising model below T_c , Gaunt and Domb (1968) used the representation

$$C_H/4kK^2 \simeq 3.1 \left(1 - \frac{u}{u_c}\right)^{-1/8} - 39.68 \left(1 - \frac{u}{u_c}\right)^{7/8} + R_{12} \left(\frac{u}{u_c}\right), \quad (2.33)$$

for the diamond lattice. The polynomial, R_{12} , is chosen so that the expansion of the right-hand side of (2.33) agrees with the exact expansion through order u^{12} . The second term in (2.33), representing a weaker coincident singularity, was suggested by the approximately linear variation with $1/n$ of the sequence A_n given by (2.23).

If the series coefficients are particularly well-behaved they can be analysed in even greater detail, and then more elaborate representations can be justified. Thus, Sykes and Fisher (1962) "subtracted-off" the dominant ferromagnetic singularity from the $\chi(w)$ expansion by writing for the square Ising lattice, for example,

$$\ln \chi(w) = -\gamma \ln(1 - 2w - w^2) + \ln \phi(w). \quad (2.34)$$

Here, $\gamma = 1\frac{1}{4}$ and the quadratic expression (which is characteristic of the theory for the square Ising lattice), contains a factor

$$\left(1 - \frac{w}{w_c}\right).$$

The series for $\phi(w)$ has coefficients which alternate in sign indicating that the dominant singularity is now on the negative real axis at the antiferromagnetic critical point $w = -w_c$. Regarding $\phi(w)$ as the basic series and re-analysing yields the representation

$$\phi(w) \simeq (D/t)(1+t)\ln(1+t) + \psi(t), \quad (t = w/w_c), \quad (2.35)$$

where $\psi(t)$ is a correction polynomial and D is a known amplitude. This result is very satisfactory since it is supported by various independent theoretical arguments (Sykes and Fisher, 1958; Fisher, 1962). From (2.34), we get

$$\chi(w) \simeq (1 - 2w - w^2)^{-\gamma} \phi(w) \quad (2.36)$$

with $\phi(w)$ given by (2.35), as the final representation valid in both the ferromagnetic and antiferromagnetic regions. The numerical evaluation of (2.36) for the antiferromagnet has been undertaken by Sykes and Fisher (1962) who worked with $\log \phi$ in place of ϕ . Analogous results have been derived for other loose-packed lattices (Sykes and Fisher, 1962; Fisher and Sykes, 1962). The above procedure was first used by Sykes and Zucker (1961) to study the antiferromagnetic susceptibilities of the triangular and kagomé lattices (which have no antiferromagnetic transition). For recent developments, see Section VI, Sykes *et al.* (1972a, b), and Domb, this volume, Chapter 6.

III. Padé Approximants

A. Background

The main short-coming of the ratio method is that in most cases it can deal with only one singularity at a time, and then only if this singularity lies on the real axis and is dominant. Of course, if the nature of the dominant singularity can be determined accurately enough, it may be subtracted-off as was done in Section II.E. Then the next-most dominant singularity (provided it too lies on the real axis) can be studied by a further application of the ratio method, and so on—in principle, at least.

Padé approximants (Padé, 1892; Wall, 1948), on the other hand, enable several singularities lying anywhere in the complex z -plane to be studied simultaneously, in a systematic manner and without reference to a particular functional form. In effect, they provide a method of approximately analytically continuing a function beyond its radius of convergence and up to the physical singularity, or beyond. For these reasons, the Padé method has been particularly successful in analysing series like (1.13), which had proved quite intractable by other methods. It can also, of course, be applied to series of all positive terms.

Padé approximants were introduced into physics by Baker and Gammel (1961) and Baker *et al.* (1961), and first applied to critical phenomena by Baker (1961). We begin our discussion by summarising, in the next subsection, some of the most important general results concerning Padé approximants. For a thorough treatment, the reader is referred to the excellent reviews by Baker (1965, 1970).

B. Theory

The $[L, M]$ Padé approximant to a function $F(z)$ is the ratio of a polynomial $P_L(z)$ of degree L to a polynomial $Q_M(z)$ of degree M ,

$$[L, M] \equiv \frac{P_L(z)}{Q_M(z)} = \frac{p_0 + p_1 z + p_2 z^2 + \dots + p_L z^L}{1 + q_1 z + q_2 z^2 + \dots + q_M z^M}. \quad (3.1)$$

The coefficients $p_0, p_1, p_2, \dots, p_L$ and q_1, q_2, \dots, q_M are chosen so that the expansion of $[L, M]$ agrees with the expansion of $F(z)$ through order $L + M$, i.e.

$$F(z) = [L, M] + O(z^{L+M+1}). \quad (3.2)$$

As shown in Baker (1965), the coefficients so chosen are unique. Although various recursive schemes for generating Padé approximants have been discussed (Baker, 1970), the direct method is often used. Thus, equating the coefficients of z^{L+1} through z^{L+M} in (3.2) gives M simultaneous linear equations for q_1 to q_M . Substituting their solution into the $(L + 1)$ linear equations obtained by equating the coefficients of z^0 through z^L in (3.2), then yields the coefficients p_0 to p_L . In practice, the solution of the corresponding matrix equations is carried out by computer, and involves the inversion of matrices. Care must be taken if low accuracy is to be avoided, since the set of equations is often "ill-conditioned". If one of the matrices is singular, the corresponding approximant does not exist.

We mention that Padé approximants can be generalized to include information about $F(z)$ at two (or more) points. This is done by modifying the linear equations which determined the coefficients of $P_L(z)$ and $Q_M(z)$, in such a way that the conditions at the other point (or points) are satisfied in addition to the conditions at $z = 0$. Unfortunately, the technique seems to have been little used or studied (Baker *et al.*, 1964; Baker, 1965; Isenberg, 1966; Gaunt and Domb, 1970), so we will not discuss it further.

If the series expansion of $F(z)$ is known through order z^N , the calculable

approximants can be arranged in a Padé table (Padé, 1892) as follows:

| | | | | | | | | |
|------------|------------|--------|---|---|---|---|------------|--------|
| [0, 0] | [1, 0] | [2, 0] | . | . | . | . | . | [N, 0] |
| [0, 1] | [1, 1] | [2, 1] | . | . | . | . | [N - 1, 1] | |
| [0, 2] | [1, 2] | [2, 2] | . | . | . | . | | |
| . | . | . | . | . | . | . | | |
| [0, N - 1] | [1, N - 1] | | | | | | | |
| [0, N] | | | | | | | | |

Note that the first row, or $[n, 0]$ sequence of approximants, simply corresponds to truncating $F(z)$ after the term of order z^n and that the poles of the $[n, 1]$ sequence in the second row are given by the ratios $a_n/a_{n+1} (= 1/\mu_{n+1})$. Some further features of the approximants along rows will be discussed in Section IV.

In general, relatively little is known about the domain and manner of convergence of Padé approximants, although several rigorous results have been proved [see Baker (1965, 1970)] for the class of functions called series of Stieltjes (Wall, 1948). By definition

$$F(z) = \sum_{r=0}^{\infty} f_r (-z)^r \quad (3.3)$$

is a series of Stieltjes, if and only if there is a bounded, non-decreasing function $\phi(w)$ taking on infinitely many values in the interval $0 \leq u < \infty$ such that

$$f_r = \int_0^{\infty} w^r d\phi(w). \quad (3.4)$$

For example, it can be shown that the $[n, n]$ and $[n - 1, n]$ Padé approximant sequences form rigorous upper and lower bounds to $F(z)$ for real positive z , and increasing n improves the bounds, which thus converge monotonically. Baker (1964, 1965) has shown how a function whose real part has a known lower bound in some region of the complex plane, and whose imaginary part satisfies a certain condition can always be converted into a series of Stieltjes. Unfortunately, as Fisher (1967) points out, such knowledge is not in general available and it may be dangerous to assume it without good evidence (Baker, 1964).

Recently, Baker (1967, 1970) has generalized Padé approximants in such a way that converging upper and lower bounds can be established for a wider class of functions than a series of Stieltjes. These generalized approxi-

mants have already proved applicable to several thermodynamic properties of the ferromagnetic Ising model (Baker, 1967).

Returning now to more general functions, it can be proved (Baker, 1965) that the diagonal $[n, n]$ approximants are invariant under the group of Euler transformations $z = aw/(1 + bw)$, which are often used to increase the rate of convergence of a series. Hence, the sequence of $[n, n]$ approximants are expected to converge at least as rapidly as the series obtained by the best Euler transformation. This is also true of any near-diagonal sequence $[n + j, n]$, since this can be reduced (Baker, 1965) to the study of the $[n, n]$ sequence for the function

$$f(z) = z^{-j} F(z) \quad (3.5)$$

if $j \leq 0$, or

$$f(z) = \left[F(z) - \sum_{n=0}^{j-1} a_n z^n \right] / z^j \quad (3.6)$$

if $j > 0$. If the behaviour of $F(z)$ at ∞ is not known, all near-diagonal sequences are *a priori* just as good. However, if $F(z) \approx z^j$ as $z \rightarrow \infty$, then the sequence of $[n + j, n]$ approximants should be considered for optimal results.

Usually the domain of convergence greatly exceeds the circle of convergence of the corresponding power series. To be specific, consider as an example a function $F(z)$ which has p poles inside its circle of meromorphy. [The circle of meromorphy is the largest circle such that all non-regular points within it are at most poles or multiple poles of $F(z)$.] Although the pole closest to the origin determines the radius of convergence, it can be rigorously proved that the $[L, M]$ sequence with $M \geq p$ converges uniformly to $F(z)$ as $L \rightarrow \infty$ everywhere inside the circle of meromorphy, except at points within small circles centred on the p poles. [See Baker *et al.*, (1961).] Throughout this region the rate of convergence is normally extremely rapid. Numerical experiments on various known functions show that convergence in the vicinity of the nearer poles is still very fast even when $M < p$. Similar results are found for diagonal and near-diagonal sequences.

Basically, the above results pertaining to the circle of meromorphy of $F(z)$ stem from the fact that poles can be represented exactly by Padé approximants. Branch point singularities, on the other hand, cannot be so represented. If $F(z)$ possesses branch point singularities, the zeros and poles of the Padé approximants begin defining a set of branch cuts, the locations of which cannot always be predicted but are usually the "obvious" choices in simple examples (Baker *et al.*, 1961; Baker, 1965). As the order of the approximants increases, the zeros and poles close up and in the limit densely populate the selected cuts. In this way, the Padé approximants (which are of

course single-valued functions of z) choose a particular branch of the many-valued function $F(z)$ and simulate the discontinuity that occurs on crossing the cut. Although convergence in the cut plane is slow near the branch cuts, particularly when the discontinuity is small, this does not prohibit rapid convergence in other regions, possibly far outside the circle of convergence of $F(z)$.

In practice, it is found that the manner of convergence is usually rather "noisy", especially for functions having several singularities. For example, increasing the order of the approximant does not necessarily improve the approximation close to the singularity of interest. Indeed, the accuracy there may actually fall as a result of increased accuracy near some more distant singularities. (In contrast, the ratio method, when it is applicable, uses extra terms to focus more and more attention on the nearest singularity.) As a second example of irregular convergence, we mention the "spurious" poles which may suddenly appear in some Padé approximants in regions close to the origin where $F(z)$ is known to be analytic. A spurious pole may be recognized by its very small residue, caused by the Padé approximant possessing an almost coincident zero. Approximants containing such pole-zero pairs are sometimes deleted from the Padé table.

Despite these unexplained features, it appears that as $n \rightarrow \infty$ at least a sub-sequence of the diagonal $[n, n]$ or near-diagonal $[n + j, n]$ approximants will converge to $F(z)$ everywhere in the complex plane, except at the singularities and on the branch cuts (Baker, 1965). As already discussed, the rate of convergence is usually very fast within the circle of meromorphy, but rather slower near the branch cuts especially if the discontinuity is small.

C. Padé method

Let us now apply the above ideas to the series for a function $F(z)$ given by

$$F(z) \approx \left(1 - \frac{z}{z_c}\right)^{-\lambda} A(z), \quad (z \rightarrow z_c^-). \quad (3.7)$$

If $A(z)$ is analytic at $z = z_c = 1/\mu$, then

$$F(z) \approx A(1 - \mu z)^{-\lambda} [1 + O(1 - \mu z)], \quad (3.8)$$

where $A = A(z_c)$ and to make precise contact with (2.6), we must write $\lambda = 1 + g$. It follows that the logarithmic derivative

$$D(z) \equiv \frac{d}{dz} \ln F(z) \approx \frac{-\lambda}{(z - z_c)} [1 + O(z - z_c)], \quad (z \rightarrow z_c), \quad (3.9)$$

has only a simple pole at z_c (Baker, 1961). Since Padé approximants can

represent simple poles exactly, approximants to the $D(z)$ series should converge much faster than approximants to the $F(z)$ series. If an approximant has a pole in the vicinity of z_c , its location will give an estimate of z_c , while the corresponding residue will be an estimate of $-\lambda$.

We mention, in passing, that the series for the logarithmic derivative of a function has been useful in other contexts (Essam and Sykes, 1963; Gaunt, 1967; Jasnow and Wortis, 1968), particularly when z_c is exactly unity since each coefficient is then an estimate of the exponent λ .

If the exact value or a good estimate of λ is available, the appropriate poles of the approximants to the series for

$$[F(z)]^{1/\lambda} \approx -\frac{z_c A^{1/\lambda}}{(z - z_c)} [1 + O(z - z_c)], \quad (z \rightarrow z_c), \quad (3.10)$$

should give a more rapidly convergent sequence of estimates for z_c (Baker, 1961). In addition, the corresponding residues yield estimates of $-z_c A^{1/\lambda}$, and hence of the amplitude A . Some workers (Baker, 1961; Gammel *et al.*, 1963; Essam and Fisher, 1963) have based their final extrapolation formula for $F(z)$ on one of the higher order approximants to this series.

Conversely, if the exact value or a good estimate of z_c is known, a better estimate of the critical exponent should be obtained by forming Padé approximants to the series

$$\lambda^*(z) \equiv (z_c - z) D(z) \approx \lambda + O(z - z_c), \quad (z \rightarrow z_c), \quad (3.11)$$

and evaluating them at $z = z_c$, where $\lambda^*(z)$ is analytic (Baker, 1961). Alternatively, and particularly if z_c is known only with moderate accuracy, the series for

$$\frac{d}{dz} \ln \frac{dF}{dz} / \frac{d}{dz} \ln F \approx \frac{\lambda + 1}{\lambda} + O(z - z_c), \quad (z \rightarrow z_c), \quad (3.12)$$

may be more useful (Baker *et al.*, 1967). Notice that the calculation of this series does not involve z_c . Thus, Padé approximants evaluated at z_c should provide estimates of λ , which one might hope to be relatively insensitive to the precise choice of z_c .

If both z_c and λ are known accurately enough, better estimates of A can be obtained (Essam and Fisher, 1963) by forming Padé approximants to the series for

$$(z_c - z) [F(z)]^{1/\lambda} \approx z_c A^{1/\lambda} + O(z - z_c), \quad (z \rightarrow z_c), \quad (3.13)$$

evaluating them at z_c , and raising the result to the power λ . In addition, one of the higher order approximants should provide an excellent extrapolation

formula for $F(z)$ over the entire range from $z = 0$ to z_c (Essam and Fisher, 1963).

Notice that according to (3.9), an error in the location of z_c leads to a first order error in λ . On the other hand, when $F(z)$ has the simple form (3.8), the more general function

$$D_p(z) \equiv \left[\left(\frac{d}{dz} \right)^p \ln F(z) \right]^{1/p}, \quad (p = 1, 2, 3, \dots), \quad (3.14)$$

behaves like

$$D_p(z) \approx - \frac{[(p-1)! \lambda]^{1/p}}{(z - z_c)} [1 + O(z - z_c)^p], \quad (z \rightarrow z_c), \quad (3.15)$$

so that an error in z_c gives only a p th order error in λ . [When $p = 1$, (3.15) coincides with (3.9).] Hence, Padé approximants to the $D_p(z)$ series should converge better for $p > 1$ than for $p = 1$. However, since each differentiation 'loses' a term, only small values of p are used in practice. To reduce the risk of being misled, only results which are consistent for different values of p are accepted.

The roots and residues of approximants to $D_p(z)$ provide estimates of both z_c and λ . When z_c is given, the appropriate generalization of (3.11) for functions of the form (3.8) is

$$\lambda_p^*(z) \equiv (z_c - z) D_p(z) \approx [(p-1)! \lambda]^{1/p} + O(z - z_c)^p, \quad (z \rightarrow z_c), \quad (3.16)$$

while if λ is known, (3.10) becomes

$$\begin{aligned} \left\{ \left(\frac{d}{dz} \right)^{p-1} [F(z)]^{1/\lambda} \right\}^{1/p} &\approx - \frac{[(p-1)! A^{1/\lambda} z_c]^{1/p}}{(z - z_c)} \\ &\times [1 + O(z - z_c)^p], \quad (z \rightarrow z_c). \end{aligned} \quad (3.17)$$

In both cases, the correction term is again of order p . Evaluating Padé approximants to (3.16) at z_c gives estimates of λ , while estimates of z_c and A are obtained from the approximants to (3.17).

This generalization ($p > 1$) of the usual Padé method ($p = 1$) was developed by Bowers and Woolf (1969) and used by them to study the critical properties of the Heisenberg model. [Padé approximants to the $D_2(z)$ series were also employed by Gammel *et al.* (1963), again for the Heisenberg model.] No further details will be given here, since the method has not, as yet, been used more widely.

We have assumed so far that $F(z)$ has simply a factorizable algebraic branch point as $z \rightarrow z_c^-$. However, most of the above procedures often seem

to work quite well for a wider class of functions; for example, for

$$F(z) \approx \left(1 - \frac{z}{z_c}\right)^{-\lambda} A(z) + B(z), \quad (z \rightarrow z_c^-) \quad (3.18)$$

where $A(z)$ and $B(z)$ are analytic at z_c , provided λ is large enough. $A(z)$ and $B(z)$ may even possess confluent (i.e. coincident) singularities at z_c , provided they are sufficiently weak compared with the dominant singularity. Of course, convergence will probably be less rapid in these cases. For example, if

$$F(z) \approx A(1 - \mu z)^{-\lambda} [1 + O(1 - \mu z)^v], \quad (z \rightarrow z_c^-),$$

where $v > 0$ and is non-integral, the correction terms to (3.15), (3.16) and (3.17) are of $O(1 - \mu z)^v$ for all values of p . Nevertheless, one might hope convergence would be especially rapid for some particular p . In summary, then, the Padé method can be expected to work reasonably well whenever $F(z)$ diverges strongly to infinity or converges strongly to zero at z_c . This appears to be the situation, for example, for the high temperature susceptibility series and the low temperature spontaneous magnetization series, respectively, of the ferromagnetic Ising model.

However, the approach may be considerably less effective when the dominant singularity is weak [for example, the high temperature specific heat of the three-dimensional Ising model (Hunter, 1969; Farrel and Meijer, 1969)], since then the coincident singularities are often of comparable strength, and/or $B(z)$ may easily be comparable in magnitude to the leading term in (3.18), except very close indeed to z_c . Even worse problems arise when $F(z)$ remains finite ($\lambda < 0$) at z_c [like the antiferromagnetic susceptibility of the Ising model in zero field (Sykes and Fisher, 1962; Fisher and Sykes, 1962)], or has a logarithmic singularity ($\lambda = 0$) there [like the zero field specific heat of the two-dimensional Ising model (Onsager, 1944)]. For example, if $F(z)$ were simply

$$F(z) = a + b(z_c - z)^\theta, \quad (\theta > 0), \quad (3.19)$$

or

$$F(z) = -a \ln(z_c - z) + b, \quad (3.20)$$

where a and b are constants, then taking the logarithmic derivative would not reduce the singularity in $F(z)$ to a simple pole. This difficulty is easily removed in such simple examples by working with the derivative function (dF/dz). In more complicated cases, however, when (3.19) and (3.20) are merely the asymptotic forms of $F(z)$ as $z \rightarrow z_c^-$, such devices are rarely successful and the convergence rate is often very slow.

If $F(z)$ has singularities at several points in the complex z -plane, the Padé method attempts to treat each of them in the above way. Thus, for example, if enough series coefficients are available, the location and exponent of every singularity may be approximated by an appropriate pole and residue of the higher-order approximants to $D(z)$. Note that if $F(z)$ is simply a product of algebraic factors, as it is for the spontaneous magnetisation of the two-dimensional Ising lattices [see (1.9) and (1.10), for example], then the Padé method will reduce all the singularities to simple poles and eventually yield the exact result. More generally, however, the convergence can be quite noisy, as was mentioned earlier. This is particularly true if the singularities are not well separated; their mutual interference may then slow down convergence quite considerably.

In spite of the above mentioned difficulties, the Padé approximant method is, in favourable circumstances, of great utility as we shall now demonstrate.

D. Applications

Let us begin, following Baker (1961), by trying the method on the high temperature susceptibility series $\chi(w)$ for the plane square and simple cubic lattices. Estimates of w_c and γ from the poles and residues of the $[n+j, n]$ approximants ($j = 0, \pm 1$) to the series for the logarithmic derivative $D(w) \equiv (d/dw) \ln \chi(w)$ are given in Tables III and IV. Several of the approximants exhibit intervening spurious poles with residues less than 10^{-3} , say. Here, and elsewhere, their presence is indicated by a superscript.

TABLE III

Estimation of the critical point w_c and critical exponent γ for the square Ising lattice from the poles and residues (in parentheses) of the $[n+j, n]$ Padé approximants to the $(d/dw) \ln \chi(w)$ series.

| n | $j = -1$ | $j = 0$ | $j = +1$ | |
|-----|-----------------------|------------|------------------------|------------|
| 1 | 0.500000 | (-2.00000) | 0.285714 | (-0.65306) |
| 2 | 0.388712 | (-1.40166) | 0.411186 | (-1.65456) |
| 3 | 0.408883 | (-1.61863) | 0.409268 | (-1.62573) |
| 4 | 0.408772 ^a | (-1.61708) | 0.416449 | (-1.79735) |
| 5 | 0.410190 | (-1.63832) | 0.412166 ^a | (-1.68234) |
| 6 | 0.414844 | (-1.77820) | 0.414125 | (-1.74584) |
| 7 | 0.4142492 | (-1.75151) | 0.4142106 | (-1.74964) |
| 8 | 0.4142141 | (-1.74983) | 0.4142133 | (-1.74978) |
| 9 | 0.4142127 | (-1.74975) | 0.4142136 ^a | (-1.74980) |
| 10 | 0.4142024 | (-1.74840) | 0.4142126 | (-1.74974) |

^a Approximant with an intervening spurious pole.

With the exception of the [9, 10] approximant, the accuracy of the last three estimates in each column for the square lattice is quite remarkable, differing from the exact result $w_c = \sqrt{2} - 1 = 0.4142135\dots$ and $\gamma = 1\frac{1}{4}$ by no more than 5×10^{-6} and 5×10^{-4} , respectively. Convergence for the simple cubic lattice seems almost as rapid. By visual inspection of the last few entries in each column, we conclude that

$$w_c = 0.218140 \pm 0.000015. \quad (3.21)$$

[Essam and Hunter (1968) have devised an (arbitrary) statistical weighting procedure for the computer examination of a Padé table.] As often happens

TABLE IV

Estimation of the critical point w_c and critical exponent γ for the simple cubic Ising lattice from the poles and residues (in parentheses) of the $[n+j, n]$ Padé approximants to the $(d/dw) \ln \chi(w)$ series.

| n | $j = -1$ | $j = 0$ | $j = +1$ |
|-----|----------------------------------|----------------------------------|---------------------|
| 1 | 0.250000 (-1.50000) | 0.190476 (-0.87075) | 0.238636 (-1.71230) |
| 2 | 0.215614 (-1.19631) | 0.216107 (-1.20482) | 0.217874 (-1.24539) |
| 3 | 0.215441 ^a (-1.19465) | 0.218968 (-1.28087) | 0.218385 (-1.25938) |
| 4 | 0.218053 (-1.24678) | 0.218151 (-1.25053) | 0.218193 (-1.25232) |
| 5 | 0.218257 (-1.25582) | 0.218165 ^a (-1.25107) | 0.218128 (-1.24922) |
| 6 | 0.218145 (-1.25018) | 0.218135 (-1.24965) | 0.218141 (-1.25000) |
| 7 | 0.218138 (-1.24979) | 0.218138 (-1.24984) | 0.218136 (-1.24962) |
| 8 | 0.218138 (-1.24980) | 0.218142 ^a (-1.25004) | |

^a Approximant with an intervening spurious pole.

[see for example, Baker *et al.* (1967); Betts *et al.* (1970)], the residues vary smoothly with the location of the poles and it appears that

$$\gamma = 1.250 \pm 0.001 \quad (3.22)$$

corresponds to the range in (3.21). The estimate (3.21) is in excellent agreement with the ratio estimate (2.27), while (3.22) reinforces (2.29) thus providing further evidence for the conjecture $\gamma = 1\frac{1}{4}$ in three dimensions.

If we accept $\gamma = 1\frac{1}{4}$ for the simple cubic lattice, a better estimate of w_c , and a first estimate of the amplitude A , can be obtained by employing (3.10). Thus, the appropriate poles and residues of $[\chi(w)]^{4/5}$ are presented in Table V, and from these we obtain

$$w_c = 0.218140 \pm 0.000003 \quad (3.23)$$

which should be compared with the preliminary estimate (3.21), and

$$w_c A^{4/5} = 0.22118 \pm 0.00003 \quad (A = 1.0166 \pm 0.0010). \quad (3.24)$$

Note that the [8, 8] approximant, for example, should make an excellent extrapolation formula for $\chi(w)$ in the range $0 < w < w_c$.

TABLE V

Estimation of the critical point w_c and amplitude A for the simple cubic Ising lattice from the poles and residues (in parentheses) of the $[n+j, n]$ Padé approximants to the $[\chi(w)]^{4/5}$ series.

| n | $j = -1$ | $j = 0$ | $j = +1$ |
|-----|-----------------------------------|-----------------------------------|-----------------------------------|
| 1 | 0.208333 (-0.20833) | 0.227273 (-0.24793) | 0.215264 (-0.21067) |
| 2 | 0.219829 (-0.22729) | 0.218718 (-0.22349) | 0.218025 (-0.22048) |
| 3 | 0.215035 (-0.19543) | 0.218041 (-0.22056) | 0.218021 ^a (-0.22046) |
| 4 | 0.218113 (-0.22100) | 0.218198 (-0.22169) | 0.218110 (-0.22093) |
| 5 | 0.218140 (-0.22119) | 0.218143 (-0.22121) | 0.218142 (-0.22120) |
| 6 | 0.218143 (-0.22120) | 0.218153 ^a (-0.221188) | 0.218141 (-0.221180) |
| 7 | 0.218141 (-0.221184) | 0.218141 (-0.221190) | 0.218141 ^a (-0.221184) |
| 8 | 0.218141 ^a (-0.221186) | 0.218140 (-0.221178) | 0.218141 ^a (-0.221188) |
| 9 | 0.218142 ^a (-0.221195) | | |

^a Approximant with an intervening spurious pole.

To gauge the consistency of our procedure, we now form Padé approximants to the $\gamma^*(w)$ series given by (3.11) and evaluate them at $w_c = 0.21813$, 0.21814 , 0.21815 . Results for the $[n, n]$ approximants only are tabulated in

TABLE VI

Estimation of the critical exponent γ for the simple cubic Ising lattice by evaluating the $[n, n]$ Padé approximants to the $\gamma^*(w)$ series for various values of w_c .

| n | $w_c = 0.21813$ | $w_c = 0.21814$ | $w_c = 0.21815$ |
|-----|---------------------|---------------------|---------------------|
| 1 | 1.2251 | 1.2252 | 1.2253 |
| 2 | 1.3025 | 1.3032 | 1.3040 |
| 3 | 1.2493 | 1.2497 | 1.2500 |
| 4 | 1.2496 | 1.2500 | 1.2505 |
| 5 | 1.2495 | 1.2499 | 1.2504 |
| 6 | 1.2493 | 1.2499 | 1.2504 ^a |
| 7 | 1.2499 ^a | 1.2500 | 1.2519 |
| 8 | 1.2492 | 1.2499 ^a | 1.2503 ^a |

^a Approximant with an intervening spurious pole.

Table VI. The sequence indicating $\gamma = 1\frac{1}{4}$ most strongly is the one based upon the central value $w_c = 0.21814$, as it should be for consistency.

Finally, using $w_c = 0.218140$ and $\gamma = 1\frac{1}{4}$, we may try and improve the preliminary estimate (3.24) of A by utilising the procedure implied by (3.13). The results, which will be found in Table VII, indicate

$$w_c A^{4/5} = 0.221172 \pm 0.000010. \quad (3.25)$$

However, allowance for the uncertainties in the critical point (3.23) will increase the final error limit to about ± 0.00002 . We remark that an alternative extrapolation formula could be based upon the [8,7] approximant, for example.

TABLE VII

Estimation of the critical amplitude A for the simple cubic Ising lattice by evaluating the $[n+j, n]$ Padé approximants to the $(0.21814-w)[\chi(w)]^{4/5}$ series at $w = w_c = 0.21814$.

| n | $j = -1$ | $j = 0$ | $j = +1$ |
|-----|-----------------------|-----------------------|-----------------------|
| 1 | 0.22892 | 0.22356 | 0.22145 |
| 2 | 0.22153 | 0.22056 | 0.22106 |
| 3 | 0.22108 | 0.221163 | 0.22120 |
| 4 | 0.22121 | 0.221183 | 0.221182 |
| 5 | 0.221182 | 0.221183 ^a | 0.221171 |
| 6 | 0.221172 | 0.221174 | 0.221173 |
| 7 | 0.221173 | 0.221175 ^a | 0.221172 |
| 8 | 0.221172 | 0.221171 | 0.221172 ^a |
| 9 | 0.221172 ^a | | |

^a Approximant with an intervening spurious pole.

The close agreement between the ratio estimates and the Padé approximant estimates for the simple cubic lattice is also found for other two- and three-dimensional lattices (Baker, 1961), and increases confidence in the essential correctness of both procedures. However, in contrast to the ratio method, we may now go on to examine the Padé approximants to the $(d/dw) \ln \chi(w)$ series for evidence of singularities other than that at w_c . For loose-packed lattices, the most striking feature is a pole on the negative real axis at $w \approx -w_c$. The $[n, n]$ approximants in Table VIII illustrate this for the square and simple cubic lattices. For the triangular and face-centred cubic lattices, on the other hand, there is no such pole. Clearly, the pole must correspond to the antiferromagnetic critical point which for the loose-packed Ising lattices is rigorously known to lie at $w = -w_c$. On closer inspection, the pole at

$w \simeq -w_c$ is seen to be the leading pole in a pole-zero sequence which is building-up along the negative real axis for $|w| \geq w_c$. Evidently, there is still a branch point singularity at $-w_c$, so that taking the logarithmic derivative has not reduced the antiferromagnetic singularity to a simple pole. This is easily understood on remembering that the antiferromagnetic susceptibility has a singularity with an asymptotic form given by (3.19) (Sykes and Fisher, 1962; Fisher and Sykes, 1962). The natural way for a Padé approximant to simulate the rapid decrease in $\chi(w)$ to some finite value χ_c as $w \rightarrow -w_c$ would be to place a zero just beyond $-w_c$. Hence, the Padé approximants to the series for the logarithmic derivative would be expected to have a pole just beyond $-w_c$ with a small positive residue. This is precisely the behaviour exhibited in Table VIII. [We mention that in Section VI an extension of the ratio method

TABLE VIII

Estimation of the antiferromagnetic critical point $-w_c$ for the square and simple cubic Ising lattices from the poles and residues (in parentheses) of the $[n, n]$ Padé approximants to the $(d/dw)\ln \chi(w)$ series.

| n | Square | Simple Cubic |
|-----|-------------------------------|-------------------------------|
| 2 | -0.4252 (0.3229) | -0.2715 (0.1325) |
| 3 | -0.4526 (0.4317) | -0.2385 (0.0829) |
| 4 | -0.4396 (0.3652) | -0.2451 (0.0953) |
| 5 | -0.4368 ^a (0.3559) | -0.2455 ^a (0.0961) |
| 6 | -0.4521 (0.4366) | -0.2345 (0.0628) |
| 7 | -0.4437 (0.3544) | -0.2267 (0.0347) |
| 8 | -0.4303 (0.1860) | -0.2279 ^a (0.0388) |
| 9 | -0.4329 ^a (0.2175) | |
| 10 | -0.4300 (0.1808) | |

^a Approximant with an intervening spurious pole.

will be considered which, unlike the basic ratio method, is capable of giving accurate information about the ferromagnetic and the antiferromagnetic singularities.] Finally, all other poles of the Padé approximants to the $(d/dw)\ln \chi(w)$ series are essentially 'cancelled' by neighbouring zeros. As an example, and to make the preceding discussion more concrete, we give in Table IX all the poles, zeros and residues of the [6,7] approximant for the simple cubic lattice.

Despite the above successes, a more important aspect of the Padé approximant method is its ability to deal with low temperature series like (1.13), whose coefficients are highly irregular in both magnitude and sign. [Indeed prior to Baker's work (Baker, 1961), no effective method of analysing

these series was known. To circumvent this difficulty, a 'more physical grouping' of the terms, corresponding to a fixed number of overturned spins, had been tried (Domb and Sykes, 1956). Although reasonably accurate estimates of the critical temperatures were made, little progress was achieved regarding the critical exponents.] Accordingly, the appropriate poles and residues of the approximants to the $(d/d\mu) \ln I(\mu)$ series are shown in Table X. Now, provided

TABLE IX

Poles, zeros and residues of the [6, 7] Padé approximant to the $(d/dw) \ln \chi(w)$ series for the simple cubic Ising lattice.

| Pole | Residue | Zero |
|---------------------------------|---------------------------------|---------------------------------|
| 0.21814 | -1.24979 | |
| -0.22230 | 0.02295 | -0.22697 |
| -0.26703 | 0.08887 | -0.31175 |
| 0.23332 \pm 0.42080 <i>i</i> | -0.03119 \pm 0.07768 <i>i</i> | 0.20781 \pm 0.40855 <i>i</i> |
| -0.23077 \pm 0.36730 <i>i</i> | 0.02733 \pm 0.00332 <i>i</i> | -0.24451 \pm 0.37274 <i>i</i> |

the critical temperature is unique, the spontaneous magnetization must vanish at the same temperature as the high temperature susceptibility diverges to infinity. We estimate from $\chi(w)$ that $w_c = 0.15611 \pm 0.00004$, which corresponds to $u_c = 0.53281 \pm 0.00009$. Happily, this value lies within 2 parts in 10^3 of the last two entries in each column of Table X.

TABLE X

Estimation of the critical point u_c and critical exponent β for the body-centred cubic Ising lattice from the poles and residues (in parentheses) of the $[n+j, n]$ Padé approximants to the $(d/d\mu) \ln I(\mu)$ series.

| <i>n</i> | <i>j</i> = -1 | <i>j</i> = 0 | <i>j</i> = +1 |
|----------|--------------------------------|--------------------------------|--------------------------------|
| 8 | 0.53059 (0.29301) | 0.53137 (0.29823) | 0.53062 (0.29286) |
| 9 | 0.53097 (0.29540) | 0.53103 (0.29579) | 0.53136 (0.29848) |
| 10 | 0.53095 ^a (0.29525) | 0.53260 (0.31447) | 0.53091 ^a (0.29535) |
| 11 | 0.53003 ^a (0.29224) | 0.53047 ^a (0.29323) | 0.53097 ^a (0.29569) |
| 12 | 0.53007 ^a (0.29227) | ^b | 0.53352 ^a (0.32921) |
| 13 | 0.53176 (0.30116) | 0.53231 (0.30772) | 0.53251 (0.31074) |
| 14 | 0.53276 (0.31502) | | |

^a Approximant with an intervening spurious pole.

^b Approximant has no pole in the vicinity of u_c .

From the residues in Table X, it appears that the critical exponent β is slightly larger than $\frac{3}{10}$. Baker's original estimate based upon much shorter series was $\beta \approx 0.30$ (Baker, 1961). A better estimate of β can be obtained by accepting the high temperature critical point as the most accurate and evaluating the approximants to $\beta^*(u)$ [defined by (3.11)] at $u_c = 0.53281$.

TABLE XI

Estimation of the critical exponent β for the body-centred cubic Ising lattice by evaluating the $[n + j, n]$ Padé approximants to the $\beta^*(u)$ series at $u = u_c = 0.53281$.

| n | $j = -1$ | $j = 0$ | $j = +1$ |
|-----|----------------------|----------------------|----------------------|
| 5 | 0.30037 | 0.29398 ^a | 0.29930 ^a |
| 6 | 0.29813 ^a | 0.28583 ^a | 0.30372 |
| 7 | 0.30172 ^a | 0.30604 | 0.30932 |
| 8 | 0.30802 | 0.31171 | 0.30784 ^a |
| 9 | 0.30275 ^a | 0.34676 | 0.31820 |
| 10 | 0.31556 | 0.31835 | 0.31821 ^a |
| 11 | 0.31679 ^a | 0.32779 ^a | 0.31730 |
| 12 | 0.31557 | 0.31470 | 0.31543 ^a |
| 13 | 0.31517 ^a | 0.31601 | 0.31605 |
| 14 | 0.31605 | | |

^a Approximant with an intervening spurious pole.

The results are displayed in Table XI. From similar sequences for this and other three-dimensional lattices, Essam and Fisher (1963) concluded that

$$0.303 \lesssim \beta \lesssim 0.318, \quad (3.26)$$

on the basis of which they conjectured $\beta = \frac{5}{16}$ for all three-dimensional Ising lattices.

As a further check on the consistency of $\beta = \frac{5}{16}$, Essam and Fisher (1963) calculated the differences between the estimates of u_c derived from the $[n, n]$ approximants to $[I(u)]^{-1/\beta}$ and the most accurate estimate of u_c obtained from the $\chi(w)$ series. Using the longer low temperature series now available and a slightly different high temperature estimate of u_c , their results for the body-centred cubic lattice may be extended as shown in Table XII. For the larger values of n , $\beta = \frac{5}{16}$ is evidently preferred to $\beta = \frac{3}{10}$. Similar results are obtained for other three-dimensional lattices.

Lastly, no special difficulties are experienced in estimating the critical amplitude and deriving extrapolation formulae for $I(u)$ in the range $0 < u < u_c$. Thus, by using the Padé approximants to the longest series for $[I(u)]^{-1/\beta}$, Baker (1961) obtained the plots shown in Fig. 7. [The curves for

the two-dimensional lattices are based upon the exact solutions (see Domb, 1960) and are given for comparison.] We have not recalculated the curves for the three-dimensional lattices, since to graphical accuracy the results would not be appreciably different to Baker's.

TABLE XII

Differences between the estimates of u_c derived from the $[n, n]$ Padé approximants to the $[I(u)]^{-1/\beta}$ series for the body-centred cubic Ising lattice and the most accurate (high temperature) estimate, $u_c = 0.53281$. (The numerical values have been multiplied by 10^5 .)

| n | $\beta = \frac{5}{16}$ | $\beta = \frac{3}{10}$ |
|-----|------------------------|------------------------|
| 5 | 4308 ^a | 3973 ^a |
| 6 | 326 | 132 |
| 7 | -86 | -244 |
| 8 | 38 | -121 |
| 9 | 125 ^a | -121 ^a |
| 10 | 58 ^a | -121 |
| 11 | -14 | -128 |
| 12 | -13 ^a | -122 |
| 13 | -22 | -62 |
| 14 | -21 ^a | -54 ^a |

^a Approximant with an intervening spurious pole.

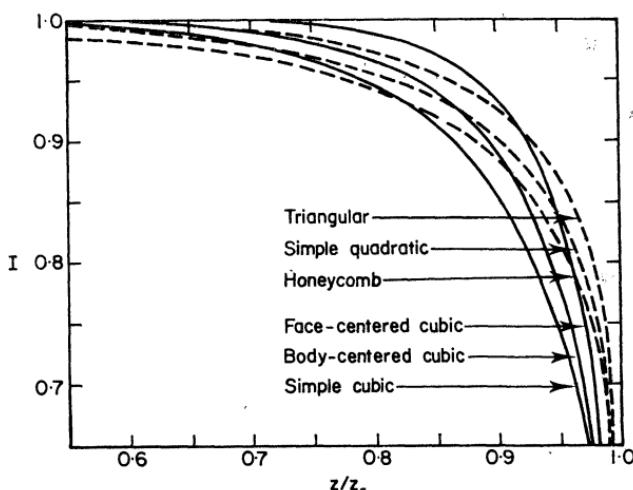


FIG. 7. Plots, versus z/z_c [where $z = \exp(-2J/kT)$], of the spontaneous magnetization of $I(\frac{1}{2})$ for various two- and three-dimensional lattices as calculated either from the exact solutions or by the Padé approximant technique. (From Baker, 1961.)

As well as a pole on the real positive axis close to u_c , the Padé approximants to the $(d/du) \ln I(u)$ series for the body-centred cubic lattice reveal a pair of poles in the complex u -plane, corresponding to singularities at (1.14), with moduli given by (1.15). Some sample results are shown in Table XIII. Of

TABLE XIII

Estimation of the non-physical singularities u_1 , u_2 and their corresponding exponent for the body-centred cubic Ising lattice from the poles and residues of the $[n, n]$ Padé approximants to the $(d/du) \ln I(u)$ series.

| n | Pole | Residue |
|-----|-----------------------|-----------------------|
| 7 | $-0.2305 \pm 0.2998i$ | $-0.0494 \pm 0.0107i$ |
| 8 | $-0.2386 \pm 0.2001i$ | $-0.0350 \pm 0.0060i$ |
| 9 | $-0.2334 \pm 0.3055i$ | $-0.0627 \pm 0.0182i$ |
| 10 | $-0.2338 \pm 0.3052i$ | $-0.0635 \pm 0.0165i$ |
| 11 | $-0.2338 \pm 0.3052i$ | $-0.0637 \pm 0.0164i$ |
| 12 | $-0.2337 \pm 0.3052i$ | $-0.0633 \pm 0.0166i$ |
| 13 | $-0.2342 \pm 0.3050i$ | $-0.0643 \pm 0.0145i$ |

course, the approximants possess many poles lying in the complex u -plane besides those at u_c , u_1 and u_2 . However, most of them are either cancelled by neighbouring zeros, or else, as the order of the approximant increases, they 'move around' the u -plane attempting to define a cut. In either case, they are usually fairly easily distinguished from the poles corresponding to the singularities at u_1 and u_2 , whose only 'movement' is that due to convergence. However, difficulties sometimes arise when there are a large number of such non-physical singularities.

Although the pattern of non-physical singularities is found to vary from lattice to lattice, the simple cubic and face-centred cubic lattices—like the body-centred cubic lattice—have non-physical singularities lying inside the "physical circle" $|u| = u_c$. Hence, series for these lattices do not converge up to the physical singularity, which explains the erratic behaviour of the coefficients in (1.13), for example. For the diamond lattice, on the other hand, the non-physical singularities appear to lie just outside the physical circle and all the coefficients are positive (Essam and Sykes, 1963; Gaunt and Essam, 1964). From a ratio analysis of the logarithmic derivative of the spontaneous magnetization series, Essam and Sykes (1963) estimated $\beta = 0.312 \pm 0.002$. This provides even closer confirmation of the conjecture $\beta = \frac{5}{16}$.

The presence of these non-physical singularities has been known for some time (e.g. Wakefield, 1951). However, our understanding of how they arise and are distributed for different lattices has only recently been advanced by

Domb and Guttmann (1970), who initiated a configurational analysis of terms in the low temperature series. Taking account of Cayley tree configurations with proper volume exclusion, they found that good approximations were obtained for the positions of all the non-physical singularities lying inside the physical circle.

The real parts of the residues in Table XIII suggest a weak divergence (with an exponent of about 0.06) at the non-physical singularities of the spontaneous magnetization, and similar results are found for other lattices (Park, 1956; Thompson *et al.*, 1969; Guttmann, 1969). Apparently, the strength of this non-physical singularity is closely related to our success in estimating β , for it turns out that when the exponents at the physical and non-physical singularities are comparable, as they seem to be for the low-temperature susceptibility (Thompson *et al.*, 1969; Guttmann, 1969), convergence is severely impaired. The situation for the low temperature specific heat is even worse, since then the non-physical singularities are considerably stronger than the rather weak physical singularity (Thompson *et al.*, 1969; Guttmann, 1969). (The non-factorisability of the physical singularity is a further unknown, complicating factor, which probably affects the spontaneous magnetization, susceptibility and specific heat, to different extents.) Consequently, present estimates of γ' and α' have rather large uncertainties (Gaunt, 1967; Thompson *et al.*, 1969; Guttmann, 1969; Guttmann *et al.*, 1970).

IV. Method of N Point Fits

In this section we study the method of “ N point fits”, recently introduced by Guttmann (1969) and Thompson *et al.* (1969), and its connection with an older method due to Park (1956). It can be shown (Gaunt and Guttmann, unpublished results) that both methods are intimately related to the Padé approximant method.

For simplicity, let us first consider the function

$$F_1(z) = A \prod_{i=1}^N (1 - \mu_i z)^{-\lambda_i}, \quad (4.1)$$

where the N factors correspond to the zeros, poles and branch-points of the function, lying in the complex z -plane at $z = z_i = 1/\mu_i$ ($i = 1, 2, \dots, N$). It is easily shown that the coefficients b_n of the series for the logarithmic derivative, namely

$$g_1(z) \equiv z(d/dz) \ln F_1(z) = \sum_{n=1}^{\infty} b_n z^n, \quad (4.2)$$

are given by

$$b_n = \sum_{i=1}^N \lambda_i \mu_i^n. \quad (4.3)$$

In fact, it can be proved that (4.3) holds *asymptotically* for a wider class of functions than (4.1), including, for example (Guttmann, 1969; Thompson *et al.*, 1969),

$$F_2(z) = z^m \prod_{i=1}^N [k_i + A_i(z) (1 - \mu_i z)^{-\lambda_i}]. \quad (4.4)$$

Hence, it is not essential that all or indeed any of the singularities should factorize, i.e. in general, the constants $k_i \neq 0$ ($i = 1, 2, \dots, N$). Unfortunately, Park (1956), who first considered the equations (4.3) for functions of the type (4.1), did not discuss this wider asymptotic validity.

Now consider the series for the logarithmic derivative of the function $F(z)$ under investigation, i.e.

$$g(z) \equiv z(d/dz) \ln F(z) = \sum_{n=1}^{\infty} c_n z^n. \quad (4.5)$$

Assuming $F(z)$ belongs to the class of functions for which (4.3) is asymptotically valid, we may write

$$c_n \approx \sum_{i=1}^N \lambda_i \mu_i^n. \quad (4.6)$$

In presenting the general solution of these equations, we will assume, following Guttmann (1969) and Thompson *et al.* (1969), that the location of the physical singularity $z = z_c$ is known either exactly or approximately from some other method. This enables us to set $\mu_1 = 1/z_c$ and form the coefficients d_n defined by

$$d_n \equiv c_n z_c^n \approx \lambda_1 + \sum_{i=2}^N \lambda_i x_i^n, \quad (4.7)$$

where $x_i = z_c/z_i$. The coefficients d_n are thus the coefficients of the logarithmic derivative of the series, normalized to a critical point of unity. The set of non-linear equations (4.7) contain N unknown exponents $\{\lambda_i\}$ ($i = 1, 2, \dots, N$) and $(N - 1)$ unknown critical points $\{z_i\}$, ($i = 2, 3, \dots, N$). After some algebra they may be linearised to yield

$$\sum_{i=0}^{N-1} t_i d_{n-i} = \lambda_1 \prod_{i=2}^N (1 - x_i), \quad (4.8)$$

where

$$\begin{aligned}
 t_0 &= 1 \\
 t_1 &= -(x_2 + x_3 + \dots + x_N) \\
 t_2 &= +(x_2 x_3 + x_2 x_4 + \dots + x_N x_{N-1}) \\
 t_3 &= -(x_2 x_3 x_4 + x_2 x_3 x_5 + \dots + x_N x_{N-1} x_{N-2}) \\
 &\vdots \\
 &\vdots \\
 &\vdots \\
 t_{N-1} &= (-1)^{N-1} x_2 x_3 x_4 x_5 \dots x_N.
 \end{aligned} \tag{4.9}$$

Defining the coefficients e_n by

$$e_n = d_n - d_{n-1}, \tag{4.10}$$

we obtain the set of linear equations

$$\sum_{i=0}^{N-1} t_i e_{n-i} = 0, \tag{4.11}$$

which may be rewritten as

$$\begin{pmatrix} e_{n-1} & e_{n-2} & \dots \dots & e_{n-N+1} \\ e_{n-2} & e_{n-3} & \dots \dots & e_{n-N} \\ e_{n-3} & e_{n-4} & \dots \dots & e_{n-N-1} \\ \vdots & & \ddots & \vdots \\ \vdots & & \ddots & \vdots \\ \vdots & & \ddots & \vdots \\ e_{n-N+1} & e_{n-N} & \dots \dots & e_{n-2N+3} \end{pmatrix} \begin{pmatrix} t_1 \\ t_2 \\ t_3 \\ \vdots \\ \vdots \\ \vdots \\ t_{N-1} \end{pmatrix} = \begin{pmatrix} -e_n \\ -e_{n-1} \\ -e_{n-2} \\ \vdots \\ \vdots \\ \vdots \\ -e_{n+2-N} \end{pmatrix} \tag{4.12}$$

Since the coefficients $\{e_i\}$ are known, it is a straightforward computing exercise to obtain the coefficients $\{t_i\}$ ($i = 1, 2, \dots, N-1$), from which all the exponents $\{\lambda_i\}$ and critical points $\{z_i\}$ follow with little difficulty. The physical critical exponent λ_1 is given by (4.8) as

$$\lambda_1 = \sum_{i=0}^{N-1} t_i d_{n-i} / \prod_{i=2}^N (1 - x_i), \tag{4.13}$$

where it follows from (4.9) that

$$\prod_{i=2}^N (1 - x_i) = \sum_{i=0}^{N-1} t_i. \tag{4.14}$$

Next, the set $\{x_i\}$ can be obtained from a slight generalization of (4.14), namely

$$\prod_{i=2}^N (x - x_i) = \sum_{i=0}^{N-1} t_i x^{N-1-i}. \quad (4.15)$$

Notice that the polynomial on the right-hand side of (4.15) has roots at $x = x_i$ ($i = 2, 3, \dots, N$). Therefore, by solving (4.15) all the x_i and hence all the critical points $z_i = z_c/x_i$ may be determined. Finally, the remaining exponents $\{\lambda_i\}$ ($i = 2, 3, \dots, N$) may be obtained from (4.7) by solving the set of equations

$$\begin{pmatrix} x_2^n & x_3^n & x_4^n & & x_N^n \\ x_2^{n-1} & x_3^{n-1} & x_4^{n-1} & \dots \dots & x_N^{n-1} \\ \vdots & \vdots & & & \vdots \\ \vdots & \vdots & & & \vdots \\ x_2^{n+2-N} & x_3^{n+2-N} & x_4^{n+2-N} & \dots \dots & x_N^{n+2-N} \end{pmatrix} \begin{pmatrix} \lambda_2 \\ \lambda_3 \\ \vdots \\ \vdots \\ \lambda_N \end{pmatrix} = \begin{pmatrix} d_n & -\lambda_1 \\ d_{n-1} & -\lambda_1 \\ \vdots & \vdots \\ \vdots & \vdots \\ d_{n-N+2} - \lambda_1 \end{pmatrix}. \quad (4.16)$$

For a given value of n , the results $\{\lambda_i\}$ ($i = 1, 2, \dots, N$), and $\{z_i\}$ ($i = 2, 3, \dots, N$) are called "the n th estimates obtained from an N point fit". (The name "N point fit" is used because the method fits the series to a functional form which assumes N factors or singular points in the complex plane.) To determine the $(2N - 1)$ unknowns requires a knowledge of the last $(2N - 1)$ series coefficients and involves only $(N - 1) \times (N - 1)$ matrices for all values of n .

It can be shown (Gaunt and Guttmann, unpublished results) that the above estimates of $\{z_i\}$ and $\{\lambda_i\}$ for $i = 2, 3, \dots, N$ are *identical* to the poles and residues, respectively, of the $[n - N, N - 1]$ Padé approximant to the $(z_c - z) (d/dz) \ln F(z)$ series. In addition, the physical exponent λ_1 is simply the value of the $[n - N, N - 1]$ approximant at $z = z_c$. Thus, the results of an N point fit for a range of values of $n = 2N - 1, 2N, 2N + 1, \dots$ can be obtained by going along the N th row of the Padé table and examining the sequence of approximants $[m, N - 1]$ with $m = N - 1, N, N + 1, \dots$. Evidently, the calculation of the $[n - N, N - 1]$ approximant requires all n series coefficients. In this way, the Padé approximant not only gives results for the N factors which are identical to the n th estimates obtained from an N point fit, but in addition, attempts to provide a better representation of the function in other regions of the complex z -plane. However, this computation involves $(n - N) \times (n - N)$ matrices, so that for long series, difficulties can arise due simply to rounding errors introduced by the computer manipulation of large matrices. In such circumstances, the N point fit method can be useful, since, as we have mentioned above, the matrices are only of order $(N - 1)$.

Let us test the N point fit method by applying it to the spontaneous magnetization series (1.13) of the spin $\frac{1}{2}$ Ising model on a body-centred cubic lattice, assuming $u_c = 0.53281$. Estimates of the critical exponent β obtained from N point fits with $N = 1, 2, \dots, 5$ are shown in Table XIV. It is seen that

TABLE XIV

Estimation of the critical exponent β for the body-centred cubic Ising lattice from an N point fit to the $I(u)$ series. The non-physical singularities u_1, u_2 are estimated from the 3 point fit.

| n | 1 point fit | 2 point fit | 3 point fit | 4 point fit | 5 point fit | Non-physical singularities u_1, u_2 |
|-----|-------------|-------------|-------------|-------------|-------------|--|
| 16 | +7.247 | +76.33 | 0.3048 | 0.3088 | 0.3073 | -0.2325 \pm 0.3030 <i>i</i> |
| 17 | -30.96 | +10.68 | 0.3124 | 0.3088 | 0.3088 | -0.2326 \pm 0.3039 <i>i</i> |
| 18 | +39.84 | -6.144 | 0.3152 | 0.3167 | 0.3088 | -0.2327 \pm 0.3038 <i>i</i> |
| 19 | -6.221 | +11.94 | 0.3050 | 0.3130 | 0.3106 | -0.2334 \pm 0.3039 <i>i</i> |
| 20 | -64.80 | +209.42 | 0.3185 | 0.3108 | 0.3115 | -0.2337 \pm 0.3045 <i>i</i> |
| 21 | +122.9 | -20.16 | 0.3126 | 0.3144 | 0.3119 | -0.2336 \pm 0.3046 <i>i</i> |
| 22 | -81.39 | +25.07 | 0.3080 | 0.2933 | 0.3126 | -0.2337 \pm 0.3046 <i>i</i> |
| 23 | -97.43 | -98.80 | 0.3213 | 0.3114 | 0.3130 | -0.2339 \pm 0.3048 <i>i</i> |
| 24 | +322.3 | -81.98 | 0.3103 | 0.3153 | 0.3134 | -0.2339 \pm 0.3049 <i>i</i> |
| 25 | -355.3 | +63.14 | 0.3109 | 0.3109 | 0.3137 | -0.2339 \pm 0.3049 <i>i</i> |
| 26 | -18.37 | -130.3 | 0.3225 | 0.3102 | 0.3140 | -0.2340 \pm 0.3049 <i>i</i> |
| 27 | +715.0 | -641.6 | 0.3102 | 0.3166 | 0.3144 | -0.2340 \pm 0.3050 <i>i</i> |
| 28 | -1170 | +187.1 | 0.3102 | 0.3102 | 0.3145 | -0.2340 \pm 0.3050 <i>i</i> |

the $N = 1$ and 2 point fits yield very ragged sequences, while for $N \geq 3$ they suddenly settle down around $\beta = 0.312 \pm 0.004$. Such behaviour suggests the presence of three singularities in the "physical disk" $|u| \leq u_c$. Besides the physical singularity at u_c , there are a conjugate pair of singularities lying closer to the origin. Clearly, their presence will render any attempt to represent the function with $N = 1$ or 2 futile. Solving the polynomial (4.15) with $N = 3$ yields, for the positions of the two non-physical singularities, the sequence in Table XIV from which we estimate $u_1, u_2 = (-0.234 \pm 0.305i) \pm (0.001 \pm 0.001i)$. This estimate and that for β are in excellent agreement with the results obtained in Section III.D by examining *diagonal* sequences of Padé approximants. Thus, it appears that *at least for this example* there is little to choose between the rows and diagonals of the Padé table. (Compare the sequences in Table XI with those in Table XIV for $N = 3, 4$ and 5). Further examples of the application of the method are given by Thompson *et al.* (1969), Guttmann (1969) and Guttmann *et al.* (1970).

Finally, it is clear that a “free N point fit” can also be defined by relaxing the constraint that the critical point is assumed known, and then solving the set of eqs (4.6) for the $2N$ unknowns $\{\mu_i\}$ and $\{\lambda_i\}$, ($i = 1, 2, \dots, N$). This was the approach envisaged by Park (1956). In essentially this way, he was able to use the series expansion for the spontaneous magnetization of the square Ising lattice to re-derive Yang’s result (1.9), for which the functional form (4.1) is exact. Although Park obtained explicit solutions only for the cases $N = 1$ and 2, the general solution can readily be obtained by an approach similar to that outlined above. [N th order matrices will replace those of order $(N - 1)$ in (4.12) and (4.16).] In this case, it can be shown (Essam and Fisher, 1963; Gaunt and Guttmann, unpublished) that the n th estimates obtained from a free N point fit (i.e. by Park’s method) are identical with the poles and residues of the $[n - N - 1, N]$ Padé approximants to the $(d/dz) \ln F(z)$ series.

V. Transformations of Expansion Variables

So far in this chapter we have studied a number of Ising model series at both high and low temperatures. The expansion variables have been $w = \tanh(J/kT)$ for the high temperature series and $u = z^2 = \exp(-4J/kT)$ for the low temperature series. There is, however, no compelling reason why these particular variables should be used in preference to any other, except that they arise naturally in the formulation of the graph counting problems (Domb, 1960 and this volume, Chapter 6). At first sight, it may appear reasonable to seek high and low temperature expansions in the variables $K = J/kT$ and K^{-1} , respectively. If, however, a function can be expanded in powers of $\exp(-2K)$, it clearly cannot be expanded in powers of K^{-1} . For high temperature series, on the other hand, an expansion in powers of $w = \tanh(J/kT)$ can certainly be re-expanded in powers of K . From the extrapolator’s point of view, however, there is little to choose between the variables w and K —at least for the Ising model—and, in practice, both variables have been used (Domb and Sykes, 1961; Sykes *et al.*, 1967).

In some cases, however, a change of expansion variable can improve the behaviour of the initial series extrapolants. Consider the Hamiltonian

$$\mathcal{H}^{(v)} = -J \sum_{\langle ij \rangle} \mathbf{s}_i^{(v)} \cdot \mathbf{s}_j^{(v)}, \quad (5.1)$$

for example, where the $\mathbf{s}_i^{(v)}$ are v -dimensional vectors, and the sum is over all nearest-neighbour pairs. For $v = 1, 2$ and 3 , $\mathcal{H}^{(v)}$ reduces to the spin $s = \frac{1}{2}$ Ising, classical planar and classical Heisenberg models, respectively (Stanley, 1968a), while as $v \rightarrow \infty$, it approaches the spherical model (Stanley, 1968b). For these four models, Stanley (1968a, c) has suggested that

the high temperature susceptibility series can be more smoothly extrapolated if they are expanded in the variable x_v , where the susceptibility of a linear chain of v -dimensional spins is given by $\chi^{(v)} = (1 + x_v)/(1 - x_v)$. In this way the usual expansion variable $x_1 = \tanh K \equiv w$ is obtained for the Ising model, but for the other models the appropriate variables are

$$x_2 = I_1(2K)/I_0(2K), \quad x_3 = \mathcal{L}(3K) \equiv \coth(3K) - 1/3K$$

and

$$x_\infty = 2K/[1 + (1 + 4K^2)^{\frac{1}{2}}],$$

where $I_n(y)$ is a modified Bessel function of the first kind and $\mathcal{L}(y)$ is the Langevin function.

For all these examples, however, the change of expansion variables does not alter the distribution of singularities in the physical disk. In the original variable, the physical singularity is the closest singularity to the origin, so that transforming the series can only improve the convergence rate if it moves singularities outside the physical disk still further away, or in some other way removes "small number" effects. For many low temperature Ising model series, however, there is clearly scope for dramatic improvement, since the series do not converge up to the physical singularity. If the series could be transformed (by an Euler transformation, for example) to some new expansion variable in which the physical singularity was closest to the origin, then the series would presumably be easier to analyse.

Before giving some specific examples of such transformations, we wish to comment on the general Euler transformation

$$x = By/(C + Dy).$$

As mentioned earlier, diagonal Padé approximants are invariant under such transformations. Hence, the diagonal (and near-diagonal) approximants might be expected to be as effective as any method based on this type of transformation. This observation is sometimes used to argue that the application of such transformations to Ising model series and the like, is rather pointless. In general, however, this conclusion is not correct because the Padé method is usually applied to the logarithmic derivative of a series, and the operations of taking the logarithmic derivative and applying an Euler transformation do not commute. It is, therefore, quite possible that the application of such a transformation could speed the convergence of the sequence of Padé approximants to the logarithmic derivative of the series.

As our first example, let us consider the $s = \frac{1}{2}$ Ising model, for which the usual low temperature expansion variable is $u = \exp(-4J/kT)$. Any other low temperature variable, x say, must clearly satisfy the condition that as $T \rightarrow 0$, x vanishes like $\exp(-c/T)$. There are, of course, a large number of

variables satisfying this condition, and one that has been used (Guttmann and Thompson, 1969; Guttmann *et al.*, 1970) is

$$x = 1 - \tanh(J/kT) = 1 - w. \quad (5.2)$$

This is related to the original variable u by the simple transformation

$$u = x^2/(2 - x)^2. \quad (5.3)$$

Note that if the original series is known through order u^N , the transformed series can be derived correct through order x^{2N+1} . Although twice as many coefficients are available for the transformed series, this is of little advantage since, as the transformation is also double-valued, there will be twice as many singularities in the x -plane as in the u -plane. There is also a spurious

TABLE XV

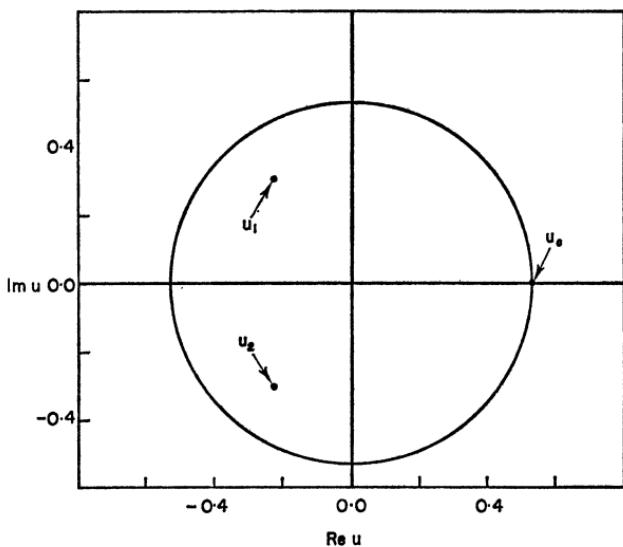
Comparison of the exact coefficients of the spontaneous magnetization series for the body-centred cubic Ising lattice expanded in the variables $u = \exp(-4J/kT)$ and $x = 1 - \tanh(J/kT)$.

| n | Coefficients of u^n | Coefficients of x^n |
|-----|-----------------------|-----------------------|
| 0 | 1 | 1 |
| 1 | 0 | 0 |
| 2 | 0 | 0 |
| 3 | 0 | 0 |
| 4 | -2 | 0 |
| 5 | 0 | 0 |
| 6 | 0 | 0 |
| 7 | -16 | 0 |
| 8 | 18 | -0.0078125 |
| 9 | 0 | -0.03125 |
| 10 | -168 | -0.0703125 |
| 11 | 384 | -0.1171875 |
| 12 | -314 | -0.1611328125 |
| 13 | -1 632 | -0.193359375 |
| 14 | 6 264 | -0.21044921875 |
| 15 | -9 744 | -0.21630859375 |
| 16 | -10 014 | -0.22174072265625 |
| 17 | 86 976 | -0.24072265625 |
| 18 | -205 344 | -0.2843017578125 |
| 19 | 80 176 | -0.3548583984375 |
| 20 | 1 009 338 | -0.44373321533203125 |
| 21 | -3 579 568 | -0.5338897705078125 |
| 22 | 4 575 296 | -0.607143402099609375 |
| 23 | 8 301 024 | -0.653301239013671875 |
| | : | : |

singularity at $x = 2$, which corresponds to $T = 0^-$, and is, therefore, of no physical significance.

If the transformation (5.3) is applied to the spontaneous magnetization

(A)



(B)

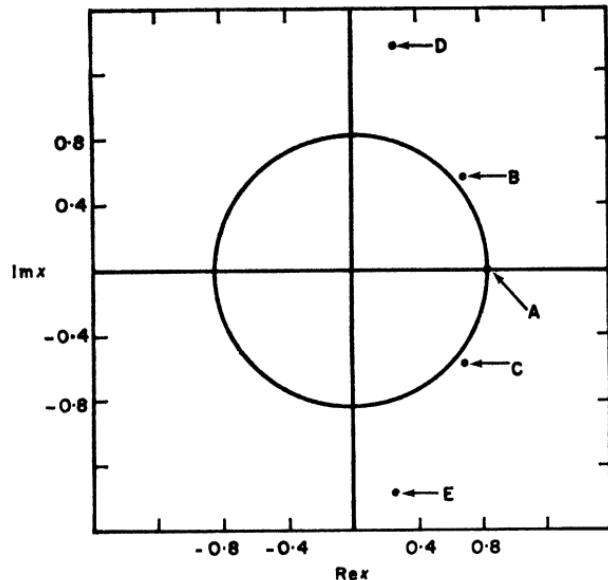


FIG. 8. Distribution of singularities in the complex u -plane (A) and complex x -plane (B) for the body-centred cubic $I(\frac{1}{2})$ lattice.

of the Ising model on a body-centred cubic lattice, the series is transformed as in Table XV. Whereas the series in the original variable u has coefficients that vary apparently randomly in sign, the series coefficients in the new variable x are of constant sign. If this trend persists, the dominant singularity must lie on the real positive x -axis. Since the physical singularity is the first singularity on the real, positive u -axis, and since the interval $0 \leq u \leq 1$ maps onto the interval $0 \leq x \leq 1$, it follows that the series in the new expansion variable now converges up to the critical point.

TABLE XVI

Estimation of the critical exponent β for the body-centred cubic Ising lattice by
 (a) evaluating the $[n, n]$ Padé approximant to the $\beta^*(x)$ series at $x = x_c$, and
 (b) by the method of N point fits. (From Guttmann *et al.*, 1970.)

| n | [n, n] approximant | 3-point fit | 4-point fit | 5-point fit | 6-point fit |
|-----|------------------------|-------------|-------------|-------------|-------------|
| 8 | 0.3114 | 0.3048 | 0.3073 | 0.3073 | 0.3087 |
| 9 | 0.2813 | 0.3052 | 0.3078 | 0.3072 | 0.3087 |
| 10 | 0.2968 | 0.3056 | 0.3087 | 0.3057 | 0.3091 |
| 11 | 0.2969 | 0.3059 | 0.3098 | | 0.3104 |
| 12 | 0.2960 | 0.3063 | 0.3110 | 0.3172 | 0.3141 |
| 13 | 0.2779 | 0.3066 | 0.3126 | 0.3389 | 0.3229 |
| 14 | 0.2995 | 0.3068 | 0.3158 | 0.3066 | 0.3146 |
| 15 | 0.3050 | 0.3071 | 0.3300 | 0.3082 | 0.3087 |
| 16 | 0.3071 | 0.3074 | 0.2573 | 0.3057 | 0.3073 |
| 17 | 0.3109 | 0.3077 | 0.2898 | 0.2982 | 0.3103 |
| 18 | 0.3021 | 0.3080 | 0.2890 | 0.2891 | 0.3184 |
| 19 | 0.3464 | 0.3083 | 0.2344 | 0.2899 | 0.3253 |
| 20 | 0.3141 | 0.3086 | 0.3277 | 0.2992 | 0.3247 |
| 21 | 0.2999 | 0.3089 | 0.3163 | 0.3065 | 0.3204 |
| 22 | 0.3148 | 0.3091 | 0.3137 | 0.3100 | 0.3168 |
| 23 | 0.3268 | 0.3094 | 0.3127 | 0.3115 | 0.3148 |
| 24 | 0.3137 | 0.3096 | 0.3124 | 0.3122 | 0.3138 |
| 25 | 0.3126 | 0.3098 | 0.3124 | 0.3124 | 0.3133 |
| 26 | 0.3132 | 0.3100 | 0.3126 | 0.3124 | 0.3131 |
| 27 | 0.3114 | 0.3102 | 0.3129 | 0.3118 | 0.3130 |
| 28 | 0.3135 | 0.3103 | 0.3132 | 0.3143 | 0.3130 |

It is of interest to see what has happened to the non-physical singularities (1.14), which previously dominated the u -expansion. The distribution of singularities in the physical disk in the u -plane is shown in Fig. 8(A), where $u_1, u_2 \approx 0.234 \pm 0.305i$ and $u_c \approx 0.53281$. Under the transformation (5.3), these singularities are mapped onto the x -plane as shown in Fig. 8(B). Their

approximate positions are as follows:

| <i>Singularity</i> | <i>Position</i> |
|--------------------|--------------------|
| <i>A</i> | 0.84387 |
| <i>B, C</i> | $0.682 \pm 0.575i$ |
| <i>D, E</i> | $0.245 \pm 1.366i$ |

Clearly, the transformation moves the non-physical singularities which lie inside the physical disk in the u -plane, outside the transformed physical disk in the x -plane. Furthermore, since the physical disk in the x -plane maps onto the u -plane in such a way that it lies entirely within the physical disk in the u -plane, it follows that singularities outside the physical disk in the u -plane cannot be transformed so that they fall inside the physical disk in the x -plane.

Now let us use the transformed series to estimate the critical exponent β . Note, first, that since

$$f(u) \approx A \left(1 - \frac{u}{u_c}\right)^{-\lambda}, \quad (u \rightarrow u_c), \quad (5.4)$$

becomes

$$f^*(x) \approx B \left(1 - \frac{x}{x_c}\right)^{-\lambda}, \quad (x \rightarrow x_c), \quad (5.5)$$

with $B = A[4/(2 - x_c)]^{-\lambda}$, the transformation (5.3) leaves critical exponents unchanged. The transformed series has been analyzed by forming diagonal Padé approximants to the

$$\beta^*(x) \equiv (x_c - x) \frac{d}{dx} \ln I(x)$$

series and evaluating these at x_c , and also by the method of N point fits for $N = 3, 4, 5$ and 6 . The results are shown in Table XVI. These sequences, particularly in the case of the N point fit method, are somewhat smoother than those obtained from the series in the original variable u , and suggest quite strongly a value around $\beta = \frac{5}{16} = 0.3125$.

As a second example, consider the low temperature susceptibility series of the Ising model on a triangular lattice,

$$\chi(u) = u^3 + 12u^5 + 4u^6 + 129u^7 + 72u^8 + \dots, \quad (5.6)$$

where the expansion is known through u^{16} [Sykes *et al.*, for details see Domb,

this volume, Chapter 6]. The ratios of successive coefficients are:

| | |
|-----|-----------------------|
| n | $\mu_n = a_n/a_{n-1}$ |
| : | : |
| 9 | 18.500000 |
| 10 | 0.720720 |
| 11 | 13.978125 |
| 12 | 0.847455 |
| 13 | 11.686598 |
| 14 | 0.951061 |
| 15 | 10.283957 |
| 16 | 1.038414 |
| : | : |

Clearly, it is not possible to estimate by the usual ratio method either the critical point (which is known to be exactly $u_c^{-1} = 3$) or the critical exponent γ' from this sequence of ratios. Let us now apply the transformation

$$u = y/(2 - 2y) \quad (5.7)$$

to the series (5.6). The critical point in the new variable is at $y_c^{-1} = 2.5$, and the ratios of successive coefficients are:

| | |
|-----|----------|
| n | μ_n |
| : | : |
| 9 | 2.680555 |
| 10 | 2.659444 |
| 11 | 2.648014 |
| 12 | 2.636994 |
| 13 | 2.627724 |
| 14 | 2.619590 |
| 15 | 2.612441 |
| 16 | 2.606098 |
| : | : |

This sequence extrapolates smoothly against $1/n$ to the correct limit 2.5, and yields a critical exponent close to the generally accepted result $\gamma' = 1\frac{1}{4}$.

Besides the two examples just considered, a number of other transformations has been used by various authors to 'map away' unwanted singularities. One of the earliest applications of a transformation to a problem in lattice statistics was the study of the antiferromagnetic behaviour of the Heisenberg model by Danielian and Stevens (1957, 1961). They used an Euler transformation to map the ferromagnetic Curie point far from the origin, in such a way that the antiferromagnetic Néel point dominated the series. A more recent application of an Euler transformation has been given by Fox and Guttmann (1970) in their study of the low temperature behaviour of the spin $s = 1$ Ising model. The transformation employed was

$$x = 2y/(1 + y), \quad (5.8)$$

where

$$y = \exp(-J/kT)$$

is the original expansion variable and

$$x = 1 - \tanh(J/2kT)$$

is the new variable. In terms of the transformed variable, all the low temperature series appeared to converge up to the critical point. Another transformation that has been used with some success is

$$K = \bar{K}/(1 \pm \bar{K}^2), \quad (5.9)$$

which was applied by Betts *et al.* (1971) to the high temperature expansion of the fluctuation in the long range order in the two-dimensional XY model.

As a last example, we mention the well-known magnetic moment transformation developed by Fisher (1959b), which relates the susceptibility χ_H of the honeycomb lattice to that of the triangular lattice, χ_T . This may be written

$$\chi_T(w) = \frac{1}{2}[\chi_H(v) + \chi_H(-v)] \equiv \chi_T(v^2), \quad (5.10)$$

where

$$v^2 = w(1 + w)(1 + w^3)^{-1}. \quad (5.11)$$

Now the high temperature expansion for the triangular lattice with antiferromagnetic interactions ($w < 0$) will only converge for temperatures corresponding to $|w| \leq w_c < 1$ (where $w = w_c$ is the critical point of the corresponding ferromagnetic lattice), even though the antiferromagnetic susceptibility is known to be analytic at all temperatures $T > 0$. However, since the honeycomb series converges for $|v| < 1/\sqrt{3}$, it follows from (5.10) that the series expansion of $\chi_T(v^2)$ will converge for $-1/3 < v^2 \leq 0$, corresponding to the antiferromagnetic temperature range $-1 < w \leq 0$ (or $T > 0$). Further details of the transformation are given by Sykes (1961), Sykes and Zucker (1961), Sykes and Fisher (1962), and Sykes *et al.* (1972a).

VI. Applications of Darboux's Theorems

A. Introduction

As we have seen in Section II, the ratio method seems to work rather well for certain series, notably the high temperature susceptibility series of the Ising model. In the usual treatment, it is assumed that the susceptibility behaves like

$$\chi(w) = \sum_{n=0}^{\infty} a_n w^n \approx A(1 - \mu w)^{-\gamma} \quad (6.1)$$

near $w = w_c = 1/\mu$, so that plotting the ratios $\mu_n = a_n/a_{n-1}$ against $1/n$ yields a straight line with gradient $\mu(\gamma - 1)$ and intercept μ . The functional form (6.1) is, however, only the leading term in the expansion of $\chi(w)$ around the critical point. With the development of much longer series expansions, it now appears possible to attempt to include higher-order terms in the expansion of $\chi(w)$.

Let us consider, therefore, the function $F(z)$, which is analytic except at a finite number of singularities $z = z_i = 1/\mu_i$. Near each singularity, $F(z)$ can be represented by

$$F(z) = A_i(z)(1 - \mu_i z)^{-\lambda_i} + B_i(z), \quad (6.2)$$

where $A_i(z)$ and $B_i(z)$ are both non-singular at z_i . These conditions are satisfied, for example, by the hypergeometric function $F(a; b; c; z)$ (Whittaker and Watson, 1940); by the high temperature susceptibility of the spherical model for three-dimensional lattices with finite range interactions (Joyce, Vol. 2, Chapter 10), and by the spontaneous magnetization and energy of the spin $\frac{1}{2}$ Ising model for two-dimensional lattices (see Domb, 1970a).

In this section, we will assume the high temperature Ising susceptibility is of the form (6.2), and use some theorems of Darboux (1878) to discuss the asymptotic form of the coefficients. It is shown that Darboux's theorems provide a powerful tool in the design of extrapolation procedures, provided of course sufficient coefficients are available to exploit them.

B. Close-packed lattices

Instead of (6.1), let us write the susceptibility as

$$\chi(w) = \sum_{n=0}^{\infty} a_n w^n \approx A(w)(1 - \mu w)^{-\gamma} + B(w), \quad (6.3)$$

where $A(w)$ and $B(w)$ are assumed regular in the neighbourhood of $w = w_c = 1/\mu$. If, in addition, both functions are regular in the physical disk

$|w| \leq w_c$, then the asymptotic form of the coefficients a_n can be obtained by substituting for the expansion of $\chi(w)$ that of $A(w_c)(1 - \mu w)^{-\gamma}$. Higher-order approximations may be obtained by replacing $\chi(w)$ by

$$\left[\sum_{r=0}^m \frac{(w - w_c)^r}{r!} A^{(r)}(w_c) \right] (1 - \mu w)^{-\gamma}, \quad (6.4)$$

the error involved in stopping at the n th term being always of $O(1/n)$ times this term. The proof of this theorem, which we denote by *DI*, is given by Darboux (1878). The expression (6.4) gives the $(m+1)$ th Darboux approximation. If $B(w) = 0$, so that the ferromagnetic singularity at $w = w_c$ factorizes, this theorem is essentially a statement that $\chi(w)$ may be expanded about w_c by multiplying $(1 - \mu w)^{-\gamma}$ by the Taylor expansion of $A(w)$ about w_c . The importance of *DI* is that it tells us that the effect of the additive function $B(w)$ becomes vanishingly small.

The application of *DI* to some two- and three-dimensional Ising model series was first discussed by Ninham (1963). For example, on applying the theorem to Yang's exact result (1.9) for the spontaneous magnetization of the square Ising lattice, which is clearly of the form (6.2), Ninham obtained the results shown in Table XVII. Here, the asymptotic form of the coefficients as obtained in the first and second Darboux approximations are compared with the exact values. Evidently, *DI* gives an asymptotic form of considerable accuracy.

TABLE XVII

Comparison between the actual coefficients of the series expansion of the spontaneous magnetization for the square Ising lattice, and those given by the first and second Darboux approximations. (From Ninham, 1963.)

| <i>n</i> | Coefficient first Darboux approximation | Coefficient second Darboux approximation | Actual coefficient |
|----------|---|--|-----------------------|
| 6 | 670 | 700 | 714 |
| 7 | 3 300 | 3 410 | 3 472 |
| 8 | 16 550 | 17 020 | 17 318 |
| 9 | 84 830 | 86 620 | 88 048 |

Returning to the form (6.3) assumed for the susceptibility, *DI* readily yields

$$\mu_n \equiv \frac{a_n}{a_{n-1}} \approx \mu \left[1 + \frac{\gamma - 1}{n} + \frac{k}{n^2} + O\left(\frac{1}{n^3}\right) \right] \quad (6.5)$$

as the asymptotic form for the ratio of successive coefficients. The expression (6.5) provides the theoretical basis for the method recently proposed by Sykes

from other considerations (Sykes *et al.*, 1972b), for obtaining better estimates for the critical parameters of the Ising model on close-packed lattices. In particular, assuming $\gamma = 1\frac{3}{4}$ for the triangular lattice, a sequence whose elements are

$$\mu_n^* \equiv \frac{n\mu_n}{n + \gamma - 1} \approx \mu \left[1 + \frac{k}{n^2} \right] + O\left(\frac{1}{n^3}\right) \quad (6.6)$$

is constructed and extrapolated against $1/n^2$. As may be seen from Fig. 2, this yields an essentially straight line for $n \geq 9$ with an intercept very close indeed to the exact value $\mu = 2 + \sqrt{3} = 3.73205 \dots$

It should be noted that (6.5) and (6.6) are identical to (2.8) and (2.22), respectively. However, since the functional form (2.6), for which (2.8) and (2.22) are valid, is a special case of our present assumption (6.3), this is not unexpected.

C. Loose-packed lattices

For loose-packed lattices, there is an antiferromagnetic singularity at $w = -w_c$, and this causes a characteristic odd-even oscillation in the ratios (see Section II.D and Fig. 3, for example). The form (6.3) may still be used [see Domb (1970b, c)], but now the function $A(w)$ is assumed regular in the disk $|w| \leq w_c$ except at $w = -w_c$, where

$$A(w) \approx A(1 + \mu w)^\phi. \quad (6.7)$$

Hence, the function $\chi(w)$ has two singularities on the circle of convergence. To determine the asymptotic behaviour of the coefficients, we make use of Darboux's second theorem (DII): Suppose a function $F(z)$ is analytic for $|z| < 1$ but has a finite number of singularities on the unit circle at $z = e^{i\phi_1}, e^{i\phi_2}, \dots, e^{i\phi_l}$. Then, if

$$F(z) \approx \sum_{v=0}^{\infty} C_v^{(k)} (1 - ze^{-i\phi_k})^{\alpha_k + v\beta_k}, \quad (\beta_k > 0, k = 1, 2, 3 \dots, l), \quad (6.8)$$

in the vicinity of $e^{i\phi_k}$, the expression

$$\sum_{v=0}^{\infty} \sum_{k=1}^l C_v^{(k)} \binom{\alpha_k + v\beta_k}{n} (-e^{-i\phi_k})^n \quad (6.9)$$

furnishes an asymptotic expansion for the coefficient of z^n in $F(z)$ in the sense that if Q is an arbitrary positive number, and a sufficiently large number of terms in the sum over v in (6.9) is taken, an expression is obtained which approximates the coefficient in question with an error of $O(n^{-Q})$. Szegő (1959)

gives the proof of this theorem for a particular choice of function $F(z)$, and his proof may readily be extended to any function satisfying the conditions stated above.

It follows from (DII) that the ratio of successive coefficients of (6.3) with $A(w)$ satisfying (6.7) is given by

$$\begin{aligned}\mu_n \equiv \frac{a_n}{a_{n-1}} &\approx \mu \left[1 + \frac{\gamma - 1}{n} + \frac{k_1}{n^2} \right. \\ &\quad \left. + O\left(\frac{1}{n^3}\right) + (-1)^n \frac{k_2}{n^{\phi+\gamma}} + O\left(\frac{1}{n^{\phi+\gamma+1}}\right) \right].\end{aligned}\quad (6.10)$$

Thus, the sequence $\{\mu_n^*\}$ has elements

$$\mu_n^* \equiv \frac{n \mu_n}{n + \gamma - 1} \approx \mu \left[1 + \frac{a}{n^2} + (-1)^n \frac{b}{n^{\phi+\gamma}} + \text{higher order terms} \right], \quad (6.11)$$

where the constants a and b are simply related to the amplitudes of the ferromagnetic and antiferromagnetic singularities (see Sykes *et al.*, 1972b).

The result (6.11), which arises quite naturally from DII, was suggested by Sykes (unpublished) from rather different considerations, and has been used by Sykes *et al.*, (1972b) to study the more complicated critical behaviour of the Ising susceptibility of loose-packed lattices. The most direct application of (6.11) requires some assumption about the nature of the antiferromagnetic singularity. It has been suggested both from configurational studies (Sykes and Fisher, 1958; Sykes, 1961; Sykes and Fisher, 1962) and from a study of pair correlations (Fisher, 1959a, 1962) that the antiferromagnetic susceptibility behaves like the energy. Accepting this result gives $\phi = 1 - \alpha$, where α is the high temperature specific heat exponent. If we use $\alpha = 0$, $\gamma = 1\frac{3}{4}$ for two-dimensional lattices and $\alpha = \frac{1}{3}$, $\gamma = 1\frac{1}{4}$ in three dimensions, the oscillatory term in (6.11) takes the forms $(-1)^n/n^{11/4}$ and $(-1)^n/n^{17/8}$, respectively. Extrapolating μ_n^* against $1/n^2$ for the square and simple cubic lattices straightens-out the plots in Figs 5(A) and (B) as shown in Figs 9(A) and (B). Because the oscillatory term is not exactly of the form $(-1)^n/n^2$, linear extrapolation of each branch results in their intersection slightly before the $1/n^2 = 0$ axis. A better estimate of μ may be obtained by neglecting the higher-order terms in (6.11) and solving for a , b and μ using three successive values of μ_n^* . The results in Tables XVIII(a) and (b) have been obtained in this way. For the square lattice, the last estimate of μ differs from the exact value $\mu = 1 + \sqrt{2} = 2.41421\dots$ by only 3 in the last place, which represents an accuracy of almost 1 in 10^5 . Similarly, estimates of μ for the simple cubic lattice appear to be rapidly converging towards a value in

substantial agreement with previous estimates. These results suggest the form (6.11) is at least a good approximation for μ_n^* and that our choice of values for γ and ϕ is correct. Furthermore, the susceptibility can be represented by

$$\chi(w) = A_0^+ (1 - \mu w)^{-\gamma} + A_1^+ (1 - \mu w)^{-\gamma+1} \\ + A_0^- (1 + \mu w)^\phi + R(w), \quad (6.12)$$

where the constants A_0^+ , A_1^+ and A_0^- follow from the values of a and b determined from Tables XVIII(a) and (b), and $R(w)$ is a correction

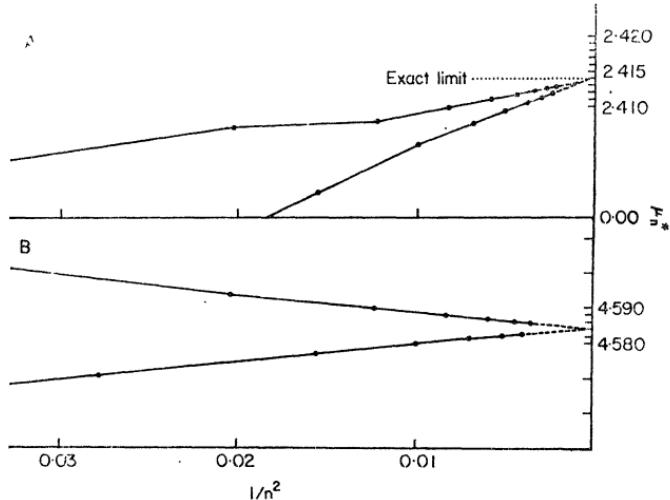


FIG. 9. Refined critical point estimates $\mu_n^* \equiv n\mu_n/(n+g)$ for the square (A) and simple cubic (B) $I(\frac{1}{2})$ lattices plotted versus $1/n^2$. (Square, $g = \frac{3}{4}$; simple cubic, $g = \frac{1}{4}$.) (Sykes and co-workers, unpublished.)

polynomial calculated from the exact coefficients of $\chi(w)$. Analogous results have been obtained for other loose-packed lattices. [Similar representations are obtained for close-packed lattices but with the term $A_0^- (1 + \mu w)^\phi$ missing.]

In the above calculations, all available information about the functional form of the susceptibility was used in estimating the critical point. However, even with less information, it is still possible to use Darboux's theorems to obtain estimates of the critical point. Let us assume, for example, that the antiferromagnetic critical exponent is not known. From the asymptotic form for μ_n^* given by (6.11), it follows immediately that we can reduce the effect of

the antiferromagnetic singularity by forming the sequence

$$\begin{aligned}\overline{\mu_n^*} &\equiv \frac{1}{2}(\mu_n^* + \mu_{n-1}^*) \\ &\approx \mu \left[1 + \frac{a}{n^2} + \frac{a'}{n^3} + (-1)^n \frac{b'}{n^{\phi+\gamma+1}} + \text{higher order terms} \right].\end{aligned}\quad (6.13)$$

The contribution of the antiferromagnetic singularity to $\overline{\mu_n^*}$ is reduced by a factor of $1/n$ compared to its contribution to μ_n^* . [An analogous result accounts for the comments made in connection with (2.26).] In Table II, values of $\overline{\mu_n^*}$ were listed for the simple cubic lattice and in Fig. 10 they are plotted against $1/n^2$. This graph is similar to Fig. 9(B) except that the two branches are now *much* closer together—notice the scales of Figs 9(B) and 10—reflecting the fact that the antiferromagnetic singularity has been considerably weakened. Extrapolating alternate $\overline{\mu_n^*}$ versus $1/n^2$ yields the sequence

| | |
|----|----------|
| 10 | 4.583811 |
| 11 | 4.584758 |
| 12 | 4.584006 |
| 13 | 4.584430 |
| 14 | 4.584064 |
| 15 | 4.584347 |
| 16 | 4.584167 |
| 17 | 4.584359 |

(6.14)

from which we estimate

$$\mu = 4.58425 \pm 0.00015 \quad (\omega_c = 0.218138 \pm 0.000007), \quad (6.15)$$

in excellent agreement with previous results.

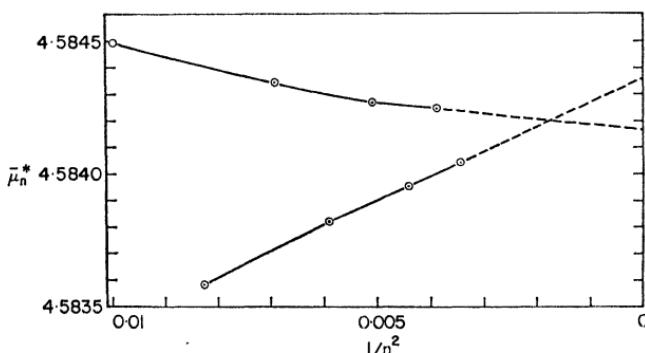


FIG. 10. Refined critical point estimates $\overline{\mu_n^*} \equiv \frac{1}{2}(\mu_n^* + \mu_{n-1}^*)$ for the simple cubic $I(\frac{1}{2})$ lattice plotted versus $1/n^2$.

D. Contour map method

As a final example, let us mention the application of Darboux's theorems to the "contour map" method. As originally developed (Guttmann *et al.*, 1968a, b), this method utilised the assumption that the ferromagnetic singularity factorizes, i.e. (6.3) and (6.7) were assumed valid but with $B(w) \equiv 0$. It then readily follows that the coefficients c_n in the series expansion of

$$A_m(w) \equiv (1 + \mu w)^m (1 - \mu w)^\gamma \chi(w) = \sum_{n=0}^{\infty} c_n (\mu w)^n, \quad (6.16)$$

where $m = 0, 1, 2, \dots$, will alternate in sign and decrease in magnitude for $m + \phi > -1$, and for n sufficiently large, i.e. for $n \geq M(m)$, where in general M is an increasing function of m . This observation suggests a criterion for determining possible values of w_c and γ , namely, the coefficients of $A_m(w)$ must alternate in sign and decrease in magnitude.

TABLE XVIII

Interference of the ferromagnetic and antiferromagnetic singularities of $\chi(w)$ for the square and simple cubic Ising lattices. (Sykes *et. al.*, 1972b.)

(a) Solution of $\mu_n^* = \mu \left[1 + \frac{a}{n^2} + (-1)^n \frac{b}{n^{11/4}} \right]$ from three points

| | | | | | Square |
|-------|----|----|---------|---------|---------------|
| Triad | | | a | b | $\mu = 1/w_c$ |
| 1 | 2 | 3 | -0.3047 | -0.2358 | 2.45491 |
| 2 | 3 | 4 | -0.0749 | -0.4133 | 2.37194 |
| 3 | 4 | 5 | -0.2854 | -0.5519 | 2.41161 |
| 4 | 5 | 6 | -0.2921 | -0.5473 | 2.41239 |
| 5 | 6 | 7 | -0.3659 | -0.5934 | 2.41823 |
| 6 | 7 | 8 | -0.2908 | -0.6409 | 2.41397 |
| 7 | 8 | 9 | -0.2302 | -0.6053 | 2.41138 |
| 8 | 9 | 10 | -0.3483 | -0.5356 | 2.41531 |
| 9 | 10 | 11 | -0.2770 | -0.4957 | 2.41341 |
| 10 | 11 | 12 | -0.3042 | -0.4805 | 2.41400 |
| 11 | 12 | 13 | -0.3186 | -0.4882 | 2.41426 |
| 12 | 13 | 14 | -0.2958 | -0.5004 | 2.41391 |
| 13 | 14 | 15 | -0.3171 | -0.5114 | 2.41419 |
| 14 | 15 | 16 | -0.3097 | -0.5151 | 2.41411 |
| 15 | 16 | 17 | -0.3117 | -0.5161 | 2.41413 |
| 16 | 17 | 18 | -0.3161 | -0.5140 | 2.41417 |
| 17 | 18 | 19 | -0.3146 | -0.5132 | 2.41416 |
| 18 | 19 | 20 | -0.3158 | -0.5126 | 2.41416 |
| 19 | 20 | 21 | -0.3177 | -0.5135 | 2.41418 |

For the close-packed lattices, $\chi(w)$ does not have a singularity at $w = -w_c$. However, the criterion can still be used if the product function $\chi(w)\chi(-w)$, which is singular at $w = -w_c$, is used instead of $\chi(w)$ in (6.16).

In practice, the method is applied as follows. Suppose one has the first N terms of the series expansion of $\chi(w)$, as well as trial values of w_c and γ , denoted by \bar{w}_c and $\bar{\gamma}$. Form the first N terms of the series expansion of $A_m(w)$, defined by (6.16), for a range of trial values \bar{w}_c and $\bar{\gamma}$, and for a range of values of m ($m = 0, 1, 2, \dots$). The factor $(1 + \mu w)^m$ accelerates the rate of convergence of the series if the exact w_c and γ are chosen, but amplifies any errors in the trial values \bar{w}_c and $\bar{\gamma}$. For each value of m , the last few terms of the series $A_m(w)$ must alternate in sign and decrease in magnitude. This requirement defines a closed region in the $\bar{w}_c - \bar{\gamma}$ plane, which includes the correct values of w_c and γ . The region so defined, for $m = r$ say, lies inside the region defined by $m = r - 1$, so that increasing the value of m results in narrower and narrower bounds on the possible values of w_c and γ . However, m cannot be increased indefinitely since when $M(m) > N$, the expected regularity cannot be observed with the available coefficients.

Typical results obtained in the above way are shown schematically in Fig. 11, which has the appearance of a contour map. It is clear that simultaneous bounds on w_c and γ may be obtained, and that if either w_c or γ

TABLE XVIII (continued)

(b) Solution of $\mu_n^* = \mu \left[1 + \frac{a}{n^2} + (-1)^n \frac{b}{n^{17/8}} \right]$ from three points

| Simple cubic | | | | | |
|--------------|----|----|---------|---------|---------------|
| Triad | | | a | b | $\mu = 1/w_c$ |
| 1 | 2 | 3 | -0.0493 | -0.0930 | 4.59917 |
| 2 | 3 | 4 | -0.0354 | -0.0991 | 4.58936 |
| 3 | 4 | 5 | -0.0645 | -0.1084 | 4.60004 |
| 4 | 5 | 6 | -0.0208 | -0.1314 | 4.58098 |
| 5 | 6 | 7 | -0.0116 | -0.1334 | 4.58236 |
| 6 | 7 | 8 | -0.0032 | -0.1306 | 4.58395 |
| 7 | 8 | 9 | -0.0065 | -0.1311 | 4.58422 |
| 8 | 9 | 10 | -0.0098 | -0.1306 | 4.58443 |
| 9 | 10 | 11 | -0.0069 | -0.1302 | 4.58428 |
| 10 | 11 | 12 | -0.0058 | -0.1303 | 4.58423 |
| 11 | 12 | 13 | -0.0051 | -0.1302 | 4.58421 |
| 12 | 13 | 14 | -0.0050 | -0.1303 | 4.58421 |
| 13 | 14 | 15 | -0.0065 | -0.1304 | 4.58424 |
| 14 | 15 | 16 | -0.0074 | -0.1303 | 4.58426 |
| 15 | 16 | 17 | -0.0089 | -0.1305 | 4.58429 |

is known exactly, the bounds on the other are considerably improved. As an example, we have applied the method to the first 17 terms of the $\chi(w)$ expansion for the simple cubic lattice (Sykes *et al.*, 1972b). We find that

$$\begin{aligned} 0.21800 < w_c < 0.21826, \quad 1.2386 < \gamma < 1.2596 \quad (m = 0), \\ 0.218121 < w_c < 0.218155, \quad 1.2484 < \gamma < 1.2512 \quad (m = 1). \end{aligned} \quad (6.17)$$

Assuming $\gamma = 1\frac{1}{4}$ leads to considerably narrower bounds on w_c , namely

$$\begin{aligned} w_c = 0.21814 \pm 0.00003 \quad (m = 0), \\ = 0.218140 \pm 0.000002 \quad (m = 1). \end{aligned} \quad (6.18)$$

These values are in excellent agreement with the estimates (2.27) and (3.23) obtained by the ratio and Padé approximant methods, respectively.

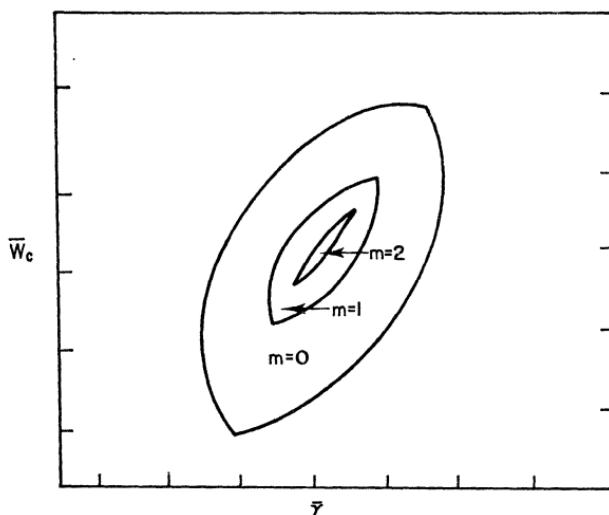


FIG. 11. Typical contour map of possible values of w_c and $\bar{\gamma}$ for successive values of m .

On setting $m = 2$, we find *no* values of $\bar{\gamma}$ and \bar{w}_c for which the coefficients of $A_m(w)$ alternate in sign and decrease in magnitude. The reason for this becomes clear if we relax the condition that the ferromagnetic singularity factorizes and consider instead that $B(w) \neq 0$ in (6.3). Then, assuming (6.7) as before, it can readily be shown that the coefficients of $A_m(w)$ alternate in sign and decrease in magnitude for

$$\min(m, m + \phi) < \gamma \quad (6.19)$$

if $B(w_c) \neq 0$. It is generally believed that for all three-dimensional loose-packed Ising lattices, $\gamma = 1\frac{1}{4}$ and $\phi = \frac{7}{8}$, so that condition (6.19) becomes $m < 1\frac{1}{4}$. This result is consistent with the above mentioned behaviour of the simple cubic lattice, which thus supports the belief that the ferromagnetic singularity of the high temperature susceptibility series does not factorize.

Further applications of the method are given by Guttmann *et al.* (1968b). However, some of the results there [notably those for which (6.19) is violated] should be discounted, since the series available at that time were too short for the non-factorizability of the physical singularity to manifest itself.

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5. Heisenberg Model

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I. Introduction

The basic Heisenberg model is defined by the Hamiltonian

$$\mathcal{H} = -2J_1 \sum_{\langle ij \rangle} \mathbf{s}_i \cdot \mathbf{s}_j - g\beta H \sum_i s_{zi}. \quad (1.1)$$

The suffices i and j refer to the sites of a crystal lattice: $\langle ij \rangle$ denotes a pair of neighbouring sites, each such pair being counted once only. \mathbf{s}_i is a spin operator at the site i , having components (s_{xi}, s_{yi}, s_{zi}) and satisfying commutation relations which may be written symbolically $\mathbf{s} \wedge \mathbf{s} = i\mathbf{s}$. J_1 is called the exchange energy between neighbouring spins: g is the gyromagnetic ratio, β the Bohr magneton, and H the external magnetic field. When, for any site, the maximum eigenvalue of s_{zi} is s , we speak of the Heisenberg model for spin s , denoted $H(s)$. The Hamiltonian still depends, of course, on the structure of the lattice; and we use the abbreviations f.c.c., b.c.c., s.c., p.t., and s.q. to denote those lattices to which we shall confine attention; namely, in three dimensions, the face-centred cubic, body-centred cubic and simple cubic, and, in two dimensions, the plane triangular and simple quadratic lattices. If the exchange operator $\mathbf{s}_i \cdot \mathbf{s}_j$ is replaced by $s_{zi}s_{zj}$ we have the corresponding Ising model, denoted $I(s)$. (See Domb this volume Chapter 6.)

For the purposes of this Chapter, (1.1) simply defines a mathematical model to be studied, for its own interest, by the method of high temperature expansions. But historically this Hamiltonian stems from the work of Heisenberg (1928) and Dirac (1929), and was first extensively used in the theory of magnetism by Van Vleck (1932). It has some theoretical validity for at any rate certain nonconducting magnetic materials; though the nearest-neighbour exchange forces may need to be supplemented by second-neighbour exchange forces. High temperature expansions have also been made including second-neighbour interactions, and in describing this work we shall use J_2 to denote the second-neighbour exchange energy. For assessing the theoretical background to (1.1), reference should be made to articles by Stevens (1963) and Anderson (1963).

There is one important respect in which the models $H(s)$ and $I(s)$ are alike. In the ferromagnetic case, that is when J_1 is positive, the ground-state energy is, in both cases,

$$-2J_1ls^2 - g\beta HNs, \quad (1.2)$$

where l is the number of nearest-neighbour pairs, and N the number of sites. For a lattice of coordination number q , this means that in the absence of an external field the ferromagnetic energy change from low to high temperatures (when the spins are uncoupled) is given by

$$\Delta E_F = NqJ_1s^2. \quad (1.3)$$

If we write this as $\frac{1}{2}NqJ$, where $J = 2J_1s^2$, then all the ferromagnetic models have the same ΔE_F "per bond", namely J . Likewise the saturation magnetisation in an external field at limitingly low temperatures is, in both cases, $Ng\beta s$, which, for comparing model with model, is conveniently written Nm . With these changes, (1.1) becomes

$$\mathcal{H} = -\frac{J}{s^2} \sum_{\langle ij \rangle} \mathbf{s}_i \cdot \mathbf{s}_j - \frac{mH}{s} \sum_i s_{zi}. \quad (1.4)$$

This form for the Hamiltonian dates, as far as high temperature expansions are concerned, from early work by Domb and Sykes (1957a, 1962). It has been used (though with J replaced by J' , which avoids confusion with the usual definition of exchange energy) in useful review articles, relating theory and experimental measurements, by Domb and Miedema (1964) and Wielinga (1970); see also Domb (1970). But, while having much to commend it, the form of Hamiltonian (1.4) by no means provides a panacea for effecting comparisons between models having different values of s ; if only because for $H(s)$ the Curie constant and paramagnetic Curie temperature are proportional to $s(s+1)$ and not to s^2 .

While still discussing the Hamiltonian, we should refer to the case of limitingly large s . Writing $s/s = t$ and letting $s \rightarrow \infty$, so that t is a unit vector (the components of which commute), (1.4) becomes

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \mathbf{t}_i \cdot \mathbf{t}_j - mH \sum_i t_{zi}. \quad (1.5)$$

This defines the "classical" Heisenberg model, (Stanley, this volume Chapter 7) which we denote by $H(\infty)$. We shall, however, write (1.5), in analogy with (1.1), as

$$\mathcal{H} = -2J_1 \sum_{\langle ij \rangle} \mathbf{t}_i \cdot \mathbf{t}_j - g\beta H \sum_i t_{zi}, \quad (1.6)$$

even though the symbols J_1 and $g\beta$ do not now have their normal physical meanings. Most high temperature work on the classical Heisenberg model

has, in fact, been based on this latter form for the Hamiltonian. We shall always use x to denote the high temperature expansion parameter J_1/kT , whether J_1 relates to (1.1) or (1.6). T denotes the absolute temperature, and k is Boltzmann's constant. In particular, x_c will denote J_1/kT_c , where T_c is the ferromagnetic Curie temperature.

Mathematically, the Hamiltonian for $H(s)$ differs from that for $I(s)$ in that (i) the individual operators do not commute and (ii) the exchange term has spherical symmetry, i.e. is isotropic. These, apparently small, changes have profound physical consequences. Before discussing the derivation of high temperature expansions, we must refer briefly to the three most important of these. They relate, respectively, and in historical sequence, to low temperature behaviour, antiferromagnetic ordering, and the properties of two-dimensional lattices.

Low temperature excitations for the Heisenberg model have to be handled by spin-wave theory, and there are no expansions involving discrete energy steps as there are for the Ising model. For the theory of spin waves, reference should be made to the article by Keffer (1966). Here we can only summarise a few results for the ferromagnetic case. In 1930, Bloch showed that the zero-field, or spontaneous magnetisation, $M(0)$, and the corresponding

TABLE I. Coefficients in eqns (7), (8), (9) and (10) for $H(\frac{1}{2})$

| | f.c.c. | b.c.c. | s.c. |
|--------|------------------------|------------------------|------------------------|
| a_1 | 2.932×10^{-2} | 5.863×10^{-2} | 1.173×10^{-1} |
| a_2 | 1.411×10^{-3} | 4.233×10^{-3} | 1.129×10^{-2} |
| a_3 | 1.85×10^{-4} | 8.68×10^{-4} | 3.26×10^{-3} |
| a_4 | 1.12×10^{-4} | 7.21×10^{-4} | 4.44×10^{-3} |
| b_1 | 2.822×10^{-2} | 5.644×10^{-2} | 1.129×10^{-1} |
| b_2 | 5.19×10^{-3} | 1.557×10^{-2} | 4.151×10^{-2} |
| b_3 | 1.37×10^{-3} | 6.40×10^{-3} | 2.404×10^{-2} |
| b_4 | 2.87×10^{-4} | 1.85×10^{-3} | 1.140×10^{-2} |
| a'_1 | 2.36×10^{-1} | 2.34×10^{-1} | 2.55×10^{-1} |
| a'_2 | 4.6×10^{-2} | 4.3×10^{-2} | 4.1×10^{-2} |
| a'_3 | 2.4×10^{-2} | 2.2×10^{-2} | 2.0×10^{-2} |
| a'_4 | 2.9×10^{-2} | 2.9×10^{-2} | 3.5×10^{-2} |
| b'_1 | 2.27×10^{-1} | 2.25×10^{-1} | 2.45×10^{-1} |
| b'_2 | 1.67×10^{-1} | 1.56×10^{-1} | 1.51×10^{-1} |
| b'_3 | 1.77×10^{-1} | 1.62×10^{-1} | 1.47×10^{-1} |
| b'_4 | 7.4×10^{-2} | 7.4×10^{-2} | 9.0×10^{-2} |

specific-heat, $C(0)$, both deviate, for three-dimensional lattices, from their values at $T = 0$ by terms proportional to $T^{3/2}$. Since the work of Dyson (1965a, b), we have known that at sufficiently low temperatures we may write in fact

$$\frac{Nm - M(0)}{Nm} = a_1 \theta^{3/2} + a_2 \theta^{5/2} + a_3 \theta^{7/2} + a_4 \theta^4 + \dots \quad (1.7)$$

and

$$\frac{C(0)}{Nk} = b_1 \theta^{3/2} + b_2 \theta^{5/2} + b_3 \theta^{7/2} + b_4 \theta^4 + \dots \quad (1.8)$$

where $\theta \equiv kT/J_1$ and the coefficients a_i and b_i depend both on the lattice and the values of s . For the particular case $s = \frac{1}{2}$, the values of the coefficients in (1.7) and (1.8), for the f.c.c., b.c.c., and s.c. lattices, are listed in Table I.

For some purposes it is more convenient to have these series in the form

$$\frac{Nm - M(0)}{Nm} = a'_1 \left(\frac{T}{T_c}\right)^{3/2} + a'_2 \left(\frac{T}{T_c}\right)^{5/2} + a'_3 \left(\frac{T}{T_c}\right)^{7/2} + a'_4 \left(\frac{T}{T_c}\right)^4 + \dots \quad (1.9)$$

and

$$\frac{C(0)}{Nk} = b'_1 \left(\frac{T}{T_c}\right)^{3/2} + b'_2 \left(\frac{T}{T_c}\right)^{5/2} + b'_3 \left(\frac{T}{T_c}\right)^{7/2} + b'_4 \left(\frac{T}{T_c}\right)^4 + \dots, \quad (1.10)$$

to obtain which, of course, we must know the appropriate values of x_c . Adopting the values suggested by high temperature susceptibility expansions, namely x_c (f.c.c.) = 0.249, x_c (b.c.c.) = 0.397 and x_c (s.c.) = 0.596, we obtain the a' and b' values also listed in Table I. These are limited to only three figures, and any subsequent modifications in the values for x_c are unlikely to change them significantly.

The coefficients we have listed are the values for $s = \frac{1}{2}$. For general spin, s , the coefficients of $\theta^{3/2}$, $\theta^{5/2}$ and $\theta^{7/2}$ in equation (1.7) have to be divided by $(2s)^{5/2}$, $(2s)^{7/2}$ and $(2s)^{9/2}$, respectively, and those in eqn (1.8) by $(2s)^{3/2}$, $(2s)^{5/2}$ and $(2s)^{7/2}$. The dependence of a_4 and b_4 on s is more complicated, though essentially they are reduced by factors $(2s)^6$ and $(2s)^4$. But we should observe that these formulae no longer make sense in the classical limit, $s \rightarrow \infty$. For, as we shall see, for large s (and fixed J_1) T_c is effectively proportional to s^2 . Thus the above rules give a'_1 proportional to $s^{1/2}$ for large s , which is nonsense when $s \rightarrow \infty$. The reason is that the range of validity of these spin-wave expansions shrinks to zero as $s \rightarrow \infty$. For them to be valid we require $T/T_c \ll 1/s$. In the spin- $\frac{1}{2}$ case they are generally regarded as useful up to $T \sim \frac{1}{2}T_c$.

Before giving the corresponding results, though in less detail, for the classical model, $H(\infty)$, it should be commented that these spin-wave expansions have a status different from that of the high temperature expansions with which we are primarily concerned. Their derivation depends on assumptions which are completely valid at sufficiently low temperatures, but cease to be valid at higher temperatures. We refer to the ignoring of bound states and kinematic interactions between spin waves, and the use of asymptotic expansions in handling mathematical integrals. For this reason, they should not be regarded as power-series expansions in $T^{1/2}$; they are more properly regarded as asymptotic expansions.

For the classical model, $H(\infty)$, the leading term in the low temperature dependence of both $M(0)$ and $C(0)$ is linear in T . The earliest discussion of the classical case was by Heller and Kramers (1934): the most recent, and thorough, is that of Loly (1970). For the saturation magnetisation we have

$$\frac{Nm - M(0)}{Nm} = a\theta + \dots = a'\left(\frac{T}{T_c}\right) + \dots \quad (1.11)$$

where for the f.c.c., b.c.c., and s.c. lattices, a equals 5.603×10^{-2} , 8.708×10^{-2} and 1.264×10^{-1} , respectively. Introducing modern estimates of x_c , from high temperature susceptibility series, namely 0.1575, 0.2435 and 0.347 we infer values of a' equal to 0.356, 0.358 and 0.364. Later terms in (1.11) involve successively higher positive integer powers of θ .

The zero-field specific heat, $C(0)$, is also linear in T , for small T ; but it starts at the value Nk rather than at the value zero. This is an unphysical feature of the classical Heisenberg model, as was observed by Fisher (1964) in his solution of the $H(\infty)$ problem for the linear chain.

Finally, before leaving spin waves, we must draw attention to the divergence, for three-dimensional lattices, of the zero-field susceptibility, $\chi(0)$; see Fisher (1967a); Vaks *et al.*, (1968). If $M(H, T)$ denotes the equilibrium magnetisation in field H at temperature T , so that $M(0, T)$ or, more accurately, $M(0+, T)$, is what we have hitherto called $M(0)$, then spin-wave theory gives

$$M(H, T) = M(0, T) + H^{1/2} M_1(T) + \dots, \quad (1.12)$$

so that, as $H \rightarrow 0$, χ diverges as $H^{-1/2}$. This is a consequence of even the first order Bloch theory. Essentially, the leading term in the free-energy, F , which produces the $T^{3/2}$ laws, has as a factor $Z_{5/2}(g\beta H/kT)$ where

$$Z_n(x) = \sum_{j=1}^{\infty} j^{-n} e^{-jx}. \quad (1.13)$$

Differentiating twice with respect to H , to find χ , yields a term proportional to $Z_{\frac{1}{2}}(g\beta H/kT)$. Thus, for any fixed T , we are faced with the sum

$$\sum_{j=1}^{\infty} \frac{e^{-cjH}}{j^{1/2}} \quad (1.14)$$

where c is a constant. Putting $cjH = y$, for sufficiently small H we can replace the sum by an integral; (1.14) then becomes

$$\frac{1}{(cH)^{1/2}} \int_0^{\infty} \frac{e^{-y}}{y^{1/2}} dy, \quad (1.15)$$

which diverges as $H^{-1/2}$ as $H \rightarrow 0$. Loly observes that one is equally faced with divergent integrals in the classical case.

We turn now to the antiferromagnetic problem, defined by (1.1) when $J_1 < 0$. As is well known, in the Ising case, for open lattices (such as the body centred cubic lattice) which can be divided into two equivalent interpenetrating sublattices, there is a symmetry which implies that the antiferromagnetic ordering temperature, or Néel temperature, occurs at the same value of $kT/|J_1|$ as would the Curie temperature were J_1 positive. In terms of the "staggered" susceptibility, defined with respect to a field H which has opposite directions on the two sublattices, the staggered susceptibility for the Ising antiferromagnetic is the same function of $kT/|J_1|$ as is the physical susceptibility for the Ising ferromagnetic. This is not true of the corresponding Heisenberg models, except in the classical limit, $s \rightarrow \infty$. Essentially, this is because whereas $s_{z1} + s_{z2}$ commutes with $\mathbf{s}_1 \cdot \mathbf{s}_2$, $s_{z1} - s_{z2}$ does not.

For just the same reason, the antiferromagnetic energy change, ΔE_A , from low to high temperatures is not given by eqn (1.3) with J_1 replaced by $|J_1|$. Indeed, the energy of the antiferromagnetic ground state is known exactly only for the $H(\frac{1}{2})$ linear chain problem, for which Hulthen (1938) proved that $\Delta E_A = 0.8863N|J_1|$, in contrast to $\Delta E_F = 0.5NJ_1$: see Mattis (1965). For other spin values and other lattices, ΔE_A is known only approximately (though fairly accurately); see Anderson (1952), Lidiard (1954). The trouble is that the spin state corresponding to alternate "up" and "down" spins is not an eigenstate of the Heisenberg Hamiltonian. Fortunately, however, neutron scattering measurements show that spin arrangements in antiferromagnetic crystals frequently do, in fact, approximate closely to the semi-classical pictures suggested, for example, by mean-field theories. This implies that the staggered susceptibilities, which are particular cases of the generalized susceptibility $\chi(\mathbf{k})$, may be expected to diverge at the Néel temperature appropriate to their particular type of ordering. $\chi(\mathbf{k})$, for any \mathbf{k} ,

can, of course, be obtained from neutron scattering experiments. For mean field theories, see Smart (1966); for types of spin ordering in ionic crystals, see Bertaut (1963); for neutron scattering by magnetic crystals, and the definition of $\chi(\mathbf{k})$, see de Gennes (1963) and Marshall and Lowde (1968).

As we have said, the third main difference between the Ising and Heisenberg models relates to the properties of two-dimensional lattices. For $I(\frac{1}{2})$, the exact solutions, due primarily to Onsager, for the zero-field specific heat and the magnetic phase boundary, $M(0, T)$ as a function of T , not only provide a firm framework against which we may judge the reliability of approximate treatments, including the use of series expansions, but conclusively establish the existence of ferromagnetic behaviour in these two-dimensional cases. For the Heisenberg model, however, we now know that there is no such ferromagnetic behaviour, for a planar lattice. This was strongly suggested by spin-wave theory, which in two dimensions is beset with divergent integrals. It was established rigorously by Mermin and Wagner (1966), who used basic inequalities to obtain

$$M < \frac{\text{constant}}{T^{1/2}} \cdot \frac{1}{|\ln H|^{1/2}} \quad (1.16)$$

Equation (1.16) shows that, for any finite T , $M \rightarrow 0$ as $H \rightarrow 0$; i.e. a two-dimensional Heisenberg model cannot exhibit spontaneous magnetisation. This holds for any value of s , including the classical limit: it is a consequence of the isotropy of the Heisenberg exchange term in the spin Hamiltonian. Mermin and Wagner's result does not, of course, rule out odd, even divergent, behaviour in the paramagnetic susceptibility; and it tells us nothing about the specific heat. We shall, in due course, comment in some detail on the apparent behaviour of high temperature susceptibility series for two-dimensional lattices.

Before closing this lengthy, but necessary, introduction, mention must be made of some very general properties which the Heisenberg models are now known to share with their Ising counterparts. All these Hamiltonians, for interactions of finite range, fall within the class for which Griffiths (1964) has proved that the free energy, defined from the partition function, Z , possesses the extensive property associated with normal thermodynamics: put crudely, for large N , F is proportional to N . Moreover, it has recently been shown, by Asano (1970a, b) for $H(s)$, and by Suzuki and Fisher (1971) for rather more general models, that, in the ferromagnetic case, these models have the property established for $I(\frac{1}{2})$ by Lee and Yang (1952), and for $I(s)$ by Griffiths (1969), namely that the zeros of Z , regarded as a function of $e^{H/kT}$, lie on the circle $|e^{H/kT}| = 1$. This implies that, at fixed T , thermodynamic functions are analytic functions of H , provided H is finite. (For a general discussion of these points, see Griffiths Vol. 1, Chapter 2.) Baker (1970) has

commented that, at least for $s = \frac{1}{2}$, an analytic result of Ginibre (1968) then ensures the validity of the theorem proved for $I(\frac{1}{2})$ by Lebowitz and Penrose (1968), namely that thermodynamic functions are necessarily analytic functions of T , near the real T axis, except when $H = 0$. These formal results not only establish that the Heisenberg ferromagnetic models behave as one intuitively, but uncritically, supposes ferromagnetic models should behave, but can also be made the basis for quantitative statements regarding critical exponents and approximations to thermodynamic functions (Baker, 1970).

Against this background, we now enter the proper territory of this Chapter: the derivation of high temperature expansions and a survey of conclusions which have been drawn from them.

II. Derivation of High Temperature Expansions

The series with which we are concerned have all been derived by one or other of three basic methods, which we shall call the moment method, the cumulant method, and the finite cluster method (see also Domb, this volume Chapter 1). A fourth method has also been used, by Wortis and coworkers, for deriving these expansions in the case of $H(\infty)$. This is a generalisation of the Horwitz and Callen (1961) approach to the Ising model, and has so far been effectively developed only for commuting operators. We shall not discuss it here, despite its power and elegance, since it is the subject of a separate survey (this volume, Chapter 3). We shall, of course, refer to coefficients which have been obtained by means of it; and give appropriate references at that time. Actually, it is only for correlation functions, and for mixed Heisenberg–Ising classical Hamiltonians, that the series so obtained are as yet appreciably more extensive than those found by the three basic methods of this chapter.

The moment, or Kramers–Opechowski, method derives from the foundation paper on high-temperature expansions for $H(\frac{1}{2})$ by Opechowski (1937). The account here, however, will follow, with some minor modifications, that given by Rushbrooke and Wood (1958) in dealing with the more general problem $H(s)$: for Opechowski's method of handling the magnetic field, H , is necessarily restricted to the case $s = \frac{1}{2}$. The basic formula of the cumulant method was first derived, for $I(\frac{1}{2})$, by Brout (1959). A particularly clear exposition was later given by Horwitz and Callen, in the paper to which we have already referred. The exposition adopted here, for non-commuting operators, is a modification of that by Rushbrooke (1964): the present approach owes something to a paper by Englert (1963). The finite cluster method, proposed originally by Domb (1960), follows immediately once the cumulant method is established: see Striebel *et al.* (1963), Rushbrooke, (1964), Sykes *et al.* (1966), Jasnow and Wortis (1967). In practice, for computational purposes, this method is restricted to the case

$s = \frac{1}{2}$: for which it has produced the longest series yet derived. Only the moment method has been used for general spin: though in fact, computationally, there is little to choose between this and the cumulant method.

A. The moment method

It is convenient to write

$$\sum_{\langle ij \rangle} \mathbf{s}_i \cdot \mathbf{s}_j \equiv P, \quad \sum_i s_{zi} \equiv Q, \quad (2.1)$$

so that $\mathcal{H} = -2J_1(P + \alpha Q)$ where $\alpha = g\beta H/2J_1$. Then the basic formulae of statistical mechanics read

$$\begin{aligned} F(H, T) &= -kT \ln Z \\ &= -kT \ln \text{Tr} \exp [2(P + \alpha Q)x] \end{aligned} \quad (2.2)$$

where $x \equiv J_1/kT$, and the trace refers to a matrix representation of the operators concerned: more precisely, the direct product of the irreducible matrix representations of the spin operators \mathbf{s}_i . Since this is of dimension $(2s + 1)^N$, where N is the number of lattice sites, we have

$$\ln Z = N \ln (2s + 1) + \ln \left[1 + \sum_{n \geq 1} \frac{2^n x^n}{n!} \mu_n \right] \quad (2.3)$$

$$= N \ln (2s + 1) + \sum_{n \geq 1} \frac{2^n x^n}{n!} \lambda_n \quad (2.4)$$

where

$$\mu_n = \frac{\text{Tr}(P + \alpha Q)^n}{(2s + 1)^N} \equiv \langle (P + \alpha Q)^n \rangle \quad (2.5)$$

and the λ 's are related to the μ 's as are cumulants to moments in the theory of statistics; i.e.

$$\left. \begin{aligned} \lambda_1 &= \mu_1 \\ \lambda_2 &= \mu_2 - \mu_1^2 \\ \lambda_3 &= \mu_3 - 3\mu_1\mu_2 + 2\mu_1^3 \\ \lambda_4 &= \mu_4 - 4\mu_3\mu_1 - 3\mu_2^2 + 12\mu_2\mu_1^2 - 6\mu_1^4 \end{aligned} \right\} \quad (2.6)$$

We note that $\lambda_n = \mu_n + (\text{nonlinear combinations of } \mu\text{'s})$. Ignoring boundary effects,[†] we shall find that the μ 's contain terms in $N, N^2 \dots$, with

[†] In language to be introduced later, we require the lattice-count of any (finite) connected interaction graph to be strictly proportional to N . One way of achieving this is by artificially imposing periodic boundary conditions. Alternatively, we can mentally recognise that besides " N " terms there are "S" terms, i.e. surface corrections, and deliberately ignore the latter. The present argument is essentially heuristic: mathematical rigour is easily provided on the basis of the Brout expansion (see Section C below).

no terms independent of N , whereas the λ 's contain terms in N only. This must be so, since the free-energy, F , is an extensive thermodynamic property (and its verification provides a check on any actual calculation). Thus

$$\lambda_n = N \text{ [coefficient of } N \text{ in } \mu_n], \quad (2.7)$$

and if we write, from (2.5),

$$\mu_n = \mu_n^{(0)} + \alpha \mu_n^{(1)} + \alpha^2 \mu_n^{(2)} + \dots \quad (2.8)$$

then

$$\lambda_n = \lambda_n^{(0)} + \alpha \lambda_n^{(1)} + \alpha^2 \lambda_n^{(2)} + \dots \quad (2.9)$$

where

$$\lambda_n^{(s)} = N \text{ [coefficient of } N \text{ in } \mu_n^{(s)}]. \quad (2.10)$$

Essentially, we are using the equation

$$f(x) = \frac{d}{dN} \exp Nf(x) \text{ at } N = 0.$$

Since

$$C_H = \left(\frac{\partial E}{\partial T} \right)_H \quad \text{where } E = kT^2 \frac{\partial}{\partial T} \ln Z$$

and

$$\chi = \left(\frac{\partial M}{\partial H} \right)_T \quad \text{where } M = kT \frac{\partial}{\partial H} \ln Z$$

we have

$$C_H = k x^2 \frac{\partial^2}{\partial x^2} \ln Z \quad (2.11)$$

and

$$\chi = \left(\frac{g\beta}{2J_1} \right)^2 kT \frac{\partial^2}{\partial \alpha^2} \ln Z. \quad (2.12)$$

Particularising to the case $H = 0$, (2.11) becomes

$$C(0) = k \sum_{n \geq 2} \frac{2^n}{(n-2)!} \lambda_n^{(0)} x^n \quad (2.13)$$

and (2.12) becomes

$$\frac{\chi(0)kT}{g^2 \beta^2} = \lambda_2^{(2)} + \sum_{n \geq 1} \frac{2^{n+1}}{(n+2)!} \lambda_{n+2}^{(2)} x^n. \quad (2.14)$$

Moreover, since the trace of any single component of spin is zero,

$$\lambda_2^{(0)} = \mu_2^{(0)} = \langle P^2 \rangle = \frac{1}{3} N q X^2 \quad (2.15)$$

$$\lambda_2^{(2)} = \mu_2^{(2)} = \langle Q^2 \rangle = \frac{1}{3} N X, \quad (2.16)$$

where $X \equiv s(s + 1)$, and the final equalities in (2.15) and (2.16) are readily established.

Since P and Q commute,

$$\mu_{n+2}^{(2)} = \frac{(n+2)(n+1)}{2} \langle P^n Q^2 \rangle. \quad (2.17)$$

Consequently (2.13) and (2.14) become,

$$\frac{C(0)}{Nk} = \frac{2}{3}qX^2x^2 \left[1 + \sum_{n \geq 1} c_n x^n \right] \quad (2.18)$$

and

$$\frac{\chi(0)kT}{Ng^2\beta^2} = \frac{1}{3}X \left[1 + \sum_{n \geq 1} a_n x^n \right], \quad (2.19)$$

where

$$c_n = \frac{6}{qX^2} \frac{2^n}{n!} \{ \text{coefficient of } N \text{ in } \langle P^{n+2} \rangle \} \quad (2.20)$$

and

$$a_n = \frac{3}{X} \frac{2^n}{n!} \{ \text{coefficient of } N \text{ in } \langle P^n Q^2 \rangle \}. \quad (2.21)$$

Before proceeding to analyse these expressions in terms of interaction graphs, we note for future reference the equations, valid for $H = 0$ only, and equivalent to (2.18),

$$\frac{E_\infty - E(T)}{NkT} = \frac{2}{3}qX^2x^2 \sum_{n \geq 0} \frac{c_n x^n}{n+1} \quad (2.22)$$

$$\frac{S_\infty - S(T)}{Nk} = \frac{2}{3}qX^2x^2 \sum_{n \geq 0} \frac{c_n x^n}{n+2} \quad (2.23)$$

and

$$\frac{1}{N} \ln Z = \ln(2s+1) + \frac{2}{3}qX^2x^2 \sum_{n \geq 0} \frac{c_n x^n}{(n+1)(n+2)}. \quad (2.24)$$

In (2.22), (2.23) and (2.24), $c_0 = 1$. E_∞ and S_∞ are the high-temperature limits of E and S : and (2.24) assumes these to be 0 and $Nk \ln(2s+1)$, respectively.

There is considerable diversity in the literature regarding notation for specific-heat coefficients, and we have here adopted the convention that c_1 introduces the first correction to the limitingly high-temperature behaviour of $C(0)$, just as a_1 introduces the first correction to the limitingly high-temperature behaviour of $\chi(0)$. And while the zero-field free energy may be mathematically more fundamental than the zero-field specific heat, it is the latter which is measured experimentally and which, by analogy with

the Ising case, may be expected to show dramatically singular behaviour at the critical point. We have therefore regarded the c 's as the zero-field thermal coefficients in which we are primarily interested.

Returning now to eqns (2.20) and (2.21), we see that we have to be able to evaluate expressions of the form $\langle P^n \rangle$ and $\langle P^n Q^2 \rangle$. Consider first $\langle P^n \rangle$, and introduce the shorthand notation (ij) for $s_i \cdot s_j$. Then we are faced with

$$\left[\sum_{\langle ij \rangle} (ij) \right]^n. \quad (2.25)$$

Any term in the expansion of (2.25) can be represented by an interaction graph localised on the lattice: but this is not a one-one correspondence. For example, if $n = 5$, when there are 5 successive factors in (2.25), the ten possible terms $(12)(12)(23)(23)(23)$, $(12)(23)(12)(23)(23)$, $(12)(23)(23)(12)(23)$, $(12)(23)(23)(23)(12)$, $(23)(12)(12)(23)(23)$, $(23)(12)(23)(12)(23)$, $(23)(23)(12)(23)$, $(23)(12)(23)(23)(12)$, $(23)(23)(12)(23)(12)$ and $(23)(23)(23)(12)(12)$, each with unit weight, would all correspond to the interaction-graph

$$\overline{\overline{1}} \quad \overline{\overline{\overline{2}}} \quad \overline{\overline{\overline{3}}}. \quad (2.26)$$

Quite generally, P^n will give rise to localised interaction graphs of order n , each graph, which is not necessarily a connected graph, having a total of n bonds, connecting neighbouring lattice sites, where any pair of neighbouring sites may be connected by more than one bond. If k bonds connect the same two sites we shall speak of a bond of multiplicity k . If the multiplicities of the bonds of the interaction graph are $k_1, k_2 \dots$, where, of course,

$$\sum_s k_s = n, \quad (2.27)$$

then the number of terms in the expansion of P^n which correspond to this (localised) graph is

$$\frac{n!}{\prod_s k_s!}. \quad (2.28)$$

We shall define the *mean trace* of a localised, or vertex-labelled, interaction graph as the trace of the sum of all the different products of (ij) operators which correspond to this graph, divided by the number of terms in the sum. In the example above, this is the sum of the traces of the products there written down explicitly, divided by ten. Now $\langle P^n \rangle$ does not just involve mean traces of products of (ij) operators; we have to remember the factor $(2s + 1)^N$ in the denominator of (2.5), and that we are working in a representation which refers to the direct-product of N $(2s + 1)$ -dimensional

manifolds, one associated with each lattice site. Since the trace of the direct product of two matrices is the product of their traces, and since any site not among the vertices of the interaction graph is associated with a unit operator, we shall have a factor $(2s + 1)$ in the numerator of (2.5) for each site not involved in the interaction-graph. Thus it is the mean trace defined above divided by $(2s + 1)^m$, where m is the number of vertices of the interaction-graph, which enters into $\langle P^n \rangle$; and we call this the *mean reduced trace*. For any graph, g , we shall use the symbol $\langle g \rangle$ to stand for this mean reduced trace. Then, from (2.5), (2.25) and (2.28),

$$\langle P^n \rangle = \sum_g n! w_g \langle g \rangle, \quad (2.29)$$

where

$$w_g \equiv 1 / \prod_s k_s! \quad (2.30)$$

and g runs over all localised interaction graphs of order n on the lattice, L .

We pause to comment on the use of $\langle \cdot \rangle$'s to denote mean reduced traces, since this convention differs from one used earlier by Rushbrooke and Wood (1963). The present usage has three merits, (i), it is equally appropriate for commuting and non-commuting operators; (ii), it facilitates the presentation of general theory, in particular the passage from the moment to the cumulant method; and (iii), it enables certain lemmas, regarding the traces of particular types of graphs, to be written very concisely. These advantages stem from two features of mean reduced traces which it is convenient to point out here, even though we shall not immediately make use of them.

First, $\langle g \rangle$ can be found by labelling the n bonds of g with n distinct symbols, $\alpha, \beta \dots \omega$; writing down $\sum_p \alpha \beta \dots \omega$, where \sum_p denotes summation over all $n!$ permutations, interpreting each term as a product of (ij) factors according to the vertex labels of g , and then using the equation

$$(2s + 1)^m \langle g \rangle = \frac{1}{n!} \text{Tr} \sum_p \alpha \beta \dots \omega. \quad (2.31)$$

Secondly, if g comprises two disconnected parts, g_1 and g_2 , of orders n_1 and n_2 , then, line-labelling these with the symbols $\alpha_1, \beta_1, \dots \omega_1$ and $\alpha_2, \beta_2, \dots \omega_2$, respectively, since

$$\text{Tr} \sum_p \alpha_1 \dots \omega_2 = \frac{n!}{n_1! n_2!} \left(\text{Tr} \sum_p \alpha_1 \dots \omega_1 \right) \left(\text{Tr} \sum_p \alpha_2 \dots \omega_2 \right), \quad (2.32)$$

we have the important result†

$$\langle g_1 + g_2 \rangle = \langle g_1 \rangle \langle g_2 \rangle. \quad (2.33)$$

† This was stated carelessly by Rushbrooke and Wood (1958), but used correctly.

After this brief digression, we return to eqn (2.29) and observe that the labels at the vertices of the interaction-graph g , (1, 2 and 3 in the example above), do not affect the value of $\langle g \rangle$. All topologically identical graphs will yield the same trace. We therefore now classify the terms in $\langle P^n \rangle$ not according to localised graphs, but according to non-localised graphs (without vertex labels). For example, when $n = 5$, the graph

$$\text{=====} \quad (2.34)$$

corresponds to all terms of the type $(ij)^2(kl)^3$, and permutations of these symbols, where no two of i, j, k, l are allowed to be equal.

If g denotes an unlabelled interaction graph, we define N_g^L as the term linear in N in the number of times that this graph can be localised on the lattice, L , of N sites, when N is regarded as so large that boundary effects can be ignored. Then, in place of (2.29), we have

$$\text{term linear in } N \text{ in } \langle P^n \rangle = \sum_g n! w_g \langle g \rangle N_g^L \quad (2.35)$$

where g runs over all topologically distinct, unlabelled, interaction-graphs of order n .

We shall have to say more about the actual calculation of $\langle g \rangle$ and N_g^L ; but defer this, and proceed to the corresponding equation for $\langle P^n Q^2 \rangle$.

In place of (2.25), we now have

$$\left[\sum_{\langle ij \rangle} (ij) \right]^n \left[\sum_i (i) \right]^2, \quad (2.36)$$

where (i) stands for s_{zi} . Thus, besides the factors previously represented by localised interaction graphs of order n , we now have two (i) symbols, which we represent by crosses. There are two types of term: those involving $(i)(j) + (j)(i) = 2(i)(j)$ since (i) and (j) commute, and those involving $(i)^2$. We indicate the corresponding interaction graphs by g^{++} and g^* , referring to $*$ as a double-cross. Then, by precisely the same arguments as we have already had, from (2.21),

$$Na_n = \frac{3}{X} 2^n \left\{ \sum_{g^{++}} 2w_g \langle g^{++} \rangle N_{g^{++}}^L + \sum_{g^*} w_g \langle g^* \rangle N_{g^*}^L \right\}, \quad (2.37)$$

where $\langle g^{++} \rangle$ and $\langle g^* \rangle$ denote mean reduced traces, the mean being with respect to all permutations of the (ij) factors, keeping the s_{zi} factors to the right-hand side; and the reduction with respect to all vertices in g^{++} or g^* . The sums are over all topologically distinguishable n th order interaction graphs of types g^{++} or g^* . As in the case of (2.29), these graphs are not

necessarily connected and $N_{g^{++}}^L$, $N_{g^*}^L$ represent the parts proportional to N in the corresponding occurrence, or localisation, factors.

With the definitions (2.1) P and Q commute, and we explicitly used this fact in invoking (2.17) to pass from (2.14) to (2.21). It is useful to consider also the formula corresponding to (2.37) when P and Q , while still having the forms

$$P = \sum_{\langle ij \rangle} (ij) \quad \text{and} \quad Q = \sum_i (i) \quad (2.38)$$

do not commute. In place of (2.17), we now have

$$\mu_{n+2}^{(2)} = \frac{\text{Tr} (\text{sum of all distinguishable sequences of } n \text{ } P\text{'s and } 2 \text{ } Q\text{'s})}{(2s + 1)^N}$$

$$\equiv \frac{(n+2)!}{n! 2!} \{P^n Q^2\} \quad (2.39)$$

where $\{ \}$ denotes the reduced trace averaged with respect to all permutations of the $n+2$ symbols within the brackets. Going through the same steps as before, in place of (2.37) we now find

$$Na_n = \frac{3}{X} 2^n \left\{ \sum_{g^{++}} 2w_g \{g^{++}\} N_{g^{++}}^L + \sum_{g^*} w_g \{g^*\} N_{g^*}^L \right\}, \quad (2.40)$$

where $\{g^{++}\}$ and $\{g^*\}$ are again mean reduced traces,[†] but this time the average is with respect to permutations of all factors involved in any localisation of the interaction-graphs: (i) symbols as well as (ij) symbols.

Now, of course, (2.40) is a valid representation of a_n even when P and Q commute. The prescriptions (2.37) and (2.40) must lead to just the same answer. But it is important to realise that there is no term by term equality between these formulae: in general, $\{g^{++}\} \neq \langle g^{++} \rangle$ and $\{g^*\} \neq \langle g^* \rangle$. In fact, for the operators in $H(s)$, the term Σ_{g^*} in (2.37) vanishes whereas the term Σ_{g^*} in (2.40) does not.

A particular case in which the more general formalism of eqn (2.40) must be used arises in the calculation of staggered susceptibilities. If the field H has opposite sign at the sites of two sublattices, A and B , then in place of Q we have Q' , where

$$Q' = \sum_a s_{za} - \sum_b s_{zb} \quad (2.41)$$

[†] In Rushbrooke and Wood (1963), brackets, $[]$, were used rather than braces, $\{ \}$, as here: but we wish to reserve $[]$ to designate cumulants—and in the earlier work the $[]$ did not refer to *mean* reduced traces. The presentation is simpler when they do.

where a and b run over the sites of A and B , respectively. P and Q' do not commute. Any particular graph g^{++} will be associated with a plus sign when the two $+$'s lie on the same sublattice, and a minus sign when they lie on different sublattices. We call the former embeddings even, the latter ones odd, and denote the corresponding occurrence numbers by $N_{g^{++}}^L(e)$ and $N_{g^{++}}^L(o)$. Then, in this case, (2.40) reads

$$Na_n' = \frac{3}{X} 2^n \left\{ \sum_{g^{++}} 2w_g \{g^{++}\} [N_{g^{++}}^L(e) - N_{g^{++}}^L(o)] + \sum_{g^*} w_g \{g^*\} N_{g^*}^L \right\}, \quad (2.42)$$

whence

$$Na_n' = Na_n - \frac{3}{X} 2^n \sum_{g^{++}} 2w_g \{g^{++}\} 2N_{g^{++}}^L(o). \quad (2.43)$$

With nearest-neighbour interactions only, and for the s.c. and b.c.c. lattices when A and B are equivalent sublattices such that all neighbours of an A site are B sites, and conversely, then instead of referring to even and odd embeddings we can speak of even and odd g^{++} graphs, and write (2.43) as

$$Na_n' = Na_n - \frac{3}{X} 2^n \sum_{g \neq (o)} 2w_g \{g_{(o)}^{++}\} N_{g^{++}}^L; \quad (2.44)$$

see Rushbrooke and Wood (1963). In this case too, since interest focuses on the antiferromagnetic ordering problem, J_1 will be negative and it is customary to define x as $|J_1|/kT$ and multiply (2.44) by $(-1)^n$. But when second neighbour interactions are also included, these considerations do not arise: see Pirnie *et al.* (1966). Even so, eqn (2.43) remains preferable to (2.42) for use in calculating staggered susceptibility coefficients, simply because, for $H(s)$, as we have said, we do not need to evaluate the quantities $\langle g^* \rangle$, and (2.43) has eliminated the quantities $\{g^*\}$.

So much for the basic moment method. It is to the mean reduced traces that we refer when we speak of moments, and the reason for this will be clarified during our discussion of the corresponding cumulant expansion. In preparation for this, we must first digress to introduce a generalised moment-cumulant transformation.

B. Generalised moment-cumulant transformation

The following mathematics has applications in many fields of theoretical physics. (See also Chapter 1, Section III.)

Suppose we have n symbols, $\alpha, \beta \dots \omega$ and have defined quantities (numbers) relating to sets of these, which we denote by enclosing the members of the set within $\langle \rangle$; i.e. we have defined quantities $\langle \alpha \rangle, \langle \beta \rangle, \dots \langle \alpha \beta \rangle, \dots \langle \alpha \beta \gamma \rangle, \dots$, where the sequence of the symbols within the $\langle \rangle$ does not matter.

The values of these quantities will depend, in general, on the symbols concerned, and not just on the number of them. And we do not allow repeated symbols.

Then, in terms of these quantities we can define others, denoted by []'s, according to the rules

$$\left. \begin{aligned} \langle\alpha\rangle &= [\alpha], \text{ any one symbol} \\ \langle\alpha\beta\rangle &= [\alpha\beta] + [\alpha][\beta], \text{ any two symbols} \\ \langle\alpha\beta\gamma\rangle &= [\alpha\beta\gamma] + [\alpha\beta][\gamma] + [\alpha\gamma][\beta] + [\beta\gamma][\alpha] + [\alpha][\beta][\gamma] \\ &\dots \end{aligned} \right\} \quad (2.45)$$

and so on, up to

$$\langle\alpha\beta\dots\omega\rangle = \sum_k \sum_{p(n,k)} [\alpha\dots\beta][\gamma\dots\delta]\dots[\varepsilon\dots\omega], \quad (2.46)$$

where $p(n, k)$ means a partition of the n symbols into k sets (with no regard to the sequence within a set, or to the sequence of the sets themselves). The eqns (2.45) are, of course, instances of (2.46) for $n = 1, 2, 3 \dots$, and hold for all possible choices of the symbols concerned. We call the [] terms *cumulants* constructed from the *moments*, $\langle \rangle$. They are also called Ursell functions constructed from the $\langle \rangle$ terms. We note that, by successive elimination, any [] is formed from $\langle \rangle$ terms of lower or equal order: so if the $\langle \rangle$ terms are defined for up to n symbols, so also are the [] terms.

Inverting these equations, we have

$$\left. \begin{aligned} [\alpha] &= \langle\alpha\rangle, \text{ any one symbol} \\ [\alpha\beta] &= \langle\alpha\beta\rangle - \langle\alpha\rangle\langle\beta\rangle, \text{ any two symbols} \\ [\alpha\beta\gamma] &= \langle\alpha\beta\gamma\rangle - \langle\alpha\beta\rangle\langle\gamma\rangle - \langle\alpha\gamma\rangle\langle\beta\rangle - \langle\beta\gamma\rangle\langle\alpha\rangle + 2\langle\alpha\rangle\langle\beta\rangle\langle\gamma\rangle \\ &\dots \end{aligned} \right\} \quad (2.47)$$

and so on up to,

$$[\alpha\beta\dots\omega] = \sum_k \sum_{p(n,k)} (-1)^{k-1}(k-1)! \langle\alpha\dots\beta\rangle\langle\gamma\dots\delta\rangle\dots\langle\varepsilon\dots\omega\rangle. \quad (2.48)$$

The eqns (2.47) are, of course, instances of (2.48) for $n = 1, 2, 3 \dots$, and hold for all possible choices of the symbols concerned. That (2.47) and (2.48) are, in fact, the inverse of (2.45) and (2.46) is readily proved by induction (on n).

To make contact with the eqns (2.6) and our original use of the words moment and cumulant, we note that if all $\langle \rangle$ -quantities referring to s symbols have the same value, μ_s , then the []-quantities for s symbols all have the value λ_s , i.e. (2.47) reduces to (2.6). This is easily established formally.

The importance of the []-functions derives from the following theorem. If the symbols $\alpha, \beta \dots \omega$ fall into two groups, $\alpha_1, \beta_1 \dots \omega_1$, and $\alpha_2, \beta_2 \dots \omega_2$, such that, for any choice of symbols,

$$\langle \alpha_1 \dots \beta_1 \alpha_2 \dots \beta_2 \rangle = \langle \alpha_1 \dots \beta_1 \rangle \langle \alpha_2 \dots \beta_2 \rangle \quad (2.49)$$

then any [] containing symbols from both groups vanishes.

The proof, by induction, is very simple. Suppose the theorem established for $< n$ symbols: and consider the case of n symbols. By (2.48)

$$[\alpha \dots \omega] = \langle \alpha \dots \omega \rangle - \sum_{k \geq 2} \sum_{p(n,k)} [\alpha \dots \beta][\gamma \dots \delta] \dots [\varepsilon \dots \omega]. \quad (2.50)$$

Suppose the left-hand side of (2.50) is $[\alpha_1 \dots \omega_1 \alpha_2 \dots \omega_2]$, with symbols from both groups. Each [] on the right-hand side has $< n$ symbols, since $k \geq 2$. So in every non-vanishing contribution to the sum, the "1" and "2" symbols occur in different []. Therefore, with a self-explanatory notation,

$$\begin{aligned} \sum_{k \geq 2} \sum_{p(n,k)} &= \sum_{k_1 \geq 1} \sum_{p(n_1, k_1)} [\alpha_1 \dots \beta_1][\gamma_1 \dots \delta_1] \dots [\varepsilon_1 \dots \omega_1] \\ &\quad \text{times} \\ &\sum_{k_2 \geq 1} \sum_{p(n_2, k_2)} [\alpha_2 \dots \beta_2][\gamma_2 \dots \delta_2] \dots [\varepsilon_2 \dots \omega_2] \\ &= \langle \alpha_1 \dots \omega_1 \rangle \langle \alpha_2 \dots \omega_2 \rangle \end{aligned}$$

which cancels with $\langle \alpha_1 \dots \omega_1 \alpha_2 \dots \omega_2 \rangle$ on account of the factorisation property of $\langle \rangle$ terms.

For small values of n , the theorem is directly verifiable from eqn (2.45).

The basic reason for the importance of this moment-cumulant transformation in the present context resides in eqns (2.31) and (2.33). Equation (2.31) shows that $\langle g \rangle$ can be written $\langle \alpha \beta \dots \omega \rangle$, where $\alpha, \beta \dots \omega$ denotes a line-labelling of g and $\langle \alpha \beta \dots \omega \rangle$ denotes the reduced trace of the corresponding product of (ij) operators, averaged over all permutations of the symbols $\alpha \beta \dots \omega$ within the $\langle \rangle$. Equation (2.33) expresses the factorisation property of these $\langle \rangle$ -functions when the graph g comprises two (or more) disconnected parts. Thus the corresponding []-functions for disconnected graphs vanish. For a connected graph the []-function, called the (bond) cumulant of g , is simply a combination of the mean reduced traces of subgraphs of g according to (2.48): we shall denote it $[g]$ or $[\alpha \beta \dots \omega]$, where $\alpha, \beta \dots \omega$ is a line-labelling of g , whichever is the more appropriate. We proceed now to show that just as Z is related to a graphical expansion involving $\langle g \rangle$ and graphs which may be either connected or disconnected, so $\ln Z$ is related to a graphical expansion involving $[g]$ and connected graphs only. In other words, we

proceed to a linked-cluster expansion of the free-energy in the form first derived, in the field of lattice-statistics, by Brout.

A rather different, and in some respects more general, development of generalised moment-cumulant transformations has been given by Kubo (1962): but the formalism of this section is fully adequate for our present purposes.

C. The cumulant method

It is convenient to write

$$\mathcal{H} = \mathcal{H}_2 + \mathcal{H}_1, \quad (2.51)$$

where $\mathcal{H}_2 = -2J_1P$ and $\mathcal{H}_1 = -g\beta HQ$, P and Q being defined by (2.1). Thus \mathcal{H}_1 refers only to single spins, and \mathcal{H}_2 to pairs of neighbouring spins. In order to have a formalism equally useful for all powers of H , we invoke the commutativity of \mathcal{H}_1 and \mathcal{H}_2 to factorise the partition function as

$$Z = Z_1 Z_2, \quad (2.52)$$

where

$$Z_1 = \text{Tr } \rho_1, \quad \rho_1 = \exp(-\mathcal{H}_1/kT) \quad (2.53)$$

and

$$Z_2 = \text{Tr} \{ \exp(-\mathcal{H}_2/kT) \cdot \rho_1 \} / \text{Tr } \rho_1 \quad (2.54)$$

$$\equiv \langle \exp(-\mathcal{H}_2/kT) \rangle_{(1)} \quad (2.55)$$

where, for any operator A ,

$$\langle A \rangle_{(1)} \equiv \text{Tr}(A\rho_1) / \text{Tr } \rho_1. \quad (2.56)$$

We refer to $\langle A \rangle_{(1)}$ as the trace of A reduced with respect to ρ_1 . Since

$$\text{Tr } \rho_1 = \left[\frac{\sinh[g\beta H(2s+1)/2kT]}{\sinh[g\beta H/2kT]} \right]^N, \quad (2.57)$$

we note that as $H \rightarrow 0$, $\rho_1 \rightarrow$ unit operator, $\text{Tr } \rho_1 \rightarrow (2s+1)^N$, and $\langle A \rangle_{(1)}$ becomes what we have previously denoted by $\langle A \rangle$.

The second small, but important, change that we shall make in this section is that we shall no longer suppose that we are necessarily dealing with an "infinite" lattice L ; rather we shall suppose that (1.1) is defined with respect to a set of sites G , N in number, between which pairs of nearest neighbours $\langle ij \rangle$ are defined. Topologically, G is just a graph, of vertices joined by (single) bonds; physically it is a cluster of interacting spins. There is no necessity for N to be large: the Brout expansion is as valid for a small finite cluster as it is for an "infinite" lattice. Having derived the Brout ex-

pansion, we can then replace G by L , if we wish to have formulae explicitly relating to an “infinite” lattice.

We now proceed to expand Z_2 in powers of $2J_1/kT$, noting that when J_1 is zero, Z_2 is unity. From (2.55), the coefficient of $(2J_1/kT)^n$ is

$$\frac{1}{n!} \left\langle \left(\sum_{\langle ij \rangle} (ij) \right)^n \right\rangle_{(1)} \quad (2.58)$$

so that, from (2.29),

$$Z_2 = 1 + \sum_{n \geq 1} \sum_g w_g \langle g \rangle_{(1)} 2^n x^n, \quad (2.59)$$

where g denotes a localised interaction graph of order n , and w_g is the bond-degeneracy factor defined in (2.30). To find $\langle g \rangle_{(1)}$ we line-label the bonds of g with symbols $\alpha, \beta \dots \omega$ and use eqn (2.31) except that now traces are reduced “with respect to ρ_1 ”. Explicitly, (2.31) is replaced by

$$\left[\frac{\sinh [g\beta H (2s+1)/2kT]}{\sinh [g\beta H/2kT]} \right]^m \langle g \rangle_{(1)} = \frac{1}{n!} \text{Tr} \sum_p \alpha \beta \dots \omega \rho_1^{(m)}, \quad (2.60)$$

where $\rho_1^{(m)}$ is just that part of ρ_1 which refers to the m sites involved in g .

Now $n! w_g$ equals the number of distinguishable labellings of the n bonds of g with the labels $\alpha, \beta \dots \omega$, where alternative labellings of the components of a multiple bond are not regarded as distinct. Consequently,

$$Z_2 = 1 + \sum_{n \geq 1} \frac{2^n x^n}{n!} \sum_g \sum_{l(g)} \langle \alpha \beta \dots \omega \rangle_{(1)} \quad (2.61)$$

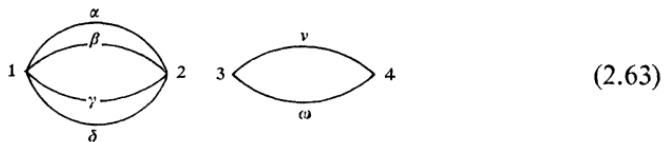
where $l(g)$ runs over the distinguishable line-labellings of g . $\langle \alpha \beta \dots \omega \rangle_{(1)}$, of course, being a mean over all permutations of the symbols, is independent of the precise line-labelling of g .

Since $\langle \alpha \beta \dots \omega \rangle_{(1)}$ has the same factorisation property for disconnected graphs as does $\langle \alpha \beta \dots \omega \rangle$, if we replace $\langle \alpha \beta \dots \omega \rangle_{(1)}$ in (2.61) by

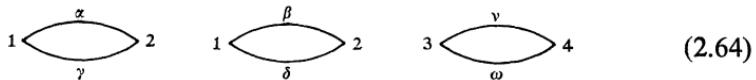
$$\sum_{\text{partitions}} [\alpha \dots \beta]_{(1)} [\gamma \dots \delta]_{(1)} \dots [\varepsilon \dots \omega]_{(1)}, \quad (2.62)$$

where the cumulant functions $[\]_{(1)}$ are related to the moment functions $\langle \rangle_{(1)}$ as are the cumulants and moments in (2.48), we obtain, for any specific line-labelling $l(g)$, a “disintegration” of g into overlapping “parts”; where each “part” is connected, since otherwise $[\]_{(1)}$ vanishes. Taking this “disintegration” apart, we have some line-labelling (with the symbols $\alpha, \beta \dots \omega$) of a set of vertex-labelled connected graphs which (without line labels) may

contain repetitions. For example, for $n = 6$, and using curved bonds to facilitate line-labelling, the partition $[\alpha\gamma][\beta\delta][\nu\omega]$ of



produces



which, as a set of vertex-labelled graphs (without line labels) contains the repetition



And, quite generally, there is a one-one correspondence between the set of "disintegrations" we obtain on "disintegrating" all alternative (distinct) labellings of the original graph (into a given set of vertex-labelled parts) and the set of distinct line-labellings (with the symbols $\alpha, \beta \dots \omega$) of these vertex-labelled parts. For these parts, when line-labelled, tell us uniquely what partition of $\alpha, \beta \dots \omega$ has been chosen in (2.62), and can be assembled uniquely into the original graph according to their vertex labels. And just as the components of multiple bonds are regarded as identical as far as labellings are concerned, so also are repeated parts (with the same vertex labels) of the "disintegrated" graph. The only distinct ways, for example, of labelling (2.65) with the symbols $\alpha, \beta, \gamma, \delta$ are those corresponding to the three partitions $[\alpha\beta][\gamma\delta]$, $[\alpha\gamma][\beta\delta]$ and $[\alpha\delta][\beta\gamma]$.

Let the symbol v identify the different vertex-labelled graphs which may result from a "disintegration" (i.e. different types of vertex-labelled connected graphs), and suppose there are r_v repetitions of type v .

Let

$$w_v = \prod_s \frac{1}{k_s!}$$

where s runs over the (multiple) bonds of v , and let $[\alpha \dots \beta]_{(1)}$ for v be denoted K_v . K_v is the reduced (bond) cumulant of v , and is a combination

of reduced traces of subgraphs of v according to the prescription (2.48). Then, since the number of distinct line-labellings of the “disintegrated” graph is

$$\frac{n!}{\prod_v r_v!} \prod_v (w_v)^{r_v},$$

(2.61) becomes

$$Z_2 = 1 + \sum_{n \geq 1} 2^n x^n \sum_g \sum_{r_v} \prod_v \frac{(w_v K_v)^{r_v}}{r_v!}, \quad (2.66)$$

where the r_v 's all take values consistent with g , which, as in (2.61), is a localised interaction-graph (not necessarily connected) of order n .

Now the three summations in (2.66) are equivalent to summing over all conceivable sets of vertex-labelled parts: since a set of vertex-labelled parts assembles uniquely into some g , for some value of n , and is a possible “disintegration” of this localised interaction-graph. And the initial term in (2.66) corresponds to $n = 0$, i.e. all $r_v = 0$. Moreover, if n_v is the order (number of bonds) of the graph v , $n = \sum_v r_v n_v$.

Thus,

$$Z_2 = \sum_{r_v} \prod_v \frac{[w_v K_v 2^{n_v} x^{n_v}]^{r_v}}{r_v!} \quad (2.67)$$

where Σ_{r_v} implies that for all v , i.e. all conceivable connected vertex-labelled graphs, r_v runs from 0 to ∞ .

Consequently,

$$Z_2 = \exp \sum_v w_v K_v \left(\frac{2J_1}{kT} \right)^{n_v}. \quad (2.68)$$

In (2.68), v runs over all connected vertex-labelled interaction-graphs which can be found (localised) on G .

Now w_v and K_v are independent of the vertex labels of the interaction-graph: they depend only on its topological structure. Connected graphs of n lines can be of various topological types and we specify such a graph by the symbol (n, t) , where t distinguishes between topologically different types. When $n = 3$, for example, $(3, t)$ runs over the set

$$(2.69)$$

Suppose now that (n, t) can be localised on G in $N_{(n,t)}^G$ ways. Then (2.68) becomes, writing Z_2^G rather than Z_2 in order to be more explicit,

$$\ln Z_2^G = \sum_{(n,t)} w_{(n,t)} K_{(n,t)} \left(\frac{2J_1}{kT} \right)^n N_{(n,t)}^G. \quad (2.70)$$

It is this eqn, (2.70), which constitutes the Brout expansion.

When, in place of G , we have a lattice, L , $N_{(n,t)}^G$ is replaced by $N_{(n,t)}^L$; and if L is so large that we can neglect boundary effects, since (n, t) is a connected graph, $N_{(n,t)}^L$ is proportional to N . Written explicitly, we have

$$\ln Z^L = \ln Z_1^L + \sum_{(n,t)} w_{(n,t)} K_{(n,t)} \left(\frac{2J_1}{kT} \right)^n N_{(n,t)}^L, \quad (2.71)$$

and this eqn, (2.71) is the basis of the cumulant method in lattice-statistics. We note that the cumulants, $K_{(n,t)}$, are functions of H/kT , since all traces are with respect to the operator ρ_1 . So also, of course, is $\ln Z_1$: see (2.57).

D. The finite cluster method

We have observed that $K_{(n,t)}$ depends only on the topological structure of the graph (n, t) , as also does $w_{(n,t)}$. The only way in which the structure of the cluster G , or lattice L , enters into eqns (2.70) and (2.71) is through the numbers $N_{(n,t)}^G$ or $N_{(n,t)}^L$. But these are by no means the simplest characteristics of G or L . Suppose (n, t) has m vertices, and we denote it more explicitly as (m, n, t) . If we temporarily label these vertices, i_1, i_2, \dots, i_m , and if the number of ways i_1, i_2, \dots, i_m can be identified with m sites of G such that if two vertices are bonded in (m, n, t) they are "nearest neighbours" on G is $X_{(m,n,t)}^G$, then $N_{(m,n,t)}^G = X_{(m,n,t)}^G / S(m, n, t)$, where $S(m, n, t)$ is the symmetry number of (m, n, t) . This symmetry number is determined by relabelling the vertices of (m, n, t) as i'_1, i'_2, \dots, i'_m , and asking in how many ways can the members of the set (i_1, i_2, \dots, i_m) be identified with the members of the set $(i'_1, i'_2, \dots, i'_m)$, *preserving the multiplicities of the bonds* between them. On the other hand $X_{(m,n,t)}^G$ does not depend on the multiplicities of the bonds in (m, n, t) , only on their existence. If the graph we obtain by suppressing the multiplicities of the bonds in (m, n, t) , i.e. by replacing multiple bonds by single bonds, is denoted (m, l, τ) , where l is the number of bonds in (m, l, τ) and τ distinguishes different topological types, then, with a self-explanatory notation, $X_{(m,n,t)}^G = X_{(m,l,\tau)}^G$ and $N_{(m,l,\tau)}^G = X_{(m,l,\tau)}^G / S(m, l, \tau)$, where $S(m, l, \tau)$ is the symmetry number of the graph (m, l, τ) . Thus

$$N_{(m,n,t)}^G = \frac{S(m, l, \tau)}{S(m, n, t)} N_{(m,l,\tau)}^G, \quad (2.72)$$

and the ratio of symmetry numbers in (2.72) depends only on the graph (m, n, t) , and not on the cluster G . The single-bond connected graphs, (m, l, τ) , are called *basic graphs*, and for these basic graphs the numbers $N_{(m, l, \tau)}^G$ or $N_{(m, l, \tau)}^L$ are called cluster constants or lattice constants. Equation (2.70) then reads

$$\ln Z_2^G = \sum_{(m, l, \tau)} \phi(m, l, \tau) N_{(m, l, \tau)}^G \quad (2.73)$$

where

$$\phi(m, l, \tau) = \sum_{(m, n, t)} w_{(m, n, t)} K_{(m, n, t)} \left(\frac{2J_1}{kT}\right)^n \frac{S(m, l, \tau)}{S(m, n, t)}, \quad (2.74)$$

and the sum in (2.74) is over all graphs (m, n, t) corresponding to the same basic graph (m, l, τ) . Thus, given the type of Hamiltonian with which we are ultimately concerned, say $H(s)$ or $I(s)$, in (2.73) $\phi(m, l, \tau)$ is entirely a property of the graph (m, l, τ) , whereas the structure of the cluster G enters only through the cluster constants $N_{(m, l, \tau)}^G$: and similarly, of course, when we are dealing with an "infinite" lattice, L .

In order to refer directly to partition functions, Z , rather than the interaction part, Z_2 , we shall rewrite (2.73) as

$$\ln Z^G = \sum_{(m, l, \tau)} \phi(m, l, \tau) N_{(m, l, \tau)}^G \quad (2.75)$$

where now among the basic graphs we include an isolated point ($m = 1, l = 0$) and the corresponding ϕ , denoted ϕ_0 , is $(1/N) \ln \text{Tr } \rho_1$: see (2.57).

The cluster G , with nearest neighbour pairs defined within it, itself constitutes a graph (of vertices connected by bonds), and if G is a connected cluster then it constitutes a basic graph. We can thus use eqn (2.75) to express the partition functions of physical clusters isomorphic in structure with basic graphs in terms of the functions $\phi(m, l, \tau)$. Let a physical cluster isomorphic with the basic graph (m, l, τ) be denoted $[m, l, \tau]$. Then (2.75) reads,

$$\ln Z [m, l, \tau] = \sum_{(m', l', \tau')} \phi(m', l', \tau') t_{(m', l', \tau')}^{[m, l, \tau]}, \quad (2.76)$$

where $t_{(m', l', \tau')}^{[m, l, \tau]}$ is the number of times we can find a subgraph of structure (m', l', τ') among the sites and bonds of $[m, l, \tau]$: it is the cluster constant for (m', l', τ') on $[m, l, \tau]$ or, in the language of Sykes *et al.* (1966), the number of weak embeddings of (m', l', τ') in $[m, l, \tau]$. We shall refer to the matrix whose elements are $t_{(m', l', \tau')}^{[m, l, \tau]}$ as the T-matrix (Rushbrooke, 1964).

The rows and columns of the T-matrix are conveniently ordered by taking either the pairs m, l or the pairs l, m in "dictionary" order: and for present purposes the latter convention is the more convenient. For given

l and m , the sequence corresponding to different choices of τ is immaterial, and can be decided quite arbitrarily.

Now the matrix T , either regarded as carried ad infinitum or truncated after a finite number of rows and columns, is not only non-singular, it is a triangular matrix with unit elements down the diagonal, for (m, l, τ) certainly occurs once and once only on $[m, l, \tau]$, and (m', l', τ') cannot occur on $[m, l, \tau]$ if either $l' > l$ or $m' > m$. Its inverse is therefore of the same form. This means that if we write the eqns (2.76) as

$$\ln Z = T \phi, \quad (2.77)$$

where $\ln Z$ is the column vector whose elements are $\ln Z[m, l, \tau]$ and ϕ is the column vector whose elements are $\phi(m', l', \tau')$, then (2.77) has the solution

$$\phi = T^{-1} \ln Z, \quad (2.78)$$

which expresses $\phi(m, l, \tau)$ as a linear combination of the logarithms of the partition functions for finite clusters $[m', l', \tau']$, where $(m', l', \tau') \leq (m, l, \tau)$ in the sense that (m', l', τ') occurs no later than (m, l, τ) in the dictionary sequence. Indeed, because of the triangular nature of T , the eqns (2.77) are very easily solved by successive elimination, and there is no need explicitly to invert the matrix T .

Nevertheless, there is one important property of the matrix T^{-1} , stemming from the graphical interpretation of the elements of T , which has yet to be mentioned. The $(m, l, \tau ; m', l', \tau')$ element of T^{-1} can be readily shown to have the value

$$(-1)^{l-l'} s_{(m', l', \tau')}^{[m, l, \tau]} \quad (2.79)$$

where $s_{(m', l', \tau')}^{[m, l, \tau]}$ is the number of (weak) embeddings of (m', l', τ') in $[m, l, \tau]$ such that all bonds of $[m, l, \tau]$ not in (m', l', τ') pass through vertices of (m', l', τ') (Essam, 1967; Rushbrooke, 1970; Domb, this Volume, Chapter 1, Section IV. B3). This implies, *inter alia*, that $\phi(m, l, \tau)$ can involve in $Z(m', l', \tau')$ only if (m', l', τ') is a subgraph of (m, l, τ) . Indeed, the whole algebra embodied in eqns (2.75)–(2.79) is unchanged if, instead of supposing that (m, l, τ) runs over all conceivable basic graphs, we confine attention to those basic graphs which in fact occur as subgraphs of G , or L .

Now, of course, if we simply substitute the ϕ 's from (2.78) into (2.77) or (2.75) we obtain only the tautology

$$\ln Z^G = \ln Z^G,$$

which is not particularly helpful. The reason why the finite cluster method provides a useful tool for the derivation of high-temperature expansions is that $\phi(m, l, \tau)$, regarded as a power-series in x , i.e. J_1/kT , necessarily contains

no power of x lower than x^l . This is shown explicitly by eqn (2.74), since (m, n, t) can correspond to the basic graph (m, l, τ) only if $n \geq l$. Thus, if we truncate the right-hand side of (2.75) by restricting (m, l, τ) to basic graphs for which $l \leq n$, and expand all ϕ 's, given by (2.78), as power series in x , then this truncated form of (2.75) will reproduce correctly the high-temperature expansion of $\ln Z^G$ up to and including the term in x^n . And it is this procedure, applied to a lattice L , which constitutes the finite cluster method.

To summarise, to find the high-temperature expansion of $\ln Z^L$ in powers of x , through the term in x^n , we require:

- (i) to consider all basic graphs, (m, l, τ) , with $l \leq n$ (which can occur on the lattice L),
- (ii) to expand $\ln Z[m, l, \tau]$, for all clusters isomorphic with this set of basic graphs, as power series in x through the terms in x^n ,
- (iii) to find the T-matrix elements, $t_{(m, l, \tau)}^{[m', l', \tau']}$, for all pairs of basic graphs in the set under consideration,
- (iv) to solve eqns (2.77) to obtain the functions $\phi(m, l, \tau)$, expanded as power series in x through the terms in x^n ,
- (v) to find the lattice constants $N_{(m, l, \tau)}^L$,
- (vi) to evaluate the scalar product

$$\sum_{(m, l, \tau) l \leq n} \phi(m, l, \tau) N_{(m, l, \tau)}^L. \quad (2.80)$$

If the coefficient of x^n in $\phi(m, l, \tau)$ is written $\phi_n(m, l, \tau)$, then $\phi_n(m, l, \tau)$ is itself a function of $g\beta H/kT$, on account of the Zeeman (single spin) term in the Hamiltonians for finite clusters. In order to deal with numbers rather than functions, we must further expand $\phi_n(m, l, \tau)$ in powers of $g\beta H/kT$, or some equivalent variable. Having done this, the terms independent of H will ultimately yield the zero-field specific heat series, those in H^2 will produce the zero-field susceptibility series, and those in higher powers of H give rise to the so-called "higher order" susceptibility series. There will be no terms involving odd powers of H , since $F(H, T)$ is necessarily an even function of H in the absence of spontaneous magnetisation.

Having now introduced the three principal methods of deriving high-temperature expansions for magnetic models based on $H(s)$, or similar Hamiltonians, we must proceed to fill in some of the details which are necessarily involved in actual calculations.

III. FULLER DETAILS ON SPECIAL TOPICS

We have outlined the basis of the three main approaches to the derivation of high-temperature expansions for the Heisenberg model, leaving aside

only the powerful Horwitz–Callen method employed by Wortis and co-workers in the classical case. But there remain several regions in which fuller details are called for, and we shall look briefly at five of these in the present section. In particular, we have to say something about, (A) occurrence factors and lattice constants; (B) the determination of mean traces for the general spin problem $H(s)$; (C) any complications introduced by including second neighbour interactions; (D) the special features of the classical Heisenberg model, $H(\infty)$; and (E) the special features of the original Heisenberg model, $H(\frac{1}{2})$. We can, however, only touch on these matters, and point to appropriate original papers for amplification.

A. Occurrence factors and lattice constants

We have seen already in eqn (2.72), that as far as connected, i.e. single-part, graphs are concerned, the numbers which primarily concern us are the occurrences for the corresponding basic graphs, in which bond-multiplicities are suppressed. If (m, l, τ) denotes such a graph, $N_{(m, l, \tau)}^L$, for an effectively infinite lattice of N sites, i.e. for a lattice large enough that boundary effects can be ignored, may be written $N n_{(m, l, \tau)}^L$, where $n_{(m, l, \tau)}^L$ is independent of N . These latter numbers, often called lattice counts (or lattice constants, this Volume, Chapter 1, Section IV), are nowadays almost invariably determined by machine calculations. It is not our present purpose to describe the computer programs which have been used (for details see Martin this Vol., Chapter 2). We comment only that if this program counts a labelled graph, of topological structure (m, l, τ) , with one point fixed on L , then to obtain $n_{(m, l, \tau)}^L$ we must divide by the symmetry number $S(m, l, \tau)$. This can normally be found without difficulty by inspection, but can also be found mechanically by counting the occurrences of a graph on itself. This last problem is, of course, just part of the larger one of finding the elements of the T-matrix, required when using the finite cluster method, which has also proved amenable to machine calculations.

It is helpful to know how many basic graphs there are, for given values of m and l . This can be found by using the Redfield–Pólya algorithm, which is conveniently accessible, together with its derivation, in the important review article of Uhlenbeck and Ford (1962) (see also this Volume, Chapter 1, Section II B). Table II, taken from Baker *et al.* (1967c), lists the numbers of such graphs for $l \leq 10$. Values for $m \leq 7$ are given by Uhlenbeck and Ford, and recently Stein and Stein (1967) have published computer calculations† extending the values to $m \leq 18$. For fixed m , of course, l runs from $l = m - 1$, for all simple trees, to $\frac{1}{2}m(m - 1)$, for the complete star graph.

As Table II shows, the number of basic graphs for which $l \leq n$ increases

† This work was performed in 1963, as were the hand calculations of Baker *et al.*, which it confirms.

rapidly with n . The number is rather more than 1000 for $n = 9$ and, from Stein and Stein, nearly 11,000 for $n = 11$. It is this proliferation of topologically distinct graphs which, more than anything else, prohibits the derivation of appreciably longer series than those yet found, by present methods. Of course, by no means all these graphs are required for finding, say, a_n by the finite cluster method. Indeed a_9 for the f.c.c. lattice involves contributions from only 473 basic graphs, the reduction from 1068 being largely due to the fact that no 9-line graphs having more than 2 nodes of order unity (vertices attached to the graph by only one bond) need be considered. Further such numerical details are given in Baker *et al.* (1967c). But for the higher-order susceptibility series all graphs must be retained, which is why at present these have not been taken beyond eighth order. And it should be noted that all 358 graphs for which $l \leq 8$ can be found, weakly embedded, on the face-centred cubic lattice.

TABLE II. Number of basic graphs with l lines and m vertices. The last two rows list totals for fixed l and cumulative totals, respectively. From Baker *et al.* (1967c)

| $m \backslash l$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|------------------|---|---|---|----|----|----|-----|-----|------|------|
| 2 | 1 | | | | | | | | | |
| 3 | | 1 | 1 | | | | | | | |
| 4 | | | 2 | 2 | 1 | 1 | | | | |
| 5 | | | | 3 | 5 | 5 | 4 | 2 | 1 | 1 |
| 6 | | | | | 6 | 13 | 19 | 22 | 20 | 14 |
| 7 | | | | | | 11 | 33 | 67 | 107 | 132 |
| 8 | | | | | | | 23 | 89 | 236 | 486 |
| 9 | | | | | | | | 47 | 240 | 797 |
| 10 | | | | | | | | | 106 | 657 |
| 11 | | | | | | | | | | 235 |
| | 1 | 1 | 3 | 5 | 12 | 30 | 79 | 227 | 710 | 2322 |
| | | 2 | 5 | 10 | 22 | 52 | 131 | 358 | 1068 | 3390 |

Even on the plane triangular lattice, 320 of these graphs occur, i.e. have non-zero lattice counts. There is, however, a big reduction in these numbers when we pass to open lattices, in which there are no triangles of nearest-neighbour sites. For the b.c.c., s.c., and s.q. lattices, respectively, the $l \leq 8$ graphs with non-vanishing lattice counts number only 162, 147 and 124. This is why derived susceptibility series for these open lattices are normally one term longer than those for close-packed lattices. Actually a_{10} for the

b.c.c. lattice involves only 271 basic graphs, as compared with the 473 required for a_9 in the f.c.c. case. Even so, the extra effort required to find the f.c.c. series, shorter though it is, is repaid by having a series whose coefficients, in fact, behave more smoothly than do those for open lattices.

We come now to the lattice counts themselves. For many years the best compilation of lattice counts was that of Domb (1960), who, to avoid listing unnecessarily many entries, made use of such, essentially transparent, formulae as

$$\boxed{\square} = 4(q - 2) \boxed{\square} - 2 \boxed{\triangle} \quad (3.1)$$

to eliminate all graphs having a node of order unity. In (3.1) each depicted graph stands for its lattice count (whatever the lattice). Equally, of course, as Domb emphasises, in as far as all lattice points are equivalent one can express the lattice count for any graph with an articulation point (i.e. point cutting at which would separate the graph into two parts) in terms of lattice counts for (vertex) irreducible graphs (i.e. graphs without articulation points) as, for example,

$$\boxed{\text{X}} = \frac{1}{2} \cdot 3p_3(3p_3 - 1) - 2 \boxed{\triangle}, \quad (3.2)$$

where p_3 is the lattice count for a simple triangle. In days when the determination of lattice counts was the major hindrance to progress, such formulae were invaluable, and more sophisticated versions are still important in deriving long series for problems, such as the self-avoiding chain problem, in which individual lattice counts dominate the situation and computers are pushed to their limits. But this is certainly not the case with basic graphs comprising up to, say, ten lines. Compact expressions for coefficients in terms of irreducible lattice constants (though, in practice, reductions of the form (3.2) are not normally employed) are useful in as far as they can be extended to situations for which the appropriate machine counts have not yet been made: and in describing the series themselves we shall draw attention to the existence of such expressions in the literature. There are occasions, however, for example with the randomly dilute problem (though we are not here concerned with this), when even reductions of the type (3.1) are ultimately out of place, and we need explicit lattice counts for all graphs, including those having nodes of order unity. For this reason, and also because it was indeed simpler so to do, Baker *et al.* made direct computer counts (for the five Bravais type lattices, f.c.c., b.c.c., s.c., p.t., and

s.q.) for all the basic graphs with which they were concerned. These are available in Baker *et al.* (1967b): a compendium which, inter alia, depicts these graphs and lists not only the lattice counts but also the corresponding T-matrix elements.[†]

Each graph depicted in this compendium, besides having its (m, l, τ) designation, is given a serial number: 1-891, 891A, which is a $(6, 10)$ graph that does not occur on any lattice, and 892-1460. They fall into five well-defined categories. I, all graphs with $l \leq 8$ (numbers 1-358); II, all graphs $l \leq 10, m \leq 7$ (numbers 359-486 and 878-1023); III, all $l = 9, m \geq 8$ graphs which do not involve circuits of odd order together with those having circuits of odd order but not more than two vertices of order unity (numbers 487-877); IV, all $l = 10, m \geq 7$ graphs which do not involve circuits of odd order, except that the only tree, $m = 11$, included is the linear chain (numbers 1024-1443); V, certain $l = 10, m = 8$ or 9, graphs having circuits of odd order but no nodes of order unity (numbers 1444-1460). Group V is not a complete topological set; they were graphs required for the calculation on hand, but do not form a useful category for other purposes. The symmetry numbers of all these graphs are listed. The T-matrix elements between all pairs of graphs are given, except that graphs 891A and 1444-1460 are omitted from consideration. But regarding lattice counts the situation is less simple, and calls for more detailed description.

Taking this first by lattices: for the simple cubic and simple quadratic lattices, the counts of all graphs in categories I, II, III and IV are listed: for the body-centred cubic lattice, the counts of all graphs in categories I, II, and III are listed, together with those for graphs in category IV having not more than two nodes of order unity. For the close-packed lattices, face-centred cubic and plane triangular, the graphs counted comprise: all in group I, those in group II for $m = 6$ and for $m = 7, l = 9$, but of those with $m = 7$ and $l = 10$ only graphs without nodes of order unity: and all in group III except that of the trees, $m = 10$, only the linear chain is counted. A few isolated examples from group IV and the members of group V are also counted on these close-packed lattices: and for the plane triangular lattice only, certain other trees from group III, but not the complete set. More simply, accurately though not quite exhaustively, we can say that, from the point of view of graphs, all basic graphs with $l \leq 8$ are counted on all five lattices, all basic graphs with $l = 9$ are counted on the open lattices and those with not more than two vertices of order unity are counted on the close-packed lattices,

[†] We are aware of only one error among the lattice counts in this compendium. The count for graph 865 on the simple quadratic lattice should read 6856 (and not 17664). We are indebted to Dr J. W. Essam for drawing our attention to this. Graph 865 a 9-line tree with 4 nodes of order unity was not required for the Heisenberg model calculations, and was counted on open lattices only. The counts for the three-dimensional, b.c.c. and s.c., lattices are correct.

and for $l = 10$ basic graphs with not more than two vertices of order unity are counted on open lattices only. It is for these categories of graphs that we believe the results most likely to prove of use to other workers.

So much regarding the lattice counts for connected graphs. In the moment method of obtaining high temperature expansions, it is necessary to find also the part proportional to N in the occurrence factors for multipart (disconnected) graphs. Consider first a two part graph, and label the parts A and B . Let simultaneous embeddings of A and B in a lattice be denoted $(A + B)$ when A and B have no vertices in common and $[AB]$ when they overlap (i.e. form one unit). Then

$$N(A)N(B) = N(A + B) + N[AB] \quad (3.3)$$

where, in (3.3), $N(A + B)$ counts all $A + B$ type embeddings, and is not just the part of this which is proportional to N . Denoting the coefficient of N in any term in (3.3) by n , we have at once,

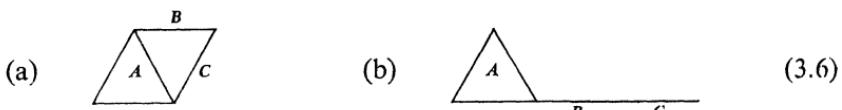
$$n(A + B) = - n[AB]. \quad (3.4)$$

Similarly, with three parts, A , B , and C , straightforward algebra yields

$$n(A + B + C) = n[[AB]C] + n[[BC]A] + n[[AC]B] - n[ABC], \quad (3.5)$$

and the corresponding expression for four parts is easily written down. In (3.5), $[[AB]C]$ implies that A and B form one unit $[AB]$, and this is united with C , whereas $[ABC]$ implies only that A , B , and C form one (overlapping) unit.

Three comments on these equations must suffice. First, every graph on the right-hand side of eqns (3.4), (3.5)... is a connected graph, so again we are ultimately concerned with lattice counts for connected, and thence basic, graphs. Secondly, if p parts are identical, A and B in (3.5) say, they should be labelled to make them distinct and the answer subsequently divided by $p!$ Finally, in practice, in hand calculations, rather than running through all the terms in an expression like the right-hand side of (3.5), it is more economical to start with a possible composite graph and ask from what terms in (3.5) it can arise. For example, of the graphs in (3.6),



(a) has weight 2, since it comes from all terms in (3.5), whilst (b) has weight 1, since it does not arise from $[[AC]B]$.

We have included these matters not only for completeness, but also because we shall later have occasion to refer to eqns (3.4), (3.5)... in another connection, when they are given a different interpretation.

B. The determination of mean traces for the general spin problem, $H(s)$

In evaluating the reduced mean trace for a given interaction graph, we are faced with two problems which may conveniently be called the sorting problem and the single-site trace problem. Logically they arise in this order, but for simplicity of exposition it is convenient to take the latter first. Both problems can be computerised, and have been: but it remains necessary to appreciate just what requires to be done.

The single-site trace problem is the problem of evaluating the trace of a product of spin operators, s_x, s_y or s_z , all referring to the same site. Then if $\alpha, \beta, \dots, \gamma$ stand for s_x, s_y or s_z in some precise assignment

$$\text{Tr}(\alpha\beta\dots\gamma) = \sum_m \sum_{m', m'', \dots} \langle m|\alpha|m'\rangle \langle m'|\beta|m''\rangle \dots \langle m''|\gamma|m\rangle \quad (3.7)$$

where, since we are at liberty to take any matrix representation, we choose $|m\rangle$ to be the eigenvector of s_z having eigenvalue m , where m runs from $-s$ to s by integer steps (and s is either an integer or half an odd integer). As is well-known (see, for example, Condon and Shortley, 1951),

$$\begin{aligned} \langle m|s_x|m'\rangle = & \frac{1}{2}\{\sqrt{(s+m)(s+1-m')}\delta_{m,m'-1} \\ & + \sqrt{(s-m')(s+1+m')}\delta_{m,m'+1}\} \end{aligned} \quad (3.8)$$

$$\begin{aligned} \langle m|s_y|m'\rangle = & \frac{i}{2}\{\sqrt{(s+m)(s+1-m')}\delta_{m,m'-1} \\ & - \sqrt{(s-m')(s+1+m')}\delta_{m,m'+1}\} \end{aligned} \quad (3.9)$$

$$\langle m|s_z|m'\rangle = m\delta_{m,m'}. \quad (3.10)$$

Therefore any route from $\langle m|$ to $|m\rangle$ in (3.7) proceeds by consecutive steps in which the quantum number either remains unchanged (when the spin component is s_z), increases by unity (an up-step) or decreases by unity (a down-step). Since we start at $\langle m|$ and return to $|m\rangle$, any up-step must be balanced by a down-step (between the same two quantum numbers) at a later stage, and eqns (3.8) and (3.9) show that, apart from factors $\frac{1}{2}, i/2$ or $-i/2$, m_1 to $m_2 = m_1 + 1$ followed subsequently by m_2 to m_1 yields the factor

$$(s+1+m_1)(s-m_1), \quad \text{i.e. } X - m_1 - m_1^2, \quad (3.11)$$

where $X \equiv s(s + 1)$, while m_1 to $m_2 = m_1 - 1$ followed subsequently by m_2 to m_1 yields the factor

$$(s + 1 - m_1)(s + m_1) \quad \text{i.e.} \quad X + m_1 - m_1^2. \quad (3.12)$$

The factors (3.11) and (3.12) arise whether the spin components are s_x or s_y , but whereas whenever s_x is involved we have a factor $\frac{1}{2}$, if s_y is involved we have the factor $i/2$ for an up-step and $-i/2$ for a down-step.

Now m_1 necessarily differs from m by an integer. So keeping m fixed and summing over all possible routes from $\langle m |$ to $| m \rangle$ we are ultimately faced with

$$\sum_{m=-s}^s \sum_n \alpha_n(X) m^n \quad (3.13)$$

where $\alpha_n(X)$ is a polynomial in X . In (3.13), n can range from zero to k , where k is the number of spin-components involved: (3.11), (3.12) and (3.10). We can now make two comments on (3.13): first, no terms with n odd survive the final summation over m ; secondly, $\alpha_0(X)$, unless it vanishes, necessarily involves X as a factor, since to obtain a term independent of m we must include either (3.11) or (3.12) with $m_1 = m$. In this case, when we sum over m , the term in (3.13) with $n = 0$ produces $XYp_0(X)$, where $Y \equiv 2s + 1$ and $p_0(X)$ is a polynomial in X . Likewise, from any other term with n even, say $n = 2r$, we obtain, after summing over m , a contribution of the form $XYp_r(X)$, where $p_r(X)$ is a polynomial in X , because

$$\sum_{m=-s}^s m^{2r} = XYf_r(X) \quad (3.14)$$

where $f_r(X)$ is a polynomial in X : see Bromwich (1931) under the heading Bernoullian functions. Thus (3.13) is always ultimately of the form $XYp(X)$, where $p(X)$ is a polynomial in X . For an alternative proof of this important result see Dalton (1968).

It is important to realise that not all traces of products of spin components need to be calculated explicitly. Many are mutually equal, or differ only in sign, and many vanish identically. To have a simple notation, let us temporarily replace the symbols s_x , s_y and s_z , respectively, by 1, 2 and 3, and denote the trace by simply enclosing the symbols within brackets. Then, from the symmetry of the commutation relations under cyclic permutation of the symbols and the invariance of traces under a change of basis, (11) = (22) = (33): and from (3.10)

$$(33) = \sum_{m=-s}^s m^2 = \frac{1}{3}XY.$$

Similarly $(12) = (23)$, and $(23) = 0$, since the step (up or down) from 2 in (3.9) cannot be balanced by a subsequent inverse step. Thus

$$(\alpha\beta) = \frac{1}{3}XY \delta_{\alpha\beta}, \quad (3.15)$$

where $\delta_{\alpha\beta} = 1$, $\alpha = \beta$, and $= 0$ otherwise. With three symbols we first observe that, for the trace not to vanish, they must all be different: for (333) vanishes because m^3 is odd, and (133) vanishes since the step (up or down) from 1 cannot be balanced by a subsequent inverse step. Moreover $(123) = (231) = (312)$, both because for finite matrices $\text{Tr } AB = \text{Tr } BA$ and because the commutation relations are invariant under cyclic permutation of the symbols; and likewise $(213) = (321) = (132)$. Since the commutation relations are invariant under the transformation $s_x \rightarrow s_y$, $s_y \rightarrow s_x$, $s_z \rightarrow -s_z$, $(213) = -(123)$. We need, therefore, only calculate (123) , which is easily found to be $\frac{1}{6}iXY$. Consequently

$$(\alpha\beta\gamma) = \frac{1}{6}iXY \varepsilon_{\alpha\beta\gamma}, \quad (3.16)$$

where $\varepsilon_{\alpha\beta\gamma}$ denotes the parity of $\alpha\beta\gamma$ as a permutation of 123.

We shall not here deal in detail with cases of more than three symbols, since it is more appropriate to refer to publications in which the necessary basic traces are tabulated. But the generalisation of the results $(12) = 0$ and $(233) = 0$ is worth stating explicitly. If in $(\alpha\beta\dots\gamma)$ there are n spin components, s_x , s_y and s_z occurring n_1 , n_2 and n_3 times, respectively, then the four integers n , $n_1 n_2$ and n_3 must either all be even or all be odd, otherwise $(\alpha\beta\dots\gamma) = 0$. Sufficient indication of the proof is given by the observation that, whatever the value of n_3 , $n_1 + n_2$ must be even if up-steps are to be balanced by down-steps.

A table of basic non-vanishing traces for $n \leq 7$ was given by Rushbrooke and Wood (1958): there are 26 of them. Since then, much more extensive tables have been published. Ambler *et al.* (1962a) list the non-vanishing traces for $n \leq 9$: unfortunately in terms of s (our notation) rather than in the form $XYp(X)$, though the conversion is not difficult. For some purposes, though not those with which we are here concerned, it is more useful to know the traces of products not of s_x , s_y and s_z but of s_+ , s_- and s_z , where $s_+ = s_x + is_y$ and $s_- = s_x - is_y$: i.e. to use the so-called spherical, rather than cartesian, basis for spin components. Ambler *et al.* (1962b) later listed the non-vanishing traces for $n \leq 9$ in this spherical basis. More recently, Dalton and Rimmer (1968), by computer calculations, have produced very extensive tables using the spherical basis. In the present context, they provide the non-vanishing polynomials $p(X)$ for $n \leq 12$; but for $n \leq 9$ they also yield reduced traces of the form (2.56), as functions of the applied field.

The $n = 8$ traces of Ambler *et al.* (1962a) were used in the calculations of Pirnie *et al.* (1966) and Stephenson *et al.* (1968), to which we shall later refer. They have subsequently been checked against the Dalton and Rimmer results, with which they agree.†

We turn now to what we have called the sorting problem. To deal with this briefly, it is convenient to take a specific example, for which we may choose the graph illustrated in (2.26). Since, for the moment, we are using 1, 2 and 3 to denote s_x , s_y and s_z , we will label the three sites involved, i , j and k . If we label the two ij bonds α and β and label the three jk bonds γ , δ and ε , then the ten possible sequences of the type $(ij)(ij)(jk)(jk)(jk)$ correspond to the ten possible sequences of the symbols α , $\beta \dots \delta$ subject to the conventions that α always precedes β and γ precedes δ which precedes ε . Since, for direct products of matrices, $(A \times B)(C \times D) = AC \times BD$, this particular sequence can be represented by

$$\begin{array}{ccc} i & j & k \\ \alpha\beta & \alpha\beta\gamma\delta\varepsilon & \gamma\delta\varepsilon \end{array} \quad (3.17)$$

where now the symbols α , $\beta \dots \varepsilon$ stand for spin-components at the sites indicated by i , j and k ; and we have adopted the summation convention for repeated symbols, each of α , $\beta \dots \varepsilon$ running over the three possibilities 1, 2 and 3. Since there are five of these symbols and ten terms of the type (3.17), this suggests that there are 10×3^5 , = 2430, cases to consider. Actually, however, in this particular example, (3.15) shows that, for a non-vanishing contribution, $\alpha = \beta$; and (3.16) shows that γ , δ and ε must all be different, i.e. 1, 2 and 3 in some sequence. By symmetry, we can choose $\alpha = 1$, and multiply the result by 3 (to account for the other cases, $\alpha = 2$ and $\alpha = 3$). This reduces the factor 3^5 above to only 6. Now for direct products, $\text{Tr}(A \times B) = (\text{Tr } A)(\text{Tr } B)$; so for any precise specification of α , $\beta \dots \varepsilon$ the trace of the matrix represented by (3.17) is the product of the three traces of matrices each referring to spin components at sites i , j and k separately. We have already discussed the possibilities at sites i and k , and reference to Rushbrooke and Wood (1958) shows that there are only two non-vanishing independent traces involving five spin-components, namely (11123) and (11213), having values $\frac{1}{30} iXY(3X - 1)$ and $\frac{1}{30} iXY(X - 2)$, respectively. Thus at site j we must have one or other of these factors, with a sign determined by the permutation rules to which we have already referred.

† Apart from one obvious misprint. The factor $(s + 1)$, our notation, in (11212212) should read $(s + 2)$. But this is indeed obvious, as was realised at the time, since otherwise the resulting expression is not a function of X . We have checked that the numerical tables of Ambler *et al.* (1962a), for specific values of s , do not embody the consequences of this misprint.

Running through the possibilities, we find that the term (3.17) contributes

$$3(\frac{1}{3}XY)(\frac{1}{6}iXY)[4(11123) - 2(11213)] \quad (3.18)$$

to the trace which we are calculating. Doing this for the 10 alternative sequences of $\alpha, \beta \dots \varepsilon$, we find that 5 of them give (3.18) and the other 5 each give

$$3(\frac{1}{3}XY)(\frac{1}{6}iXY)[2(11123) + 4(11213)]. \quad (3.19)$$

Combining (3.18) and (3.19), with these weights, the trace corresponding to the graph (2.26) is found to be

$$3(\frac{1}{3}XY)(\frac{1}{6}iXY)[30(11123) + 10(11213)] \quad (3.20)$$

i.e.

$$-X^3Y^3(10X - 5)/18.$$

Ultimately, however, we are interested in mean reduced traces, i.e. for $\langle \overline{\text{=====}} \rangle$ we must divide by Y at each vertex and by the number of distinct sequences of pair operators, in this case 10. Thus, finally,

$$\langle \overline{\text{=====}} \rangle = -X^3(2X - 1)/36. \quad (3.21)$$

We have given this example in some detail both to clarify what is involved and to emphasise its essentially simple, but tedious, character. The expression (3.20), however, is not fully typical of the general case, since it is only for vertices of orders 2 and 3 (i and k above) that we have single expressions like (3.15) and (3.16): for vertices of higher order there are several inequivalent basic traces. So in place of (3.20) we shall generally have a sum of products of basic traces (with no common factors throughout, other than the XY factors which arise at every vertex). Fortunately, as we have said, all this sorting process can be computerised. This was done by Eve for 8-line graphs, in connection with the work already mentioned (Pirnie *et al.*, 1966; Stephenson *et al.*, 1968). See Dalton and Rimmer (1969), for corresponding work on the mixed Heisenberg–Ising general spin problem.

Since single-vertex traces always contain a single factor Y , the zero-field specific heat and zero-field susceptibility coefficients, which involve reduced traces, are necessarily functions of X only: which is equally true in the mixed, Heisenberg–Ising, case.

So far, in this section, we have dealt with the problem of computing the mean reduced trace of a given interaction graph. There remains the question of how many such graphs have to be dealt with in the course of finding some specific expansion coefficient. Table II does not directly help us here, since in the moment method we are concerned with multi-line graphs, and not solely with basic graphs. We are also concerned with disconnected graphs,

though, since we shall already know the traces for all components of these in any systematic procedure, they add little to the labour as far as the trace problem is concerned.

Since our aim is to emphasise that certain simple theorems, or lemmas, greatly reduce the number of graphs whose traces require separate calculation, it is convenient first to enunciate these lemmas and then illustrate their value by looking in some detail at the calculation of $\langle P^5 Q^2 \rangle$ and $\{P^5 Q^2\}$: see Section II.A above. This will serve also to show why staggered susceptibility coefficients are harder to determine than are normal susceptibility coefficients.

We present the lemmas in part diagrammatically, with the following conventions: a circle represents any graph, connected or disconnected; lines shown explicitly are not multiple bonds unless depicted as such; any crosses are depicted explicitly.

The first two theorems are trivial, but so basic that they warrant mention: (i) since the trace of any single component of spin vanishes, graphs with a node of order unity can be ignored; (ii) the trace of any term (sequence of (ij) and (i) operators) containing an odd number of (i) operators vanishes. We see this most readily by applying the transformations $s_x \rightarrow s_y$, $s_y \rightarrow s_x$, $s_z \rightarrow -s_z$ to each spin variable concerned. An immediate consequence is that graphs with two (separate) crosses contribute to $\langle P^n Q^2 \rangle$ or $\{P^n Q^2\}$ only when the two crosses lie on the same component of the interaction graph.

We come now to the lemmas, which are less fundamental but none the less valuable. They are simpler and more transparent when presented, as here, in terms of mean reduced traces than in their original forms (Rushbrooke and Wood, 1958, 1963). In our shorthand notation, these read:

1.

$$\left\langle \begin{array}{c} \text{circle} \\ \text{---} \\ \text{circle} \end{array} \right\rangle = 0.$$

2.

$$\left\langle \begin{array}{c} i \\ \text{circle} \\ j \\ k \end{array} \right\rangle = 0.$$

irrespective of coincidences between i , j and k .

3.

$$\left\langle \begin{array}{c} i \\ \text{circle} \\ j \end{array} \right\rangle = \frac{1}{3} X \left\langle \begin{array}{c} i \\ \text{circle} \\ j \end{array} \right\rangle$$

whether i and j coincide or not.

4. $\langle \text{---} \text{---} \rangle = \frac{1}{9} X \langle \text{---} \text{---} \rangle$

5. $\langle \text{---} \text{---} \text{---} \rangle = \frac{1}{3} \langle \text{---} \text{---} \rangle$

6. $\langle \text{---} \text{---} \text{---} \rangle = \frac{1}{X} \langle \text{---} \text{---} \text{---} \rangle$

7. $\langle \text{---} \text{---} \text{---} \rangle = \langle \text{---} \text{---} \text{---} \rangle$

In the interpretation of these formulae, we note that at vertices off the circle there must be no more interaction lines than those shown. Equations (5) and (6) are unaffected by direct links between the crosses within the graph represented (on both sides) by the circle.

We note that lemmas 1 and 2 enable us to discard certain graphs without further consideration; lemmas 3 and 4 express the traces of particular graphs of order n in terms of those of related graphs of order $n - 1$ (presumably already known); lemmas 5 and 6 express traces required for $\langle P^n Q^2 \rangle$ and $\{P^n Q^2\}$ in terms of traces pertaining to $\langle P^{n+1} \rangle$ and $\langle P^{n+2} \rangle$, respectively; and lemma 7, combined with eqn (3.4), implies that in computing $\langle P^n Q^2 \rangle$ we can ignore double-cross graphs. We have no counterpart to lemma 7 in the way that 6 is a counterpart to 5: but we have seen already, in eqn (2.44), that double-cross graphs can be circumvented when evaluating staggered susceptibility coefficients.

Once stated, these lemmas are easily established, and our comments will be minimal. Thus, 1 follows from 5 together with theorem (ii) above; 2, 3 and 4 rely on eqns (3.15) and (3.16); 5 and 6 depend on the isotropy of the spin Hamiltonian (in that the crosses on the left hand sides could equally represent s_x or s_y instead of s_z). The proof of lemma 7 also relies on this isotropy, which enables an ending 33 in an expression of the type (3.17) to be replaced by a multiple ($X/3$) of the unit operator. Lemma 7 is not valid for the general spin Ising problem, $I(s)$, though it does hold for $I(\frac{1}{2})$ (Morgan and Rushbrooke, 1961). The need to take explicit account of double-cross graphs in the case of dipolar interactions has been noted by Marquand (1967).

In illustrating the relevance of these lemmas to the calculation of $\langle P^n Q^2 \rangle$ and $\{P^n Q^2\}$ we shall confine attention to connected graphs. There are 22

connected graphs of order 5 with no more than two nodes of order unity; but decorating these with two crosses so as to suppress all nodes of order unity yields 51 topologically different g^{++} graphs. Application of lemma 5 in the case of $\langle P^5 Q^2 \rangle$ yields 25 topologically different connected graphs of order 6; 2 of these have zero trace by lemma 1 and 2 more by lemma 2: of the remainder, 6 reduce to graphs of lower order by lemma 3, and one more so reduces by lemma 4. We are left with just 14 connected graphs of order 6 whose traces have to be evaluated. In the case of $\{P^5 Q^2\}$, application of lemma 6 yields 39 topologically different connected graphs of order 7; 3 of these have zero trace by lemma 1 and 6 more by lemma 2: of the remainder, 14 reduce to graphs of lower order by lemma 3, and one more so reduces by lemma 4. We are left with just 15 connected graphs of order 7 whose traces have to be evaluated. It is primarily because these are seventh order graphs, rather than sixth order graphs, that the calculation of $\{P^5 Q^2\}$ is appreciably more laborious than that of $\langle P^5 Q^2 \rangle$.

We have referred to 14 connected graphs of order 6 whose traces have to be calculated *ab initio*. These are in fact the only graphs arising in the calculation of $\langle P^6 \rangle$ whose traces must be so calculated: the traces of all other (connected) graphs of order 6 either vanish (by theorem (i) or lemmas 1 and 2) or reduce to those of lower order graphs (by lemmas 3 and 4). Indeed, on account of these lemmas, the mean reduced traces of all multiline interaction graphs (without crosses) of order ≤ 8 can be found easily in terms of the corresponding traces, in powers of X , of 1 graph of order 2, 1 of order 3, 2 of order 4, 4 of order 5, 14 of order 6, 33 of order 7, and 101 of order 8. These basic traces derived by Wood, Rushbrooke, Pirnie and Stephenson, are listed in Appendix I. They suffice for the calculation of the zero-field specific heat coefficients, $c_1 \dots c_6$, the zero-field susceptibility coefficients, $a_1 \dots a_7$, and the staggered susceptibility coefficients, $a_1 \dots a_6$, for any $H(s)$ model, whatever the range of the interactions.

C. Second-neighbour interactions

To include second-neighbour, as well as first-neighbour, interactions the basic Hamiltonian (1.1) is generalised to become

$$\mathcal{H} = -2 \sum_{\langle ij \rangle} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j - g\beta H \sum_i s_{zi}, \quad (3.22)$$

where now $\langle ij \rangle$ runs over both nearest and next-nearest pairs of sites on the lattice (each such pair, of either type, being counted once only), and J_{ij} equals J_1 or J_2 according as i and j are first or second neighbours. In order to have a single dimensionless expansion parameter, it is convenient still

to define x as J_1/kT , and to denote J_2/J_1 by α . Then, in any high-temperature expansion, we may think of the pair-operator $s_i \cdot s_j$ as always carrying the factor x , and carrying also an extra factor α when i and j are second-neighbours, rather than first-neighbours, on the lattice. Thus, the trace, or cumulant parts of any calculation are essentially unaffected by the inclusion of second-neighbour interactions; the only difference is that as regards the interaction graphs themselves the bonds are now of two types, conveniently labelled 1 or 2 according as they relate to first-neighbour or second-neighbour distances. The zero-field susceptibility expansion coefficient a_n , being determined by n th order interaction graphs, will now be polynomial of degree n in α , since each interaction line can, in principle, be of either type. Equations such as (2.37), (2.40) and (2.71) are unchanged except that now g , or (n, t) refers to graphs whose lines bear the labels 1 or 2. All components of a multiple bond must bear the same label (since two sites cannot at the same time be both first and second neighbours): thus the weight factors, w_g , are unaffected by these labels. Again we are ultimately concerned with lattice counts for basic graphs (m, l, τ) , though now the l bonds are of two types, distinguished by the labels 1 and 2.

To say that only the counting problem is affected would, however, ignore two things which concern mean traces. First, the distinction between open and close-packed lattices disappears: when second-neighbour bonds are allowed, graphs with circuits of odd order (e.g. triangles) can occur on simple-cubic and body centred cubic lattices. So the longest series for open lattices cannot be generalised to include second neighbour interactions without further mean traces being computed. Secondly, there are corresponding additional complexities in the calculation of staggered susceptibilities: to which we shall refer in a moment. But these matters apart, it is only the counting problem which is affected.

It is affected in two ways. First, because there are vastly more graphs necessarily under consideration, and secondly because any counting technique must distinguish between first and second neighbour bonds. On the former point, any basic graph of order l with symmetry number unity will give rise to 2^l distinguishable graphs when the bonds are labelled either 1 or 2. We do not wish to enter into details of counting techniques (which are being dealt with elsewhere in Chapter 2 of this volume), but add only that for connected basic graphs, with bonds labelled either 1 or 2, the problem for cubic lattices has been programmed for computer calculations by Eve and the results were used in the susceptibility calculations, through a_6 , of Pirnie *et al.* (1966). Equivalent data, though necessitating the use of equations of type (3.1), have been published by Dalton (1965, 1966).

In the particular case $\alpha = 1$, i.e. when all exchange interactions are equal we can drop the labels 1 and 2 on the interaction lines and simply count

unlabelled basic graphs on a lattice whose topology is governed by the first and second neighbour structure of the lattice concerned. The counting problem is simplified, if only because less book-keeping is entailed. This particular case is known as the equivalent neighbour model, and the lattice structure, for first and second neighbour interactions, denoted f.c.c.(12), b.c.c.(12), s.c.(12). These lattices have coordination numbers 18, 14 and 18 respectively: though f.c.c.(12) and s.c.(12) are not topologically equivalent. Moreover, although all sites in any one of these lattices are topologically equivalent, this is not true of their bonds. The corresponding generalisations to include also third neighbour interactions are denoted f.c.c.(123), b.c.c.(123) s.c.(123): they have coordination numbers 42, 26 and 26, respectively. Basic equivalent neighbour lattice counts for $l \leq 7$ for (12)-type lattices and for $l \leq 6$ for (123)-type lattices have been published by Domb and Dalton (1966).

We turn finally to the additional complexities which arise in the calculation of staggered susceptibility series. Rushbrooke and Wood (1963) considered only the most obvious type of anti-ferromagnetic ordering on s.c. and b.c.c. lattices, since this can occur with nearest neighbour interactions

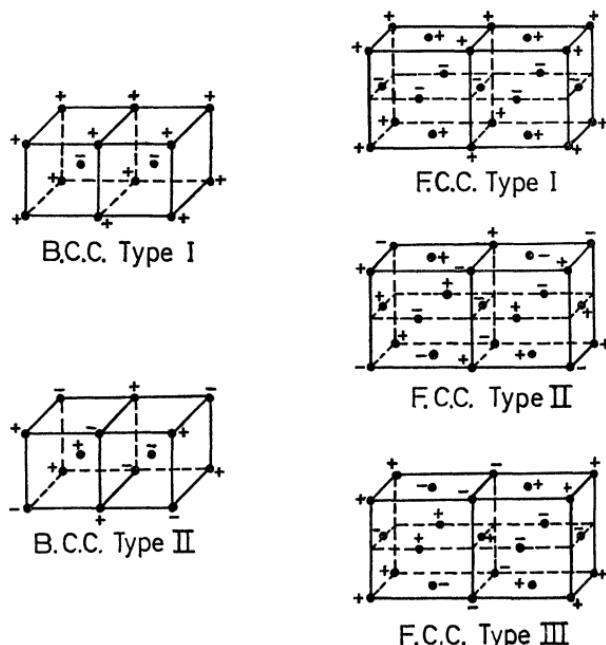


FIG. 1. The five types of antiferromagnetic ordering considered by Pirnie *et al.* (1966).

only. Pirnie *et al.* (1966), by including also second neighbour interactions, were able to discuss a greater variety of possible orderings, and indeed examined the two types of ordering on the b.c.c. lattice and the three types of ordering on the f.c.c. lattice suggested by mean-field considerations: see Smart (1966). These structures are depicted symbolically in Fig. 1, where the lines refer, of course, to second-neighbour distances. The corresponding staggered susceptibility series are instances of series for the generalised susceptibility $\chi(\mathbf{k})$, for particular choices of \mathbf{k} . Thus for the b.c.c. lattice, I and II refer, respectively, to $\mathbf{k} = [0, 0, 1]$ and $\mathbf{k} = [\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$; while for the f.c.c. lattice, I, II and III refer, respectively, to $\mathbf{k} = [0, 0, 1]$, $\mathbf{k} = [\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ and $\mathbf{k} = [0, \pm\frac{1}{2}, 1]$; see Bertaut (1963).

We have seen already that in calculating staggered susceptibility series we can avoid double-cross graphs by using eqn (2.43), in which $N_{g^{++}}^L(o)$ denotes the term linear in N in those embeddings of g^{++} on L in which the two crosses lie on different sublattices: more accurately, on sites of opposite parity. In the simple cases discussed by Rushbrooke and Wood, the only g^{++} graphs capable of such "odd" embeddings were those in which the two crosses were an odd number of links apart: and all embeddings of such graph were necessarily "odd". They could thus refer to odd g^{++} graphs, $g_{(o)}^{++}$, and replace (2.43) by (2.44). And it was only for the $g_{(o)}^{++}$ graphs that the {}-traces had to be calculated. But this is no longer the case when second-neighbour interactions are involved. As reference to Fig. 1 shows, any g^{++} graph is now capable of both even and odd embeddings; and thus the {}-traces have to be calculated for all g^{++} graphs†, which appreciably increases the magnitude of the computation.

The counting problem too is correspondingly more complex. In the simple case of Rushbrooke and Wood (1963), since all embeddings of a given g^{++} graph were necessarily either all even embeddings or all odd embeddings, $N_{g^{++}}^L$ was simply the ferromagnetic lattice count for g^{++} . This differs from N_g^L only by the extent to which g^{++} has a different symmetry number from g . But when a given g^{++} graph is capable of both even and odd embeddings (for any given assignment of the labels 1 and 2 among its bonds), then besides the ferromagnetic lattice counts $N_{g^{++}}^L$ we require also the "staggered occurrences" $N_{g^{++}}^L(o)$: for use in eqn (2.43). To obtain these, Eve modified his earlier counting program, so as to count separately, for each lattice structure, the g^{++} embeddings in which the two crosses are on sites of opposite parity. The detailed values of these lattices count have not been published, but are to be found in Pirnie (1966): as are also the "staggered occurrences" for multipart graphs. Nearly 1200 basic graphs (including multipart graphs), each with two crosses, require consideration, on each of

† This is stated misleadingly in the text of Pirnie *et al.* (1966).

the five structures of Fig. 1, in order to find the staggered susceptibility coefficients $a_1' \dots a_6'$ as functions of α .

D. Special features of the classical model, $H(\infty)$

The theory so far has been outlined in terms appropriate to the general spin Heisenberg model, $H(s)$: in this section and the next we wish to refer specifically to those features of the models for $s = \frac{1}{2}$ and $s = \infty$ which have enabled longer series to be obtained in these cases. And we take first the classical case, $s = \infty$.

Perhaps no series have been derived by such a variety of different methods as have the high-temperature expansions for the classical Heisenberg model. As we said earlier, we shall not deal explicitly here with the powerful method employed by Wortis and coworkers (Chapter 3 of this Volume). It is a generalisation of the Horwitz–Callen–Englert approach to the Ising model made practicable by the commutivity of the Heisenberg operators in the classical limit. But all methods, whatever they are, rely in large measure for their success on two properties of the mean traces of classical interaction graphs. These are that

- (A) $\langle g \rangle = 0$ unless every vertex of g is of even order, and
- (B) if g has an articulation point, so that it can be written symbolically $g_1 \cdot g_2$, then $\langle g \rangle = \langle g_1 \rangle \langle g_2 \rangle$.

These basic theorems refer to reduced mean traces in zero magnetic field; and all authors have recognised their validity. For their proof we can use either† the discrete representation approach, in which $H(\infty)$ is regarded as referring to the highest powers of X in expansions appropriate to $H(s)$, or the continuous representation approach, in which (1.6) is written

$$\mathcal{H} = -2J_1 \sum_{\langle ij \rangle} \cos \theta_{ij} - g\beta H \sum_i \cos \theta_i \quad (3.23)$$

where θ_i is the angle between \mathbf{t}_i and \mathbf{H} , and θ_{ij} is the angle between \mathbf{t}_i and \mathbf{t}_j . Perhaps the discrete representation affords the simplest proof of (A), and the continuous representation the simplest proof of (B).

To prove (A), we note that if g_n is an n th order interaction graph then the highest possible power of X in $\langle g_n \rangle$ is X^n , this power certainly being realised for a polygon, in which each vertex is of order 2. The sum of the orders of the vertices of g_n is always $2n$, and if each vertex is of even order we shall still obtain a term in X^n : on the other hand, as the discussion below eqn (3.13) indicates, vertices of odd order will lower the order of the highest power of X . Thus, in the classical limit, we are concerned only with

† For the equivalence of these two approaches see Millard and Leff (1971).

graphs all of whose vertices are of even order. Indeed, as the argument below (3.16) indicates, at each vertex we must have even numbers of s_x , s_y and s_z components.

To prove (B), it is necessary only to observe that when $H = 0$ the right-hand side of (2.33) involves only the relative orientations of neighbouring unit vectors, and thus, whatever the orientation of the vector at the articulation point of g , an integral over the orientations of the remaining vectors involved in $\langle g \rangle$ necessarily factorises into the product of the integrals involved in $\langle g_1 \rangle$ and $\langle g_2 \rangle$. Integrating over all orientations of the unit vector at the articulation point yields, in all three cases, a factor 4π , which is cancelled on passing from traces to reduced traces. In the continuous representation, of course, instead of dividing by $2s + 1$ at each vertex we divide by 4π (in order that the unit operator may have reduced trace unity).

We have discussed only the reduced traces $\langle g \rangle$ for graphs without crosses. For susceptibility graphs, g^{++} , we can use lemma 5 above to return to graphs without crosses but with an extra link. Since this link does not necessarily correspond to a nearest neighbour bond on the lattice it is often most conveniently represented by a dotted line.

Precisely how (A) and (B) are reflected in the details of actual calculations depends on the techniques employed. Thus Wood and Rushbrooke (1966), using the discrete representation and moment method to find susceptibility series, made use of (A) and (B) in the calculation of reduced traces, and (B) again to simplify the counting problem. The point here is that all susceptibility graphs (involving one dotted line) which decompose into the same set of fragments on cutting at their articulation points have the same reduced trace. Thus, for example, the set



now stands not just for a 3-part graph, but also for 3 2-part graphs, and 6 connected graphs, which can be constructed from these pieces. We can thus use eqn (3.5) to find the coefficient of N in the sum of the corresponding occurrence factors, provided we now interpret $[AB]$ as signifying at least two-point contact between the parts A and B. This greatly reduces the length of the calculation.

Taking next the finite cluster method, used by Joyce and Bowers (1966a, b), theorem (B) implies that the only $[m, l, \tau]$ clusters which contribute to $C(0)$ are those represented by star graphs (see also Domb and Wood, 1965; Domb this Volume, Chapter 1, Section IV B), while those which contribute to $\chi(0)$ correspond either to star graphs or to those graphs with articulation points which can be made into star graphs by the addition of one extra (dotted) line.

Midway between these two approaches stand the methods used by Stanley (1967a, b) [see also Stanley this Volume, Chapter 7; Stanley and Kaplan, (1966a)], and by Stephenson and Wood (1968). Essentially, these both employ the cumulant approach, eqn (2.71). But whereas Stephenson and Wood use eqn (2.50) to construct cumulants from moments, iteratively, Stanley uses this equation in the alternative form

$$[\alpha \dots \omega] = \langle \alpha \dots \omega \rangle - \sum_{p(n,2)} [\alpha \dots \beta] \langle \gamma \dots \omega \rangle, \quad (3.24)$$

where, in the sum on the right-hand side, neither the $[]$ -bracket nor the $\langle \rangle$ -bracket is empty (and we can always arrange for a given symbol, say α , to occur in the $[]$ -bracket).

Regarding the calculation of traces in the continuous representation, Joyce (1967), in an elegant paper, has shown how these or, more precisely, how the zero-field partition functions of finite clusters, can be expressed as sums of products of Wigner's $3n - j$ symbols. But this method becomes unduly complicated when $H \neq 0$, and the more direct approach of Stephenson and Wood, simply substituting

$$\cos \theta_{ij} = \cos \theta_i \cos \theta_j + \sin \theta_i \sin \theta_j \cos (\phi_j - \phi_i)$$

in (3.23), enables field-dependent high-temperature expansions to be obtained without difficulty. Specifically, Stephenson and Wood calculate traces $\langle g \rangle_{(1)}$ which are "reduced" with respect to the operator $\rho_1 \equiv \exp [g\beta H \cos \theta / kT]$ at each site, and thence generate the corresponding cumulants $[g]_{(1)}$. We note that

$$\langle \rho_1 \rangle = 4\pi \frac{\sinh y}{y}, \quad \text{where } y \equiv \frac{g\beta H}{kT}. \quad (3.25)$$

By expanding both numerators and denominators in powers of y , Stephenson and Wood obtain a free-energy expansion of the form

$$F = -NkT \sum_{r \geq 0} \sum_{n \geq 0} a_{2r,n} y^{2r} x^n. \quad (3.26)$$

For $r = 2, 3, 4$ and 5 , they derive the coefficients $a_{2r,n}$ for $n \leq 7$. These are the so called "higher order" susceptibility series. We note that the zero-field specific heat and susceptibility coefficients, c_n and a_n of (2.18) and (2.19), are given by $c_n = (n+1)(n+2)a_{0,n+2}/2a_{0,n}$ with $a_{0,2} = q/3$, and $a_n = 6a_{2,n}$, respectively. The factors X^2 and X in (2.18) and (2.19) disappear on account of the new definitions of J_1 and $g\beta$ in the classical limit. For these cases, $r = 0$ and $r = 1$, Stephenson was able to obtain appreciably longer series by utilising the consequences of theorem (B), to which we have already referred (Stephenson, 1969; Stephenson and Wood, 1970). The numbers of

classical interaction graphs listed, together with their traces and cumulants, by Stephenson as required to determine the coefficients $c_0, c_1, c_2 \dots c_8$ for $H(\infty)$, f.c.c. lattice, are 1, 1, 2, 2, 5, 7, 18, 32 and 86, respectively.

E. Special features of the original Heisenberg model, $H(\frac{1}{2})$

Although many different techniques have, in fact, been used for finding high-temperature expansion coefficients for the $H(\frac{1}{2})$ model, perhaps the only one demanding specific mention here is that employed in the finite cluster method. For spin $\frac{1}{2}$, the Hamiltonian (1.1) is conveniently written

$$\mathcal{H} = -\frac{1}{2}J_1 \sum_{\langle ij \rangle} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j - \mu H \sum_i \sigma_{zi} \quad (3.27)$$

where the components of $\boldsymbol{\sigma}_i$ are the Pauli spin matrices, $\boldsymbol{\sigma}_i = 2\mathbf{s}_i$, and we have replaced $\frac{1}{2}g\beta$ by the magnetic moment μ . The Dirac identity

$$\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j = 2P_{ij} - 1 \quad (3.28)$$

is now used to replace the pair interaction terms (themselves essentially a consequence of the Pauli exclusion principle) by a sum of permutation (interchange) operators; and we can invoke the standard theory of representations of the symmetric group to reduce the size of the matrices, traces of powers of which are ultimately required. For finding $H(\frac{1}{2})$ series by the moment method, Domb and Sykes invoked (3.28) in 1956 as an alternative to the algebraic approach (based on the commutation rules) employed by Rushbrooke and Wood (1955); but its use in the context of the finite cluster method dates from the early 1960's when Domb and coworkers (notably Wood, D. W.) and Baker, Rushbrooke and coworkers, seem simultaneously to have appreciated its possibilities. The earliest published papers are Domb and Wood (1964) and Baker *et al.* (1964); but fuller references are given in the next section.

With a finite cluster $[m, l, \tau]$, we are initially faced with matrices of order 2^m , representing operators in a space conveniently spanned by the 2^m vectors (kets) $\alpha(1)\alpha(2)\dots\alpha(m), \alpha(1)\dots\alpha(m-1)\beta(m), \dots, \beta(1)\alpha(2)\dots\alpha(m), \alpha(1)\dots\beta(m-1)\beta(m), \dots, \beta(1)\beta(2)\dots\alpha(m), \dots, \beta(1)\beta(2)\dots\beta(m)$, where $\alpha(i)$ and $\beta(i)$ represent the two possible spin states at site i . The permutation operator P_{ij} acting on these, interchanges the spin states at sites i and j ; and thus the subspaces defined by given numbers of α 's and β 's are invariant under these operators. These invariant manifolds are of dimension $\binom{m}{k}$, where the corresponding value of $\Sigma_i \sigma_{zi}$ is $(m-2k)$, and $k = 0, 1, 2 \dots m$. They provide representations $\Delta^{(k)}$ of the symmetric group, but these are not irreducible representations (except for $k=0$ and $k=m$). $\Delta^{(k)}$ and $\Delta^{(m-k)}$ are, of course, equivalent representations. The crux of the

matter is that, for $k = 1, 2 \dots [m/2]$, $\Delta^{(k)}$ is the direct sum of $\Delta^{(k-1)}$ and an irreducible representation $D^{(k)}$: see, for example, Wigner (1959). Thus $D^{(k)}$, of dimension

$$\binom{m}{k} - \binom{m}{k-1},$$

occurs $m + 1 - 2k$ times in the original representation of order 2^m : being associated successively with values $m - 2k, m - 2k - 2, \dots, -m + 2k$ of the operator $\Sigma_i \sigma_{z_i}$.

The irreducible representations $D^{(k)}$ are, in fact, those irreducible representations of the symmetric group S_m whose Young diagrams have at most two horizontal rows, the second row having k squares. For their explicit construction see, for example, Hamermesh (1962). Once we know the matrix representation of P_{ij} provided by $D^{(k)}$, we simply use (3.28) to construct the corresponding matrix for $\Sigma_{ij} \sigma_i \cdot \sigma_j$ appropriate to the cluster $[m, l, \tau]$: for which purpose, of course, we label the sites of the cluster $1, 2, \dots, m$. We call this matrix Γ_k . A better, but more cumbersome notation, would be $\Gamma_k[m, l, \tau]$.

The dimensions of the largest Γ_k matrices, for $m = 2, 3 \dots, 11$, are 1, 2, 3, 5, 9, 14, 28, 48, 90 and 165 respectively. If we had not performed the second reduction above, from $\Delta^{(k)}$ to $D^{(k)}$, the corresponding largest sizes would have been 2, 3, 6, 10, 20, 35, 70, 126, 252 and 462 (with the same number of matrices to be dealt with). Since we are ultimately concerned with finding the traces of powers of these matrices, the saving in computer time produced by the second reduction is appreciable.

It follows immediately, from (2.2), that for any cluster $[m, l, \tau]$ the partition function, $Z(H, T)$, is given by

$$Z_{[m, l, \tau]} = \sum_{n=0}^{\infty} \frac{x^n}{2^n n!} \left\{ \sum_{k=0}^{[m/2]} \text{Tr} (\Gamma_k^n) \sum_{p=k}^{m-k} \exp [(m-2p)y] \right\} \quad (3.29)$$

where $x \equiv J_1/kT$ and $y \equiv \mu H/kT$. We note that $Z_{[m, l, \tau]}$ is an even function of y . The coefficients in the double power-series expansion of Z in terms of x and y^2 are readily determined and by taking the logarithm (by machine calculation) we find the coefficients $A(r, n)$ in the expansion

$$\ln Z_{[m, l, \tau]} = \sum_{r \geq 0} \sum_{n \geq 0} A(r, n) y^{2r} x^n. \quad (3.30)$$

We then apply the standard procedure of the finite cluster method (Section II.D above) to find the corresponding expansion of $\ln Z$ for any given lattice. In this way we find not only series in powers of x for $C(0)$ and $\chi(0)$, but also for the higher order susceptibilities defined by (3.26). [Note: although

y appears to be defined slightly differently for $H(\infty)$ and $H(\frac{1}{2})$, it is mH/kT in both cases, where m denotes the saturation magnetisation per lattice site.]

As a digression, we may comment that, as an immediate consequence of (3.29), the zero-field susceptibility of the cluster $[m, l, \tau]$ is given explicitly by

$$\frac{\chi(0)kT}{2} = \frac{\sum_{k=0}^{[m/2]} (m-2k)(m-2k+1)(m-2k+2) \text{Tr} \exp\left(\frac{x}{2}\Gamma_k\right)}{3 \sum_{k=0}^{[m/2]} (m-2k+1) \text{Tr} \exp\left(\frac{x}{2}\Gamma_k\right)} \quad (3.31)$$

where, if d_k denotes the dimensionality of Γ_k and λ_i , $i = 1, 2 \dots d_k$, are its eigenvalues,

$$\text{Tr} \exp\left(\frac{x}{2}\Gamma_k\right) = \sum_i \exp(x\lambda_i/2).$$

Instances of eqn (3.31) are to be found in Rushbrooke and Morgan (1961), Elliott and Heap (1962), Morgan and Rushbrooke (1963) and Heap (1963). Complete results for $m \leq 6$ have been tabulated by Muse (1969). While of value in discussing randomly dilute ferromagnets, these closed form expressions are not helpful for finding high-temperature expansions. It is much easier to compute the traces of powers of a matrix than to find its eigenvalues and then expand exponentials.

Quite apart from its connection with representations of the symmetric group, the $H(\frac{1}{2})$ model has another property which simplifies work based on high-temperature expansions. This feature, recognised by Opechowski (1937), and shared also by the corresponding spin- $\frac{1}{2}$ Ising model, results from the simple identity $\sigma_{zi}^2 = 1$. For, as a consequence of this identity,

$$\begin{aligned} \exp(y\sigma_{zi}) &= \cosh y + \sigma_{zi} \sinh y \\ &= \cosh y (1 + t\sigma_{zi}) \end{aligned} \quad (3.32)$$

where $t \equiv \tanh y$. Thus if we were deriving the high-temperature expansion for the partition function, Z^L , of an infinite lattice by the moment method, we should be faced with interaction graphs (not necessarily connected) of lines and crosses, each line corresponding to a factor $x/2$, i.e. $J_1/2kT$ (since the (i,j) operators are written $\sigma_i \cdot \sigma_j$), and each cross to a factor t . But with this interpretation of the crosses, based on (3.32), we cannot have more than one cross at any site; and graphs with isolated crosses have zero trace, since $\text{Tr } \sigma_{zi} = 0$. Thus there cannot be more t -factors than there are sites involved in interaction lines. The greatest number of such sites in a graph g_n is $2n$, which arises when, and only when, g_n comprises n separate lines.

Thus, the highest power of t associated with x^n is t^{2n} : and since we pass from Z^L to $\ln Z^L$ by picking out the term linear in N , this result holds also for $\ln Z^L$. More precisely, we can write

$$\frac{1}{N} \ln Z^L = \ln (2 \cosh y) + \sum_{j \geq 0} \sum_{n \geq 1} \frac{x^n}{2^n n!} f(n, j) t^{2j} \quad (3.33)$$

where

$$f(n, j) = 0 \quad \text{when } n < j. \quad (3.34)$$

From the above argument it is elementary to show that $f(n, n)$ equals $n!$ times the coefficient of N in the occurrence factor for n separate bonds on L , which has sign $(-1)^{n-1}$.

We note that the zero-field specific heat and susceptibility coefficients are given by $2^n n! c_n = f(n+2, 0)/f(2, 0)$ and $2^n n! a_n = 2f(n, 1)$, respectively.

Baker *et al.* (1970) have shown that the property expressed in (3.33) and (3.34) holds not only for an infinite lattice but also for any finite cluster, $[m, l, \tau]$. Indeed they established (3.33) and (3.34) in this unnecessarily sophisticated way.

IV. High Temperature Series Expansions

We must now briefly, but systematically, review the literature, covering rather more than thirty years, in which the high-temperature series with which we are here concerned have been progressively developed. Departing, however, from strict historical sequence, we shall take first papers concerned with the general spin model, $H(s)$, then those relating to the classical model, $H(\infty)$, and then those for the original model, $H(\frac{1}{2})$. Sections A, B, and C, relate, respectively, to these three cases; and cover not only thermodynamic series but also those for "staggered" susceptibilities. We defer till section F mention of correlation functions and second-moment series: on which there has been relatively little work. Section D introduces anisotropic spin Hamiltonians; and section E relates (very briefly) to spinel structures and the extension of the Heisenberg model to cover the phenomenon of ferrimagnetism.

A. Series for the general spin model, $H(s)$

These series effectively begin with a paper by Brown and Luttinger in 1955, in which $a_1 \dots a_4$ were presented for the five lattices, f.c.c., b.c.c., s.c., p.t. and s.q. Brown (1956) added a_5 for open lattices (b.c.c., s.c., and s.q.). In 1957, Wood and Rushbrooke derived $a_1 \dots a_5$ in terms of general lattice

parameters (revealing a small error in Brown's values for a_5); and in 1958 the same authors extended this work to include also a_6 and the specific heat coefficients $c_1 \dots c_5$. Numerical values of $a_1 \dots a_6$ are tabulated for $s = \frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}$ and 3 for the f.c.c. and b.c.c. lattices.[†] In 1968, Stephenson *et al.* added a_7 and c_6 : presenting these as polynomials in X for all five lattices.[‡] And, to date, these are the longest series for the general spin model.

Higher-order susceptibility series have been barely considered for $H(s)$, but Fechner (1969) discusses the field dependence of the first four susceptibility coefficients.

The work described above was confined to nearest-neighbour interactions. Second-neighbour interactions were introduced in 1964 when Wojtowicz gave $c_1(\alpha) \dots c_3(\alpha)$ and Wojtowicz and Joseph gave $a_1(\alpha) \dots a_4(\alpha)$ in terms of general lattice parameters: α standing for the ratio J_2/J_1 . The following year, Pirnie and Wood (1965) gave $a_5(\alpha)$ for f.c.c., b.c.c., and s.c. lattices: and Dalton, see also Dalton (1966), gave $c_1(\alpha) \dots c_4(\alpha)$ and $a_1(\alpha) \dots a_5(\alpha)$ in terms of lattice parameters (which are tabulated). The most extensive second-neighbour series are those of Pirnie *et al.* (1966), who published $a_1(\alpha) \dots a_6(\alpha)$, as polynomials in X and α , for the three cubic lattices.

Staggered susceptibility series were introduced by Rushbrooke and Wood (1963), who gave $a'_1 \dots a'_6$ as polynomials in X for nearest neighbour interactions only on the b.c.c. and s.c. lattices. This work was appreciably generalised by Pirnie *et al.* (1966), who introduced second-neighbour interactions and considered the five antiferromagnetic orderings depicted in Fig. 1, deriving $a'_1(\alpha) \dots a'_6(\alpha)$, in each case. As we have observed already, these staggered susceptibilities are particular instances of the generalised susceptibility, $\chi(\mathbf{k})$. For nearest neighbour interactions only, the first four coefficients, $a_1(\mathbf{k}) \dots a_4(\mathbf{k})$ of $\chi(\mathbf{k})$ have been presented recently by Collins (1970) in terms of general lattice parameters.[§]

Of these $H(s)$ coefficients, we present in Appendix II the expressions of Pirnie *et al.* (1966) for $a_1(\alpha) \dots a_6(\alpha)$ for the three cubic lattices, and the generalised susceptibility coefficients $a_1(\mathbf{k}) \dots a_4(\mathbf{k})$ of Collins (1970).

B. Series for the classical model, $H(\infty)$

The earliest series is that of Barker (1954), who derived $c_1 \dots c_6$ for the s.c. lattice (the odd coefficients, c_{2n+1} , vanish). From then till 1966, work on $H(\infty)$ is embraced exclusively in that for $H(s)$. Then Wood and Rushbrooke

[†] There is one misprint: for $H(3/2)$, b.c.c., $a_3 = 5685.3333$ and not 5683.3333.

[‡] There is one misprint: in a_7 , b.c.c., the coefficient of X^7 should read 42335.155814 and not 42334.144814.

[§] The factor $\Sigma_2/(z - 1)$ in Collins's expression for $a_4(\mathbf{k})$ should read Σ_1 (Rushbrooke and Pirnie, unpublished); and this correction has been made in Appendix II.

(1966) published $a_1 \dots a_8$ for the three cubic lattices, and Joyce and Bowers (1966b) added a_9 for the open lattices (b.c.c. and s.c.). Joyce and Bowers also gave $c_1 \dots c_7$ for f.c.c. and $c_1 \dots c_8$ for b.c.c. and s.c. (when the odd coefficients vanish). Stanley (1967b) gave $a_1 \dots a_7$ in terms of general lattice constants, and $a_1 \dots a_9$ for open lattices; and later (1967c) added a_8 for close-packed lattices (evaluating this for the p.t. lattice). In this second paper, Stanley also converted from series in x to series in u , where $u = \coth 2x - 1/2x$ [see also Stanley (1969)]. In 1968, Jasnow and Wortis reported confirmation of all the above susceptibility coefficients. Stephenson and Wood (1970) quote a_9 for the f.c.c. lattice, and indeed Stephenson (1969) gives c_8 f.c.c., a_9 f.c.c. and p.t., and $a_{10}\dagger$ b.c.c. and s.c. Moore (1969) confirms $a_1 \dots a_9$, p.t. lattice, and adds a_{10} [it is necessary to multiply Moore's coefficients by $(2/3)^n$ to preserve the normal meaning of J_1]. Recently Stephenson's value of a_9 , f.c.c. lattice, has been confirmed by Ferer *et al.* (1971), who have added a_{10} and $c_9\dagger$.

The higher-order susceptibility coefficients, $a_{2r,n}$ of eqn (3.26), for $r = 2, 3, 4, 5$ and $n \leq 7$ were published by Stephenson and Wood in 1968, for both open and close-packed lattices. In their 1971 paper, Ferer *et al.* give $a_{4,n}$, $n \leq 8$, f.c.c. lattice.‡

Regarding second-neighbour interactions, Bowers and Woolf (1969) give $a_1(\alpha) \dots a_7(\alpha)$ in the particular case $\alpha = 1$ for the cubic lattices, i.e. $a_1 \dots a_7$ for the equivalent neighbour models f.c.c. (12), b.c.c.(12) and s.c.(12). The first six of these are fully confirmed by the more general expressions of Pirnie *et al.* (1966).

In Appendix III we list a_n coefficients for f.c.c., b.c.c., s.c., p.t., s.q., f.c.c. (12), b.c.c.(12) and s.c.(12) lattices; and c_n coefficients for the three cubic lattices.

C. Series for the spin- $\frac{1}{2}$ model, $H(\frac{1}{2})$

In his pioneer paper of 1937, Opechowski gave the $f(n,j)$ coefficients of eqn (3.33) for $n \leq 4$, for the f.c.c. lattice: and thus, in particular, expressions

† Dr. Ferer (private communication) has employed the computer program of Ferer *et al.* (1971) to find a_{10} for these open lattices, and obtains values which differ from Stephenson's by about 1 in 10^5 , b.c.c. lattice, and 3 in 10^5 , s.c. lattice. We believe these values are more likely to be correct than those of Stephenson, and are indebted to Dr. Ferer for permission to quote his values in Appendix III.

‡ This work reveals errors of order 1 in 10^5 in Stephenson and Wood's values of $a_{4,5}$ and $a_{4,7}$, f.c.c. lattice. We have tracked these to a single parity fault (subsequently located as a typing error). This fault will not affect Stephenson and Wood's higher-order coefficients for open lattices, but must affect their $a_{2r,n}$ coefficients, $r \geq 2$, $n \geq 5$, for close-packed lattices (f.c.c. and p.t.). Fortunately, we believe the errors are small enough to have negligible effect on the calculation by Stephenson and Wood (1970) of the magnetic phase boundary for $H(\infty)$, f.c.c. lattice, to which we refer in Section V.C below.

for $a_1 \dots a_4$. Opechowski (1939) made corrections to $f(4, j)$, and Zehler (1950) further corrected a_4 f.c.c., and added $a_1 \dots a_4$ s.c. In 1955, Rushbrooke and Wood gave $a_1 \dots a_5$, and $c_1 \dots c_4$, in terms of general lattice parameters (specified for common lattices), and Domb and Sykes (1956) added a_6 . Domb and Sykes (1957b) gave a_6 for the hexagonal close-packed lattice (which is about 2 in 10^5 larger than for the f.c.c. lattice: see also Rushbrooke and Wood (1958)).

Progress then awaited the development of the finite-cluster method. Domb and Wood (1964) gave a_7 and a_8 , c_6 and c_7 in terms of lattice parameters for open lattices; see Domb *et al.* (1964) for some numerical evaluations. Wood (1965) added a_9 for open lattices, and the same year Domb and Wood, in a definitive paper on this work, gave a_7, a_8, a_9, c_5, c_6 and c_7 for open lattices and a_7, c_5 and c_6 for close-packed lattices: all in terms of general lattice parameters. (A minor error in their numerical evaluation of c_6 , f.c.c. does not invalidate the general expression.)

The parallel work of Baker *et al.* begins with the publication (1964) of $a_1 \dots a_{10}$ and $c_1 \dots c_{19}$ for the linear chain, a study undertaken to examine the feasibility of including clusters of up to 11 spins. In the particular case of the linear chain, lemma 1 of Section III.B implies a specific heat series of twice the normal length. Later (1966a) Baker *et al.* gave a_7, a_8, a_9, c_6 and c_7 for the f.c.c. lattice, and $a_7, a_8, a_9, a_{10}, c_6, c_7$ and c_8 for b.c.c. and s.c. lattices (the numbers actually presented being $2f(n, 1)$ and $f(n + 2, 0)$ of eqn (3.33), as also in Domb and Wood (1965): these numbers are integers). Their final results, presented the following year, added c_8 for close-packed lattices and included also the higher-order susceptibility coefficients, $a_{2r,n}$ of (3.26) for $r = 2, 3, 4$ and $n \leq 8$. See Baker *et al.* (1967a) for coefficients pertaining to planar lattices and Baker *et al.* (1967c) for a thorough discussion of the three-dimensional cubic lattices.

In one respect, however, Baker *et al.* later took this work further. For they reverted to the procedure of Opechowski and discussed (though by the finite-cluster method, rather than the original moment method) not the higher-order susceptibility series of (3.26) but the t -expansion coefficients of eqn (3.33). All $f(n, j)$ of (3.33) for $n \leq 8$ were determined, for the f.c.c., b.c.c., s.c., p.t. and s.q. lattices. In their publication (1970), Baker *et al.* did not list these coefficients explicitly, only expressions derived from them: we therefore give them here in Appendix IV.† With them, the $a_{2r,n}$ coefficients of (3.26) can be evaluated, $n \leq 8$, for all r .

Second-neighbour interactions were considered by Dalton and Wood (1965), who gave expressions for $a_1(\alpha) \dots a_5(\alpha)$, $c_1(\alpha) \dots c_3(\alpha)$ for cubic lattices. For the equivalent neighbour models f.c.c.(12), b.c.c.(12), s.c.(12),

† We note that $f(4, 2)$ f.c.c. does not accord with Opechowski, but has the value derived recently by Fechner (1969).

f.c.c.(123), b.c.c.(123) and s.c.(123) they added an extra term to each of these series. The coefficients are repeated in Domb and Dalton (1966), a paper which also gives the corresponding Ising-model series. The susceptibility coefficients for f.c.c.(12), b.c.c.(12) and s.c.(12) follow also from Pirnie *et al.* (1966) on putting $\alpha = 1$ and $X = 3/4$. More recently, Bowers and Woolf (1969) have added a_7 for these (12)-lattices.

In Appendix IV, besides the $f(n, j)$ coefficients already referred to, we list a_n coefficients for f.c.c., b.c.c., s.c., p.t., s.q., f.c.c.(12), b.c.c.(12), and s.c.(12) lattices; and c_n coefficients for the three cubic lattices.

It is very satisfactory that many coefficients, for $H(\frac{1}{2})$ as well as for $H(\infty)$, have been derived independently by more than one group of workers. Where this is not so, we print the coefficients in italics. We have not, however, adopted this convention with the $f(n, j)$'s.

D. Anisotropic spin-Hamiltonians

The Hamiltonian

$$\mathcal{H} = -2J_1 \sum_{\langle ij \rangle} [a_x s_{xi} s_{xj} + a_y s_{yi} s_{yj} + a_z s_{zi} s_{zj}] - g\beta H \sum_i [b_x s_{xi} + b_y s_{yi} + b_z s_{zi}], \quad (4.1)$$

where the a 's and b 's are constants, embraces not only the Heisenberg and Ising models but other possibilities as well, In particular

$$a_x = a_y = a_z = 1, \quad b_x = b_y = 0, \quad b_z = 1 \quad \text{yields } H(s) \quad (4.2)$$

$$a_x = a_y = 0, \quad a_z = 1, \quad b_x = b_y = 0, \quad b_z = 1 \quad \text{yields } I(s) \quad (4.3)$$

and

$$a_x = a_y = 1, \quad a_z = 0, \quad b_x = 1, \quad b_y = b_z = 0 \quad \text{defines } XY(s). \quad (4.4)$$

The XY -model has been studied for both $s = \frac{1}{2}$ (see Betts this Volume, Chapter 8) and $s = \infty$ classical XY -model). The case

$$a_x = a_y, \quad a_z \neq 0, \quad b_x = b_y = 0, \quad b_z = 1 \quad \text{defines } HI(s), \quad (4.5)$$

the so called mixed Heisenberg-Ising Hamiltonian.

We shall not here discuss at all the Ising model (for which, of course, very extensive series are known; see Chapter 6 by Domb in this Vol.): we confine attention to the other possibilities. Moreover, the models can, with advantage, be defined solely by the pairwise interactions part of the Hamiltonian; but we have included the field part explicitly to emphasise that

interest normally centres on that direction of applied field which produces the maximum response at the critical point.

For general spin, we know only of the work of Dalton and Rimmer (1969), who give $a_1 \dots a_4$ for $HI(s)$ as functions of $(a_x + a_y)/a_z$. But for $s = \frac{1}{2}$ and $s = \infty$ there is a larger literature.

For the classical models ($s = \infty$), the most general study, not confined to the Hamiltonians (4.2)–(4.5), is that of Jasnow and Wortis (1968). The series they publish for anisotropic cases are of eighth order, and relate to $I(\infty)$, $XY(\infty)$, and $HI(\infty)$ for $a_x = a_y = a_z/2$, on the f.c.c. lattice. We know of no explicit study of $XY(\infty)$ on a two-dimensional lattice. A related, though distinct, model is the planar classical model, $P(\infty)$, defined by

$$H = -2J_1 \sum_{\langle ij \rangle} \mathbf{t}_i \cdot \mathbf{t}_j \quad (4.6)$$

where now \mathbf{t}_i and \mathbf{t}_j are unit vectors constrained to lie in a plane (and the field, H , also lies in this plane, for maximum response). Series for $P(\infty)$ through eighth order on the f.c.c. and other cubic lattices have been given by Bowers and Joyce (1967) and Stanley (1968), who gives also a_9 for open lattices; and for the plane triangular lattice Moore (1969) gives $P(\infty)$ series through tenth order. The strict absence of long-range order (spontaneous magnetisation) for $P(\infty)$, and other classical Hamiltonians, for two-dimensional lattices, has been proved by Mermin (1967).

For $HI(\frac{1}{2})$, Obokata *et al.* (1967) give $a_1 \dots a_7$ as functions of $a_x (= a_y)$ and a_z . They refer to the case $a_z = 0$ as the XY -model, but are not calculating the susceptibility with H in the x - y plane. $XY(\frac{1}{2})$ as defined by (4.4) has been extensively studied by Betts and coworkers. Since $\Sigma_i \sigma_{xi}$ does not commute with $\Sigma_{\langle ij \rangle} [\sigma_{xi} \sigma_{xj} + \sigma_{yi} \sigma_{yj}]$, Betts does not consider the susceptibility itself, and high-order susceptibilities, but rather the related fluctuations,

$$Y \equiv \langle M_x^2 \rangle / Nm^2 \quad (4.7)$$

and

$$Y_2 \equiv [3\langle M_x^2 \rangle^2 - \langle M_x^4 \rangle] / 2Nm^2 \quad (4.8)$$

where

$$M_x \equiv \sum_i \sigma_{xi}. \quad (4.9)$$

These should exhibit the same critical behaviour as the corresponding susceptibilities (Falk and Bruch, 1969). Betts *et al.* (1970a) find series for Y through $(J_1/kT)^9$ for the three cubic lattices, and Ditzian and Betts (1970) give the f.c.c. series for Y_2 through sixth order. Betts *et al.* (1971) have extended this work to the plane triangular lattice, giving Y again to ninth order and Y_2 to seventh order.

E. Ferrimagnets and spinel structures

We regard these as essentially outside the scope of this review, and so make but brief reference to the more important papers. Mathematically, since we are always working in a direct-product representation, there is no need for the spins s_i , and related magnetic moments, to have the same value for all sites i . If their values and, in particular, their associated magnetic moments, differ as between two sublattices, then the model can exhibit ferrimagnetism. Physically, ferrimagnetic behaviour and ordering in spinel-type structures are closely associated: which is why we group these papers together.

The earliest work is that of Wojtowicz (1960) and Fechner (1961, 1963). The most extensive is due to Wojtowicz (1967), who gives general fifth order susceptibility series, which are then particularised to spinel- and garnet-type structures. Longer, eighth order, series for classical ($\text{spin } \infty$) ferrimagnetics on cubic structures have been discussed by Freeman and Wojtowicz (1968). Series for classical ferromagnets, defined by $H(\infty)$, $I(\infty)$ and $XY(\infty)$ on B-type spinel structures, through eighth order, have been given by Jasnow and Moore (1968).

F. Correlation functions and second moment series

For paramagnetic substances, with no zero-field magnetisation, it is convenient to define the correlation function $\Gamma(\mathbf{r})$ as

$$\Gamma(\mathbf{r}) = \langle s_{zi} s_{zj} \rangle \quad (4.10)$$

where in (4.10), as in (4.7) and (4.8) above, $\langle \rangle$ stands for the equilibrium thermal average in zero field, and \mathbf{r} is the vector distance (usually measured in lattice spacings) between sites i and j . In the absence of long-range order (i.e. for a magnetic substance above its Curie point), $\Gamma(\mathbf{r}) \rightarrow 0$ as $\mathbf{r} \rightarrow \infty$. In terms of $\Gamma(\mathbf{r})$ the correlation moments, μ_t , are defined† by

$$\mu_t = \sum_{\mathbf{r}} r^t \Gamma(\mathbf{r}). \quad (4.11)$$

The zeroth moment, corresponding to $t = 0$, is, of course, related simply to $\chi(0)$, the zero-field susceptibility: for, from (2.12), the absence of spontaneous magnetisation in zero field, and the commutivity of P and Q ,

$$\chi(0) = kT \frac{\partial^2 Z}{\partial H^2} \cdot \frac{1}{Z}$$

† Note that these μ 's are not the μ 's of Section II.A; but no confusion should arise.

i.e.

$$\frac{\chi(0)kT}{g^2 \beta^2} = \langle Q^2 \rangle = \left\langle \left(\sum_i s_{zi} \right) \left(\sum_j s_{zj} \right) \right\rangle \\ = N \sum_j \langle s_{zi} s_{zj} \rangle$$

or

$$\frac{\chi(0)kT}{Ng^2 \beta^2} = \sum_{\mathbf{r}} \Gamma(\mathbf{r}) = \mu_0. \quad (4.12)$$

There has been no detailed study of correlation functions for the Heisenberg model comparable with that of Fisher and Burford (1967) for the Ising model, $I(\frac{1}{2})$. Almost all work is confined to high-temperature series for μ_2 for classical models. The earliest reference to such work is by Fisher (1966), but full details were not then published; see also Bowers and Woolf (1969). Jasnow and Wortis (1968) give eighth order second-moment series for $H(\infty)$, $I(\infty)$, $XY(\infty)$, and $HI(\infty)$ with $a_x = a_y = a_z/2$, for the f.c.c. lattice. Moore (1969) gives ten terms of the second-moment series for $H(\infty)$ and $P(\infty)$ on the plane triangular lattice. Recently Ferer *et al.* (1971) have obtained correlation moments through tenth order for $H(\infty)$. f.c.c. lattice. Also for $H(\infty)$, Stanley (1967a) has given general expressions for $\langle \mathbf{s}_i \cdot \mathbf{s}_j \rangle$ through eighth order for close-packed lattices and ninth order for open lattices. For more general Heisenberg models the only published work we know of relates to five term series for $H(s)$ by Binder (1969). (Correlations will be considered in detail by Fisher and Jasnow in Vol. 4 of this publication.)

V. Properties Derived from High Temperature Expansions

There is little point in calculating successive coefficients in the high-temperature expansion of a thermodynamic function, or any other quantity defined by an initial Hamiltonian, without the intention of drawing physical conclusions from the series concerned. Since, however, it has not yet proved possible to say anything rigorously about the general term in such a series for the Heisenberg model, these conclusions have necessarily to be approached with caution. Mathematically, of course, nothing at all can be inferred from the initial terms of an infinite series. It is only the belief that the initial terms in fact do some justice to the underlying physics, and that the more terms we have the more justice is done, that encourages us to base physical predictions on the only knowledge we have. That this is not an entirely empty belief, may be illustrated by the observation that the first susceptibility coefficient, a_1 , defines the linear asymptote to a plot of $1/\chi$ against T ; this line intersecting the temperature axis at $kT/J_1 = a_1 (= \frac{3}{4}qX)$. This is the paramagnetic Curie temperature predicted by mean-field theory;

the asymptote itself corresponds to the Curie-Weiss law. And although this Curie-Weiss law is true neither of the Heisenberg model nor of real magnetic substances it is certainly not physically nonsense (at least, not for three-dimensional lattices).

The conclusions we draw are best regarded as produced by extrapolation from a sequence of successive approximations. When ratio methods and Neville tables (see below) are used, this characteristic is quite explicit. But when series are analysed by the method of Padé approximants, since we do not normally extrapolate on the entries in a Padé table it is less obvious that extrapolation is involved. In one sense, however, it certainly is; for a Padé approximant extends a series in the light of what is already known about it. And this is just what is also done by an extrapolation on the ratios of successive coefficients.

We are concerned with series of the type

$$f(x) = 1 + a_1x + a_2x^2 + \dots + a_nx^n + \dots \quad (5.1)$$

which are believed to be singular at $x = x_c$. We shall normally suppose that near $x = x_c$

$$f(x) \sim \frac{A}{(x_c - x)^p} \quad (5.2)$$

where A is a function of x sufficiently slowly varying that it may be treated as a constant, and p is an exponent whose value is of interest to us. That the singularity in $f(x)$ at x_c is of the type (5.2) is an assumption which underlies almost all analysis of power series in this field. As a working hypothesis, it is partially, but by no means completely, justified by (a) its simplicity, (b) some rather long series in other areas of crystal statistics, where ratios of successive coefficients, a_n/a_{n-1} , rapidly approach convincing linearity when plotted against $1/n$, (c) certain exact results on the two-dimensional Ising model.[†]

We do not intend here either to embark on a fresh analysis of the Heisenberg series or to recapitulate in detail analyses which have already been published. (A detailed exposition of the analysis of series expansions is given by Gaunt and Guttmann in Chapter 4 of this volume). But some limited comments are certainly appropriate, and to make them intelligible we need first to summarise, and label for easy reference, the different analytical techniques which have been used.

[†] A logarithmic singularity (as with the two-dimensional Ising model specific-heat) demands special attention; but in no Heisenberg case is there any evidence of purely logarithmic singularities.

Taking first those involving Padé approximants, we denote by $[D, N]$ the Padé approximant (*PA*) to (5.1) whose denominator is of degree D in x and numerator of degree N .† If n coefficients in (5.1) are known, we normally form all *PA*'s for which $D + N \leq n$, and the corresponding quantities of interest pertaining to these *PA*'s (such as the smallest positive real roots of their denominators) are said to constitute the complete Padé table (of this quantity) for (5.1). A Padé table is regarded as well-converged when this quantity appears to be rather unambiguously predicted by the later diagonals, $D + N = n$, $n - 1$ and $n - 2$, in this table. It is sometimes necessary to ignore *PA*'s for which either D or N is small, say ≤ 2 . We now distinguish the following well-known procedures:

P(a). Assuming a value for x_c , *PA*'s to

$$(x - x_c) \frac{d}{dx} \ln f(x)$$

evaluated at $x = x_c$ provide estimates of p .

P(b). Assuming a value for p , the smallest positive real roots of the denominators of *PA*'s to $f(x)^{1/p}$ provide estimates of x_c .

We know, see particularly Baker *et al.* (1967c), that P(a) and P(b) are highly correlated, and far from discriminatory. Moreover, roughly speaking and for the Heisenberg series, a 1% change in x_c produces a 10% change in p .‡

P(1). We form *PA*'s to $(d/dx) \ln f(x)$. The smallest positive real roots of their denominators provide estimates of x_c , and the residues at these roots are simultaneously estimates of $-p$. We regard this as the basic Padé method; and comment only that the $[1, N]$ estimates form the basis of an early extrapolatory procedure due to Park (1956). Plotted against $1/N$, the $[1, N]$ estimates of x_c should, on the basis of (5.2), approach the $1/N = 0$ axis horizontally.

P(2). We form *PA*'s to $[d^2 \ln f(x)/dx^2]^{1/2}$. The smallest positive real roots of their denominators provide estimates of x_c , and the residues at these roots are simultaneously estimates of $p^{1/2}$. This method was first used by Gammel *et al.* (1963), and has more recently been used by Bowers and Woolf (1969). Just as P(1) sacrifices the first coefficient, a_1 , in (5.1), for the sake of turning a branch point into a simple pole, so P(2) sacrifices the first two coefficients of (5.1). The possible advantage of discarding untypical coefficients (which do not yet significantly reflect asymptotic behaviour) may be offset by then having shorter series to deal with.

† A more recent notation, with much to commend it, is $[N/D]$. But we have kept consistently to the older convention in this chapter.

‡ See Hunter and Baker (1973) for an analysis of this correlation.

P(3). We evaluate PA 's to

$$\left(\frac{d}{dx} \ln \frac{df}{dx} \right) / \frac{d}{dx} \ln f(x) \quad \text{at } x = x_c,$$

thereby obtaining estimates of $(p + 1)/p$. At first sight this method is akin to P(a), in that it demands an estimate of x_c . We classify it, however, with P(1) and P(2) since the estimates of p so obtained are normally very much less sensitive to the choice of x_c than are those from P(a). It was used by Baker *et al.* (1967c) in an analysis of the $H(\frac{1}{2})$ series.

We turn now to ratio methods, which can be used when the coefficients in (5.1) are positive. These methods stem from the important early Ising model papers by Domb and Sykes (1957a, 1961).

R(1). On the basis of (5.2), the ratios $r_n = a_n/a_{n-1}$, plotted against $1/n$ will tend, as $1/n \rightarrow 0$, to $1/x_c$ (which we denote by θ_c). The limiting gradient of this plot is $(p - 1)\theta_c$.

R(2). The ratios $na_n/(n + p - 1)a_{n-1}$ plotted against $1/n$ will, for the correct choice of p , approach the $1/n = 0$ axis horizontally, cutting it at θ_c .

R(3). For the correct choice of x_c ,

$$n[x_c(a_n/a_{n-1}) - 1] \rightarrow p - 1 \quad \text{as } n \rightarrow \infty.$$

Again, in using R(3), we plot successive estimates against $1/n$ and extrapolate. The extrapolations involved in R(1), R(2) and R(3) are most conveniently performed numerically by drawing up Neville tables.[†]

There is some evidence that R(2) and R(3) are inter-correlated in the same sense as are P(a) and P(b).

Finally, we refer to two methods which contrast the behaviour of a pair of series.

Q(1). If $f(x) = 1 + a_1x + a_2x^2 + \dots + a_nx^n + \dots \sim \frac{A}{(x_c - x)^p}$

and

$g(x) = 1 + b_1x + b_2x^2 + \dots + b_nx^n + \dots \sim \frac{B}{(x'_c - x)^{p'}}$

[†] The Neville table method was brought to the attention of one of us (G.S.R.) by Dr. H. I. Scoins in 1954. An early and interesting application of this extrapolation technique, though in a different field of physics, is that of Bolton and Scoins (1956). It was used by Rushbrooke and Wood (1955, 1958), though without an adequate reference to its source (Hartree, 1952). This was supplied, together with a detailed description of the method, by Baker *et al.* (1967c): for which reason we do not repeat it here. It has been used extensively by Wortis and coworkers. For "smooth" sequences of positive coefficients, it is commendable for its directness and simplicity.

then the ratios $b_n a_{n-1} / b_{n-1} a_n$ plotted against $1/n$ will tend to $x_c/x'_c = \theta'_c/\theta_c$, with a limiting gradient $(p' - p)x_c/x'_c$.

Q(2). If $x_c = x'_c$, i.e. if $f(x)$ and $g(x)$ are known to become singular at the same critical point, then the series

$$1 + c_1x + c_2x^2 + c_nx^n + \dots, \quad (5.3)$$

where $c_n = b_n/a_n$, will diverge at $x = 1$, having a singularity of strength $p' - p + 1$; whence, by R(3),

$$n \left[\frac{c_n}{c_{n-1}} - 1 \right] \rightarrow p' - p.$$

In one form or another, Q(1) has a long history. In particular for the Heisenberg model, it was used by Rushbrooke and Wood (1963) for discussing staggered susceptibility series; see also Morgan and Rushbrooke (1961). Although Q(2) is only a version of Q(1) it is noteworthy as enabling the determination of critical indices (or their differences) without having a prior estimate of the critical temperature itself, and so warrants separate mention. It has been so used by Ferer *et al.* (1971), who refer to it as the method of “ T_c -renormalisation”: cf. Fisher and Hiley (1961) and Fisher and Burford (1967). We shall denote the series (5.3) by “ $g(x):f(x)$ ”.

Against this background, we now proceed to review conclusions which have been reached for the Heisenberg model from high temperature series expansions.

A. Critical temperatures

Although the values of critical temperatures and critical exponents are closely inter-related, we can usefully say something about the former without committing ourselves too closely on the latter, provided we assign reasonably wide confidence limits to the critical temperatures and this is our policy in the present section. We have, in fact, examined all the $H(\frac{1}{2})$ and $H(\infty)$ susceptibility series for the cubic lattices, and the (12)-cubic lattices, by methods P(1), P(2) and P(3), and have used ratio methods on the f.c.c. series. We shall later make a few limited comments on the extent to which these methods do or do not support particular values of the susceptibility exponent. Meanwhile, we believe the values we quote for the critical temperatures are within sufficiently broad limits to satisfy most workers. Of course, in default of knowledge of the general term in the susceptibility series, these limits are necessarily subjective: we can only say (and ultimately it is a personal matter) that we should be surprised if the critical temperature did not actually lie within these bounds. If they should not, then the terms

in the susceptibility series that have so far been calculated are misleading in their implications: but there is no good reason why they should not be.

In their 1958 paper, analysing six-term susceptibility series, for the three cubic lattices and for many spin values, Rushbrooke and Wood concluded that θ_c , i.e. kT_c/J_1 , was linear in X and proportional to $q - 1$. More precisely, they observed that the equation

$$\theta_c = (q - 1)(0.579X - 0.072) \quad (5.4)$$

adequately summarised their results. Although unexpected, the form of (5.4) should not have been too surprising, since, as we have just observed, mean field theories predict $\theta_c = 2qX/3$.

TABLE III. Estimates of values of $x_c (= J_1/kT_c)$ and $\theta_c (= kT_c/J_1)$ for $H(\frac{1}{2})$ and $H(\infty)$

| Lattice | $H(\frac{1}{2})$ | | $H(\infty)$ | |
|------------|---------------------|------------------|---------------------|------------------|
| | x_c | θ_c | x_c | θ_c |
| f.c.c. | 0.249 \pm 0.001 | 4.02 \pm 0.02 | 0.1575 \pm 0.0003 | 6.35 \pm 0.015 |
| b.c.c. | 0.396 \pm 0.002 | 2.53 \pm 0.015 | 0.2435 \pm 0.001 | 4.11 \pm 0.015 |
| s.c. | 0.595 \pm 0.003 | 1.68 \pm 0.01 | 0.346 \pm 0.002 | 2.89 \pm 0.02 |
| f.c.c.(12) | 0.1475 \pm 0.0005 | 6.78 \pm 0.03 | 0.098 \pm 0.001 | 10.2 \pm 0.01 |
| b.c.c.(12) | 0.205 \pm 0.005 | 4.88 \pm 0.12 | 0.1315 \pm 0.001 | 7.60 \pm 0.01 |
| s.c.(12) | 0.1475 \pm 0.0005 | 6.78 \pm 0.03 | 0.098 \pm 0.001 | 10.2 \pm 0.01 |

Table III lists the values we should today favour for the $H(\frac{1}{2})$ and $H(\infty)$ models in the light of longer series. It will be observed that (5.4) fits the (central) values for the nearest neighbour lattices to within 1.5% except only for $H(\frac{1}{2})$, s.c. lattice, when it is about 7% out. For values of spin other than $\frac{1}{2}$ and ∞ , we are in no position to improve on (5.4), regarded as being accurate to within 1 or 2%.

For the equivalent neighbour models, however, (5.4) is not particularly satisfactory, and, for spin $\frac{1}{2}$, the equation of Dalton and Wood (1965) (see also Domb and Dalton, 1966), namely

$$x_c = \frac{2}{q} + \frac{12}{q^2} \quad (5.5)$$

fits estimates on these lattices, including the (123)-cubic lattices, to within 1%. Equation (5.5) also adequately covers $H(\frac{1}{2})$, f.c.c. lattice; and so may be regarded as valid for $q \geq 12$. The first term on the right-hand side of (5.5) is the mean field value.

For comparing one model with another, it is physically more meaningful to look not at θ_c but at $RT_c/\Delta E_F$, where ΔE_F , the total energy change from low to high temperatures, is given by eqn (1.3), or by NqJ_1 in the classical case. The corresponding estimates of $RT_c/\Delta E_F$, based on the central values of Table III, are listed in Table IV, together with some corresponding results for the Ising model. Without needing to claim high accuracy for these figures, three things are apparent (all of which might have been presupposed intuitively). For ferromagnetic models with the same overall energy-change (from low to high temperatures), for a given lattice and given spin-value, the Heisenberg model is more "difficult to magnetise" than the Ising model; the higher the spin value the more "difficult to magnetise" is the model; and the lower the coordination number the more "difficult to magnetise" is the model. By more "difficult to magnetise" we mean that we have to cool to a lower (relative) temperature before the susceptibility diverges.

TABLE IV. Estimates of $RT_c/\Delta E_F$. For $H(\frac{1}{2})$ and $H(\infty)$ these correspond to the central estimates of Table III. The $I(\frac{1}{2})$ values are derived from Domb and Dalton (1966), and the $I(\infty)$ f.c.c. value from Domb and Sykes (1962)

| Lattice | q | $H(\frac{1}{2})$ | $H(\infty)$ | $I(\frac{1}{2})$ | $I(\infty)$ |
|------------|-----|-------------------|-------------|------------------|-------------|
| f.c.c. | 12 | 1.34 | 0.529 | 1.63 | 0.583 |
| b.c.c. | 8 | 1.26 ₅ | 0.514 | 1.59 | |
| s.c. | 6 | 1.12 | 0.482 | 1.50 | |
| f.c.c.(12) | 18 | 1.51 | 0.567 | 1.72 | |
| b.c.c.(12) | 14 | 1.39 | 0.543 | 1.66 | |
| s.c.(12) | 18 | 1.51 | 0.567 | 1.72 | |

Before discussing in greater detail the influence of second-neighbour interactions, it is convenient next to look at the anti-ferromagnetic ($J_1 < 0$) nearest neighbour model. Confining attention to the b.c.c. and s.c. lattices and by considering the staggered susceptibility series, Rushbrooke and Wood (1963) concluded that, for equal values of $|J_1|$, Néel temperatures, T_N , were rather higher than the corresponding Curie temperatures, T_c , as is also predicted by certain closed-form approximations, such as the constant-coupling approximation of Kasteleijn and van Kranendonk (1956). More precisely, for equal values of $|J_1|$, they derived the equation

$$\frac{T_N - T_c}{T_c} \approx \frac{0.63}{qX} \quad (5.6)$$

(though the coefficient 0.63 might better be written 0.65 ± 0.05). We note that the Ising model symmetry is regained as $s \rightarrow \infty$ and the spin-variables

commute. Although based on only six-term series, the ratio method Q(1) gave rather convincing results; and, incidentally, as Table I of that paper illustrates, strongly suggested that the staggered susceptibility diverges at T_N with the same exponent ($p \equiv \gamma$) as does the susceptibility at T_c .

At that time it was not completely clear that, for negative J_1 , the susceptibility series itself would be singular at $x = J_1/kT_N$. That it is so, is strongly suggested by the later work of Baker *et al.* (1967c) on the 10-term susceptibility series for $H(\frac{1}{2})$, b.c.c. lattice. This was examined by first subtracting out the ferromagnetic singularity, and then differentiating before forming Padé approximants. We shall not repeat the details here, though there was unexpectedly close agreement between T_N as so located and that obtained from the staggered susceptibility. And if χ is indeed singular at $x = -|J_1|/kT_N$, then the ferromagnetic singularity at $|J_1|/kT_c$ is not the singularity lying closest to the origin in the complex x -plane, and thus the a_n coefficients will not indefinitely remain positive. We would likewise expect the staggered susceptibility to have a weak singularity at x_c . Nevertheless,

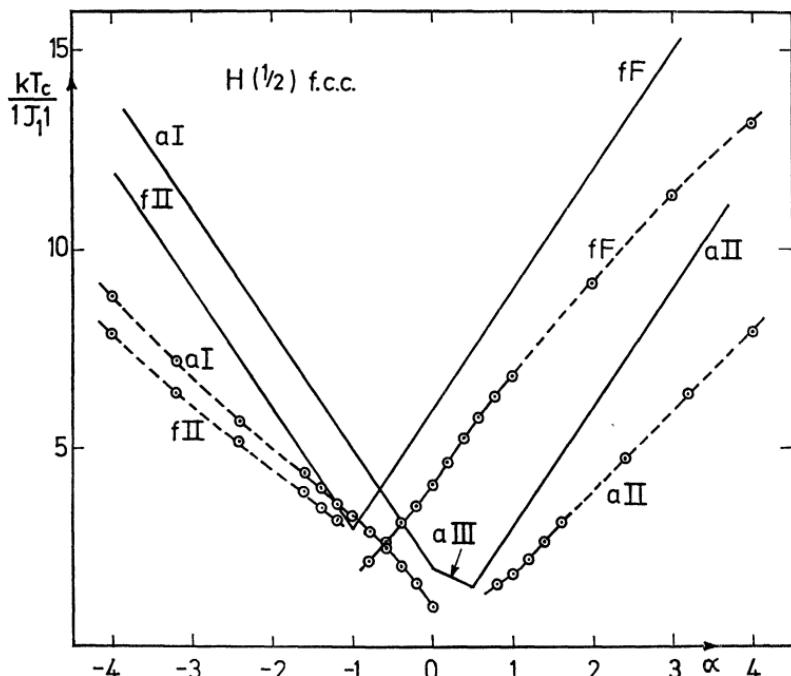


FIG. 2. Ferromagnetic and antiferromagnetic critical temperatures for $H(\frac{1}{2})$ f.c.c. lattice, with first and second neighbour interactions, compared with predictions (full lines) of mean-field theory. F, I, II, and III refer, respectively, to ferromagnetic ordering and the three antiferromagnetic orderings of Fig. 1. α denotes J_2/J_1 . f implies $J_1 > 0$ and a implies $J_1 < 0$. Adapted from Pirnie *et al.* (1966).

we are not unhappy about applying ratio tests to the early terms of these series, believing that the unwanted singularity is too weak to mask the influence of the dominant singularity on the early coefficients. (Domb *et al.*, 1964.)

After this digression, we turn to examine in more detail the effect of second-neighbour interactions on critical temperatures. The most elaborate series treatment has been that of Pirnie *et al.* (1966) who, for general first and second neighbour interactions on the f.c.c. and b.c.c. lattices, considered not only the susceptibility series (appropriate to ferromagnetic ordering) but the staggered susceptibility series appropriate to the five types of ordering illustrated in Fig. 1. Here we confine attention to the f.c.c. lattice and spin $\frac{1}{2}$.[†] Figure 2 shows their results, and compares them with those of mean-field theory, taken from Smart (1966). The circled points result from PA analyses of the corresponding series. The labels F, I, II, III, refer, respectively to ferromagnetic ordering and the three f.c.c. antiferromagnetic orderings of Fig. 1. The symbols f and a refer to the sign of J_1 : f when $J_1 > 0$ and a when $J_1 < 0$. As always, α stands for J_2/J_1 . It will be observed that no Padé approximant evidence for anti-ferromagnetic ordering of type III is presented: this is because the denominators of PA's to the type III staggered susceptibility series had no sufficiently consistent real roots (too many such roots were involved for any to be located accurately). Apart from this, the ordering temperatures depend on α qualitatively very much as predicted by mean-field theory. In particular, we draw attention to the markedly linear dependence of T_c on α .

For ferromagnetic ordering, and over the range $0 \leq \alpha \leq 1$, this linearity has been examined in greater detail by Dalton and Wood (1965), for all three cubic lattices. The curves are not, of course, quite strictly linear, but the comparatively short series do not allow the curvature to be found with any precision. Writing

$$T_c(\alpha) = T_c(0)[1 + m_1\alpha + \dots], \quad (5.7)$$

Dalton and Wood infer, for f.c.c., b.c.c., and s.c., lattices, $m_1 = 0.76$, 0.99 and 2.74 , respectively, in contrast with the mean-field values, which are 0.5 , 0.75 , and 2.00 . However, we think there is a slip[‡] in the value (2.74) quoted by Dalton and Wood for the s.c. lattice, and that the value their work indicates is in fact closer to 3.1 .

Before leaving the matter of critical temperatures, we must comment on the position regarding two-dimensional lattices. We know that there

[†] Pirnie *et al.* (1966) present detailed results also for $H(\infty)$, and for the b.c.c. lattice. Our Figure differs from theirs in that we have plotted $kT_c/|J_1|$, whereas Pirnie *et al.* plotted the inverse of this scaled by the mean-field ferromagnetic Curie temperature.

[‡] $m_1 = 2.74$ does not seem consistent either with the Curie points, for $\alpha = 0$ and 1 , quoted by Dalton and Wood, or with Fig. 6 of their paper.

can be no spontaneous magnetisation, but this does not necessarily rule out a pseudo-Curie point at which the paramagnetic susceptibility diverges. Without discussing here experimental evidence from layered substances (see, for example, de Jongh *et al.* (1969); de Jongh and van Amstel (1971)), we must briefly mention the evidence from high-temperature expansions. For a relevant Green's function theory, see Mubayi and Lange (1969).

There has long been some suggestion that Curie points can be located from susceptibility series for two-dimensional lattices. Thus Brown and Luttinger (1955) discussed four-term series for planar lattices; and Rushbrooke and Wood (1958) with six-term series, observed that for all spin values the series for the plane triangular lattice suggested a Curie temperature approximately two thirds of that for the three-dimensional simple cubic lattice (which has the same coordination number). Stanley and Kaplan (1966b), using the same series data, inferred

$$\theta_c \simeq \frac{1}{3}(q - 1)[2X - 1] \quad (5.8)$$

for $s > \frac{1}{2}$. For $s = \frac{1}{2}$ there must, indeed, be considerable uncertainty. Appendix IV shows that even the known susceptibility coefficients are no longer all positive (which precludes the use of ratio tests), and Padé approximant studies do not convincingly locate a Curie point; see, for example, Baker *et al.* (1970). Nine-term susceptibility series for the classical model, $H(\infty)$, for both triangular and quadratic lattices, have been analysed by Stephenson (1969). While ratio tests can be held to suggest $\theta_c \sim 1.7$ and 1.1 for p.t. and s.q. lattices, respectively, Stephenson observes that complete Padé tables for x_c have a marked tendency to exhibit complex roots (this being particularly true of those PA's which utilise the later coefficients), and is sceptical of the possibility of drawing convincing conclusions. Moore (1969) gives $\theta_c \sim 1.6$ as the value suggested, by ratio tests, on the ten-term series for the p.t. lattice; but a P(1) analysis still gives $x_c \sim 0.54 \pm 0.13i$ as the best defined singularity (indeed, the only singularity which is at all well defined). And one might comment further that the $[1, N]$ estimates of x_c , for $N = 1, 2 \dots 8$, are 0.4545, 0.4950, 0.5183, 0.5424, 0.5831, 0.6333, 0.6814, 0.7458, which certainly give no indication of convergence.

We must conclude therefore that Heisenberg model series for two-dimensional lattices have so far done more to draw attention to an interesting theoretical possibility than to establish clear evidence for it. At the same time, we must refer to work on two related models (for the plane triangular lattice). Thus Moore (1969) presents series evidence, stronger than for $H(\infty)$, that $P(\infty)$ has a pseudo-Curie point; and Betts *et al.* (1971) have given rather convincing evidence that this is true of the model $XY(\frac{1}{2})$ (see Betts this Volume, Chapter 8). Their analysis is of interest in that a direct application of

$P(1)$ led to complex x_c much as with $H(\infty)$, but there was a second pair of well-defined complex roots (of denominators of PA 's) no further from the origin and close to the imaginary axis. On applying a conformal transformation to the susceptibility series so as to diminish the influence of this non-physical pair, x_c was determined as real and well-defined. As Betts *et al.* (1971) remark, if $I(\frac{1}{2})$ and $XY(\frac{1}{2})$ both have Curie points (or a pseudo-Curie point) it might seem likely that this would be true also of $H(\frac{1}{2})$, since $I(\frac{1}{2})$ and $XY(\frac{1}{2})$ are opposite extremes of the anisotropic Hamiltonian (4.1).

B. Thermodynamic properties, $T > T_c$

Critical temperatures have been located by examining the divergence of the susceptibility series. We must now say something about the magnitude of the susceptibility itself, at temperatures greater than T_c . We shall refer here also to quantities related to the zero-field specific heat series, although we defer discussion of the precise form of the magnetic specific heat anomaly near T_c until after reviewing the present position regarding critical exponents.

Since $\chi(0)$ diverges at T_c , we shall consider the numerical value of $1/\chi(0)$, $T > T_c$; and follow the precedent of Rushbrooke and Wood (1958) in scaling this so that the linear asymptote has unit gradient. Denoting this scaled value by $1/\bar{\chi}(0)$, we note from (2.19) that the scaling factor is, in general,

$$\frac{s(s+1)}{3s^2} \frac{Nm^2}{kT_c} \quad (5.9)$$

where m is the saturation magnetic moment per lattice site. This reduces to Nm^2/kT_c when $s = \frac{1}{2}$ and $Nm^2/3kT_c$ for the classical model. In all cases

$$\bar{\chi}(0) = \frac{T_c}{T} \left[1 + \sum_{n \geq 1} a_n x^n \right], \quad (5.10)$$

where the a_n 's are the zero-field susceptibility coefficients.

Since $1/\bar{\chi}(0)$ is finite (zero) at T_c , it might be thought practicable to invert the right-hand side of (5.10), so obtaining a power series (in x) which could be examined numerically by simply forming PA 's to it and evaluating these for various values of $x, < x_c$. Unfortunately, if in eqn (5.2) the exponent p (denoted by γ for the susceptibility series) is not unity, PA 's to $1/f(x)$ do not converge well to $(x_c - x)^\gamma$ in the neighbourhood of the branch point. For this reason, for plotting $1/\bar{\chi}(0)$, we have preferred to write

$$\frac{1}{\bar{\chi}(0)} = \frac{T}{T_c} \left[PA \text{ to } \left(1 + \sum_{n \geq 1} a_n x^n \right)^{1/\gamma} \right]^{-\gamma}. \quad (5.11)$$

With the expression (5.11), we find good convergence between the numerical values of alternative PA 's provided $T/T_c \geq 1.05$, i.e. $x \leq 0.95 x_c$.

In using eqn (5.11) we have, of course, to assign a value to γ . In plotting the curves of Fig. 3, which relate to the f.c.c. lattice, we took† $\gamma = 1.43$ for $H(\frac{1}{2})$ and $\gamma = 1.375$ for $H(\infty)$. Though there is now rather convincing evidence that for $H(\infty)$ $\gamma \approx 1.40$, we believe the structure of (5.11) is such

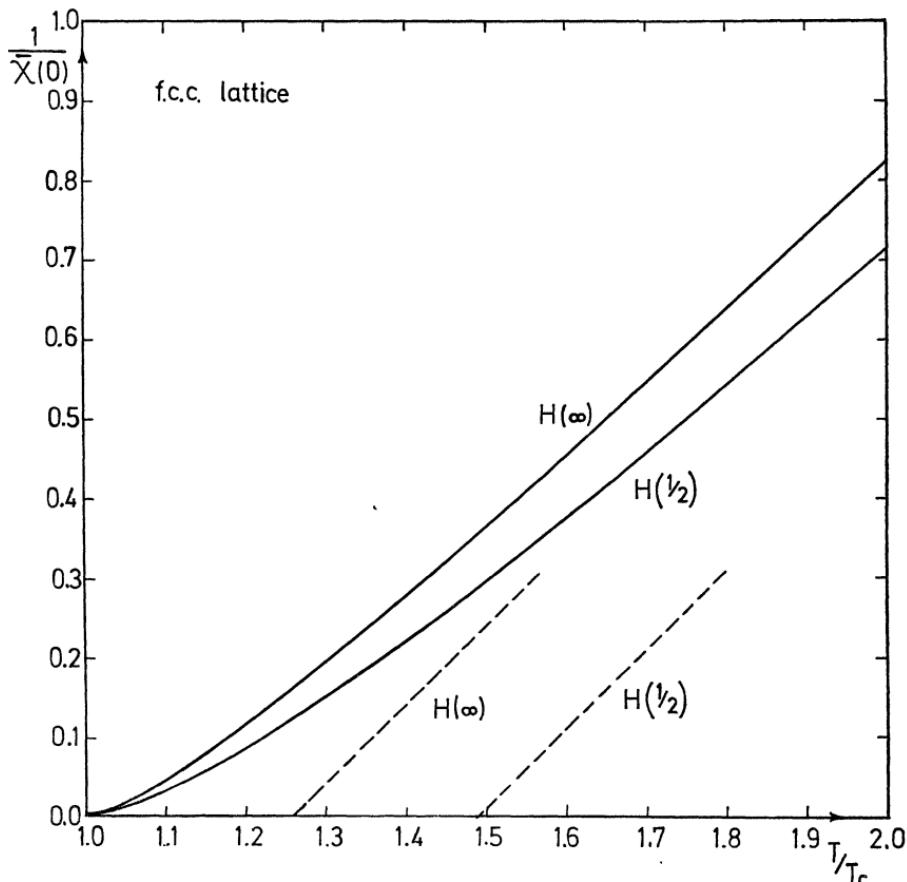


FIG. 3. Inverse susceptibilities for $H(\frac{1}{2})$ and $H(\infty)$, f.c.c. lattice, and their linear asymptotes. $\chi(0)$ is scaled so that the asymptote has unit gradient.

† In their 1967 paper, Baker *et al.* concluded that for $H(\frac{1}{2})$, f.c.c. lattice,

$$\frac{1}{\chi}(0) \sim \frac{T}{T_c} \frac{(1 - T_c/T)^{1.43}}{1.07}$$

for T near T_c . It is of interest to compare this asymptotic formula with the predictions of (5.11). For $T/T_c = 1.05, 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.7$ and 1.8 , equation (5.11) gives $0.012, 0.033, 0.087, 0.151, 0.221, 0.296, 0.375, 0.457$ and 0.541 , whereas the asymptotic formula gives $0.013, 0.033, 0.087, 0.149, 0.218, 0.291, 0.368, 0.448$ and 0.528 . We believe that for $T/T_c \leq 1.05$ an asymptotic formula obtained as in Baker *et al.* (1967c) will do the better justice to numerical values of $1/\chi(0)$; but that for $T > 1.3T_c$ the asymptotic formula no longer gives the true value of $1/\chi(0)$ to better than one percent.

that its predictions will not be sensitive to the precise choice of γ . Figure 3 shows also the linear asymptotes. If the linear asymptote cuts the temperature axis at T_c^* , sometimes called the paramagnetic Curie temperature, then for $H(\frac{1}{2})$ $T_c^*/T_c = \frac{1}{2}qx_c$ and for $H(\infty)$ $T_c^*/T_c = \frac{3}{2}qx_c$.

We comment only that all features of Fig. 3 are, of course, independent of the value of the exchange interaction, J_1 .

The other thermodynamic quantities to which we would refer here are $E(\infty) - E(T_c)$ and $S(\infty) - S(T_c)$, given by eqns (2.22) and (2.23), respectively, with $x = x_c$. These equations involve the zero-field specific heat coefficients c_n . Accurate estimates of these energy and entropy changes probably demand an analytic form for the specific-heat anomaly itself, more accurate than is yet available. In default of this, however, it is possible, as many authors have done, to estimate $E(\infty) - E(T_c)$ and $S(\infty) - S(T_c)$ by attempting to sum the right hand sides of (2.22) and (2.23), each term being evaluated at $x = x_c$. For smooth sequences of coefficients, as with $H(\infty)$, a convenient method is to form the sequence of successive partial sums and extrapolate on these by drawing up the appropriate Neville table. With irregular coefficients, however, it is difficult to do better than evaluate the series, at $x = x_c$, by the method of Padé approximants.

TABLE V. Estimates of $[E(\infty) - E(T_c)]/[E(\infty) - E(0)]$. The $H(\frac{1}{2})$ values are derived from Dalton and Wood (1965). The $H(\infty)$ values are derived from Bowers and Woolf (1969). The $I(\frac{1}{2})$ values are derived from Domb and Dalton (1966), and the $I(\infty)$ value from Domb and Sykes (1962).

| Lattice | q | $H(\frac{1}{2})$ | $H(\infty)$ | $I(\frac{1}{2})$ | $I(\infty)$ |
|------------|-----|------------------|-------------|------------------|-------------|
| f.c.c. | 12 | 0.58 | 0.25 | 0.25 | 0.10 |
| b.c.c. | 8 | 0.58 | 0.27 | 0.27 | |
| s.c. | 6 | 0.67 | 0.33 | 0.33 | |
| f.c.c.(12) | 18 | 0.47 | | 0.17 | |
| b.c.c.(12) | 14 | 0.50 | | 0.21 | |
| s.c.(12) | 18 | 0.47 | | 0.17 | |

Table V gives estimates of $[E(\infty) - E(T_c)]/[E(\infty) - E(0)]$ for the three cubic lattices, and equivalent neighbour (12)-lattices, for $H(\frac{1}{2})$ and $H(\infty)$; and compares these with the corresponding values for the Ising models, $I(\frac{1}{2})$ and $I(\infty)$. We have preferred to give the fraction of the total energy-change, ΔE_F , which is released above the Curie point, rather than $[E(\infty) - E(T_c)]/RT_c$: and where authors have listed the latter values we have used the values of $RT_c/\Delta E_F$ of Table IV to effect the conversion. The sources of the values quoted are given in the legend to the table.

Table VI gives the corresponding values of $S(\infty) - S(T_c)$. It is inappropriate to refer to relative entropy changes in this case, since $S(\infty) - S(0)$ is always $Nk \ln(2s + 1)$, which diverges for the classical models.

TABLE VI. Estimates of $[S(\infty) - S(T_c)]/Nk$. Sources are as for Table V except that for $H(\frac{1}{2})$, f.c.c., the value of Baker *et al.* (1967c) has been taken.

| Lattice | q | $H(\frac{1}{2})$ | $H(\infty)$ | $I(\frac{1}{2})$ | $I(\infty)$ |
|------------|-----|------------------|-------------------|-------------------|-------------|
| f.c.c. | 12 | 0.24 | 0.31 | 0.10 | 0.13 |
| b.c.c. | 8 | 0.24 | 0.34 | 0.11 | |
| s.c. | 6 | 0.26 | 0.41 ₅ | 0.13 | |
| f.c.c.(12) | 18 | 0.19 | | 0.06 ₅ | |
| b.c.c.(12) | 14 | 0.21 | | 0.09 | |
| s.c.(12) | 18 | 0.19 | | 0.06 ₅ | |

While we have quoted what we believe are the best current estimates of these quantities, it will be noted that we have not given more than two significant figures. For the Ising model, $I(\frac{1}{2})$, greater precision would certainly be justified; but for $H(\frac{1}{2})$ and $H(\infty)$ we would suggest that the second digit has an uncertainty of ± 1 (or, possibly, even ± 2). Nevertheless, what does emerge from these Tables is certainly of significance. For they indicate clearly that the energy and entropy changes above T_c are proportionately greater for the Heisenberg models than for the corresponding Ising models, and show too how ferromagnetic second-neighbour interactions assist the onset of magnetisation.

C. The magnetic phase boundary, $T < T_c$

For the Heisenberg models, in contrast to the Ising models, we can say nothing from series expansions of the behaviour, $T < T_c$, of $\chi(0)$ and $C(0)$. The only expansions we have are the low-temperature expansions of spin-wave theory: and we have already noted that this theory suggests that $\chi(0)$ itself does not exist. Fortunately, however, from the high-temperature expansions it is possible to locate the magnetic phase-boundary, i.e. the dependence on T , for $T < T_c$ of the zero-field spontaneous magnetisation $M(0)$. To do this, we require not only the high-temperature expansion of $\chi(0)$ but also the high-temperature expansions of sufficiently many of the higher-order susceptibilities: more precisely, we need an expansion of the free-energy, $F(H, T)$, in powers of H as well as of reciprocal temperature.

The procedure is slightly different in the two cases which have been investigated, $s = \frac{1}{2}$ and $s = \infty$. For $H(\frac{1}{2})$ we follow Baker *et al.* (1970).

Starting from the expansion (3.33), using the basic equation

$$M = kT(\partial/\partial H) \ln Z,$$

and writing† \bar{m} for M/Nm , we obtain

$$\bar{m} = tb_0(x) + t^3 b_1(x) + \dots + t^{17} b_8(x) + \dots \quad (5.12)$$

where

$$b_0(x) = 1 + 2 \sum_{n=1}^{\infty} \frac{x^n}{2^n n!} f(n, 1) \quad (5.13)$$

and

$$b_j(x) = 2 \sum_{n=1}^{\infty} \frac{x^n}{2^n n!} [(j+1)f(n, j+1) - jf(n, j)], \quad j \geq 1. \quad (5.14)$$

We note, from (3.34), that $b_j(x)$ starts with a term in x^j ; and that the series $b_1(x) \dots b_8(x)$ are known through terms in x^8 (see Section IV.C and Appendix III).

As the discussion at the end of Section III.E indicated, $b_0(x)$ is simply the basic high-temperature expansion of the zero-field susceptibility $\chi(0)$, which diverges at $x = x_c$. The $b_j(x)$, $j \geq 1$, are combinations of the higher-order susceptibility series (see eqn (3.30)), each of which also is presumed to diverge at $x = x_c$. For this reason alone we cannot use (5.12) as it stands to find \bar{m} when $x > x_c$. But we note also that the magnetic phase-boundary in which we are interested corresponds to $H \rightarrow 0$, i.e. $t \rightarrow 0$, since t stands for $\tanh(mH/kT)$. Thus, as it stands, (5.12) implies $m \rightarrow 0$ as $H \rightarrow 0$; i.e. it relates to the paramagnetic situation, $T > T_c$.

To make progress, we first revert eqn (5.12), so obtaining t as a double power-series in x and \bar{m} , i.e. we infer

$$t = \bar{m} c_0(x) + \bar{m}^3 c_1(x) + \dots + \bar{m}^{17} c_8(x) + \dots \quad (5.15)$$

Fuller details of this reversion are given in Baker *et al.* (1970), but essentially one could substitute (5.15) in (5.12) and equate the coefficients, on each side, of like powers of \bar{m} . The functions $c_0(x) \dots c_8(x)$ are then known, as expansions in powers of x , through terms in x^8 . Of course

$$c_0(x) = [b_0(x)]^{-1}, \quad (5.16)$$

and $c_j(x)$, like $b_j(x)$, starts with a term in x^j . Finally, in (5.15), we group together like powers of x , obtaining

$$t = \bar{m} g(x, \bar{m}^2) \quad (5.17)$$

where

$$g(x, \bar{m}^2) = 1 + \sum_{n \geq 1} \frac{x^n}{2^n n!} p_n(\bar{m}^2), \quad (5.18)$$

† Since m is already in use for the saturation magnetisation per lattice site, we must use \bar{m} for the reduced magnetisation M/Nm . The spontaneous magnetisation is the limit of \bar{m} as $H \rightarrow 0$, $T < T_c$: which we denote $\bar{m}(0)$.

$p_n(\bar{m}^2)$ being a polynomial in \bar{m}^2 of degree n . For $n \leq 8$ these polynomials are known exactly, and are listed in Baker *et al.* (1970). They have the property that $p_n(1) = 0$, all n .

Equation (5.17) is essentially a magnetic equation of state, portraying the interdependence of H , T and \bar{m} . As $H \rightarrow 0$, i.e. $t \rightarrow 0$, there are two solutions: $\bar{m} = 0$ and $g(x, \bar{m}^2) = 0$. The solution $\bar{m} = 0$ always exists, but is presumably unstable, as in mean-field theory, for $T < T_c$. There remains the solution

$$g(x, \bar{m}^2) = 0 \quad (5.19)$$

which defines, implicitly, the magnetic phase boundary $\bar{m}(0)$ as a function of x .

We can immediately make two comments on this phase boundary. Any point on the phase boundary corresponding to $\bar{m} = 1$, i.e. to saturation magnetisation, necessarily corresponds to $T = 0$ since, as we have noted, $p_n(1) = 0$, all n . Secondly, when we put $\bar{m} = 0$ in (5.19), eqns (5.17), (5.15), and (5.16) show that the equation $g(x, 0) = 0$ is simply the equation $[(b_0(x))]^{-1} = 0$, i.e. $[\chi(0)]^{-1} = 0$. Thus the phase boundary necessarily intersects the temperature axis at the Curie point as determined from the divergence of the paramagnetic susceptibility.

To plot the phase-boundary explicitly, between $\bar{m} = 0$ and $\bar{m} = 1$, since, for any such \bar{m} , $g(x, \bar{m}^2)$ is known as a power series in x (through the term in x^8) we might suppose it convenient simply to form PA's to $g(x, \bar{m}^2)$ and examine for what values of x their numerators vanish. Baker *et al.* (1970) did this, but also observed that more consistent results were obtained not from the zeros of numerators of PA's to $g(x, \bar{m}^2)$, but from zeros of denominators of PA's to

$$\frac{d}{dx} \ln g(x, \bar{m}^2): \quad (5.20)$$

and they adopted this second method. Why this should be so is particularly clear when $\bar{m} = 0$. For then $g(x, 0)$ is simply $[(b_0(x))]^{-1}$, which we believe behaves like $(x_c - x)^\gamma$, i.e. has a branch point at $x = x_c$. Taking the logarithmic derivative turns this branch point into a simple pole, to which PA's can do good justice. We believe similar considerations apply for $\bar{m} > 0$; which is why it is better to consider PA's to (5.20) rather than to $g(x, \bar{m}^2)$ itself.

For further details, reference must be made to the original paper. The resulting phase-boundary, for the f.c.c. lattice, is shown in Fig. 4, and for the range $0.7 \geq \bar{m} \geq 0.45$ the authors believe T/T_c is reliable to within 1%. It will be noted that the phase boundary appears to approach the asymptotic, low-temperature, $T^{3/2}$ curve from below—as we should expect

from eqn (1.9) and Table I. It is, indeed, virtually indistinguishable from that predicted by second-order Green's function theory (Cooke and Gersch, 1967). Repeating the analysis for the b.c.c. lattice, Baker *et al.* found remarkable coincidence with the f.c.c. case: though this becomes less surprising if we compare the coefficients $a_1' \dots a_4'$ of Table I for these two lattices. For the s.c. lattice convergence, between the predictions of different PA's, was less satisfactory; but for given \bar{m} , T/T_c seemed to be some 5 or 6% lower than for the f.c.c. lattice (\bar{m} between 0.55 and 0.75): roughly in accordance with second-order Green's function theory. Applying the method to the series for the plane triangular lattice did not lead to acceptable convergence, which is satisfactory in that we know there can be no magnetic phase-boundary for two-dimensional lattices.

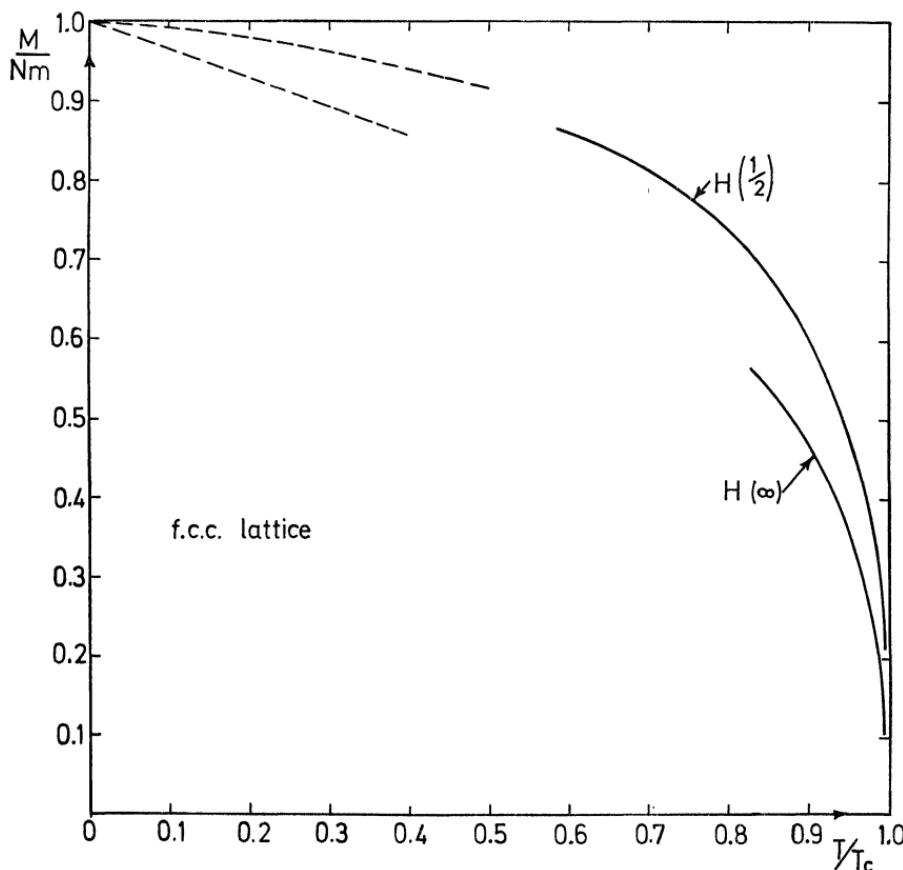


FIG. 4. Magnetic phase boundaries, and low temperature asymptotes, for $H(\frac{1}{2})$ and $H(\infty)$, f.c.c. lattice. Curves from Baker *et al.* (1970) and Stephenson and Wood (1970).

For the classical model, $H(\infty)$, a rather different procedure must be adopted, since there is now no simple field variable analogous to t , satisfying the Opechowski equation (3.34). However, differentiating eqn (3.26) with respect to H yields

$$\bar{m} = \sum_{r \geq 1} \sum_{n \geq 0} 2r a_{2r,n} y^{2r-1} x^n. \quad (5.21)$$

Stephenson and Wood (1970) now avoided the difficulty of working with a doubly infinite sum, essentially by summing the array diagonally. Writing

$$\frac{y}{x} \equiv h = \frac{mH}{J_1}, \quad (5.22)$$

(5.21) becomes

$$\frac{\bar{m}}{x} = \sum_{r \geq 1} \sum_{n \geq 0} 2r a_{2r,n} h^{2r-1} x^{2r+n-2}, \quad (5.23)$$

which reverts to give

$$h = \frac{\bar{m}}{x} \sum_{r \geq 0} x^r \beta_r \left(\frac{\bar{m}}{x} \right), \quad (5.24)$$

where β_r is a finite polynomial in $(\bar{m}/x)^2$. The first ten of these polynomials, i.e. β_0 to β_9 , can be found from the coefficients $a_{2r,n}$ of Stephenson and Wood (1968) supplemented by the susceptibility coefficients $a_{2,8}$ and $a_{2,9}$; indeed the diagonal summation necessarily sacrifices some of the known higher-order susceptibility coefficients, and only 20 of the 32 found by Stephenson and Wood are used, namely $a_{4,0} \dots a_{4,7}$, $a_{6,0} \dots a_{6,5}$, $a_{8,0} \dots a_{8,3}$, $a_{10,0}$ and $a_{10,1}$. The equation analogous to (5.19) is now

$$g(x) \equiv \sum_{r \geq 0} x^r \beta_r \left(\frac{\bar{m}}{x} \right) = 0, \quad (5.25)$$

and for $\bar{m} = 0$ this is again equivalent to $[\chi(0)]^{-1} = 0$. Thus, following Stephenson and Wood, we now choose a value for \bar{m}/x , say c , and examine the roots of denominators of PA's to $d \ln g(x)/dx$. Geometrically, this corresponds to finding the intersections of the magnetic phase-boundary with the rectangular hyperbola $mkT/J_1 = c$. It was found that for c greater than about 3 there are no real roots, implying that the hyperbola ceases to intersect the phase-boundary. For $c < 3$, instead of there being two real roots, as might be expected, there is only one, which merges with T_c as $c \rightarrow 0$. Thus the method locates only the lower part of the magnetic phase-boundary: up to about $\bar{m} = 0.6$. Nevertheless, as Fig. 4 shows, this is enough

to stress the difference between the phase-boundaries for $H(\frac{1}{2})$ and $H(\infty)$, and the classical boundary appears to be heading satisfactorily towards the low-temperature linear asymptote: eqn (1.11). Stephenson and Wood confined their analysis to the f.c.c. lattice.

D. Critical indices

The earliest work on critical indices for the Heisenberg model was that of Domb and Sykes (1962) and Gammel *et al.* (1963). Both papers discuss the susceptibility exponent, γ , on the basis of the six-term series of Rushbrooke and Wood (1958). Domb and Sykes confined attention to $H(\infty)$, f.c.c. lattice, and used a ratio method. Gammel *et al.* applied the Padé methods, P(1) and P(2), to the series for all three cubic lattices and for many spin values, including $s = \frac{1}{2}$ and $s = \infty$. The conclusion of both papers was that $\gamma = 1.33$. The papers are important as indicating rather clearly that for the Heisenberg model γ is greater than for the spin- $\frac{1}{2}$ Ising model ($\gamma = 1.25$), though the actual evidence for the value 1.33 was perhaps never very strong.[†]

Today the susceptibility series for $H(\frac{1}{2})$ and $H(\infty)$, for the three cubic lattices, are of tenth order, except in the case of $H(\frac{1}{2})$, f.c.c. lattice, which is of order nine. In discussing the status of current estimates of γ , we shall confine attention to three papers; Baker *et al.* (1967c), Bowers and Woolf (1969), and Ferer *et al.* (1971).

Baker *et al.* (1967c) still provides the most extensive and detailed analysis of the $H(\frac{1}{2})$ series. Starting with the classic Padé approach (Baker, 1961) based on P(1), P(a) and P(b), the paper demonstrated that, over the

[†] The Padé evidence of Gammel *et al.* (1963) certainly supported $\gamma = 1.33$ for the b.c.c. lattice, whether $s = \frac{1}{2}$ or $s = \infty$. For the f.c.c. lattice (which should not be troubled by an antiferromagnetic singularity, however weak) with $s = \frac{1}{2}$ there is really no convergence in the Padé estimates. For higher spin values, in particular for $s = \infty$, the central Padé estimates are appreciably higher than 1.33. For $H(\infty)$, f.c.c. lattice, with method P(1) the [2, 2], [2, 3] and [3, 2] values of γ are all 1.36 ± 0.01 , and the [2, 2] estimates from P(2) is 1.38. Domb and Sykes (1962) confined attention to this $H(\infty)$, f.c.c. series. Rather than using $R(3)$, which is sensitive to the choice of x_c , they considered the sequence of estimates

$$\gamma_n = 1 + n(r_n/l_n - 1)$$

where $r_n = a_n/a_{n-1}$ and l_n is the linear extrapolant $nr_n - (n-1)r_{n-1}$. For $n = 2, 3, \dots, 6$, the values found for γ_n are 1.2, 1.2575, 1.2898, 1.3104 and 1.3216. Paying attention, perhaps, to the rate at which the differences between successive estimates of γ decrease, Domb and Sykes concluded $\gamma = 1.33$. On the other hand, if these values of γ_n are extrapolated against $1/n$, either visually or by a Neville table, one infers $\gamma = 1.38 \pm 0.01$. It seems worth commenting that if $\chi(0)$ were precisely $A/(x_c - x)^\gamma$, with A a constant, every value of γ_n would equal γ . But if in place of A we write $A + a(x_c - x)$, then γ_n will approach γ linearly in $1/n$. Perhaps a conservative estimate from the 6-term $H(\infty)$, f.c.c. series would be 1.37 ± 0.02 . If, using the more recent coefficients the Domb and Sykes sequence is extended, $n = 7, 8, \dots, 10$, the new γ_n values are 1.3292, 1.3359, 1.3418, 1.3466. They increase only slowly, but extrapolation against $1/n$ now suggests a value close to 1.40.

range of uncertainty in x_c , $P(a)$ and $P(b)$ are so highly correlated as to have little diagnostic value. The Padé method $P(3)$ was therefore investigated, and pointed to the conclusion $\gamma = 1.43 \pm 0.01$ for all three lattices. It would be mistaken, however, to suppose that support for this value comes only from method $P(3)$. This value was also suggested by the central Padé estimates from $P(1)$, and corresponds to a range in which $P(a)$ and $P(b)$ are exceptionally concordant.

The paper by Bowers and Woolf (1969), though primarily concerned with the $H(\infty)$ series, then of ninth order for the open lattices and eighth order in the f.c.c. case, considered not only the nearest neighbour models, but also the equivalent neighbour (12)-lattices for both $H(\infty)$ and $H(\frac{1}{2})$. Their analysis was extensive, and we single out what seem their strongest arguments. Thus method $P(2)$ gave an impressively well-converged Padé table for $H(\infty)$, f.c.c. lattice (Table V of their paper) corresponding to $\gamma = 1.375$. They argued, not unconvincingly though relying rather heavily on $R(2)$ and $R(3)$, that $\gamma = 1.375$ is equally appropriate to the $H(\infty)$ (12)-cubic lattices.† Finally, they presented an impressively well converged Padé table (XXIV of their paper) for $H(\frac{1}{2})$, (12)-f.c.c. lattice, based on method $P(1)$, which again predicted‡ $\gamma = 1.375$. They were therefore led to advocate the universal value $\gamma = 1.375$ for both $H(\infty)$ and $H(\frac{1}{2})$, and could point to some indications of this in the analysis of Baker *et al.*, while conceding that 1.43 was perhaps the most reasonable inference from that work.

Since 1969, two new terms have been added to the susceptibility series for $H(\infty)$, f.c.c. lattice, and Ferer *et al.* (1971) now conclude that, for $H(\infty)$, $\gamma = 1.405 \pm 0.02$. Their analysis is interesting in that it never considers the susceptibility series directly (by itself), but employs ratio tests and Neville table extrapolations on “ T_c -renormalised” series; see Q(1) and Q(2) above. The other series employed for this “ T_c -renormalisation” are the spherical moment series (4.11), for $t = -1, -\frac{1}{2}, \frac{1}{2}, \dots, 2$, and the analogues of these for the first of the higher-order susceptibility series§. This analysis, which

† Were this not so, we should be faced with an unexpected lattice-dependence of critical indices. Second-neighbours on the f.c.c. lattice themselves form an s.c. lattice and it is natural to suppose that for the general second-neighbour problem, involving J_1 and J_2 , γ is independent of the ratio J_2/J_1 , since in the two extreme cases $J_1 = 0$ or $J_2 = 0$ we have the familiar nearest neighbour models.

‡ We find this is supported also by method $P(3)$. $P(2)$ gives a rather less well converged Padé table. But if, following Baker and Gaunt (1967) we omit from consideration PA's having “defects”—for which see Hunter and Baker (1973)—any evidence for $\gamma = 1.375$ for $H(\frac{1}{2})$ models is much weakened.

§ The susceptibility series itself is so “smooth” that a Neville table extrapolation of the ratios a_n/a_{n-1} , can be taken to third order and suggests $\theta_c = 6.350 \pm 0.003$. Taking $\theta_c = 6.350$, similar extrapolation on $R(3)$ gives $\gamma = 1.405 \pm 0.005$, while taking $\theta_c = 6.353$ leads to $\gamma = 1.392 \pm 0.005$. Combining these estimates we infer $\gamma = 1.405 \pm 0.02$, precisely as given by Ferer *et al.* (1971). Their estimate of θ_c is 6.3506 ± 0.0040 .

serves also to give other critical indices (see below), is, we find, in fact supported by more direct approaches. For example, the method P(2) which led Bowers and Woolf to infer $\gamma = 1.375$ now indicates a value close to 1.40: to the entries in their Padé Table V we can add the two diagonals [6, 1], [5, 2] ... [1, 6] and [7, 1], [6, 2] ... [1, 7], which read 1.410, 1.383, 1.397, 1.382, 1.412, 1.397, and 1.399, 1.396, 1.406, 1.406, 1.396, 1.399, 1.399. We must conclude, therefore that the estimates of γ provided by the equivalent neighbour models are unacceptably low, and might ascribe this to the fact that the comparatively short series (only seven terms) have to accommodate an antiferromagnetic singularity, however weak; see Fig. 2.

Leaving unresolved the question of the universality (spin-independence) of γ for Heisenberg models, we turn to summarise more briefly conclusions drawn for other exponents. Historically, the next to be estimated was the high-temperature gap parameter, 2Δ , for the model $H(\frac{1}{2})$. If, from (3.26), we write

$$\sum_{n \geq 0} a_{2r,n} x^n \equiv F_r(x)$$

then Baker *et al.* (1966b, 1967c) examined $F_2(x)$, $F_3(x)$ and $F_4(x)$ by R(1) and found that these eight-term series clearly diverged at the same critical temperature, x_c , as had been indicated, more precisely, by the susceptibility series $F_1(x)$. With x_c taken from the susceptibility work, Neville table extrapolations based on R(3) then indicated that

$$F_r(x) \sim \frac{A_r}{(x_c - x)^{\gamma + 2\Delta(r-1)}} \quad (5.26)$$

where $2\Delta = 3.63 \pm 0.03$, for both f.c.c.[†] and b.c.c. lattices.

For $H(\frac{1}{2})$, γ and Δ are the only thermodynamic exponents that can be directly extracted from high-temperature series. For $H(\infty)$, the specific-heat series permit an estimate of the corresponding exponent α , but we defer discussion of the specific heat anomalies for the next section.

Of the correlation function indices, v and η , for present purposes v may be regarded as defined through (4.11) by

$$\mu_t \sim \frac{\text{constant}}{(x_c - x)^{\gamma + vt}}, \quad (5.27)$$

[†] For $H(\frac{1}{2})$, f.c.c. lattice, we have recently examined the series " $F_2:F_1$ ", " $F_3:F_2$ " and " $F_4:F_3$ ", i.e. have attempted to determine 2Δ by " T_c -renormalisation". Q(2) and a Neville table extrapolation does not give satisfactory convergence when applied to " $F_2:F_1$ ": but from " $F_3:F_2$ " we infer $2\Delta = 3.60$ and from " $F_4:F_3$ " we infer $2\Delta = 3.61$, with a confidence of perhaps one unit in the last digit. These estimates are (just) within the confidence limits of Baker *et al.* (1967c) but have the advantage that they in no way invoke the susceptibility series.

and η as then given by the Fisher equation

$$\gamma = v(2 - \eta). \quad (5.28)$$

For more careful definitions, and the relation of these indices to the asymptotic behaviour of the correlation function itself, reference must be made to Fisher (1967b).

For the model $H(\frac{1}{2})$, there does not seem to have yet been any direct estimate made of the index v ; but for $H(\infty)$, Fisher (1967b) ascribes the estimate $v = 0.692 \pm 0.012$ to work by himself and Burford. Bowers and Woolf (1969), examining μ_2 , infer $v = 0.70 \pm 0.0215$ and Ferer *et al.* (1971) find $v = 0.717 \pm 0.007$. In fact Ferer *et al.* determined γ from the two equations $v = 0.717 \pm 0.007$ and $2v - \gamma = 0.029 \pm 0.006$: on which account they can use (5.28) to infer approximately, $\eta = 0.040 \pm 0.008$.

So much for direct determination of critical exponents (with the exception of α for the classical model). If we take γ and Δ as basic, then the scaling law equations (see Fisher, 1967b).

$$\alpha = 2 - 2\Delta + \gamma \quad (5.29)$$

$$\beta = \Delta - \gamma, \quad \delta = \Delta/(\Delta - \gamma) \quad (5.30)$$

$$v = (2\Delta - \gamma)/3, \quad \eta = (4\Delta - 5\gamma)/(2\Delta - \gamma), \quad (5.31)$$

where β is the exponent for the magnetic phase boundary and δ the degree of the critical isotherm, can be used to predict the remaining indices; these are listed in Table VII. The $H(\frac{1}{2})$ column is taken from Baker *et al.* (1967c); β and δ for $H(\infty)$ are quoted by Ferer *et al.* (1971). The estimates of v and η for $H(\infty)$ in Table VII are clearly less reliable than those of Ferer *et al.* which we have already quoted.

TABLE VII. Critical exponents derived from estimates of γ and Δ and application of the scaling laws

| | $H(\frac{1}{2})$ | $H(\infty)$ |
|----------------------|-------------------|-------------------|
| γ | 1.43 ± 0.01 | 1.405 ± 0.02 |
| 2Δ | 3.63 ± 0.03 | 3.54 ± 0.03 |
| α from (5.29) | -0.20 ± 0.04 | -0.14 ± 0.04 |
| β from (5.30) | 0.385 ± 0.025 | 0.365 ± 0.035 |
| δ from (5.30) | 4.73 ± 0.27 | 4.90 ± 0.54 |
| v from (5.31) | 0.735 ± 0.015 | 0.712 ± 0.016 |
| η from (5.31) | 0.05 ± 0.05 | 0.00 ± 0.05 |

We comment only that these estimates of β are not inconsistent with "effective" β 's obtained by Baker *et al.* (1970) and Stephenson and Wood (1970) from their phase-boundaries. For $H(\frac{1}{2})$, Baker *et al.* found $\beta = 0.35 \pm 0.05$ for $0.4 \leq \bar{m} \leq 0.7$, and for $H(\infty)$ Stephenson and Wood quote $\beta = 0.38 \pm 0.03$ for $0.1 \leq \bar{m} \leq 0.4$. Likewise Baker *et al.* (1970), attempting to analyse the critical isotherm not too close to $H = 0$ inferred $\delta = 5.0 \pm 0.2$. But we would emphasise that no method is known for determining either β or δ accurately for Heisenberg models, other than by application of the scaling laws.

E. The specific heat anomaly

We have said that for $H(\infty)$ the specific heat exponent, α , can be determined by direct analysis of the $C(0)$ high-temperature series. This is perhaps to overstate the case, but several authors, Joyce and Bowers (1966b), Bowers and Woolf (1969), and Ferer *et al.* (1971), have used R(3) to examine α , for the f.c.c. lattice, and all have found the later estimates to be negative. Unfortunately, successive values are sensitive to choice of x_c and, in any case, not particularly suited to a convincing extrapolation. Joyce and Bowers are the first to have pointed to the possibility that $C(0)$ might be finite at T_c . Bowers and Woolf (taking $x_c = 0.157225$) concluded $-1/8 \leq \alpha \leq -1/16$, and Ferer *et al.* (with $x_c = 0.15747$) infer $\alpha = -0.14 \pm 0.06$. This direct support for negative α , independent of (5.29), is gratifying; though of all the scaling laws (5.29), which simply extrapolates (5.26) to $r = 0$, is perhaps the most transparently plausible.

If α is negative, then $C(0)$ is not infinite at T_c , and near T_c we may write

$$C(0)/Nk = A - B \left(1 - \frac{T_c}{T}\right)^{|\alpha|}. \quad (5.32)$$

For $H(\infty)$, f.c.c. lattice, it seems probable that A and B could be found with acceptable accuracy provided α were known precisely. Thus Domb and Bowers (1969), taking $\alpha = -1/16$, concluded $A = 10.00$ and $B = 10.85$. Starting from (2.18) and assuming a value for x_c , Domb and Bowers transformed the known specific heat series to the form

$$C(0)/Nk = \sum_{n \geq 2} k_n t^n \quad (5.33)$$

where $t = x/x_c = T_c/T$. Expanding $(1 - t)^{|\alpha|}$ as $1 - \sum_{n \geq 1} h_n t^n$, they examined the sequence of ratios k_n/h_n , $n \geq 2$. For $H(\infty)$, f.c.c. lattice, with $\alpha = -1/16$, for $n = 6, 7 \dots 11$, k_n/h_n is always in the range 10.84 to 10.91. Domb and

Bowers took 10.85 as the value thus predicted for the constant B in (5.32). Then (5.33) can be written

$$C(0)/Nk = B - B(1-t)^{|\alpha|} - \phi(t) \quad (5.34)$$

where $\phi(t)$ is a correction polynomial whose terms, even for $t = 1$, rapidly decrease; consequently $\phi(t)$ can be summed, and A in (5.32) is simply $B - \phi(1)$. The method works because k_n/h_n reaches a steady value (or a predictable limit); but this is very sensitive to choice of α .[†] Domb and Bowers themselves observe that for $\alpha = -1/8$ the maximum is reduced from about 10.0 to about 5.7.

Unfortunately this method seems not to be applicable to the $H(\frac{1}{2})$ problem, even for the f.c.c. lattice; not because an early c_n coefficient is negative, but because the ratios k_n/h_n do not approach a sufficiently well-defined limit. In their 1967 paper, Baker *et al.*, taking $\alpha = -0.20$ (see Table VII), fitted PA estimates of $C(0)$ over the range $0.70 \leq T_c/T \leq 0.96$ with an expression of the form

$$C(0)/Nk = (T_c/T)^2 [A - B(1 - T_c/T)^{0.20}] \quad (5.35)$$

and inferred, for the f.c.c. lattice, $A = 1.206$, $B = 0.966$. But this method (even for a correct α) probably underestimates the height of the maximum in $C(0)$. For Stephenson (1969) applied it to $H(\infty)$, f.c.c. lattice, taking[‡] $\alpha = -1/16$, and obtained $A = 5.75$ in contrast to the Domb and Bowers value of 10.0. Nevertheless, even this method is preferable to simply evaluating $C(0)$ by forming PA's to (2.18), since these PA's fail to give $C(0)$ an infinite gradient at T_c . Direct PA's make A only 1.61 for $H(\infty)$ and 0.80 for $H(\frac{1}{2})$.

Despite the difficulty in determining the height of the specific heat maximum, particularly for the model $H(\frac{1}{2})$, it does, however, seem certain that for $H(\frac{1}{2})$ the maximum is appreciably less than for $H(\infty)$, even if the two models have the same exponent α . Table VIII shows numerical values of $C(0)$, for both $H(\frac{1}{2})$ and $H(\infty)$, f.c.c. lattice, for temperatures at which the series for $C(0)$ can be convincingly evaluated, both by Padé evaluation and by extrapolation on partial sums, to an accuracy of one unit in the last digit quoted. It will be noted that for large T the $H(\frac{1}{2})$ specific heat exceeds that for $H(\infty)$: this must be so, since the limiting expressions are $0.28(T_c/T)^2$ and $0.20(T_c/T)^2$, respectively. But the curves cross at about $T/T_c = 1.5$, and when $T/T_c = 1.1$ the $H(\infty)$ value is 50% higher than that for $H(\frac{1}{2})$.

[†] For given α , A is not particularly sensitive to small changes in x_c or to the value adopted for B .

[‡] Actually Stephenson took $\alpha = -0.07$, but this should make relatively little difference.

TABLE VIII. $C(0)$, f.c.c. lattice

| T/T_c | $H(\frac{1}{2})$ | $H(\infty)$ |
|---------|--------------------|-------------------|
| 1.1 | 0.50 | 0.75 |
| 1.2 | 0.37 | 0.47 |
| 1.3 | 0.29 | 0.34 |
| 1.4 | 0.23 ₃ | 0.25 ₄ |
| 1.5 | 0.20 ₋₄ | 0.20 ₁ |
| 1.6 | 0.166 | 0.163 |
| 1.7 | 0.143 | 0.135 |
| 1.8 | 0.125 | 0.115 |
| 1.9 | 0.110 | 0.098 |
| 2.0 | 0.098 | 0.085 |
| 3.0 | 0.039 | 0.031 |
| 4.0 | 0.021 | 0.016 |

Although the precise value of α is not known, there is little reason to doubt that it is negative.[†] If this is so, then not only is $C(0)$ always finite, but the Heisenberg models will not be subject to exponent renormalisation in Fisher's sense, due to impurities or other hidden variables in thermodynamic equilibrium with the magnetic lattice (Fisher, 1968). Indeed, one set of $H(\frac{1}{2})$ indices proposed by Baker *et al.* (1967c), namely $\gamma = 10/7$, $2\Delta = 25/7$, $\alpha = -1/7$, $\beta = 5/14$, $\delta = 5$, are just the renormalised $I(\frac{1}{2})$ values. It is however, difficult to advance a plausible physical reason why the $H(\frac{1}{2})$ model should be regarded as a renormalised $I(\frac{1}{2})$ model.

F. Discussion

In this brief review of properties which can be derived from high-temperature expansions, we have deliberately kept to those things which seem perhaps most firmly established and have omitted matters which, though not uninteresting, are necessarily speculative. In this latter category fall, for example, the discussions of antiferromagnetic susceptibilities given by Baker *et al.* (1967c) and Bowers and Woolf (1969). We have also refrained from supplementing published work on critical exponents with more than minor comments. But there are two recent suggestions regarding these indices which, while inevitably still subjudice, are sufficiently important to demand mention. They were both advanced at the International Conference on Magnetism at Grenoble, 1970, and both relate to the issue of whether or not the $H(s)$ critical exponents are independent of the value of s .

[†] To the direct evidence for $H(\infty)$, and the support of Table VII, should be added the detailed $H(\frac{1}{2})$ discussion in Baker *et al.* (1967c).

Thus Betts *et al.* (1970b) and also Stanley and Betts (1971), making the assumption of spin independence, have sought simple expressions for these indices which shall cover present estimates for a wide range of three dimensional physical models and depend only on the spin dimensionality, D , of the underlying Hamiltonian. We note that $D = 1$ for $I(s)$, $D = 2$ for $XY(\frac{1}{2})$ or $P(\infty)$, $D = 3$ for $H(s)$, and, as Stanley (1968b) has shown, the limit $D \rightarrow \infty$, $s = \infty$, yields the so-called spherical model. For $I(\frac{1}{2})$ there is strong series support for $\gamma = 5/4$; for $XY(\frac{1}{2})$ Betts *et al.* (1970a) have, from series analysis, inferred $\gamma = 4/3$; for the spherical model $\gamma = 2$; and these three values are covered by the simple expression

$$\gamma = \frac{8 + 2D}{7 + D}. \quad (5.36)$$

For the spherical model $\delta = 5$; for $I(\frac{1}{2})$ δ is certainly close to 5; and we have already referred to the suggestion, Baker *et al.* (1970), that $\delta \sim 5$ for $H(\frac{1}{2})$. If $\delta = 5$ for all three-dimensional lattice models (with interactions of finite range) then the scaling laws, (5.29), (5.30), and (5.31), together with (5.36), enable all exponents to be predicted. Indeed, if $\delta = 5$ the scaling laws imply

$$\alpha = \frac{4 - 3\gamma}{2}, \quad \beta = \frac{1}{4}\gamma, \quad 2\Delta = \frac{5}{2}\gamma \quad (5.37)$$

$$\nu = \frac{1}{2}\gamma \quad \text{and} \quad \eta = 0$$

so that (5.36) immediately yields the other exponents. On putting $D = 3$ we find

$$\begin{aligned} \gamma &= 1.4, & \alpha &= -0.1, & \beta &= 0.35, & 2\Delta &= 3.5 \\ \nu &= 0.7 & \text{and} & \eta &= 0. \end{aligned} \quad (5.38)$$

The question, therefore, now arises whether or not these values are tenable for the Heisenberg models, $H(\frac{1}{2})$ and $H(\infty)$.

The recent work on $H(\infty)$ to which we have already referred has certainly produced index values extraordinarily close to the predictions (5.38). Admittedly the values of ν and $2\nu - \gamma$ quoted by Ferer *et al.* (1971) would seem to exclude $\eta = 0$: but if necessary we can accept (5.29) and (5.30) without being committed to (5.31). With the crucial indices γ and 2Δ , the present estimates for $H(\infty)$ can hardly be held to be in conflict with (5.38).

For the model $H(\frac{1}{2})$, the present position is less simple. Baker *et al.* (1967c) gave $\gamma = 1.43 \pm 0.01$ and $2\Delta = 3.63 \pm 0.03$. As reference to their published Padé tables shows, had they said $\gamma = 1.41 \pm 0.04$ they would have covered several more estimates of γ and no present conflict would arise; but, while

accepting what Ferer *et al.* have called "the natural tendency to have too much confidence in one's analysis", we believe the 1967 work did in fact point to values of γ and 2Δ higher than those predicted in (5.38). Recently Lee and Stanley (1970), see also Stanley and Betts (1971), have suggested that this is due to "interference" from certain "non-physical" singularities to whose existence Baker *et al.* had drawn attention in their 1967 paper. Applying conformal transformations aimed at diminishing this "interference", they have concluded $\gamma = 1.36 \pm 0.04$ and $2\Delta = 3.50 \pm 0.2$.

Without having seen details of this analysis, we are in no strong position to comment on it. But we can say why, rightly or wrongly, Baker *et al.* were not worried about this "interference" at the time of their 1967 paper. Before doing so, we must specify these "non-physical" singularities more precisely.

As Baker *et al.* observed, *PA*'s to $d \ln \chi / dx$ for the three cubic lattices have rather well-defined poles not only at $x = x_c$ but at certain other points in the complex x -plane. For the f.c.c. lattice, many *PA*'s have poles at about $x = 0.19 \pm 0.35i$, and for the s.c. lattice, apart from the antiferromagnetic singularity, there are persistent poles at about $x = -0.075 \pm 0.50i$. For the b.c.c. lattice, Baker *et al.* (1967c) were rather non-committal, but there is perhaps some evidence of "non-physical" poles near $x = \pm 0.4i$.

Since the f.c.c. lattice does not have an antiferromagnetic singularity, we shall confine attention to this case. Then one possible way of judging whether there is interference from the non-physical poles is by forming *PA*'s to

$$(x^2 - 0.38x + 0.16) \frac{d \ln \chi}{dx}. \quad (5.39)$$

We have done this and find that not only do the non-physical poles disappear, but that the [1, 5], [1, 6], [1, 7], [2, 4], [2, 5], [2, 6], [3, 3], [3, 4], [3, 5], [4, 3], [4, 4], [5, 2], [5, 3] and [6, 1] *PA*'s all yield γ estimates in the range 1.430 ± 0.003 . Moreover, small changes in the quadratic factor in (5.39) can certainly be made without disturbing the conclusion $\gamma = 1.43 \pm 0.01$. And Baker *et al.* were aware of this before publishing their 1967 paper.

One comment must, however, be made. Most *PA*'s to (5.39) have $x^2 - 0.456x + 0.164$ as a quadratic factor of their numerators. Indeed, all the non-physical poles to which we have drawn attention are closely balanced by nearby zeros. It is for this reason, of course, that they are "weak" singularities. We do not know their origin; whether they are "genuine" features of the susceptibility function χ , or are formed by applying a Padé analysis to a function not quite of the form (5.2), and not entirely well-suited to Padé approximant representation. The method of conformal transformations, by displacing both the poles and the associated zeros,

may have its merits; but we are not yet in a position to judge this. At present, the conjecture (5.36), striking though it is, cannot claim strong support from the $H(\frac{1}{2})$ model.

This is one question which has still to be resolved. Another, as we have seen, is the existence or otherwise of pseudo-Curie points for Heisenberg models based on two-dimensional lattices. Perhaps in both cases we need further experience in the analysis of series even more than extra terms in the series themselves. Meanwhile, despite these open questions, we believe that the Heisenberg model series work with which this chapter has been concerned has provided sufficiently firm predictions of thermodynamic functions for meaningful comparisons to be made with experimental data.

Appendix I

We list the reduced mean traces, defined by eqn (2.31), for those interaction graphs of order ≤ 8 for which they have to be calculated *ab initio*. The trace of any other interaction graph of order ≤ 8 can be found from these by use of the lemmas of Section III.B: as explained at the end of that section. These basic traces, which have not been published previously, were derived by Wood, Rushbrooke, Pirnie and Stephenson.

The tables give (i) a descriptive numeral, of which the first integer denotes the order of the graph; (ii) a depiction of the graph in which bonds are labelled according to their multiplicities (when greater than unity); (iii) the reduced mean trace as a polynomial in X , where $X \equiv s(s+1)$.

$$(2.1) \quad \overline{^2} \quad \frac{1}{3}X^2$$

$$(3.1) \quad \overline{^3} \quad -\frac{1}{6}X^2$$

$$(4.1) \quad \overline{^4} \quad \frac{1}{15}X^2(3X^2 - 2X + 2)$$

$$(4.2) \quad \overline{^2 ^2} \quad \frac{1}{27}X^3(3X - 1)$$

$$(5.1) \quad \overline{^5} \quad -\frac{1}{6}X^2(2X^2 - 2X + 1)$$

$$(5.2) \quad \overline{^3 ^2} \quad -\frac{1}{36}X^3(2X - 1)$$

$$(5.3) \quad \begin{array}{c} \triangle \\ 3 \end{array} \quad \frac{1}{180}X^3(12X^2 - 8X + 3)$$

$$(5.4) \quad \begin{array}{c} \triangle \\ 2 \quad 2 \end{array} \quad 0$$

$$(6.1) \quad \begin{array}{c} \underline{\quad 6 \quad} \\ - \end{array} \quad -\frac{1}{105}X^2(15X^4 - 30X^3 + 88X^2 - 87X + 32)$$

$$(6.2) \quad \begin{array}{c} \underline{\quad 4 \quad} \quad \underline{\quad 2 \quad} \\ - \end{array} \quad \frac{1}{90}X^3(6X^3 - 8X^2 + 8X - 3)$$

$$(6.3) \quad \begin{array}{c} \underline{\quad 3 \quad} \quad \underline{\quad 3 \quad} \\ - \end{array} \quad \frac{1}{90}X^3(3X - 2)$$

$$(6.4) \quad \begin{array}{c} \triangle \\ 4 \end{array} \quad -\frac{1}{45}X^3(3X^2 - 3X + 1)$$

$$(6.5) \quad \begin{array}{c} \triangle \\ 3 \quad 2 \end{array} \quad -\frac{1}{180}X^4(2X - 1)$$

$$(6.6) \quad \begin{array}{c} \triangle \\ 2 \quad 2 \\ 2 \end{array} \quad \frac{1}{450}X^3(22X^3 - 22X^2 + 9X - 1)$$

$$(6.7) \quad \begin{array}{c} \diagup \quad \diagdown \\ 2 \quad 2 \\ \diagdown \quad \diagup \\ 2 \end{array} \quad \frac{1}{81}X^4(3X^2 - 3X + 1)$$

$$(6.8) \quad \begin{array}{c} \diagup \quad \diagdown \\ 2 \quad 2 \\ \diagdown \quad \diagup \\ 2 \end{array} \quad \frac{1}{405}X^4(15X^2 - 10X + 2)$$

$$(6.9) \quad \begin{array}{c} \square \\ 2 \end{array} \quad \frac{1}{810}X^4$$

$$(6.10) \quad \begin{array}{c} \square \\ 2 \quad 2 \end{array} \quad \frac{1}{540}X^4$$

$$(6.11) \quad \begin{array}{c} \triangle \\ 2 \quad \quad \quad 2 \end{array} \quad -\frac{1}{810}X^4(5X - 1)$$

$$(6.12) \quad \begin{array}{c} \square \\ 2 \quad \quad \quad 2 \end{array} \quad -\frac{1}{1620}X^4$$

$$(6.13) \quad \begin{array}{c} \square \\ 2 \quad \quad \quad 2 \end{array} \quad \frac{1}{1620}X^4(36X^2 - 24X + 5)$$



$$(6.14) \quad \frac{1}{3240}X^4$$

$$(7.1) \quad \frac{7}{60}X^2(30X^4 - 88X^3 + 171X^2 - 148X + 46)$$

$$(7.2) \quad \frac{5}{270}X^3(30X^3 - 59X^2 + 51X - 16)$$

$$(7.3) \quad \frac{4}{900}X^3(30X^3 - 54X^2 + 61X - 26)$$



$$(7.4) \quad \frac{1}{378}X^3(18X^4 - 36X^3 + 65X^2 - 54X + 16)$$



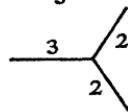
$$(7.5) \quad \frac{1}{2700}X^3(16X^2 - 9X - 1)$$



$$(7.6) \quad \frac{1}{1800}X^3(72X^4 - 120X^3 + 108X^2 - 41X + 3)$$



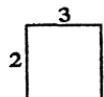
$$(7.7) \quad -\frac{1}{2700}X^3(66X^3 - 80X^2 + 33X - 4)$$



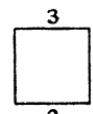
$$(7.8) \quad -\frac{1}{810}X^4(15X^2 - 22X + 9)$$

$$(7.9) \quad \begin{array}{c} 3 \\ \diagup \quad \diagdown \\ 2 \quad 2 \end{array} \quad -\frac{1}{1620}X^4(30X^2 - 25X + 6)$$

$$(7.10) \quad \begin{array}{c} 2 \\ \diagup \quad \diagdown \\ 3 \quad 2 \end{array} \quad -\frac{1}{810}X^4(15X^2 - 15X + 4)$$



$$(7.11) \quad -\frac{1}{1620}X^4(6X^2 - 5X + 2)$$



$$(7.12) \quad -\frac{1}{3240}X^4(12X^2 - 8X + 5)$$

$$(7.13) \quad \begin{array}{c} 2 \\ \boxed{} \\ 2 \end{array} \quad -\frac{1}{1944}X^4$$

$$(7.14) \quad \begin{array}{c} 2 \\ \triangle \\ 2 \quad 2 \end{array} \quad -\frac{1}{2430}X^4(2X-1)$$

$$(7.15) \quad \begin{array}{c} 2 \\ \triangle \\ 2 \quad 2 \end{array} \quad \frac{1}{9720}X^4$$

$$(7.16) \quad \begin{array}{c} 2 \\ \triangle \\ 3 \\ 2 \end{array} \quad \frac{1}{1620}X^4(36X^3 - 48X^2 + 31X - 8)$$

$$(7.17) \quad \begin{array}{c} 3 \\ \triangle \\ 2 \end{array} \quad \frac{1}{1620}X^4(36X^3 - 36X^2 + 17X - 2)$$

$$(7.18) \quad \begin{array}{c} 2 \\ \triangle \\ 2 \quad 3 \end{array} \quad \frac{1}{3240}X^4(10X - 3)$$

$$(7.19) \quad \begin{array}{c} 3 \\ \square \\ \diagup \quad \diagdown \end{array} \quad -\frac{1}{1620}X^4(18X^2 - 18X + 5)$$

$$(7.20) \quad \begin{array}{c} 3 \\ \square \\ \diagup \quad \diagdown \end{array} \quad -\frac{1}{1620}X^4(X - 1)$$

$$(7.21) \quad \begin{array}{c} 2 \\ \square \\ \diagup \quad \diagdown \end{array} \quad \frac{1}{48600}X^4(792X^3 - 792X^2 + 304X - 31)$$

$$(7.22) \quad \begin{array}{c} 2 \\ \square \\ \diagup \quad \diagdown \end{array} \quad \frac{1}{4860}X^4$$

$$(7.23) \quad \begin{array}{c} 2 \\ \square \\ \diagup \quad \diagdown \end{array} \quad \frac{1}{2430}X^5$$

$$(7.24) \quad \begin{array}{c} 2 \\ \square \\ \diagup \quad \diagdown \end{array} \quad -\frac{1}{4860}X^4(18X^2 - 11X + 1)$$

(7.25)

$$\frac{1}{2916}X^5$$

(7.26)

$$-\frac{1}{1458}X^5(3X - 1)$$

(7.27)

$$\frac{1}{729}X^5(9X^2 - 6X + 1)$$

(7.28)

$$-\frac{1}{19440}X^4(8X - 1)$$

(7.29)

$$\frac{1}{7290}X^5$$

(7.30)

$$-\frac{1}{7290}X^5$$

(7.31)

$$-\frac{1}{9720}X^5$$

(7.32)

$$\frac{1}{1215}X^5(9X^2 - 6X + 1)$$

(7.33)

$$\frac{1}{29160}X^5$$

(8.1) 8 $\frac{1}{45}X^2(5X^6 - 20X^5 + 116X^4 - 330X^3 + 534X^2 - 408X + 114)$

(8.2) 6 2 $\frac{1}{630}X^3(30X^5 - 90X^4 + 264X^3 - 429X^2 + 328X - 92)$

(8.3) 5 3 $\frac{1}{1260}X^3(84X^3 - 211X^2 + 206X - 70)$

(8.4) 4 4 $\frac{1}{7875}X^3(315X^5 - 840X^4 + 1512X^3 - 1657X^2 + 1114X - 336)$

$$(8.5) \quad \begin{array}{c} \triangle \\ 6 \end{array} \quad -\frac{1}{1260}X^3(150X^4 - 440X^3 + 687X^2 - 508X + 138)$$

$$(8.6) \quad \begin{array}{c} 5 \\ \triangle \\ 2 \end{array} \quad -\frac{1}{3780}X^3(30X^4 - 46X^3 + 35X^2 - 3X - 6)$$

$$(8.7) \quad \begin{array}{c} 4 \\ \triangle \\ 3 \end{array} \quad -\frac{1}{15750}X^3(630X^4 - 1379X^3 + 1304X^2 - 503X + 42)$$

$$(8.8) \quad \begin{array}{c} 2 \\ \triangle \\ 2 \\ 4 \end{array} \quad \frac{1}{9450}X^3(306X^5 - 714X^4 + 994X^3 - 740X^2 + 255X - 30)$$

$$(8.9) \quad \begin{array}{c} 3 \\ \triangle \\ 3 \\ 2 \end{array} \quad -\frac{1}{63000}X^3(420X^4 - 1092X^3 + 992X^2 - 379X + 56)$$

$$(8.10) \quad \begin{array}{c} 2 \\ \diagup \\ 4 \\ \diagdown \\ 2 \end{array} \quad \frac{1}{14175}X^4(315X^4 - 735X^3 + 1022X^2 - 798X + 248)$$

$$(8.11) \quad \begin{array}{c} 3 \\ \diagup \\ 2 \\ \diagdown \\ 3 \end{array} \quad \frac{1}{890}X^4(21X^2 - 42X + 20)$$

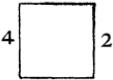
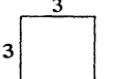
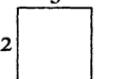
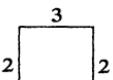
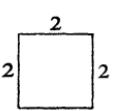
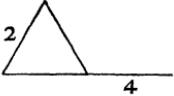
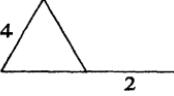
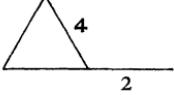
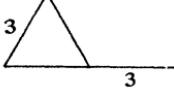
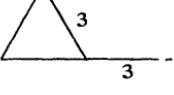
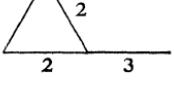
$$(8.12) \quad \begin{array}{c} 4 \\ \diagup \\ & 2 \\ \diagdown & \\ 2 & 2 \end{array} \quad \frac{1}{28350}X^4(630X^4 - 1050X^3 + 1148X^2 - 627X + 127)$$

$$(8.13) \quad \begin{array}{c} 2 \\ \diagup \\ & 4 \\ \diagdown & \\ 2 & 2 \end{array} \quad \frac{1}{28350}X^4(630X^4 - 1260X^3 + 1596X^2 - 1054X + 259)$$

$$(8.14) \quad \begin{array}{c} 3 \\ \diagup \\ & 3 \\ \diagdown & \\ 2 & 2 \end{array} \quad \frac{1}{2520}X^4(28X^2 - 33X + 10)$$

$$(8.15) \quad \begin{array}{c} 3 \\ \diagup \\ & 2 \\ \diagdown & \\ 2 & 3 \end{array} \quad \frac{1}{1080}X^4(10X^2 - 10X + 3)$$

$$(8.16) \quad \begin{array}{c} 4 \\ \square \\ 2 \end{array} \quad \frac{1}{56700}X^4(252X^2 - 293X + 103)$$

- (8.17)  $\frac{1}{28350}X^4(133X^2 - 137X + 57)$
- (8.18)  $\frac{1}{37800}X^4(504X^4 - 840X^3 + 756X^2 - 352X + 71)$
- (8.19)  $\frac{1}{5400}X^4(72X^4 - 96X^3 + 68X^2 - 24X + 7)$
- (8.20)  $\frac{1}{16200}X^4(12X^2 - 13X + 8)$
- (8.21)  $\frac{1}{113400}X^4(182X^2 - 198X + 83)$
- (8.22) 
$$\begin{aligned} &\frac{1}{425250}X^4(5922X^4 - 7896X^3 + 4508X^2 \\ &- 1284X + 252 \end{aligned}$$
- (8.23)  $-\frac{1}{56700}X^4(210X^3 - 224X^2 + 216X - 61)$
- (8.24)  $-\frac{1}{14175}X^4(315X^3 - 406X^2 + 194X - 24)$
- (8.25)  $-\frac{1}{28350}X^4(630X^3 - 1239X^2 + 931X - 246)$
- (8.26)  $-\frac{1}{1080}X^4(12X^3 - 14X^2 + 7X - 1)$
- (8.27)  $-\frac{1}{18900}X^4(210X^3 - 378X^2 + 287X - 82)$
- (8.28)  $\frac{1}{11340}X^4(7X - 4)$

$$(8.29) \quad \begin{array}{c} 2 \\ \diagdown \quad \diagup \\ 3 \end{array} \quad -\frac{1}{22680}X^4(X-2)$$

$$(8.30) \quad \begin{array}{c} 2 \\ \diagup \quad \diagdown \\ 3 \quad 2 \end{array} \quad -\frac{1}{28350}X^4(105X^3 - 154X^2 + 56X + 4)$$

$$(8.31) \quad \begin{array}{c} 3 \\ \diagup \quad \diagdown \\ 2 \end{array} \quad -\frac{1}{11340}X^4(42X^3 - 42X^2 + 10X + 1)$$

$$(8.32) \quad \begin{array}{c} 2 \\ \diagup \quad \diagdown \\ 2 \end{array} \quad -\frac{1}{56700}X^4(210X^3 - 189X^2 + 51X - 1)$$

$$(8.33) \quad \begin{array}{c} 2 \\ \diagup \quad \diagdown \\ 2 \quad 2 \end{array} \quad \begin{aligned} &-\frac{1}{170100}X^4(2772X^4 - 4620X^3 + 3402X^2 \\ &\quad - 1132X + 129) \end{aligned}$$

$$(8.34) \quad \begin{array}{c} 2 \\ | \\ 2 \quad 2 \\ | \\ 2 \end{array} \quad \frac{1}{405}X^5(5X^3 - 10X^2 + 9X - 3)$$

$$(8.35) \quad \begin{array}{c} 2 \\ | \\ 2 \quad 2 \\ | \\ 2 \end{array} \quad \begin{aligned} &\frac{1}{25515}X^5(315X^3 - 420X^2 + 224X - 43) \end{aligned}$$

$$(8.36) \quad \begin{array}{c} 2 \quad 2 \\ \diagup \quad \diagdown \\ 2 \quad 2 \end{array} \quad \frac{1}{25515}X^5(315X^3 - 315X^2 + 119X - 17)$$

$$(8.37) \quad \begin{array}{c} 4 \\ \diagup \quad \diagdown \\ 2 \quad 2 \end{array} \quad \frac{1}{28350}X^4(450X^4 - 900X^3 + 1107X^2 - 718X + 178)$$

$$(8.38) \quad \begin{array}{c} 4 \\ \diagup \quad \diagdown \\ 2 \quad 2 \end{array} \quad -\frac{1}{11340}X^4(14X^2 - 23X + 11)$$

$$(8.39) \quad \begin{array}{c} 2 \\ \diagup \quad \diagdown \\ 2 \quad 2 \end{array} \quad \frac{1}{113400}X^4(42X^2 - 13X - 12)$$

$$(8.40) \quad \begin{array}{c} 3 \quad 2 \\ \diagup \quad \diagdown \\ 2 \quad 2 \end{array} \quad \begin{aligned} &\frac{1}{113400}X^4(1512X^4 - 2520X^3 + 2044X^2 \\ &\quad - 750X + 77) \end{aligned}$$

$$(8.41) \quad \begin{array}{c} 2 \\ \boxed{3} \\ 2 \end{array} : \quad -\frac{1}{113400}X^4(924X^3 - 1134X^2 + 473X - 52)$$

$$(8.42) \quad \begin{array}{c} 3 \\ \boxed{2} \\ 2 \end{array} : \quad -\frac{1}{22680}X^4(14X^2 - 9X + 3)$$

$$(8.43) \quad \begin{array}{c} 2 \\ \boxed{2} \\ 3 \end{array} : \quad -\frac{1}{113400}X^4(42X^2 - 43X + 23)$$

$$(8.44) \quad \begin{array}{c} 2 \\ \boxed{2} \\ 2 \end{array} : \quad \frac{1}{170100}X^4(126X^2 - 99X + 14)$$

$$(8.45) \quad \begin{array}{c} 2 \\ \boxed{2} \\ 2 \end{array} : \quad -\frac{1}{340200}X^4(924X^3 - 1092X^2 + 380X - 39)$$

$$(8.46) \quad \begin{array}{c} 2 \\ \boxed{2} \\ 2 \end{array} : \quad \frac{1}{340200}X^4(322X^2 - 218X + 43)$$

$$(8.47) \quad \begin{array}{c} 2 \\ \boxed{2} \\ 2 \end{array} : \quad -\frac{1}{170100}X^4(462X^3 - 483X^2 + 203X - 20)$$

$$(8.48) \quad \begin{array}{c} 2 \\ \boxed{3} \\ 2 \end{array} : \quad -\frac{1}{9720}X^5(12X^2 - 8X + 3)$$

$$(8.49) \quad \begin{array}{c} 2 \\ \boxed{2} \\ 2 \end{array} : \quad -\frac{1}{204120}X^5$$

$$(8.50) \quad \begin{array}{c} 2 \\ \boxed{2} \\ 2 \end{array} : \quad -\frac{1}{34020}X^5$$

$$(8.51) \quad \begin{array}{c} 2 \\ \boxed{3} \\ 3 \end{array} : \quad \frac{1}{1944}X^5(2X - 1)$$

$$(8.52) \quad \begin{array}{c} 3 \\ \boxed{2} \\ 2 \end{array} : \quad \frac{1}{4860}X^5(36X^3 - 36X^2 + 17X - 3)$$

$$(8.53) \quad \begin{array}{c} 2 \\ | \\ \square \\ | \\ 2 & 2 \end{array}$$

$$\frac{1}{204120}X^5(84X - 43)$$

$$(8.54) \quad \begin{array}{c} 2 \\ | \\ \square \\ | \\ 2 & 2 \end{array}$$

$$\frac{1}{204120}X^5(126X - 67)$$

$$(8.55) \quad \begin{array}{c} 2 \\ | \\ \square \\ | \\ 2 & 2 \end{array}$$

$$\frac{1}{51030}X^5(21X - 13)$$

$$(8.56) \quad \begin{array}{c} 2 \\ | \\ \square \\ | \\ 2 & 2 \end{array}$$

$$\frac{1}{17010}X^5(7X - 3)$$

$$(8.57) \quad \begin{array}{c} \triangle \\ | \\ \square \\ | \\ 3 & 2 \end{array}$$

$$-\frac{1}{972}X^5(6X^2 - 5X + 1)$$

$$(8.58) \quad \begin{array}{c} \triangle \\ | \\ \square \\ | \\ 2 & 2 & 2 \end{array}$$

$$-\frac{1}{20412}X^5(42X^2 - 42X + 11)$$

$$(8.59) \quad \begin{array}{c} \triangle \\ | \\ \square \\ | \\ 2 & 2 & 2 \end{array}$$

$$-\frac{1}{102060}X^5(210X^2 - 147X + 19)$$

$$(8.60) \quad \begin{array}{c} \triangle \\ | \\ \times \\ | \\ 2 & 2 & 2 \end{array}$$

$$-\frac{1}{51030}X^5(105X^2 - 77X + 19)$$

$$(8.61) \quad \begin{array}{c} \triangle \\ | \\ \square \\ | \\ 2 & 2 & 2 \end{array}$$

$$-\frac{1}{51030}X^5(105X^2 - 56X + 8)$$

$$(8.62) \quad \begin{array}{c} \square \\ | \\ \times \\ | \\ 3 \end{array}$$

$$\frac{1}{226800}X^4(98X^2 - 52X + 17)$$

$$(8.63) \quad \begin{array}{c} \square \\ | \\ \times \\ | \\ 2 & 2 \end{array}$$

$$-\frac{1}{340200}X^4(196X^2 - 194X + 39)$$

$$(8.64) \quad \begin{array}{c} 2 \\ \diagup \quad \diagdown \\ \square \quad \square \\ \diagdown \quad \diagup \\ 2 \end{array} \quad \frac{1}{850500} X^4 (9324X^4 - 12432X^3 + 6706X^2 - 1458X + 139)$$

$$(8.65) \quad \begin{array}{c} 2 \\ \diagup \quad \diagdown \\ \triangle \quad \triangle \\ \diagdown \quad \diagup \\ 2 \end{array} \quad \frac{1}{510300} X^5 (2772X^3 - 2772X^2 + 1064X - 151)$$

$$(8.66) \quad \begin{array}{c} 2 \\ \diagup \quad \diagdown \\ \triangle \quad \triangle \\ \diagdown \quad \diagup \\ 2 \end{array} \quad -\frac{1}{34020} X^5$$

$$(8.67) \quad \begin{array}{c} 2 \\ \diagup \quad \diagdown \\ \triangle \quad \triangle \\ \diagdown \quad \diagup \\ 2 \end{array} \quad \frac{1}{51030} X^5 (7X - 4)$$

$$(8.68) \quad \begin{array}{c} 2 \\ \diagup \quad \diagdown \\ \triangle \quad \triangle \\ \diagdown \quad \diagup \\ 3 \end{array} \quad -\frac{1}{9720} X^5$$

$$(8.69) \quad \begin{array}{c} 2 \\ \diagup \quad \diagdown \\ \triangle \quad \triangle \\ \diagdown \quad \diagup \\ 2 \end{array} \quad \frac{1}{25515} X^5$$

$$(8.70) \quad \begin{array}{c} 2 \\ \diagup \quad \diagdown \\ \triangle \quad \triangle \\ \diagdown \quad \diagup \\ 2 \end{array} \quad \frac{1}{40824} X^5$$

$$(8.71) \quad \begin{array}{c} 2 \\ \diagup \quad \diagdown \\ \triangle \quad \triangle \\ \diagdown \quad \diagup \\ 2 \end{array} \quad \frac{1}{22680} X^5$$

$$(8.72) \quad \begin{array}{c} 2 \\ \diagup \quad \diagdown \\ \triangle \quad \triangle \\ \diagdown \quad \diagup \\ 2 \end{array} \quad -\frac{1}{102060} X^5 (126X^2 - 105X + 25)$$

$$(8.73) \quad \begin{array}{c} 2 \\ \diagup \quad \diagdown \\ \triangle \quad \triangle \\ \diagdown \quad \diagup \\ 2 \end{array} \quad -\frac{1}{204120} X^5 (252X^2 - 168X + 47)$$

$$(8.74) \quad \begin{array}{c} 2 \\ \diagup \quad \diagdown \\ \triangle \quad \triangle \\ \diagdown \quad \diagup \\ 2 \end{array} \quad -\frac{1}{22680} X^5$$

$$(8.75) \quad \begin{array}{c} 2 \\ \diagup \quad \diagdown \\ \triangle \quad \triangle \\ \diagdown \quad \diagup \\ 2 \end{array} \quad -\frac{1}{34020} X^5$$

$$(8.76) \quad \begin{array}{c} \text{Diagram: Two triangles sharing a common base, each with a side labeled 2.} \\ \frac{1}{20412} X^5 (7X - 1) \end{array}$$

$$(8.77) \quad \begin{array}{c} \text{Diagram: A square divided into four triangles by a diagonal from the top-left corner to the bottom-right corner. The side length is labeled 3.} \\ \frac{1}{9720} X^5 \end{array}$$

$$(8.78) \quad \begin{array}{c} \text{Diagram: A square divided into four triangles by a diagonal from the top-left corner to the middle of the right side. The side length is labeled 2.} \\ -\frac{1}{204120} X^5 (42X - 25) \end{array}$$

$$(8.79) \quad \begin{array}{c} \text{Diagram: A square divided into four triangles by a diagonal from the top-left corner to the middle of the bottom side. The side length is labeled 2.} \\ \frac{1}{102060} X^5 (756X^3 - 756X^2 + 273X - 29) \end{array}$$

$$(8.80) \quad \begin{array}{c} \text{Diagram: A square divided into four triangles by a diagonal from the top-left corner to the bottom-right corner. The side length is labeled 2.} \\ -\frac{1}{102060} X^5 (21X - 8) \end{array}$$

$$(8.81) \quad \begin{array}{c} \text{Diagram: A square divided into four triangles by a diagonal from the top-left corner to the middle of the right side. The side length is labeled 2.} \\ -\frac{1}{20412} X^5 (7X - 4) \end{array}$$

$$(8.82) \quad \begin{array}{c} \text{Diagram: A square divided into four triangles by a diagonal from the top-left corner to the middle of the bottom side. The side length is labeled 2.} \\ \frac{1}{102060} X^5 (756X^3 - 1008X^2 + 539X - 104) \end{array}$$

$$(8.83) \quad \begin{array}{c} \text{Diagram: A square divided into four triangles by a diagonal from the top-left corner to the bottom-left corner. The side length is labeled 2.} \\ -\frac{1}{34020} X^5 (7X - 4) \end{array}$$

$$(8.84) \quad \begin{array}{c} \text{Diagram: A regular hexagon with all sides labeled 2.} \\ \frac{1}{8748} X^6 \end{array}$$

$$(8.85) \quad \begin{array}{c} \text{Diagram: A regular pentagon with all sides labeled 2.} \\ -\frac{1}{4374} X^6 (3X - 1) \end{array}$$

$$(8.86) \quad \begin{array}{c} \text{Diagram: A rectangle with a horizontal top edge labeled 2 and a vertical right edge labeled 2.} \\ \frac{1}{2187} X^6 (9X^2 - 6X + 1) \end{array}$$

$$(8.87) \quad \begin{array}{c} \text{Diagram of a pentagon with vertices labeled 1, 2, 3, 4, 5 clockwise from top-left.} \\ \text{A diagonal connects vertex 1 to vertex 3.} \end{array} \quad -\frac{1}{2041200}X^5(11088X^3 - 11088X^2 + 3976X - 439)$$

$$(8.88) \quad \begin{array}{c} \text{Diagram of a pentagon with vertices labeled 1, 2, 3, 4, 5 clockwise from top-left.} \\ \text{A diagonal connects vertex 1 to vertex 4.} \end{array} \quad -\frac{1}{102060}X^5(14X - 9)$$

$$(8.89) \quad \begin{array}{c} \text{Diagram of a pentagon with vertices labeled 1, 2, 3, 4, 5 clockwise from top-left.} \\ \text{A diagonal connects vertex 1 to vertex 5.} \end{array} \quad -\frac{1}{102060}X^5(7X - 2)$$

$$(8.90) \quad \begin{array}{c} \text{Diagram of a pentagon with vertices labeled 1, 2, 3, 4, 5 clockwise from top-left.} \\ \text{A diagonal connects vertex 2 to vertex 5.} \end{array} \quad -\frac{1}{81648}X^5$$

$$(8.91) \quad \begin{array}{c} \text{Diagram of a pentagon with vertices labeled 1, 2, 3, 4, 5 clockwise from top-left.} \\ \text{Two diagonals connect vertex 1 to vertices 3 and 4.} \end{array} \quad -\frac{1}{102060}X^5(126X^2 - 91X + 13)$$

$$(8.92) \quad \begin{array}{c} \text{Diagram of a pentagon with vertices labeled 1, 2, 3, 4, 5 clockwise from top-left.} \\ \text{Two diagonals connect vertex 1 to vertices 3 and 5.} \end{array} \quad -\frac{1}{34020}X^5(42X^2 - 42X + 11)$$

$$(8.93) \quad \begin{array}{c} \text{Diagram of a pentagon with vertices labeled 1, 2, 3, 4, 5 clockwise from top-left.} \\ \text{Three diagonals connect vertex 1 to vertices 3, 4, and 5.} \end{array} \quad -\frac{1}{81648}X^5$$

$$(8.94) \quad \begin{array}{c} \text{Diagram of a pentagon with vertices labeled 1, 2, 3, 4, 5 clockwise from top-left.} \\ \text{Three diagonals connect vertex 2 to vertices 3, 4, and 5.} \end{array} \quad -\frac{1}{204120}X^5(14X - 3)$$

$$(8.95) \quad \begin{array}{c} \text{Diagram of a pentagon with vertices labeled 1, 2, 3, 4, 5 clockwise from top-left.} \\ \text{Four diagonals connect vertex 2 to vertices 3, 4, 5, and 1.} \end{array} \quad -\frac{1}{408240}X^5$$

$$(8.96) \quad \begin{array}{c} \text{Diagram of a square with vertices labeled 1, 2, 3, 4 clockwise from top-left.} \\ \text{All four diagonals of the square are drawn.} \end{array} \quad -\frac{1}{68040}X^5(7X - 4)$$

$$(8.97) \quad \begin{array}{c} \text{Diagram of a pentagon with vertices labeled 1, 2, 3, 4, 5 clockwise from top-left.} \\ \text{Three diagonals connect vertex 3 to vertices 1, 2, and 4.} \end{array} \quad -\frac{1}{408240}X^5(56X - 15)$$

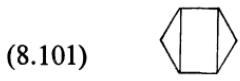
$$(8.98) \quad \begin{array}{c} \text{Diagram of a pentagon with vertices labeled 1, 2, 3, 4, 5 clockwise from top-left.} \\ \text{Three diagonals connect vertex 4 to vertices 1, 2, and 3.} \end{array} \quad -\frac{1}{204120}X^5(7X - 2)$$



$$(8.99) \quad \frac{1}{3645} X^6 (9X^2 - 6X + 1)$$



$$(8.100) \quad \frac{1}{87480} X^6$$



$$(8.101) \quad \frac{1}{43740} X^6$$

Appendix II

The susceptibility coefficients $a_n(\alpha)$ for $H(s)$ with first and second neighbour interactions for the three cubic lattices: see Section III.C. α denotes J_2/J_1 . These expressions are taken from Pirnie *et al.* (1966).

They are followed by the generalised susceptibility coefficients $a_1(\mathbf{k}) \dots a_4(\mathbf{k})$ as derived by Collins (1970), with a small correction in $a_4(\mathbf{k})$ made by Rushbrooke and Pirnie; see Section IV.A.

Face-centred cubic (f.c.c.) lattice

$$a_0 = 1$$

$$a_1 = 4X(2 + \alpha)$$

$$a_2 = \frac{2X}{3} \cdot \begin{array}{c|cc} 1 & X \\ \hline \alpha & -6 & +88 \\ \alpha^2 & & +96 \\ & -3 & +20 \end{array} \quad a_3 = \frac{8X}{45} \cdot \begin{array}{c|ccc} 1 & X & X^2 \\ \hline \alpha & +12 & -382 & +2328 \\ \alpha^2 & & -240 & +3960 \\ \alpha^3 & & -180 & +1920 \\ & +6 & -81 & +244 \end{array}$$

$$a_4 = \frac{2X}{135} \cdot \begin{array}{c|cccc} 1 & X & X^2 & X^3 \\ \hline \alpha & -90 & +4704 & -52\,864 & +192\,736 \\ \alpha^2 & & +1584 & -68\,064 & +446\,976 \\ \alpha^3 & & +2376 & -42\,096 & +349\,824 \\ \alpha^4 & & +1152 & -24\,192 & +104\,448 \\ \alpha^5 & -45 & +1020 & -4880 & +9200 \end{array}$$

$$a_5 = \frac{8X}{14\,175} \cdot \begin{array}{c|ccccc} 1 & X & X^2 & X^3 & X^4 \\ \hline \alpha & +1728 & -120\,240 & +2\,105\,760 & -13\,511\,984 & +34\,402\,464 \\ \alpha^2 & & -29\,736 & +1\,976\,184 & -26\,256\,832 & +101\,245\,312 \\ \alpha^3 & & -39\,312 & +1\,620\,108 & -21\,078\,624 & +110\,157\,824 \\ \alpha^4 & & -42\,840 & +1\,116\,360 & -11\,994\,080 & +53\,820\,480 \\ \alpha^5 & & -18\,900 & +606\,060 & -4\,438\,560 & +11\,303\,040 \\ & 864 & -25\,974 & +188\,016 & -552\,200 & +752\,240 \end{array}$$

| | 1 | X | X^2 | X^3 | X^4 | X^5 |
|-----------------------------------|---------|------------|--------------|----------------|-----------------|-----------------|
| $a_6 = \frac{2X}{127575} \cdot 1$ | -52 164 | +4 407 480 | -104 294 484 | +975 204 216 | -4 304 586 048 | +8 336 670 720 |
| α | | +882 576 | -73 516 896 | +1 554 114 816 | -11 169 411 072 | +29 767 523 328 |
| α^2 | | +1 174 824 | -75 302 136 | +1 314 699 120 | -11 864 832 000 | +41 595 499 008 |
| α^3 | | +1 016 064 | -50 518 944 | +982 267 776 | -7 663 246 080 | +28 576 450 560 |
| α^4 | | +1 244 808 | -43 389 432 | +525 145 248 | -3 492 822 528 | +9 911 394 048 |
| α^5 | | +497 664 | -19 859 904 | +213 895 296 | -897 707 520 | +1 579 991 040 |
| α^6 | -26 082 | +941 436 | -9 367 506 | +36 934 092 | -78 518 688 | +83 019 648 |

Body-centred cubic (b.c.c.) lattice

$$a_0 = 1$$

$$a_1 = \frac{4}{3}X(4 + 3\alpha)$$

| | 1 | X | 1 | X | X^2 |
|------------------------------|-----|------|--------------------------------|------|------------|
| $a_2 = \frac{2X}{9} \cdot 1$ | -12 | +112 | $a_3 = \frac{8X}{135} \cdot 1$ | +24 | -444 +1936 |
| α | | +192 | α | -540 | +4920 |
| α^2 | -9 | +60 | α^2 | -360 | +3840 |
| | | | α^3 | +18 | -243 +732 |

| | 1 | X | X^2 | X^3 |
|--------------------------------|------|-------|---------|----------|
| $a_4 = \frac{2X}{405} \cdot 1$ | -180 | +5568 | -38 528 | +103 232 |
| α | | +3600 | -84 960 | +357 120 |
| α^2 | | +4968 | -75 888 | +427 392 |
| α^3 | | +2304 | -48 384 | +208 896 |
| α^4 | -135 | +3060 | -14 640 | +27 600 |

| | 1 | X | X^2 | X^3 | X^4 |
|-----------------------------------|---------|------------|-------------|-------------|-------------|
| $a_5 = \frac{16X}{42525} \cdot 1$ | +1728 | -70 848 | +726 312 | -3 124 880 | +5 980 000 |
| α | | -35 154 | +1 317 456 | -9 844 128 | +25 790 688 |
| α^2 | -40 068 | +1 160 712 | -12 591 936 | +42 630 336 | |
| α^3 | -45 360 | +1 138 410 | -9 245 040 | +32 508 000 | |
| α^4 | -18 900 | +606 060 | -4 438 560 | +11 303 040 | |
| α^5 | +1296 | -38 961 | +282 024 | -828 300 | +1 128 360 |

| | 1 | X | X^2 | X^3 | X^4 | X^5 |
|-----------------------------------|---------|------------|-------------|--------------|----------------|----------------|
| $a_6 = \frac{2X}{127575} \cdot 1$ | -34 776 | +1 712 592 | -23 917 320 | +138 297 936 | -423 384 192 | +623 838 208 |
| α | | +716 688 | -32 598 720 | +383 870 592 | -1 731 319 296 | +3 254 587 392 |
| α^2 | | +816 480 | -35 616 672 | +489 291 264 | -2 914 437 120 | +6 774 421 248 |
| α^3 | | +692 496 | -27 445 824 | +434 206 080 | -2 775 010 560 | +7 195 840 512 |
| α^4 | | +886 464 | -30 544 992 | +315 390 528 | -1 645 174 656 | +3 959 963 136 |
| α^5 | | +331 776 | -13 239 936 | +142 596 864 | -598 471 680 | +1 053 327 360 |
| α^6 | -26 082 | +941 436 | -9 367 506 | +36 934 092 | -78 518 688 | +83 019 648 |

ic (s.c.) lattice

$$a_0 = 1$$

$$a_1 = 4X(1 + 2\alpha)$$

$$a_2 = \frac{2X}{3} \cdot \begin{array}{c|cc} 1 & X \\ \hline -3 & +20 \\ \alpha & +96 \\ \alpha^2 & -6 & +88 \end{array}$$

$$a_3 = \frac{8X}{45} \cdot$$

$$\begin{array}{c|ccc} 1 & X & X^2 \\ \hline +6 & -81 & +244 \\ \alpha & -240 & +1800 \\ \alpha^2 & -180 & +4080 \\ \alpha^3 & +12 & -382 & +2328 \end{array}$$

$$a_4 = \frac{2X}{405} \cdot \begin{array}{c|cccc} 1 & X & X^2 & X^3 \\ \hline -135 & +3060 & -14\,640 & +27\,600 \\ \alpha & +4752 & -86\,112 & +281\,088 \\ \alpha^2 & +7128 & -155\,088 & +991\,872 \\ \alpha^3 & +3456 & -161\,856 & +1\,430\,784 \\ \alpha^4 & -270 & +14\,112 & -158\,592 & +578\,208 \end{array}$$

$$= \frac{16X}{42\,525} \cdot \begin{array}{c|ccccc} 1 & X & X^2 & X^3 & X^4 \\ \hline +1296 & -38\,961 & +282\,024 & -828\,300 & +1\,128\,360 \\ \alpha & -44\,604 & +1\,263\,276 & -7\,230\,048 & +14\,477\,568 \\ \alpha^2 & -58\,968 & +1\,791\,342 & -22\,455\,216 & +71\,129\,856 \\ \alpha^3 & -64\,260 & +2\,906\,820 & -32\,793\,600 & +161\,461\,440 \\ \alpha^4 & -28\,350 & +2\,014\,740 & -33\,193\,440 & +167\,700\,960 \\ \alpha^5 & +2592 & -180\,360 & +3\,158\,640 & -20\,267\,976 & +51\,603\,696 \end{array}$$

$$\begin{array}{c|cccccc} 1 & X & X^2 & X^3 & X^4 & X^5 \\ \hline -26\,082 & +941\,436 & -9\,367\,506 & +36\,934\,092 & -78\,518\,688 & +83\,019\,648 \\ \alpha & +882\,576 & -30\,382\,560 & +270\,922\,752 & -909\,519\,360 & +1\,296\,807\,936 \\ \alpha^2 & +1\,174\,824 & -48\,010\,536 & +721\,420\,560 & -4\,024\,204\,800 & +8\,085\,654\,528 \\ \alpha^3 & +1\,016\,064 & -55\,433\,952 & +1\,057\,246\,848 & -8\,923\,224\,576 & +25\,693\,495\,296 \\ \alpha^4 & +1\,244\,808 & -84\,160\,512 & +1\,447\,525\,728 & -11\,276\,275\,968 & +42\,385\,014\,528 \\ \alpha^5 & +497\,664 & -44\,426\,880 & +1\,093\,443\,840 & -9\,966\,546\,432 & +33\,954\,757\,632 \\ \alpha^6 & -52\,164 & +4\,407\,480 & -104\,294\,484 & +975\,204\,216 & -4\,304\,586\,048 & +8\,336\,670\,720 \end{array}$$

Generalised susceptibility coefficients

$$a_1(\mathbf{k}) = \frac{2}{3}X \Sigma_1$$

$$a_2(\mathbf{k}) = \frac{1}{9}X[4X \Sigma_2 - \Sigma_1 - 2q]$$

$$a_3(\mathbf{k}) = \frac{1}{27}X[\frac{3}{5}(12X^2 - 8X + 3)\Sigma_1 + 3q + 8X^2\Sigma_3 - 4X\Sigma_2 + 8X(3X - 1)(q - 1)\Sigma_1 - 12X^2(2q - 1)\Sigma_1 - 4Xp_1q]$$

$$a_4(\mathbf{k}) = \frac{2}{81}X[-\frac{9}{5}(3X^2 - 3X + 1)\Sigma_1 - \frac{9}{10}(4X^2 - 4X + 3)q - 3X(2X - 1)(q - 1)(3\Sigma_1 + 2q) + \frac{3}{5}X(56X^2 - 24X + 3)p_1\Sigma_1 + \frac{18}{5}Xp_1q - 4X^2p_2q + 8X^2(3X - 1)(q - 3)p_1\Sigma_1 + 8X^2(3X - 1)(q - 1)\Sigma_2 + \frac{6}{5}X(12X^2 - 8X + 3)\Sigma_2 + 4X^2(3X - 1)(q - 2)\Sigma_2 - 6X^2\Sigma_3 + 8X^3\Sigma_4 + 3X^2(2q - 1)(3\Sigma_1 + 2q) - 24X^3(q - 1)p_1\Sigma_1 - 12X^3(3q - 2)\Sigma_2 - \frac{3}{5}Xq(q - 1) + \frac{3}{5}X\Sigma_2].$$

Here q is the lattice coordination number. For the f.c.c., b.c.c., and s.c. lattices, $p_1 = 4, 0$, and 0 , respectively, and $p_2 = 22, 12$, and 4 , respectively. Σ_r is the sum of the cosines of the scalar product of \mathbf{k} and the end points of all self-avoiding walks of r steps on the lattice, starting from the origin. In terms of p_3 and p_4 , the lattice constants for triangles and quadrilaterals, respectively, $p_1 = 6p_3/q$ and $p_2 = 8p_4/q$.

Appendix III

a_n coefficients for $H(\infty)$, defined through eqns (1.6) and (2.19)

| n | a_n [f.c.c.] | a_n [b.c.c.] | a_n [s.c.] |
|-----|----------------|----------------|--------------|
| 1 | 8 | 5.3333 | 4 |
| 2 | 58.6667 | 24.8889 | 13.3333 |
| 3 | 413.8667 | 114.7259 | 43.3778 |
| 4 | 2855.3481 | 509.7877 | 136.2963 |
| 5 | 19415.8527 | 2249.9706 | 424.5446 |
| 6 | 130694.4263 | 9779.9445 | 1301.5034 |
| 7 | 873209.9636 | 42335.1558 | 3967.8674 |
| 8 | 5800796.3979 | 181758.3614 | 11998.0391 |
| 9 | 38359707.246 | 778141.1625 | 36150.6748 |
| 10 | 252725807.32 | 3314373.4145 | 108371.9900 |

| <i>n</i> | a_n [p.t.] | a_n [s.q.] |
|----------|--------------|--------------|
| 1 | 4 | 2.66667 |
| 2 | 13.3333333 | 5.33333 |
| 3 | 39.8222222 | 9.95556 |
| 4 | 110.696296 | 16.9086 |
| 5 | 292.309559 | 27.2404 |
| 6 | 741.855191 | 42.2122 |
| 7 | 1822.0514 | 63.0670 |
| 8 | 4351.6776 | 91.6638 |
| 9 | 10144.7594 | 129.4967 |
| 10 | 23151.5426 | |

| <i>n</i> | a_n [f.c.c.(12)] | a_n [b.c.c.(12)] | a_n [s.c.(12)] |
|----------|--------------------|--------------------|------------------|
| 1 | 12 | 9.333333333 | 12 |
| 2 | 136 | 80.88888889 | 136 |
| 3 | 1502.577778 | 677.2148148 | 1502.577778 |
| 4 | 16343.46667 | 5551.802469 | 16343.46667 |
| 5 | 175904.8240 | 44901.74683 | 175897.2388 |
| 6 | 1878903.364 | 359709.9354 | 1878666.201 |
| 7 | 19953997.26 | 2861309.552 | 19948988.53 |

c_n coefficients for $H(\infty)$, defined through eqns (1.6) and (2.18)

| <i>n</i> | c_n [f.c.c.] | c_n [b.c.c.] | c_n [s.c.] |
|----------|----------------|----------------|--------------|
| 1 | 5.33333 | 0 | 0 |
| 2 | 28.53333 | 15.2 | 4.53333 |
| 3 | 151.70370 | 0 | 0 |
| 4 | 807.30300 | 177.10052 | 29.74251 |
| 5 | 4372.35358 | 0 | 0 |
| 6 | 24146.78317 | 2211.96010 | 170.47494 |
| 7 | 135432.72998 | 0 | 0 |
| 8 | 768679.3903 | 29380.88102 | 1100.28851 |
| 9 | 4404582.6807 | | |

Appendix IV

The coefficients $f(n, j)$ of eqn (3.33), for $n \leq 8$. For given n , the coefficients are listed sequentially, $0 \leq j \leq n$. Available values of $f(9, 0)$, $f(9, 1)$, $f(10, 0)$ and $f(10, 1)$ are added for completeness.

| <i>n</i> | f.c.c. lattice |
|----------|---|
| 1 | 0, 6 |
| 2 | 18, 120, -138 |
| 3 | 108, 3312, -11172, 7752 |
| 4 | 180, 117360, -838656, 1441872, -720756 |
| 5 | -5040, 5104416, -66190560, 208511040 -242164080, 94744224 |
| 6 | 162000, 263405088, -5631588672, 28529880864, -57308461200, 50330952000, -16184350080 |
| 7 | 14565600, 15717292800, -518612953152, 3916735549440, -12014728917408, 17682684163200, -12492230849280, 3410421148800 |
| 8 | 563253408, 1063892512512, -51595772643456, 552101473737984, -2409974307485952, 5261160226823424, -6105026127070080, 3608165330784000, -855895279911840 |
| 9 | 17544639744, 80532234584064 |
| 10 | 750651187968 |

| <i>n</i> | b.c.c. lattice |
|----------|--|
| 1 | 0, 4 |
| 2 | 12, 48, -60 |
| 3 | -24, 832, -3000, 2192 |
| 4 | 168, 18400, -140224, 254112, -132456 |
| 5 | 1440, 504384, -6905280, 22945920, -27859680, 11313216 |
| 6 | 24480, 16313280, -367155456, 1961681856, -4127298720, 3771964800, -1255530240 |
| 7 | -297024, 610699520, -21150914176, 168356308736, -541590616896, 831155673600, -609253747200, 171872893440 |

| <i>n</i> | b.c.c. lattice |
|----------|---|
| 8 | 28 017 216, 25 867 292 160, -1 316 934 235 392, 14 841 714 362 880, -67 990 992 892 416, 155 016 652 718 592, -187 008 013 382 400, 114 451 513 505 280, -28 019 835 385 920 |
| 9 | -533 681 664, 1 229 543 182 336 |
| 10 | 41 156 316 672, 64 541 249 655 808 |

| <i>n</i> | s.c. lattice |
|----------|--|
| 1 | 0, 3 |
| 2 | 9, 24, -33 |
| 3 | -18, 264, -1 122, 876 |
| 4 | -162, 3 960, -34 992, 69 480, -38 286 |
| 5 | 2 520, 74 928, -1 153 680, 4 244 160, -5 527 080, 2 359 152 |
| 6 | 33 192, 1 584 624, -41 192 208, 244 696 272, -557 497 800, 540 973 440, -188 597 520 |
| 7 | -1 019 088, 38 523 264, -1 590 250 368, 14 145 677 952, -49 610 005 200, 81 472 184 640, -63 034 403 040, 18 579 291 840 |
| 8 | -7 804 944, 1 115 604 864, -66 219 927 360, 838 945 907 328, -4 213 375 823 616, 10 344 814 558 848, -13 257 834 206 400, 8 530 825 806 720, -2 178 264 115 440 |
| 9 | 723 961 728, 35 969 253 888 |
| 10 | 2 596 523 904, 1 223 162 767 104 |

| <i>n</i> | p.t. lattice |
|----------|---------------------------------------|
| 1 | 0, 3 |
| 2 | 9, 24, -33 |
| 3 | 18, 204, -1 086, 864 |
| 4 | -306, 1 800, -29 952, 65 304, -36 846 |

| <i>n</i> | p.t. lattice |
|----------|---|
| 5 | -3 240, 21 168, -805 680, 3 608 640, -5 018 760, 2 197 872 |
| 6 | 49 176, 390 864, -22 285 440, 179 644 560, -460 937 880, 472 220 640, -169 081 920 |
| 7 | 1 466 640, 6 823 008, -648 694 368, 8 632 346 688, -36 157 021 488, 64 886 401 440, -52 677 233 280, 15 955 911 360 |
| 8 | -13 626 000, 45 446 784, -19 872 971 712, 412 819 334 784, -2 630 801 650 560, 7 334 198 815 104, -10 113 012 463 680, 6 802 189 833 600, -1 785 552 718 320 |
| 9 | -1 172 668 032, -899 102 208 |
| 10 | 75 256 704 |

| <i>n</i> | s.q. lattice |
|----------|---|
| 1 | 0, 2 |
| 2 | 6, 8, -14 |
| 3 | -12, 32, -252, 232 |
| 4 | -84, 208, -3 712, 9 840, -6 252 |
| 5 | 1 200, 2 272, -55 200, 299 840, -483 600, 235 488 |
| 6 | 3 120, 11 744, -893 312, 8 255 328, -24 871 920, 28 929 600, -11 434 560 |
| 7 | -249 312, -103 808, -15 118 656, 222 650 624, -1 088 666 208, 2 246 549 760, -2 045 957 760, 680 895 360 |
| 8 | 920 928, 2 102 528, -252 642 688, 6 036 996 864, -44 349 816 064, 142 753 373 952, -223 345 557 120, 167 225 667 840, -48 071 046 240 |
| 9 | 86 274 816, 99 147 776 |
| 10 | -1 232 035 584, -1 287 219 712 |

a_n coefficients for $H(\frac{1}{2})$, defined through eqns (1.1) and (2.19)

| n | a_n [f.c.c.] | a_n [b.c.c.] | a_n [s.c.] |
|-----|----------------|----------------|--------------|
| 1 | 6 | 4 | 3 |
| 2 | 30 | 12 | 6 |
| 3 | 138 | 34.666666667 | 11 |
| 4 | 611.25 | 95.833333333 | 20.625 |
| 5 | 2658.55 | 262.7 | 39.025 |
| 6 | 11432.5125 | 708.04166667 | 68.777083333 |
| 7 | 48726.726190 | 1893.2896825 | 119.42976190 |
| 8 | 206142.36741 | 5012.1086310 | 216.16227679 |
| 9 | 866895.50635 | 13235.513272 | 387.19383267 |
| 10 | | 34737.965232 | 658.34153977 |

| n | a_n [p.t.] | a_n [s.q.] |
|-----|---------------|----------------|
| 1 | 3 | 2 |
| 2 | 6 | 2 |
| 3 | 8.5 | 1.333333333 |
| 4 | 9.375 | 1.083333333 |
| 5 | 11.025 | 1.183333333 |
| 6 | 16.964583333 | 0.50972222222 |
| 7 | 21.152678571 | -0.32182539683 |
| 8 | 8.8058779762 | 0.40739087302 |
| 9 | -9.6784556878 | 1.0672839506 |
| 10 | | -0.69281883818 |

| n | a_n [f.c.c.(12)] | a_n [b.c.c.(12)] | a_n [s.c.(12)] |
|-----|--------------------|--------------------|------------------|
| 1 | 9 | 7 | 9 |
| 2 | 72 | 42 | 72 |
| 3 | 548 | 234.6666667 | 548 |
| 4 | 4059.375 | 1262.958333 | 4059.375 |
| 5 | 29570.075 | 6663.225 | 29565.575 |
| 6 | 212951.7396 | 34736.11042 | 212869.1229 |
| 7 | 1520865.135 | 179510.349 | 1519860.768 |

c_n coefficients for $H(\frac{1}{2})$, defined through eqns (1.1) and (2.18).

| n | c_n [f.c.c.] | c_n [b.c.c.] | c_n [s.c.] |
|-----|----------------|----------------|--------------|
| 1 | 3 | -1 | -1 |
| 2 | 1.25 | 1.75 | -2.25 |
| 3 | -5.83333333 | 2.5 | 5.83333333 |
| 4 | 23.4375 | 5.3125 | 9.60416667 |
| 5 | 210.729165 | -6.44583333 | -29.4875 |
| 6 | 679.076736 | 50.6677083 | -18.8197917 |
| 7 | 1510.88512 | -68.9382937 | 124.690278 |
| 8 | 4040.22156 | 332.272780 | 27.9504836 |

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Note Added in Proof

This chapter was effectively closed July 1971. Since then several papers have appeared to which detailed reference would be made were it being written today. Here we must be more cursory than some of these papers deserve. Appropriate references to sections of this chapter are given in square brackets.

Lee and Stanley (1971): this is the definitive version of work to which we have referred [V.F]. It should be noted that x_c and γ are determined from the transformed susceptibility series by unsophisticated ratio tests. A Padé analysis of the transformed series would have continued to yield $\gamma = 1.43$. That for certain series ratio tests can be more satisfactory than Padé analyses has been demonstrated by Hunter and Baker (1973). In the Lee and Stanley work, everything turns on the values chosen for x_c . New methods for analysing series with competing singularities have recently been devised by Baker and Hunter (1973), but so far have been applied only to Ising model series.

Menyuk *et al.* (1971), examining sixth order susceptibility series for $H(\frac{1}{2})$ with first and second neighbour interactions found that γ apparently decreases with increasing α [IV.A, V.D]. Paul and Stanley (1972) have examined the corresponding series for $I(\frac{1}{2})$, $P(\infty)$ and $H(\infty)$. For $H(\infty)$ the series are now of eighth order (available on request). The decrease persists for $\alpha \lesssim 10$; but they dismiss it as a short-series effect, because it is paralleled by series work on the spherical model (for which we know $\gamma = 2$, all α).

Ritchie and Fisher (1972): this paper, on critical point scattering and correlations for Heisenberg models, closes a gap to which we have referred [IV.F]. Coefficients of the first six powers of x in the expansion of the second spherical moment, μ_2 , are tabulated (from general expressions derived by Burford) for $s = 1/2, 1, 3/2, 5/2$ and ∞ . Where longer series are known, they are used. The authors favour universality of critical exponents (with increased uncertainty for low spin), but adopt slightly lower values for γ and ν than did Ferer *et al.* (1971) [V.D]. Their value for η is 0.043 ± 0.014 . The paper follows the lines of Fisher and Burford (1967), particularly as regards the temperature dependence of scattering intensity for fixed momentum transfer. For other work on correlation functions for $H(\infty)$, see Ferer (1971).

Milošević and Stanley (1972a, b), in two interesting papers, have used high-temperature series expansions of $H(T, M)$ [IV.B, C; V.C] to calculate the scaling function $h(\xi)$, defined by

$$H(\varepsilon, M) = M^\delta h(\varepsilon/M^{1/\beta}) \quad \text{where} \quad \varepsilon \equiv (T - T_c)/T_c.$$

For the cubic lattices, they consider in detail $I(\frac{1}{2})$, $H(\frac{1}{2})$ and $H(\infty)$, and concentrate emphasis on the reduced function $h(\xi)/h(0)$. For $I(\frac{1}{2})$ their functions agree closely with those derived by Gaunt and Domb (1970), using low-temperature expansions. The reduced functions for $H(\frac{1}{2})$ and $H(\infty)$ are almost identical (within the uncertainty of the method), but easily distinguished from that for $I(\frac{1}{2})$. Comparison is made with experimental measurements.

Wood and Dalton (1972), for the model $HI(s)$, have published $a_1 \dots a_6$ and (effectively) $c_1 \dots c_5$ in terms of general lattice parameters [IV.D].

Yamaji and Kondo (1973), for the model $H(s)$, have determined $a_1 \dots a_8$ and $c_1 \dots c_7$ for the three planar lattices, triangular, quadratic and honeycomb. They have analysed these series for several values of s (including $\frac{1}{2}$ and ∞), by both ratio and PA methods, and conclude that the weight of the evidence is against the existence of pseudo-Curie points [5.A] for these two-dimensional lattices.

Finally, to the few exact Heisenberg model results mentioned in Section I of this chapter, must now be added the recent work of Baxter (1972), who has determined the ground-state energy of the general anisotropic spin- $\frac{1}{2}$ Heisenberg infinite linear chain, by relating this problem to the eight-vertex model.

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6. Ising Model

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I. Introduction

A. Historical survey

In 1925 Uhlenbeck and Goudsmit put forward the hypothesis that the electron possesses a spin $s = \frac{1}{2}$, and that in a magnetic field its direction is quantized so that it orients either parallel or antiparallel to the field. In the same year

Lenz suggested to his student Ising (1925) that if an interaction was introduced between spins so that parallel spins in a crystalline lattice attracted one another, and antiparallel spins repelled one another, then at sufficiently low temperatures the spins would all be aligned, and the model might provide an atomic description of ferromagnetism. The Hamiltonian corresponding to this model can be written in the form

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - mH \sum_i \sigma_i. \quad (1.1)$$

Here $J (> 0)$ represents the interaction between spins, H is the magnetic field, m the magnetic moment of a single spin, and σ_i is a dummy variable which can take the values ± 1 . The suffix i runs over all sites of the lattice, and $\langle ij \rangle$ over all pairs of sites i and j which are nearest neighbours.

The criterion with which to test the model is whether it gives rise to the characteristic pattern of singularities associated with ferromagnetism, and more particularly whether a Curie temperature, T_c , can be defined with the property that there exists a non-zero spontaneous magnetization for $T < T_c$. Ising was able to solve the problem in one dimension only, and he found that the solution is analytic without any singularities† (see Thompson, Vol. 1, Chapter 5). Ten years elapsed before Peierls (1936) showed that the two-dimensional model does have a non-zero spontaneous magnetization, and can therefore be regarded as a valid model of a ferromagnet (see Griffiths, Vol. 1, Chapter 2).

In an important investigation in 1941 Kramers and Wannier discovered a transformation which enabled them to conjecture the exact value of the Curie temperature of an s.q. lattice. They also showed how to develop exact power series expansions for the partition function at high and low temperatures. The high temperature series followed the method which had been introduced by Opechowski (and Kramers) in 1937 for the Heisenberg model, the expansion variable being βJ ($\beta = 1/kT$). The low temperature series in powers of $\exp - 2\beta J$ corresponded to successive excitations above the lowest energy ground state, and had no direct counterpart for the Heisenberg model. (See Rushbrooke *et al.* this volume Ch. 5.).

Kramers and Wannier's paper was a precursor to Onsager's fundamental calculation in 1944 of the partition function of the s.q. lattice in zero field, which has served as a landmark in the theory of critical behaviour. During subsequent years a reservoir of exact information was steadily built up on the Ising model as calculations were extended to the spontaneous magnetization (e.g. Onsager, 1949; Yang, 1952), correlations (e.g. Kaufman and Onsager,

† This is the only paper Ising ever published and the result he obtained is relatively trivial; nevertheless, the "Ising model" now has a very extensive associated literature! For a historical review see Brush (1967).

1949; Wu, 1966), and susceptibility (e.g. Fisher, 1959a; Kadanoff, 1966a; Wu, 1966); solutions also became available for a variety of additional two-dimensional lattices (e.g. Temperley, 1950; Utiyama, 1951; Syozi, 1955). (For a general review of exact information available in two dimensions see Domb, 1960; Green and Hurst, 1964; and Syozi, Vol. 1, Chapter 7.).

In the few years following the publication of Onsager's solution there was considerable optimism that methods would be found of extending the treatment to three dimensions and removing the restriction of zero magnetic field. Despite many efforts and a number of premature claims the 30 years which have elapsed have seen virtually no progress towards such a solution. However, a number of rigorous general theorems have been established (see Griffiths, Vol. 1, Chapter 2), the most notable being that of Yang and Lee (1952) on the zeros of the grand partition function.

In the absence of exact solutions the two alternative approaches available were closed form approximations and series expansions. The former had been developed in the 1930s by Bragg and Williams (1934), Bethe (1935), Guggenheim (1935) and others; however, a comparison by Kramers and Wannier (1941) of these closed form results with exact series expansions showed that even the best approximations available gave only a few terms correctly. These authors suggested therefore that such approximations were probably unreliable in the critical region, and this suggestion was beautifully substantiated by Onsager (1944). (For a general account of closed form approximations see Burley, Vol. 2, Chapter 9).

Series expansions had been introduced by Kramers and Wannier (1941) with the aim of testing the validity of closed form approximations. However, the present author suggested (Domb, 1949) that if expansions of sufficient length could be derived they might provide a direct assessment of critical behaviour.

Such expansions were derived in two dimensions for the s.q. lattice by Domb (1949) and in three dimensions for the s.c. lattice by Wakefield (1951). The calculations were extended to a variety of two- and three-dimensional lattices (Domb and Potts, 1951; Domb, 1952; Domb and Sykes, 1956, 1957a) and methods of extracting information regarding critical behaviour were steadily improved.

Series for the initial susceptibility at high temperatures provided the smoothest and most regular pattern of behaviour of coefficients; they were all found to be positive in sign, and the ratio method (see Gaunt and Guttman, this volume Chapter 4) was used to estimate the Curie temperatures and critical exponents. For the s.q. and p.t. lattices in two dimensions the Curie temperatures were known exactly, and hence a more accurate estimate could be made of the critical exponents. Domb and Sykes (1957a) suggested the value $\gamma = 1.75$ for the susceptibility exponent of these lattices and this

was later justified rigorously (see references quoted above). For three dimensional lattices the corresponding estimate was 1.25 (Domb and Sykes, 1961a). However, the low temperature series in three dimensions alternated in sign and it was clear that spurious non-physical singularities were masking the true critical behaviour. Although it was possible to improve the convergence by suitable grouping of terms (metastable approximations, Domb and Sykes, 1956) only rough estimates could be provided of critical exponents at low temperatures.

A dramatic step forward was taken by Baker in 1961 who applied the Padé approximant (see Gaunt and Guttmann, this volume, Chapter 4) to these Ising series. For series with positive terms his results were in excellent accord with those of the ratio method. But for the low temperature series he could by-pass the spurious singularities and was able to provide estimates for the critical exponent β of the spontaneous magnetization. In all subsequent work on estimating critical behaviour from series expansions the Padé approximant has been a tool of major importance.

Another significant development at this time was the application of computers to the problems of lattice constant enumerations (see Domb, this volume, Chapter 1). The first steps were taken by Eve at the University of Newcastle for simple polygons (Rushbrooke and Eve, 1959) and by Martin at the National Physical Laboratory for self-avoiding walks (Martin, 1962). Subsequently more comprehensive programmes were developed for other lattice constants, particularly by Martin at King's College, and these are described in Chapter 2 of this volume.

Two other developments which helped significantly in extending series expansions are worthy of record. The introduction of the "code" method for low temperature series by Sykes *et al.* (1965); and the use of the finite cluster method at high temperatures, particularly in the form which eliminates the need to subtract subgraphs (see Domb, Chapter 1, Section IV.B4).

Because of the existence of exact solutions and the possibility of deriving extensive series expansions both at low and high temperatures, the Ising model of spin $\frac{1}{2}$ has served as a pioneer in the exploration of critical behaviour, and many important results in the theory of critical phenomena started with an application to the Ising model. These include accurate estimates of critical exponents (e.g. Domb and Sykes, 1961a; Essam and Fisher, 1963; Essam and Sykes, 1963; Sykes *et al.*, 1967), accurate estimates of critical values of thermodynamic functions (Domb, 1960), the observation that dimension rather than lattice structure determines critical behaviour (Domb, 1960), critical behaviour of antiferromagnets (Sykes and Fisher, 1958), critical amplitudes (e.g. Fisher, 1963), critical equation of state (Domb and Hunter 1965; Domb, 1968b), critical correlations (Fisher and Burford, 1967),

surface and finite size effects (Watson, Vol. 2, Chapter 4), lattice-lattice scaling (Betts *et al.*, 1971), correction terms in the equation of state (Domb, 1971c), the crossover exponent (e.g. Liu and Stanley, 1972). A number of puzzling features which have not yet been adequately resolved were also revealed by numerical studies of series expansions for the Ising model of spin $\frac{1}{2}$; for example, in three dimensions the apparent failure of the exact scaling relation for the correlation exponent (e.g. Domb, 1968a), the failure of strong scaling (Moore *et al.*, 1969) and the possibility that the critical exponent δ is exactly 5 (Gaunt and Sykes, 1972).

When the spin value s differs from $\frac{1}{2}$ many of the simplifying features disappear, and the numerical data available were far more limited. Nevertheless, even here the Ising model has played a pioneering role; in 1962 Domb and Sykes noted that the susceptibility exponent γ remained $5/4$ for all s , and this was an important step in the chain leading to the "Universality Hypothesis" (Domb, 1971d; Kadanoff, 1971) and "Smoothness Postulate" (Griffiths, 1970, 1971).

B. Physical applications

1. Ferromagnetism

The partition function corresponding to the Hamiltonian (1.1) is given by

$$\begin{aligned} Z_N^I &= \sum \exp - \beta \mathcal{H} \\ &= \sum_{\langle ij \rangle} \prod \exp(K\sigma_i\sigma_j) \prod \exp(\beta m H \sigma_i) \quad (K = \beta J, J > 0) \end{aligned} \quad (1.2)$$

the sum being taken over all nearest-neighbour pairs i and j and over all $\sigma_i = \pm 1$, i ranging over N sites of the lattice or net. The extension to distant neighbour interactions is immediate if we replace the single interaction parameter K by a family of interaction parameters K_{ij} and sum over all neighbour pairs $\langle ij \rangle$. For the most part we shall be concerned in this article with the nearest neighbour interaction model of spin $\frac{1}{2}$ which we shall denote by $I(\frac{1}{2})$ and term the *simple Ising model*; when we make no specific qualification we shall have this model in mind.

For general spin s we replace the Hamiltonian (1.1) by

$$\mathcal{H} = - \frac{J}{s^2} \sum_{\langle ij \rangle} s_{zi} s_{zj} - \frac{mH}{s} \sum_i s_{zi}. \quad (1.3)$$

This is normalized so that the maximum interaction between two parallel spin, $\uparrow\uparrow$, remains constant, and the maximum interaction with the external magnetic field remains constant. The s_{zi} are standard spin operators taking $(2s + 1)$ values $-s, -(s - 1), \dots, (s - 1), s$; when $s = \frac{1}{2}$, $s_i = \frac{1}{2}\sigma_i$.

For general s we write for the partition function

$$Z_{N,s}^I = \sum_{\langle ij \rangle} \prod \exp(K s_i s_j / s^2) \prod \exp(\beta m H s_i / s). \quad (1.4)$$

Thermodynamic properties can be derived from the partition function in the standard manner by forming the free energy

$$F_N^I = -kT \ln Z_N^I. \quad (1.5)$$

However we must remember that this free energy is a function of H and T and corresponds to

$$F = U - TS + MH. \quad (1.6)$$

The internal energy and specific heat are given by

$$U = -\frac{\partial}{\partial \beta} [\ln Z(\beta, H)], \quad (1.7)$$

$$C_H = k\beta^2 \frac{\partial^2}{\partial \beta^2} [\ln Z(\beta, H)]. \quad (1.8)$$

The magnetization and susceptibility are given by

$$M = \frac{1}{\beta} \frac{\partial}{\partial H} (\ln Z), \quad (1.9)$$

$$\chi = \frac{1}{\beta} \frac{\partial^2}{\partial H^2} (\ln Z). \quad (1.10)$$

For the simple Ising model we can use (1.2) to write these thermodynamic quantities as averages of the σ_i operators as follows:

$$M = m \sum_i \langle \sigma_i \rangle, \quad (1.11)$$

$$\chi = \beta m^2 \left[N + 2 \sum_{\langle ij \rangle} \langle \sigma_i \sigma_j \rangle \right], \quad (1.12)$$

$$U = -J \sum_{\langle ij \rangle} \langle \sigma_i \sigma_j \rangle - mH \sum_i \langle \sigma_i \rangle. \quad (1.13)$$

The general expression for C_H is more complicated but in zero field it reduces to

$$C_H = kK^2 \sum_{\langle ij \rangle \langle kl \rangle} \langle \sigma_i \sigma_j \sigma_k \sigma_l \rangle - k\beta^2 U^2 \quad (1.14)$$

Here the average of an operator P is defined by

$$\langle P \rangle = \sum P \exp(-\beta \mathcal{H})/Z. \quad (1.15)$$

Corresponding expressions in terms of the s_{zi} operators can readily be derived for general s .

The above formulae apply to an arbitrary net of spins. The case of most general interest is that of a lattice of N sites (N large) satisfying periodic boundary conditions. For this case it is sometimes convenient (particularly at low temperature) to take out the zero energy terms and write

$$Z_N^I = y^{-N/2} u^{-qN/8} \Lambda_N^I, \quad (1.16)$$

where

$$y = \exp(-2\beta mH), u = \exp(-4K), \quad (1.17)$$

and q is the coordination number of the lattice.

2. Antiferromagnetism and Ferrimagnetism

The Ising antiferromagnet corresponds to $J < 0$. All the formulae of the previous section remain valid, but for even lattices (e.g., s.q., s.c., b.c.c.) the lowest energy state corresponds to an alternating order of up and down spins. It is therefore convenient in this case to differentiate between "odd" and "even" sites by using different magnetic fields H_+ , H_- for these sites. This is equivalent to a model with different magnetic moments m_+ , m_- at these sites, i.e. the Ising model of a ferrimagnet. We thus take as our general Hamiltonian

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - m_+ H_+ \sum_{i^+} \sigma_{i^+} - m_- H_- \sum_{i^-} \sigma_{i^-}. \quad (1.18)$$

We can now define the sub-lattice magnetizations:—

$$M_+ = \frac{1}{\beta} \frac{\partial}{\partial H_+} (\ln Z_N^I) = m_+ \sum_{i^+} \langle \sigma_{i^+} \rangle, \quad (1.19)$$

$$M_- = \frac{1}{\beta} \frac{\partial}{\partial H_-} (\ln Z_N^I) = m_- \sum_{i^-} \langle \sigma_{i^-} \rangle.$$

Similarly three different susceptibilities can be defined, χ_{++} , χ_{+-} , χ_{--} which can likewise be expressed in terms of correlations of type $\langle \sigma_{i^+} \sigma_{j^+} \rangle$, $\langle \sigma_{i^+} \sigma_{j^-} \rangle$, $\langle \sigma_{i^-} \sigma_{j^-} \rangle$.

In zero magnetic field it is easy to show that the partition function of an antiferromagnet is identical with that of a ferromagnet (e.g. Domb, 1960). In fact the $\langle \sigma_{i^+} \sigma_{j^+} \rangle$ and $\langle \sigma_{i^-} \sigma_{j^-} \rangle$ are the same for both models whereas

the $\langle \sigma_i + \sigma_j - \rangle$ have opposite signs. However for non-zero H the behaviour is very different, and it is useful to introduce the "staggered" susceptibility which is the second derivative corresponding to $m_+ = m_-$, $H_+ = -H_-$, or equivalently $m_+ = -m_-$, $H_+ = H_-$. We then find that the normal susceptibility of an antiferromagnet is given (in terms of the ferromagnet correlations) by

$$\chi = \chi_{++} + \chi_{--} - 2\chi_{+-} = \sum \langle \sigma_i + \sigma_j + \rangle + \sum \langle \sigma_i - \sigma_j - \rangle - 2 \sum \langle \sigma_i + \sigma_j - \rangle, \quad (1.20)$$

whilst the staggered susceptibility is given by

$$\chi' = \chi_{++} + \chi_{--} + 2\chi_{+-} = \sum \langle \sigma_i + \sigma_j + \rangle + \sum \langle \sigma_i - \sigma_j - \rangle + 2 \sum \langle \sigma_i + \sigma_j - \rangle. \quad (1.21)$$

In zero field the *staggered* susceptibility of an *antiferromagnet* is thus identical with the normal susceptibility of a *ferromagnet*. However in non-zero field the ferromagnet has no transition whereas the antiferromagnet does have a transition (see next section); the staggered susceptibility is then a convenient quantity for locating this transition.

By analogy with (1.16) and (1.17) we can remove the lowest energy terms of a ferrimagnet and write

$$Z_N^I = y_+^{-N/4} y_-^{-N/4} u^{-qN/8} \Lambda_N^I, \quad (1.22)$$

where

$$y_+ = \exp(-2\beta m_+ H_+), y_- = \exp(-2\beta m_- H_-), u = \exp(-4K). \quad (1.23)$$

3. Solutions and order-disorder transitions

A regular solution is a lattice model in which sites are occupied by *A* or *B* atoms which interact by means of central forces (it is usual to take only nearest neighbour interactions into account). We shall see that a regular solution is equivalent to a simple Ising model but care is needed in specifying the partition functions for the two models. Let J_{AA} , J_{AB} , J_{BB} represent the interaction energies between the atoms. We identify a site occupied by an atom *A* with a \uparrow spin and a site occupied by an atom *B* with a \downarrow spin. It is clear that there is a (1-1) correspondence between Ising and solution configurations, but to obtain a partition function for the solution parallel to Z_N^I we need to average over all possible numbers N_A , N_B of the two constituents; we shall therefore obtain a grand partition function.

To establish the exact relationship we follow Fisher (1965) and define variables

$$\begin{aligned} \tau_{Ai} &= \frac{1}{2}(1 + \sigma_i) \\ \tau_{Bi} &= \frac{1}{2}(1 - \sigma_i). \end{aligned} \quad (1.24)$$

Thus when $\sigma_i = +1$, $\tau_{Ai} = 1$ and $\tau_{Bi} = 0$; when $\sigma_i = -1$, $\tau_{Ai} = 0$ and $\tau_{Bi} = 1$; the τ_i correspond to the occupation of sites by *A* and *B* atoms. The energy of any configuration is

$$\begin{aligned}\mathcal{E}(\sigma_i, \sigma_j) &= \sum_{\langle ij \rangle} J_{AA} \tau_{Ai} \tau_{Aj} + J_{AB} (\tau_{Ai} \tau_{Bj} + \tau_{Bi} \tau_{Aj}) + J_{BB} \tau_{Bi} \tau_{Bj} \\ &= \frac{N}{4} (J_{AA} + 2J_{AB} + J_{BB}) + \frac{q}{4} (J_{AA} - J_{BB}) \sum_i \sigma_i \\ &\quad + \frac{1}{4} (J_{AA} + J_{BB} - 2J_{AB}) \sum_{\langle ij \rangle} \sigma_i \sigma_j.\end{aligned}\quad (1.25)$$

The grand partition function for the solution is given by

$$\Xi_N = \sum_{\langle ij \rangle} \lambda_A^{N_A} \lambda_B^{N_B} \exp[-\beta \mathcal{E}(\sigma_i, \sigma_j)]. \quad (1.26)$$

$$\sigma_i, \sigma_j = \pm 1$$

Since the numbers of *A* and *B* atoms are given by

$$\begin{aligned}N_A &= \sum_i \tau_{Ai}, \\ N_B &= \sum_i \tau_{Bi},\end{aligned}\quad (1.27)$$

we can rewrite this in a form parallel to (1.2),

$$\begin{aligned}\Xi_N &= \Lambda_0^N \sum_{\langle ij \rangle} \Pi \exp(\beta J^* \sigma_i \sigma_j) \Pi \exp(\beta \mu_{AB} \sigma_i), \\ &= \Lambda_0^N Z_N^I (K^*, H^*)\end{aligned}\quad (1.28)$$

where

$$J^* = \frac{1}{4}(2J_{AB} - J_{AA} - J_{BB})$$

$$mH^* = \mu_{AB} = \frac{1}{2}kT \ln \lambda_A/\lambda_B + \frac{q}{4} (J_{BB} - J_{AA}) \quad (1.29)$$

$$\ln \Lambda_0 = \frac{1}{2} \ln(\lambda_A \lambda_B) - \frac{\beta}{4} (J_{AA} + J_{BB} + 2J_{AB}).$$

For $J^* > 0$ the behaviour is analogous to a ferromagnet and at low temperatures the solution separates into two phases. For $J^* < 0$ the behaviour is analogous to an antiferromagnet, and the system can undergo

an order-disorder transition. To derive the behaviour of a solution with a fixed ratio of A to B atoms, we use the formulae

$$N_A = \lambda_A \frac{\partial}{\partial \lambda_A} (\ln \Xi_N)$$

$$N_B = \lambda_B \frac{\partial}{\partial \lambda_B} (\ln \Xi_N).$$

We can then relate the singularities associated with phase separation to those of a ferromagnet, and the singularities associated with the onset or disappearance of long range order with those of an antiferromagnet (see e.g. Domb, 1960).

4. Lattice gas

It was pointed out by Cernuschi and Eyring in 1939 that if the A atoms in the above treatment are molecules and the B atoms are holes we obtain a crude model of liquid-vapour behaviour. Although we could not expect any refined agreement with experiment, we are at least presented with a means of exploring the liquid-vapour phase transition and the nature of the critical point. This "lattice gas" model of condensation has in fact been very effectively used for this purpose.

To convert the formulae of the previous section into those appropriate to a lattice gas we put J_{AB} , J_{BB} equal to zero and λ_B equal to 1. We then find that (1.29) reduces to

$$J^* = -\frac{1}{4} J_{AA}$$

$$mH^* = \frac{1}{2} kT \ln \lambda_A - \frac{q}{4} J_{AA} \quad (1.30)$$

$$\ln \Lambda_0 = \frac{1}{2} \ln \lambda_A - \frac{\beta}{4} J_{AA}.$$

Thus the magnetic field is closely related to the chemical potential of the lattice gas.

We must remember in comparing (1.28) with the conventional grand partition function that N is a fixed quantity for all configurations of the ensemble and really corresponds to volume V ; N_A is the variable which determines the density of the fluid.[†]

[†] In Domb (Chapter 1) we used \mathcal{N} for the fixed number of sites (here denoted by N) and N for the variable number of fluid particles (here denoted by N_A).

The above interpretation is valid for attractive intermolecular forces ($J_{AA} < 0$). However for repulsive forces ($J_{AA} > 0$) we return to the anti-ferromagnetic picture which we can use as a model of melting (Domb, 1951, 1958; Runnels, Vol. 2, Chapter 8).

C. Types of series expansion

We have shown above that the Ising model provides a basis for the discussion of a number of physical problems. For convenience we shall always use magnetic language in deriving the behaviour of the model. The transformation to appropriate variables for the other problems can then be made in a straightforward manner (see also Vicentini-Missoni, Vol. 2, Chapter 2).

1. Ferromagnet

We first quote theorems for the Ising model which have established the general form of singularities of the partition function in the (H,T) plane when we proceed to the thermodynamic limit $N \rightarrow \infty$ (see Griffiths, Vol. 1, Chapter 2).

- (i) At sufficiently low temperatures there is a discontinuity in magnetization M as $H \rightarrow 0$; the limiting value of M as $H \rightarrow 0$, M_0 ($\neq 0$), is termed the *spontaneous magnetization*.

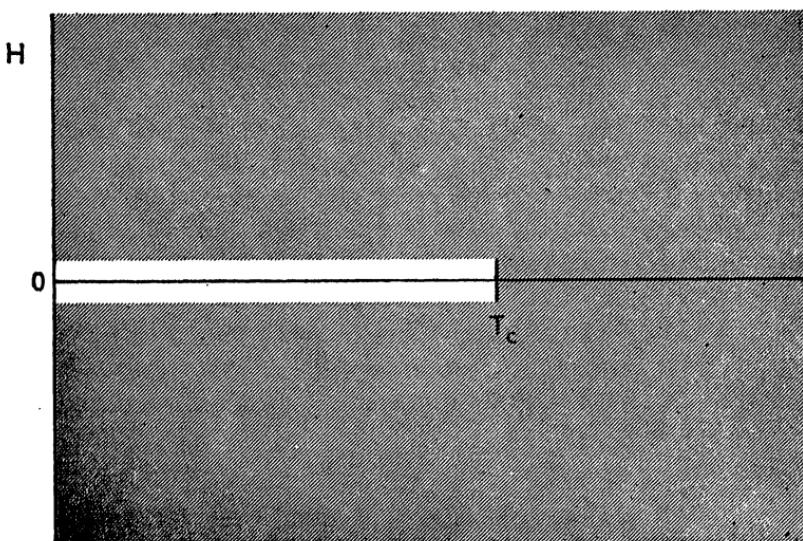


FIG. 1. Partition function is analytic everywhere in shaded region.

(ii) For $H > 0$ the partition function has no singularities and is analytic; for sufficiently large T it is analytic even when $H = 0$. We thus see that the singularities are confined to the low temperature side of the $H = 0$ axis, and the function is analytic in the shaded region in Fig. 1.

For many two-dimensional lattices exact solutions for the simple Ising model are available for $H = 0$ which show that there is a unique critical temperature T_c characterized by singularities in the thermodynamic functions. Hence for $H = 0$ these functions are analytic for $T > T_c$. It is believed that this property holds for the more general Ising model in two or more dimensions. However, it is known to be untrue for the dilute Ising model (Griffiths, 1969).

There are basically three different types of series expansion which have been used to elucidate the physical behaviour of the simple Ising model, and these are illustrated in Fig. 2.

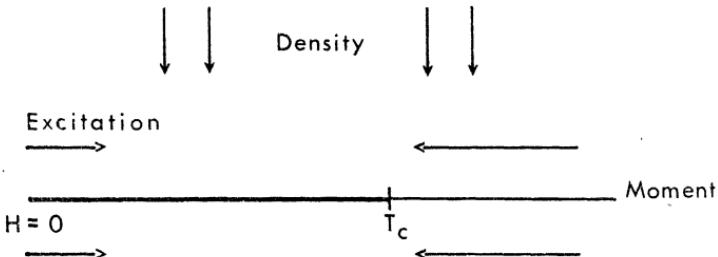


FIG. 2. Types of series expansion for a ferromagnet.

(a) *High temperature expansions of "moment" or "cumulant" type.* At very high temperatures the configurations are completely random. As the temperature is lowered deviations from randomness occur which can be systematically taken into account by means of a series expansion in $\beta = 1/kT$. In the primitive form the partition function Z_N is expanded as

$$Z_N = \langle \exp - \beta \mathcal{H} \rangle = 1 - \beta \langle \mathcal{H} \rangle + \frac{\beta^2}{2!} \langle \mathcal{H}^2 \rangle - \frac{(\beta)^3}{3!} \langle \mathcal{H}^3 \rangle + \dots \quad (1.31)$$

where $\langle \rangle$ now denotes the trace or sum over all configurations. This is of the form of a moment expansion in statistics, and in fact $Z_N(\beta, H)$ is effectively identical with the moment generating function for the distribution

of \uparrow spins and $\uparrow\downarrow$ contacts on the lattice (Domb, 1964). Hence if we expand $\ln Z_N$ we will obtain a cumulant expansion:

$$\begin{aligned}\ln Z_N = & -\beta \langle \mathcal{H} \rangle + \frac{\beta^2}{2!} [\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2] - \frac{\beta^3}{3!} \\ & [\langle \mathcal{H}^3 \rangle - 3 \langle \mathcal{H}^2 \rangle \langle \mathcal{H} \rangle + 2 \langle \mathcal{H} \rangle^3] + \dots \quad (1.32)\end{aligned}$$

A general discussion of expansions like (1.31) and (1.32) is given in this volume, Chapter 1. For the simple Ising model there are a number of simplifications which will be discussed in detail in Section II. It is sometimes useful to take alternative variables to $K (= \beta J)$, e.g. $w = \tanh K$, $f = u^{-1} - 1 = \exp 4K - 1$, $\zeta = 1 - u$.

Because of the magnetic symmetry of the model all odd derivatives of $\ln Z$ with respect to H vanish in these expansions. A particularly convenient form of this type of expansion of the simple Ising model for any net is

$$\ln Z_N^I = N \ln (2 \cosh \beta m H) + L \ln \cosh K + \sum_{r=1}^{\infty} w^r \Psi_r(\tau). \quad (1.33)$$

Here L is the number of links in the net,

$$\tau = (1 - y) / (1 + y) = \tanh \beta m H, \quad (1.34)$$

and the polynomials $\Psi_r(\tau)$ contain only even powers of τ ,

$$\Psi_r(\tau) = A_r^{(0)} + A_r^{(2)} \tau^2 / 2! + A_r^{(4)} \tau^4 / 4! + \dots \quad (1.35)$$

The zero field partition function is then given by

$$\ln Z_{N0}^I = N \ln 2 + L \ln \cosh K + \sum_{r=1}^{\infty} A_r^{(0)} w^r \quad (1.36)$$

and the zero field susceptibility from (1.10), by

$$\chi_{N0} = \beta m^2 \left[N + \sum_{r=1}^{\infty} A_r^{(2)} w^r \right]. \quad (1.37)$$

The even derivatives of χ_{N0} can be related similarly to

$$\sum_{r=1}^{\infty} A_r^{(2s)} w^r. \quad (1.38)$$

In the thermodynamic limit of large N we expect that

$$\Psi_r(\tau) \sim N \psi_r(\tau)$$

We then have for the thermodynamic quantities *per site*

$$\ln Z^I = \ln(2 \cosh \beta mH) + \frac{q}{2} \ln \cosh K + \sum_{r=1}^{\infty} \psi_r(\tau) w^r \quad (1.39)$$

$$\begin{aligned} \ln Z_0^I &= \ln 2 + \frac{q}{2} \ln \cosh K + \sum_{r=1}^{\infty} a_r^{(0)} w^r \\ - U_0^I/J &= \frac{1}{2} q w + \sum_{r=2}^{\infty} u_r w^r \quad (u_r = (r+1)a_{r+1}^{(0)} - (r-1)a_{r-1}^{(0)}) \\ \chi_0 &= \beta m^2 \left(1 + \sum_{r=1}^{\infty} a_r^{(2)} w^r \right). \end{aligned} \quad (1.40)$$

A transformation to any of the other "high temperature" variables mentioned above is elementary, and numerical work can readily be programmed for a computer.

(b) *Density expansions of "cluster" type.* For this type of expansion we start with the state of complete alignment of spins in a very large magnetic field, and allow the field to decrease giving rise at any particular temperature to groups of 1, 2, 3 . . . overturned spins. The expansions correspond to the cluster integral expansions for a condensing gas (this volume Chapter 1, Section 3).

If we use the expansion variable y , we obtain the analogue of activity expansions,

$$\ln Z_N^I = -\frac{N}{2} \ln y - \frac{qN}{8} \ln u + \sum_{r=1}^{\infty} y^r G_r(u). \quad (1.42)$$

We here assume that N is sufficiently large for the configurations in which nearly *all* spins are overturned to be ignored. For finite nets in which this is not the case the expansion can be suitably modified (see Section II B3). Taking the thermodynamic limit we find for the partition function *per site*

$$\ln Z^I = -\frac{1}{2} \ln y - \frac{q}{8} \ln u + \sum_{r=1}^{\infty} y^r g_r(u), \quad (1.43)$$

where for large N ,

$$G_r(u) \sim N g_r(u). \quad (1.44)$$

The magnetization is given, from (1.9), by

$$\begin{aligned} M_N = \frac{1}{\beta} \frac{\partial}{\partial H} (\ln Z_N^I) &= -2my \frac{\partial}{\partial y} (\ln Z_N^I) = m \left[N - 2y \frac{\partial}{\partial y} \ln \Lambda_N^I \right] \\ &= m \left[N - 2 \sum_{r=1}^{\infty} y^r G_r(u) \right] \end{aligned} \quad (1.45)$$

In the thermodynamic limit we obtain for the magnetization *per site*

$$M = m \left[1 - 2y \frac{\partial}{\partial y} \ln \Lambda^I \right] = m \left[1 - 2 \sum_{r=1}^{\infty} y^r g_r(u) \right], \quad (1.46)$$

and for the spontaneous magnetization

$$M_0 = m \left[1 - 2 \sum_{r=1}^{\infty} g_r(u) \right]. \quad (1.47)$$

We shall find that for any dimension $d \geq 2$, M_0 is non-zero for sufficiently small u , but $M_0 = 0$ for $u \sim 1$ (small ζ).

Virial expansions analogous to those involving irreducible cluster integrals are used only in the thermodynamic limit. We then change to the variable

$$\rho = y \frac{\partial}{\partial y} \ln \Lambda^I = \frac{1}{2} (1 - M/m) \quad (1.48)$$

and obtain

$$\ln Z^I = \sum_{r=1}^{\infty} \rho^r k_r(u). \quad (1.49)$$

The variable ρ represents the density of overturned spins starting from a zero energy state in which they are all aligned.

(c) *Low temperature expansions of “excitation” type.* At sufficiently low temperatures the spins will all align even in zero field. We can then consider excited states arising from groups of overturned spins having configurations with more and more $\uparrow\downarrow$ bonds. In zero field the lowest energy state is doubly degenerate and we obtain an expansion

$$\ln Z_N^I = \ln 2 - \frac{qN}{8} \ln u + \sum_{r=1}^{\infty} B_r^{(0)} u^r. \quad (1.50)$$

For practical applications it is convenient to split the degeneracy by taking a small magnetic field which singles out one energy state, and ignoring the

second state in which all the spins are overturned. We then obtain in a general field H ,

$$\ln Z_N^I = -\frac{N}{2} \ln y - \frac{qN}{8} \ln u + \sum_{r=1}^{\infty} F_r(y) u^r, \quad (1.51)$$

and in the thermodynamic limit,

$$\ln Z^I = -\frac{1}{2} \ln y - \frac{q}{8} \ln u + \sum_{r=1}^{\infty} f_r(y) u^r. \quad (1.52)$$

The series (a) (b) (c) above are not independent. It is easy to see that (1.52) is merely a rearrangement of (1.43), and we shall see in Section II.B2 that (1.39) can also be readily derived from (1.43). In many respects (1.43) is the fundamental expansion, although for the particular cases represented by (1.40) and (1.41) it is easier to derive extensive terms of the expansion.

The same types of expansion can be derived for the Ising model of general spin s . However, the relationship of type (b) expansions to a condensing gas is more sophisticated; for many purposes it is convenient to take arbitrary energy levels for each individual spin, and to pursue the analogy with a multicomponent gas.

2. Antiferromagnet and ferrimagnet

We can change from ferromagnet to antiferromagnet if we replace J by $-J$ and keep the convention $J > 0$. Type (a) expansions can be adapted immediately, and for example in (1.39), (1.40) and (1.41) we merely have to multiply the r th term by $(-1)^r$. Likewise for type (b), expansion (1.43) remains valid but the variable u ranges between 1 and ∞ instead of between 0 and 1. However, type (c) expansions are completely different since the lowest energy state for "even" lattices is one of alternating order. If in this case we write $u' = u^{-1}$ (so that u' goes from 0 to 1) equation (1.50) in zero field remains valid with u' replacing u . However, when $H \neq 0$ instead of (1.52) we have

$$\ln Z^I = -\frac{1}{2} \ln y - \frac{q}{8} \ln u + \sum_{r=1}^{\infty} f_r^{(a)}(y) u^r, \quad (1.53)$$

where the function $f_r^{(a)}(y)$ is completely different from $f_r(y)$, the two having the same value only when $y = 1$ (the superscript a denotes antiferromagnet).

The pattern of singularities in the (H, T) plane differs from that of a ferromagnet. There are fewer rigorous theorems, but from the existence or non-

existence of long range order we can conjecture the form indicated in Fig. 3 (Domb, 1960).

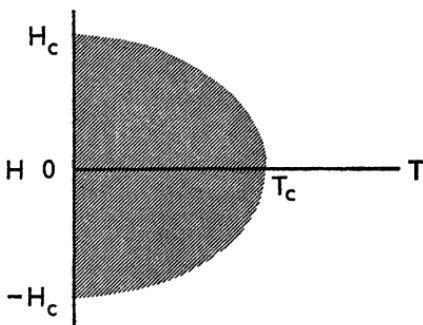


FIG. 3. Line of singularities for an antiferromagnet for the s.q., s.c., b.c.c., and d. lattices. The shaded region corresponds to long-range order.

The model of a ferrimagnet corresponds to an alternation of magnetic moments m_+ and m_- . As long as m_+ and m_- are both positive the general theorems for a ferromagnet remain valid, and we can obtain series of type (a), (b) and (c) as in the previous section. For example, we can write as a generalization of (1.43), (1.52) respectively

$$\ln Z^I = -\frac{1}{4} \ln y_+ - \frac{1}{4} \ln y_- - \frac{q}{8} \ln u + \sum_{r,s=1}^{\infty} y_+^r y_-^s g_{rs}(u), \quad (1.54)$$

$$\ln Z^I = -\frac{1}{4} \ln y_+ - \frac{1}{4} \ln y_- - \frac{q}{8} \ln u + \sum_{r=1}^{\infty} f_r^{(a)}(y_+, y_-) u^r. \quad (1.55)$$

It was pointed out by Sykes† (unpublished) that the series for an antiferromagnet can conveniently be obtained by taking $m_- = -m_+$. This is remarkable since it provides a mechanism for circumventing the line of singularities in Fig. 3, and getting the series for the ordered state (1.55) from those for the disordered state (1.54).

For “odd” lattices the situation of the antiferromagnet at low temperatures is much more complicated because of the large degeneracy of the lowest energy state. The triangular lattice has so many states that there is a finite entropy at $T = 0$. There is no transition when $H = 0$, and it is very difficult to derive any low temperature expansions. Most of the current information available has come from extrapolation of high temperature expansions (Sykes and Zucker, 1961; Sykes *et al.*, 1972a). The conjectured pattern of singularities

† This method was applied in deriving the series used by Bienenstock and Lewis (1967) and Rapaport and Domb (1971).

is shown in Fig. 4 (Domb, 1960; see also Burley, Vol. 2, Chapter 9). For the f.c.c. there is no longer a finite entropy at $T=0$, and the system has a two-dimensional type of order (Danielian, 1961, 1964; Betts and Elliott, 1965). Low temperature expansions are still difficult to derive; the conjectured pattern of singularities is shown in Fig. 5.

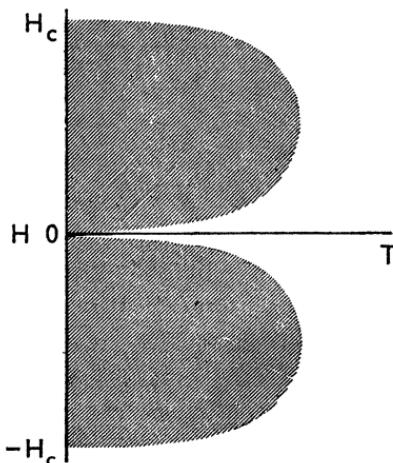


FIG. 4. Line of singularities for p.t. lattice, the shaded region corresponding to long-range order. There is no long-range order when $H = 0$.

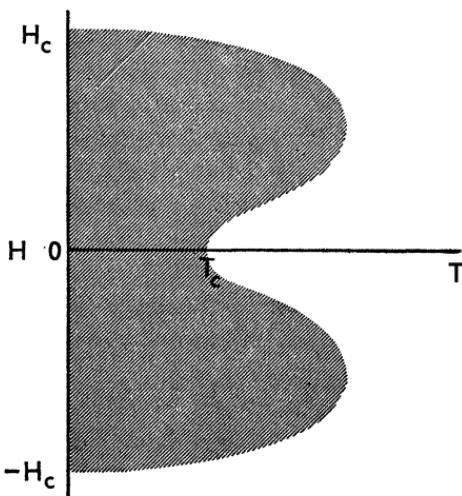


FIG. 5. Line of singularities for f.c.c. lattice, the shaded region corresponding to long-range order. There is a two-dimensional ordering when $H = 0$.

II. Derivation of Series Expansions

A. High temperature expansions

The earliest derivations of series expansions used the method of lattice constants and embeddings described in Chapter 1 of this volume. For many years this was the only practical method available. An elegant formalism had been developed by Brout (1959, 1960, 1961), Horwitz and Callen (1961), Englert (1963) and others using the general perturbation methods of quantum field theory which were based on free graph (or random walk) enumerations. However, the formalism was used in practice to provide closed form approximations by summing partial sets of graphs of different types. To use the method for exact enumerations of terms in a series expansion it was necessary to take account of a rapidly increasing number of contributions which gave rise to formidable computational difficulties. A major break-through was provided by Wortis and his collaborators at the University of Illinois who used an integral equation (which could be solved by computer) to deal with the most numerous sets of configurations, and evaluated the few remaining configurations individually. A detailed description of this approach is given in Chapter 3 of this volume.

The first method is better equipped to take advantage of specific simplifying features of the lattice or model. Thus for the simple Ising model where such features exist very extensive series expansions have been possible. We shall now describe in more detail how they were derived. The second method is more useful for general problems, and has been particularly powerful for spin s which can be tackled with no more difficulty than spin $\frac{1}{2}$. It has also been put to very effective use for the calculation of spin-spin correlations which will be described in Vol. 4.

1. Primitive method

We shall first introduce a transformation originally due to van der Waerden (1941) which eliminates all multiple bonds for the simple Ising model. Noting that the $\sigma_i \sigma_j$ satisfy the relation

$$\begin{aligned} (\sigma_i \sigma_j)^2 &= (\sigma_i \sigma_j)^4 = \dots = 1 \\ (\sigma_i \sigma_j) &= (\sigma_i \sigma_j)^3 = (\sigma_i \sigma_j)^5 = \dots , \end{aligned} \quad (2.1)$$

we can write

$$\begin{aligned} \exp K(\sigma_i \sigma_j) &= \cosh K + \sigma_i \sigma_j \sinh K = \cosh K(1 + w \sigma_i \sigma_j) \\ &\quad (w = \tanh K). \end{aligned} \quad (2.2)$$

Hence we can expand the first product in (1.2) for any net in the form

$$\begin{aligned} \sum_{\langle ij \rangle} \Pi \exp(K\sigma_i\sigma_j) &= \cosh^L K \sum_{\langle ij \rangle} \Pi (1 + w\sigma_i\sigma_j) \\ &= \cosh^L K \sum_{\langle ij \rangle \langle kl \rangle \dots} [1 + w(\sigma_i\sigma_j) \\ &\quad + w^2(\sigma_i\sigma_j)(\sigma_k\sigma_l) + \dots] \end{aligned} \quad (2.3)$$

where $\langle ij \rangle \langle kl \rangle \dots$ are any different interacting pairs of the net. This can be interpreted topologically. The first term, $(\sigma_i\sigma_j)$, corresponds to any one of the L interaction links of the net; the second term, $(\sigma_i\sigma_j)(\sigma_k\sigma_l)$, corresponds to any of the $L(L-1)/2!$ non-identical pairs; and so on (see Fig. 6).

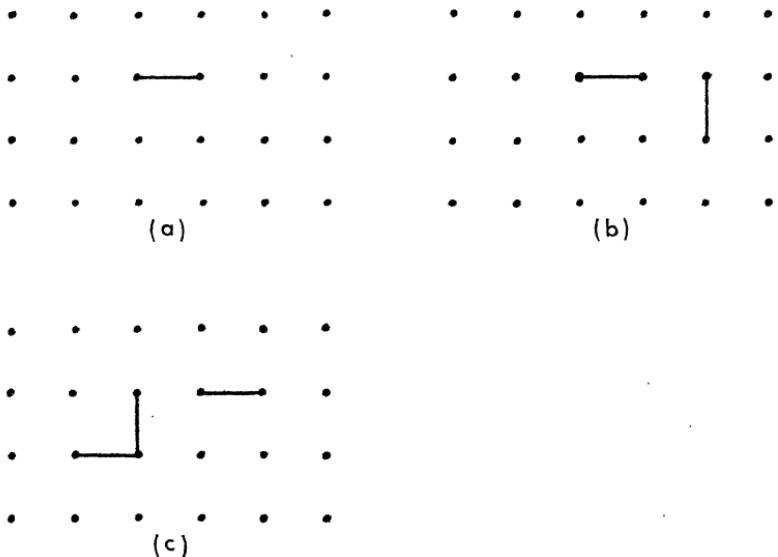


FIG. 6. Typical contributions to the high-temperature expansion.
 (a) First term L contributions, (b) Second term $L(L-1)/2!$ contributions, (c) Third term $L(L-1)(L-2)/3!$ contributions.

We can expand the second product in (1.2) in a similar manner

$$\begin{aligned} \prod_i \exp(\beta mH\sigma_i) &= \prod_i (\cosh \beta mH + \sigma_i \sinh \beta mH) = \cosh^N \beta mH \prod_i (1 + \tau \sigma_i) \\ &= \cos^N \beta mH \left[1 + \tau \sum_i \sigma_i + \tau^2 \sum_{ij} \sigma_i \sigma_j + \dots \right] (\tau = \tan \beta mH). \end{aligned} \quad (2.4)$$

When we now group the σ_i together and sum over all $\sigma_i = \pm 1$ it is easy to see that each graph in Fig. 6 makes only one non-zero contribution; a graph

with l links and s odd vertices contributes $2^N w^l \tau^{2s}$ (the number of odd vertices on a graph is always even). Hence we can write

$$Z_N^{(I)} = \cosh^L K (2 \cosh \beta m H)^N [X_{N0} + \tau^2 X_{N2} + \tau^4 X_{N4} + \dots]. \quad (2.5)$$

The term X_{N0} contains contributions from all even-vertexed graphs (which

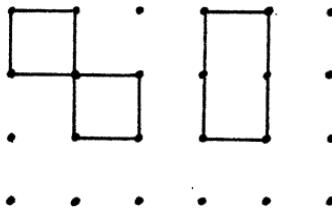


FIG. 7. A typical zero field graph.

are usually termed *zero field graphs*, Fig. 7). We can write

$$\left. \begin{aligned} X_{N0} &= \sum D_l^{(N)} w^l \\ D_l^{(N)} &= \sum_x p_{lx}^{(N)} \end{aligned} \right\} \quad (2.6)$$

Here $p_{lx}^{(N)}$ represents a typical even-vertexed graph of l lines, x being a graph-distinguishing suffix.

The term X_{N2} contains contributions from all graphs with two odd vertices

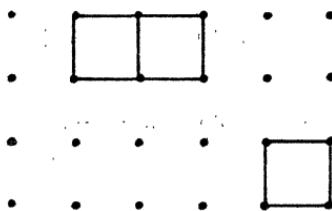


FIG. 8. A typical magnetic graph.

(usually termed *magnetic graphs*, Fig. 8). We can write

$$\left. \begin{aligned} X_{N2} &= \sum E_l^{(N)} w^l \\ E_l^{(N)} &= \sum_x q_{lx}^{(N)} \end{aligned} \right\} \quad (2.7)$$

where $q_{lx}^{(N)}$ represents a typical magnetic graph of l lines. Similarly for X_{N4}, X_{N6}, \dots for which the contributing graphs are termed *hypermagnetic* (Fig. 9).

It is important to note that all the above expansions can be generalised to deal with different interactions between different links of the net and different magnet fields acting on different spins of the net. We merely replace any term w^l by $w_1^{l_1} w_2^{l_2} w_2^{l_3} \dots$ and a τ^{2s} by $\tau_1^{s_1} \tau_2^{s_2} \tau_3^{s_3} \dots$.

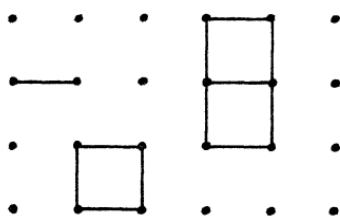


FIG. 9. A typical hypermagnetic graph with 4 odd vertices.

To use the primitive method to obtain the partition function per site in the thermodynamic limit, we follow the procedure outlined in Chapter 1 (Section IV. B.1) evaluating *all* lattice constants of appropriate type for a lattice with a cyclic boundary, and obtaining X_{Nt} as a polynomial in N . If we take the coefficient of N in this polynomial we obtain $\ln Z^I$, and if we put N equal to 1 we obtain Z^I . Thus we find that the zero field partition function is given by

$$\ln Z_0^I = \ln 2 + \frac{L}{N} \ln \cosh K + \sum_l d_l w^l, \quad (2.8)$$

where d_l is the coefficient of N in $D_l^{(N)}$; and the initial susceptibility is given by

$$\chi_0 = \beta m^2 \left[1 + 2 \sum_l e_l w^l \right], \quad (2.9)$$

where e_l is the coefficient of N in $E_l^{(N)}$. A comparison of (2.7) and (2.9) with (1.12) indicates that the contribution to χ_0 from diagrams with odd vertices at a, b represents the correlation $\langle \sigma_a \sigma_b \rangle$; this can best be established by evaluating $\ln Z^I$ for a magnetic field which acts only on the spins a, b .

Corresponding results can readily be derived for the even derivatives of χ_0 with respect to H in terms of hypermagnetic graphs and multiple correlations.

Comparing (2.8) with (1.40) we can identify $a_l^{(0)}$ with d_l ; similarly comparing (2.9) with (1.41) we identify $a_l^{(2)}$ with $2e_l$.

2. Susceptibility coefficients. Counting theorem.

To calculate the partition function in zero field (2.8) the only graphs which need be considered have even vertices and are thus "closed". The lattice constants of such graphs (see Chapter 1, Section IV) are not too

numerous, and the expansion can be pursued for some way even without computer enumerations. However, to calculate the initial susceptibility, “open” graphs with two vertices of odd degrees are needed, and their lattice constants are often much more numerous and difficult to calculate directly. From the point of view of accurate estimation of the critical temperature the susceptibility expansion plays a central role, and it is important to obtain as many terms as possible.

A counting theorem due to Sykes (1961) shows how to formulate the coefficients of the susceptibility series (2.7) (2.9) as lattice coefficients of closed graphs. The general procedure parallels that used for the *chain counting theorem* (Chapter 1, Section IV.A6), and derives a difference equation for e_l of the form

$$e_l - 2\sigma e_{l-1} + \sigma^2 e_{l-2} = \sum_{n \leq l} p_{nx}, \quad (l \geq 3) \quad (\sigma = q-1) \quad (2.10)$$

where p_{nx} are the lattice constants of closed graphs. As a result of (2.10) the *reduced susceptibility* $\chi(w) = \chi_0/\beta m^2$ can be expressed in the form

$$\chi(w) = (1 - \sigma w)^{-2} \left[1 - (\sigma - 1)w - \sigma w^2 + \sum_3^\infty f_l w^l \right]. \quad (2.11)$$

From the coefficients f_l it is convenient to subtract an “energetic” contribution $-2ld_l$, leaving finally the formula

$$\chi(w) = (1 - \sigma w)^{-2} [1 - (\sigma - 1)w - \sigma w^2 - 2wU(w) + G(w)]. \quad (2.12)$$

The terms in (2.12) have the following meaning. $U(w)$ is the *reduced energy*

$$U(w) = w \frac{d}{dw} (\ln Z_0^{-1} - \frac{q}{2} \ln \cosh K) = \sum l d_l w^l. \quad (2.13)$$

$G(w)$ termed the *residual correlation function* is given by

$$G(w) = 8(1 + w)^2 \sum_l g_l w^l. \quad (2.14)$$

The g_l are linear sums of lattice constants (connected and disjoint) of closed graphs which satisfy the following conditions:

- (i) only lattice constants with l lines occur in g_l ;
- (ii) only zero field and magnetic lattice constants occur.

The coefficients g_l can be written in the form

$$g_l = \sum_x w_{lx} p_{lx}, \quad (2.15)$$

where w_{lx} is the *counting weight* of the associated configuration determined by the following rules. For a zero-field graph with vertices of degree $2q_1, 2q_2 \dots 2q_v$,

$$w_{lx} = \sum_{i=1}^v \frac{q_i(q_i - 1)}{2}; \quad (2.16)$$

hence only graphs with at least one vertex of degree four need be considered, and the vertices of degree 2 make no contribution. To take typical examples for a graph with one vertex of degree 4, $w_{lx} = 1$, for two vertices of degree 4, $w_{lx} = 2$, for one vertex of degree 6, $w_{lx} = 3$. For a magnetic graph with odd vertices of order $(2r_1 + 1)$ and $(2r_2 + 1)$.

$$w_{lx} = r_1 r_2. \quad (2.17)$$

As typical examples for a graph with two odd vertices of degree 3, $w_{lx} = 1$, for one vertex of degree 3 and one of degree 5, $w_{lx} = 2$.

Although Sykes was able to establish the above results rigorously, his formal proof was never published; an elegant proof was given subsequently

TABLE I. Susceptibility coefficients $a_r^{(2)}$ for two-dimensional lattices (eqn. 1.41). (Data from Sykes *et al.*, 1972a).

| $r/lattice$ | p.t. | s.q. | h.c. | $r/lattice$ | h.c. |
|-------------|-------|--------|------------|-------------|---------------|
| 1 | | 6 | 4 | 3 | 22 348998 |
| 2 | | 30 | 12 | 6 | 23 403840 |
| 3 | | 138 | 36 | 12 | 24 299018 |
| 4 | | 606 | 100 | 24 | 25 677840 |
| 5 | | 2586 | 276 | 48 | 26 13 635630 |
| 6 | | 10818 | 740 | 90 | 27 24 206220 |
| 7 | | 44574 | 1972 | 168 | 28 43 092888 |
| 8 | | 181542 | 5172 | 318 | 29 76 635984 |
| 9 | | 732678 | 13492 | 600 | 30 135 698970 |
| 10 | 2 | 935218 | 34876 | 1098 | 31 240 199320 |
| 11 | 11 | 687202 | 89764 | 2004 | 32 426 144654 |
| 12 | 46 | 296210 | 229628 | 3696 | |
| 13 | 182 | 588850 | 585508 | 6792 | |
| 14 | 717 | 395262 | 1 486308 | 12270 | |
| 15 | 2809 | 372302 | 3 763460 | 22140 | |
| 16 | 10969 | 820358 | 9 497380 | 40224 | |
| 17 | — | — | 23 918708 | 72888 | |
| 18 | — | — | 60 080156 | 130650 | |
| 19 | — | — | 150 660388 | 234012 | |
| 20 | — | — | 377 009300 | 421176 | |
| 21 | — | — | 942 105604 | 756624 | |

by Nagle and Temperley (1968). The counting theorem has proved to be of great practical use in extending susceptibility series for the simple Ising model, and it was subsequently generalized by Stanley to the D-dimensional classical vector model (Stanley, 1967; see this volume, Chapter 7). Even though the method requires the use of disjoint lattice constants, this does not become a serious handicap until terms of quite high order. As a result the coefficients $a_r^{(2)}$ in (1.41) have now been calculated as far as $r = 16$ for the p.t. (plane triangular), $r = 21$ for the s.q. (simple quadratic), and $r = 32$ for the h.c. (plane honeycomb) lattice in two dimensions, and $r = 17$ for the s.c. (simple cubic), $r = 15$ for the b.c.c. (body centred cubic) and $r = 12$ for the f.c.c. (face centred cubic) lattices in three dimensions (Sykes *et al.*, 1972 a, b). For the diamond lattice a subsequent calculation by Sykes and Gaunt (1973) gives coefficients up to $r = 22$. These susceptibility coefficients are reproduced in Tables I and II.

For the p.t. and h.c. lattices a "star-triangle" type of transformation discovered by Fisher (1959b) (see Syozi Vol. 1, Chapter 7) provides a useful

TABLE II. Susceptibility coefficients $a_r^{(2)}$ for three-dimensional lattices (eqn. 1.41). (Data from Sykes *et al.*, 1972b; Gaunt and Sykes, 1973.)

| $r/\text{lattice}$ | f.c.c. | b.c.c. | s.c. | d. |
|--------------------|-----------------|-----------------|---------------|--------------|
| 1 | 12 | 8 | 6 | 4 |
| 2 | 132 | 56 | 30 | 12 |
| 3 | 1404 | 392 | 150 | 36 |
| 4 | 14652 | 2648 | 726 | 108 |
| 5 | 151116 | 17864 | 3510 | 324 |
| 6 | 1 546332 | 118760 | 16710 | 948 |
| 7 | 15 734460 | 789032 | 79494 | 2772 |
| 8 | 159 425580 | 5 201048 | 375174 | 8076 |
| 9 | 1609 987708 | 34 268104 | 1 769686 | 23508 |
| 10 | 16215 457188 | 224 679864 | 8 306862 | 67980 |
| 11 | 162961 837500 | 1472 595144 | 38 975286 | 196548 |
| 12 | 1 634743 178420 | 9619 740648 | 182 265822 | 566820 |
| 13 | | 62823 141192 | 852 063558 | 1 633956 |
| 14 | | 409297 617672 | 3973 784886 | 4 697412 |
| 15 | | 2 665987 056200 | 18527 532310 | 13 501492 |
| 16 | | | 86228 667894 | 38 742652 |
| 17 | | | 401225 391222 | 111 146820 |
| 18 | | | | 318 390684 |
| 19 | | | | 911 904996 |
| 20 | | | | 2608 952940 |
| 21 | | | | 7463 042916 |
| 22 | | | | 21328 259716 |

relation between the susceptibilities $\chi_t(w)$ and $\chi_h(w)$,

$$\chi_t(w) = \frac{1}{2}[\chi_h(w^*) + \chi_h(-w^*)]. \quad (2.18)$$

$$w^{*2} = w(1+w)/(1+w^3).$$

3. Connected and star lattice constant expansions

Following the general procedure described in Chapter 1 (Section IV.B2, 3) we now eliminate disjoint lattice constants. We can then write for any net G

$$\ln Z^I(G) = \sum_i (c_i; G) \kappa_i(w, y), \quad (2.19)$$

where for convenience we have replaced the variables, β, F, H of Chapter 1, eqn. (4.44), by w and y . The sum is taken over all connected sub-graphs c_i of G , and the κ_i depend only on the c_i and not on G . The κ_i can be determined from the partition functions of finite clusters; in fact the general formula is (Chapter 1 eqn. (4.60))

$$\kappa(c_j) = \sum_i t_{ij}^* \ln Z^I(c_i) \quad (2.20)$$

$$t_{ij}^* = (-1)^{l_i - l_j} (c_i; c_j)^F.$$

Here the sum is taken over all connected subgraphs c_i of c_j , and $(c_i; c_j)^F$ denotes the full perimeter lattice constant. From (2.20) the $\kappa(c_j)$ can easily be expanded as power series in w , and if we take G to be a lattice of N sites with a cyclic boundary condition we can use (2.19) to derive a power series expansion for $\ln Z_N^I$ in terms of connected lattice constants. Each such lattice constant is proportional to N .

This is the method which has been effectively used for the Heisenberg model of spin $\frac{1}{2}$ (see this volume, Chapter 5). The limitation of the number of terms which can be obtained arises principally from the large number of connected lattice constants which must be calculated. Such a limitation does not apply to $\ln Z_N^I$ in zero field for which only star lattice constants enter (Chapter 1, Section IV.B4). We can then write instead of (2.19)

$$\ln Z^I(G) = \sum_i (s_i; G) \kappa_i(w), \quad (2.21)$$

where $\kappa(s_i)$ is similar in form to (2.20) but involves only partition functions of star subgraphs. Although no explicit expression has been found for t_{ij}^* in the case of star graphs, the coefficients can be determined quite readily in practice by direct inversion of the equations (4.89) of Chapter 1. The partition functions $Z^I(s_i)$ can be written down easily using (2.5), and can be put in a form which depends only on the topology of the s_i .

We illustrate by showing how to calculate $\kappa_i(w)$ for a number of star topologies. The general scheme of Chapter 1 eqn. (4.89) operates with the weights given as follows:

$$\begin{aligned}
 w(a)_p &= \ln Z^I[(a)_p] = \ln(1 + w^a) \\
 w(a,b,c)_\theta &= \ln Z^I[(a,b,c)_\theta] = \ln(1 + w^{a+b} + w^{b+c} + w^{c+a}) \\
 w(a,b;c,d;e,f)_\alpha &= \ln Z^I[(a,b;c,d;e,f)_\alpha] = \ln(1 + w^{a+d+e} + w^{a+c+f} \\
 &\quad + w^{b+c+e} + w^{b+d+f} + w^{a+c+b+d} + w^{a+e+b+f} + w^{c+e+d+f}) \\
 w(a,b;c,d;e,f)_\beta &= \ln Z^I[a,b;c,d;e,f]_\beta = \ln(1 + w^{a+b} + w^{c+d} \quad (2.22) \\
 &\quad + w^{a+f+d+e} + w^{b+f+d+e} + w^{a+f+c+e} + w^{b+f+c+e} + w^{a+b+c+d}) \\
 w(a,b;c,d;e)_\gamma &= \ln Z^I[a,b;c,d;e]_\gamma = \ln(1 + w^{a+b} + w^{c+d} + w^{a+d+e} \\
 &\quad + w^{b+d+e} + w^{a+c+e} + w^{b+c+e} + w^{a+b+c+d}) \\
 w(a,b,c,d)_\delta &= \ln Z^I[a,b,c,d]_\delta = \ln(1 + w^{a+b} + w^{a+c} + w^{a+d} + w^{b+c} \\
 &\quad + w^{b+d} + w^{c+d}).
 \end{aligned}$$

Each of the $\ln Z^I(s_i)$ can be expanded as a power series in w , and the corresponding $\kappa(s_i)$ determined successively from Chapter 1 (4.89) as power series in w by subgraph subtraction. Following Sykes and Hunter (1973) we refer to the coefficients of powers of w in the expansion of $\kappa(s_i)$ as the λ -weights of s_i , the coefficient of w^l being the primary λ -weight, the coefficient of w^{l+1} the secondary λ -weight, ... w^{l+m} the $(m+1)$ th order λ -weight (l is the number of lines in the star s_i , and we have seen in Chapter 1, Section IV.B2 that the coefficients w^t are zero for $t < l$). The parameter m above is sometimes referred to as the *entry parameter* (Domb and Wood, 1965). Denoting the $(m+1)$ th λ -weight of a star s_i by $w_\lambda(s_i; m)$, the coefficient $a_r^{(0)}$ in the expansion (1.40) for a lattice L is given by

$$a_r^{(0)} = \sum_{m \geq 0} (s_i; L) w_\lambda(s_i; m), \quad (l = r - m), \quad (2.23)$$

the sum being taken over all star graphs s_i of r lines or less.

We now introduce the simplification discussed in Chapter 1, Section IV.B4 which enables us to *ignore the subgraphs and subtraction process*. The letters $a, b, c \dots$ relating the star graph s_i to a particular topology have referred to the number of lines in a link between two principal points of the topology. We change the model so that this link consists of a single line of interaction J_a . Then because of the property discussed in Section II.A1

equations (2.22) remain valid for the new model provided that we replace w^a , w^b , $w^c \dots$ by w_a , w_b , $w_c \dots$ ($w_a = \tanh \beta J_a$ etc.). For example, the partition function for the θ topology is

$$\ln Z^I(\theta) = \ln(1 + w_a w_b + w_b w_c + w_c w_a) \quad (2.24)$$

which is denoted in an obvious shorthand notation by $\ln(1 + ab + bc + ca)$. Following the procedure of Chapter 1, Section IV.B4, (2.24) is expanded and only terms containing abc are retained as follows:

$$\begin{aligned} -a^2bc - b^2ca - c^2ab + (a^3b^2c + a^2b^3c + ab^2c^3 + ab^3c^2 + a^3bc^2 \\ + a^2bc^3) + 2a^2b^2c^2 + \dots \end{aligned} \quad (2.25)$$

Each of these terms can be described as a *bonding* of the θ topology, the coefficient of which represents the *weight* of the bonding; each bonding can then be re-interpreted in terms of the original model ($w_a \rightarrow w^a$ etc.). Thus each bonding weight makes its contribution to an appropriate λ -weight, and as a particular example the term $a^r b^s c^t$ contributes to $w_\lambda(\theta; r+s+t-3)$.

In Chapter 1, Section IV.B4 a brief description is also given of a new method of calculating the bonding weights (Domb, 1972b) using the device of replacing a single interaction J by a parallel pair of interactions J' , J'' for "ladder" topologies, and making a suitably chosen interaction infinite for non-ladder topologies. This appreciably facilitates the calculation of individual weights and enables a number of general theorems to be enumerated.

The method of different interactions described above can readily be computerized and has been used to calculate the coefficients $a_r^{(0)}$ in (1.40) for the standard three-dimensional lattices. Results are reproduced in Table III as far as $r = 14$ for the f.c.c. lattice, $r = 16$ for the b.c.c. lattice, $r = 18$ for the s.c. lattice, and $r = 22$ for the d . lattice.

For the standard two-dimensional lattices exact formulae are available for $\ln Z^I$, and there is no difficulty in calculating a substantial number of terms of $a_r^{(0)}$. This calculation has been much facilitated by a recent development due to Guttmann and Joyce (1972) (following a suggestion of Sykes). One of these authors (Joyce, 1974) has been able to determine differential equations for U_0^I in (1.40) from which the coefficients u_r can readily be found by means of a recurrence relation. Table IV lists the first 20 non-zero coefficients u_r for the standard two-dimensional lattices.

To calculate the zero field susceptibility for any net G we can make use of

TABLE III. Zero field $\ln Z_0^I$ coefficients $a_r^{(0)}$ for three-dimensional lattices (eqn. 1.40). (Data from Sykes *et al.*, 1972c; Sykes (private communication).)

| r/lattice | f.c.c. | b.c.c. | s.c. | d. |
|-----------|----------------------|------------|-------------------------|---------------------|
| 3 | 8 | — | — | — |
| 4 | 33 | 12 | 3 | — |
| 5 | 168 | — | — | — |
| 6 | 930 | 148 | 22 | 2 |
| 7 | 5664 | — | — | — |
| 8 | 37018 $\frac{1}{2}$ | 2496 | 187 $\frac{1}{2}$ | 3 |
| 9 | 254986 $\frac{2}{3}$ | — | — | — |
| 10 | 1 827768 | 52168 | 1980 | 24 |
| 11 | 13 520328 | — | — | — |
| 12 | 102 807720 | 1 242078 | 24044 | 69 |
| 13 | 795 503400 | — | — | — |
| 14 | 6279 937374 | 32 262852 | 319170 | 486 |
| 15 | | — | — | — |
| 16 | | 892 367762 | 4 514757 $\frac{3}{4}$ | 2087 $\frac{1}{2}$ |
| 17 | | | — | — |
| 18 | | | 67 003469 $\frac{1}{3}$ | 13678 $\frac{2}{3}$ |
| 19 | | | — | — |
| 20 | | | | 72420 |
| 21 | | | | — |
| 22 | | | | 466238 |

equation (1.12) which tells us that χ_0 is the sum of $\langle \sigma_i \sigma_j \rangle_0$ for all pairs i, j of the lattice. Each $\langle \sigma_i \sigma_j \rangle_0$ can be derived from a $\ln Z^I$ calculation for a net G' consisting of the original net G with an additional bond J' connecting i and j . We then have

$$\langle \sigma_i \sigma_j \rangle = \lim_{K' \rightarrow 0} \frac{\partial}{\partial K'} \ln Z^I(G') = \lim_{w' \rightarrow 0} \frac{\partial}{\partial w'} \ln Z^I(G'). \quad (2.26)$$

If we expand $\ln Z^I(G')$ in terms of bonded topologies as above, we need only take account of bondings with a single line along J' .

The graphs contributing to $\chi_0(G)$ can therefore be derived from stars by breaking the whole or part of any line joining two principal points. Examples of such graphs derived from a θ -topology are shown in Fig. 10. We denote all graphs of this type derived from a parent star s_i as $c_t(s_i)$. The $\kappa(s_i)$ can be calculated for the parent star s_i (with the dashed part corresponding to an interaction J') by one of the methods described above,

TABLE IV. Zero field coefficients u_r for two-dimensional lattices (eqn. 1.40).

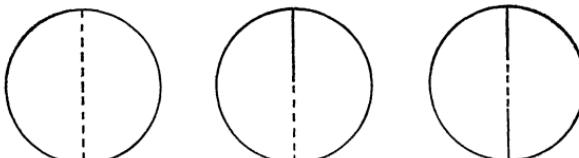
| $r/\text{lattice}$ | $\text{h.c.}(u_{2n})$ | $\text{s.q.}(u_{2n})$ | $\text{p.t.}(u_n)$ |
|--------------------|-----------------------|-----------------------|--------------------|
| 1 | 1.5 | | 3 |
| 2 | 0 | 4 | 6 |
| 3 | 3 | 8 | 12 |
| 4 | -3 | 24 | 24 |
| 5 | 15 | 84 | 54 |
| 6 | -24 | 328 | 138 |
| 7 | 93 | 1 372 | 378 |
| 8 | -180 | 6 024 | 1080 |
| 9 | 639 | 27 412 | 3186 |
| 10 | -1368 | 128 228 | 9 642 |
| 11 | 4 653 | 613 160 | 29 784 |
| 12 | -10 605 | 2 985 116 | 93 552 |
| 13 | 35 169 | 14 751 592 | 297 966 |
| 14 | -83 664 | 73 825 416 | 960 294 |
| 15 | 272 835 | 373 488 764 | 3 126 408 |
| 16 | -669 627 | 1 907 334 616 | 10 268 688 |
| 17 | 2 157 759 | 9 820 757 380 | 33 989 388 |
| 18 | -5 423 280 | 50 934 592 820 | 113 277 582 |
| 19 | 17 319 837 | 265 877 371 160 | 379 833 906 |
| 20 | -44 354 277 | 1 395 907 472 968 | 1 280 618 784 |

and expanded as a power series, the coefficient of w' being denoted by $\sigma[c_t(s_i)]$. If σ is now expanded as a power series in w , the coefficients of powers of w can conveniently be referred to as the χ -weights of $c_t(s_i)$, the coefficient of w^{l+m} being the $(m+1)$ th order χ -weight denoted by $w_\chi(c_t; m)$ (l is the number of lines in c_t). We then have as a parallel to (2.23)

$$a_r^{(2)} = \sum_{m \geq 0} (c_t(s_i); L) w_\chi(c_t; m) \quad (l = r - m) \quad (2.27)$$

the sum being taken over all derived graphs c_t of r lines or less. From the discussion of the previous paragraph we see that the χ -weights can be obtained from the set of bonding weights of star topologies.

The above procedure can be generalized to deal with $a_r^{(4)}$ and higher derivatives.

FIG. 10. Connected susceptibility graphs derived from a θ -topology.

For $a_r^{(4)}$ the contributing graphs can be derived from parent stars by breaking two sections of line joining principal points of the star. Again the appropriate weights can be obtained from the bonding weights of star topologies.

In practice, however, formulae like (2.27) have not been much used for calculating coefficients because of the difficulty of determining lattice constants of open graphs. For $a_r^{(2)}$ the method of the previous section has proved more useful, and for higher derivatives density expansions can be conveniently transformed as will be shown shortly. We shall later (Section II. B3) describe a procedure by which *all* series expansions for the simple Ising model can be expressed in terms of star lattice constants; this introduces complications in the weight calculations, but does offer the possibility of extending high temperature series expansions for the susceptibility and its derivatives.

4. General spin s

For spin s we use the Hamiltonian (1.3) and the partition function is given by (1.4) which we rewrite in the form

$$Z_{N,s}^I = \sum_{s_{zi}=-s}^s \prod_{\langle ij \rangle} \exp(4\bar{K}s_{zi}s_{zj}) \prod_i \exp(2\bar{L}s_{zi}) \quad (2.28)$$

where

$$\bar{K} = K/4s^2, \quad \bar{L} = \beta m H / 2s.$$

When $s = \frac{1}{2}$, \bar{K} is identical with K , and $\bar{L} = \beta m H$. To apply the primitive method we expand each term of the first product as follows:

$$\exp(4Ks_{zi}s_{zj}) = 1 + 4\bar{K}s_{zi}s_{zj} + \frac{(4\bar{K})^2}{2!}(s_{zi}s_{zj})^2 + \frac{(4\bar{K})^r}{r!}(s_{zi}s_{zj})^r + \dots \quad (2.29)$$

The reduction of all the terms of (2.29) to single-bonded graphs is possible only for $s = \frac{1}{2}$, and for general s multiply-bonded graphs must be taken into account. Relation (2.2) can be generalized, and means that for spin s all bondings of order $(2s+1)$ or more can be eliminated. For lower values of s (particularly $s = 1$) this transformation might produce a simplification, but

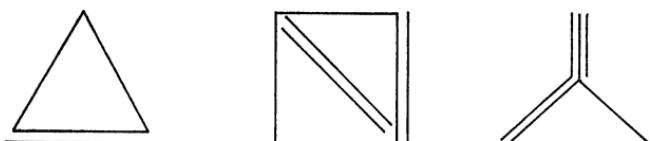


FIG. 11. Typical multiply-bonded graphs which enter into expansions for general s .

in practice it has not been much used. Typical multiply-bonded graphs which enter are shown in Fig. 11. For each such graph we identify a *silhouette* $g^{(s)}$ reducing all the multiple bonds to single bonds, and it is the lattice constant of $g^{(s)}$ which is relevant to the calculation.

When we substitute (2.29) into (2.28) and pick out the term in $(4\bar{K})^l$, we obtain a contribution from every possible multiply-bonded graph of l lines; every such graph is associated with an appropriate product of $s_{zi}, s_{zj}, \dots, s_{zk}$, there being one $s_{zi}s_{zj}$ for each bond. We must now multiply these products by $\exp(2\bar{L}s_{zi}) \dots$ and sum over values of $s_{zi} \dots$ equal to $-s, -(s-1), \dots, (s-1), s$.

It is convenient for this purpose to define

$$\begin{aligned} t_0 &= \sum_{s_{zi}=-s}^s \exp(2\bar{L}s_{zi}) = y^{-s} + y^{-(s-1)} + \dots + y^{(s-1)} + y^s \\ t_a &= \sum_{s_{zi}=-s}^s s_{zi}^a \exp(2\bar{L}s_{zi}) = s^a y^{-s} + (s-1)^a y^{-(s-1)} + \dots \\ &\quad (-s+1)^a y^{(s-1)} + (-s)^a y^s. \\ (y &= \exp - 2\bar{L} = \exp(-\beta mH/s)). \end{aligned} \quad (2.30)$$

Then in any multiply-bonded graph constructed from the N vertices of the net G each vertex of order zero gives rise to a factor t_0 , and each vertex which is the meeting point of a lines gives rise to a factor t_a . We denote as usual the lattice constant of the silhouette graph by $(g^{(s)}; G)$. Consider a configuration in which the bonds of g have multiplicities $\alpha, \beta, \gamma \dots$ and the vertices have multiplicities a, b, c, \dots [$\alpha + \beta + \gamma + \dots = \frac{1}{2}(a+b+c+\dots) = l$]. We can then write

$$Z_{N,s}^I = t_0^N \left[1 + \sum_{l=1}^{\infty} (\bar{K})^l \sum_{g^{(s)}, \alpha, \beta, \gamma} (g^{(s)}; G) \hat{t}_a \hat{t}_b \hat{t}_c \dots / \alpha! \beta! \gamma! \right] (\hat{t}_a = t_a / t_0). \quad (2.31)$$

In zero magnetic field \hat{t}_a are zero for odd a , and only configurations, all of whose vertices are even, contribute. For the zero field susceptibility, configurations with not more than two odd vertices contribute. To evaluate this susceptibility we must expand each \hat{t}_a as far as the second power of H and pick out the coefficient of H^2 in (2.31). The coefficients in these expansions are given by successive derivatives of $t_0 = \sinh(2s+1)\bar{L}/\sinh \bar{L}$ at $\bar{L}=0$ and can readily be obtained from the Taylor expansion of t_0

about $L = 0$. For example,

$$\hat{t}_1 = -\frac{2X}{3} L \quad (2.32)$$

$$\hat{t}_2 = \frac{X}{3} \left[1 + \frac{8X-6}{15} L^2 + \dots \right] \quad (2.33)$$

$$\hat{t}_3 = -\frac{2X}{3} \left[\frac{3X-1}{5} L + \dots \right] \quad X = s(s+1). \quad (2.34)$$

The zero-field partition function for a torus can be derived in the standard manner. We can conveniently write for the partition function *per site* in zero field by analogy with (1.40)

$$\ln Z_{0,s}^I = \ln(2s+1) + \frac{q}{2} \sum_{r=2}^{\infty} \hat{a}_r^{(0)}(s) \bar{K}^r / s^{2r} r! \quad (2.35)$$

and for the zero field susceptibility by analogy with (1.41)

$$\chi_{0,s} = \frac{\beta m^2(s+1)}{3s} \sum_{r=0}^{\infty} \hat{a}_r^{(2)}(s) \bar{K}^r / s^{2r}. \quad (2.36)$$

Early calculations by Domb and Sykes (1957a, 1962) using the primitive method determined $\hat{a}_r^{(0)}$ as far as $r = 8$, and $\hat{a}_r^{(2)}$ as far as $r = 6$ for a variety of lattices. These coefficients are reproduced for the f.c.c. lattice (for which convergence is most rapid) in Table V.

It would be feasible to proceed to a cumulant expansion, using the finite cluster method for deriving coefficients, and hence extending the above series appreciably. However, the free graph technique described by Wortis in Chapter 3 has proved more effective in tackling the problem of general spin s , and numerical values of the coefficients for higher r and for a variety of values of s are given in Table VI.

B. Density expansions

We have mentioned in Section I.C1(b) that these expansions parallel the cluster expansions for a condensing gas. We start from a zero energy state in which the spins are all aligned in a magnetic field, and consider at a given temperature the excited states corresponding to 1, 2, ... r ... overturned spins. The r overturned spins may all be connected or may consist of t disjoint groups; configurations arising for the case $r = 3$ are illustrated in Fig. 12. It will be seen that the energy of excitation of an individual over-

TABLE V. Zero-field $\ln Z_0^I$ and susceptibility coefficients for general spin s (eqns. 2.35 and 2.36). (Data from Domb and Sykes 1962.)

| | |
|---|---|
| $\hat{a}_2^{(0)}(s) = X^2/9$ | |
| $\hat{a}_3^{(0)}(s) = 8X^3/27$ | |
| $\hat{a}_4^{(0)}(s) = (X^2/225)(514X^2 - 116X + 1)$ | |
| $\hat{a}_5^{(0)}(s) = \left(\frac{48X^3}{405}\right)(184X^2 - 56X + 1)$ | |
| $\hat{a}_6^{(0)}(s) = (X^2/297675)(83599648X^4 - 36144288X^3 + 4664376X^2 - 118584X$ | + 675) |
| $\hat{a}_7^{(0)}(s) = (8X^3/14175)(7996592X^4 - 4275072X^3 + 817524X^2 - 35076X + 435)$ | |
| $\hat{a}_8^{(0)}(s) = (X^2/212625)(18568249616X^6 - 11735319488X^5 + 3100557664X^4$ | |
| | $- 343347552X^3 + 14868306X^2 - 246780X + 945)$ |
| $\hat{a}_0^{(2)}(s) = 1$ | |
| $\hat{a}_1^{(2)}(s) = 4X$ | |
| $\hat{a}_2^{(2)}(s) = (2X/5)(38X - 1)$ | |
| $\hat{a}_3^{(2)}(s) = (2X/75)(2124X^2 - 136X + 1)$ | |
| $\hat{a}_4^{(2)}(s) = (X/3150)(656648X^3 - 70772X^2 + 2322X - 15)$ | |
| $\hat{a}_5^{(2)}(s) = (X/330750)(251682608X^4 - 39096208X^3 + 2440236X^2 - 49104X$ | + 225) |
| $\hat{a}_6^{(2)}(s) = (X/1984500)(5480403392X^5 - 1125263472X^4 + 105206144X^3$ | |
| | $- 4607196X^2 + 79290X - 315)$ |

turned spin is $2mH + 2qJ$. However, for every bond between two overturned spins energy $2J$ is lost. Thus for a configuration of r overturned spins with m connecting bonds the energy of excitation is

$$2rmH + 2(qr - m)J , \quad (2.37)$$

and the corresponding Boltzmann factor is

$$(yz^q)^r z^{-2m} \quad (z = u^{\frac{1}{2}} = \exp - 2\beta J) . \quad (2.38)$$

The number of excited energy states of this kind is the number of different configurations with r spins and m bonds that can be constructed from the net G . This is precisely the sum of strong lattice constants $[g_r; G]$ of all graphs g_r with r vertices and m bonds (see this volume Chapter 1, Section IV.A2). As in the case of high temperature expansions we can employ a primitive method which uses all lattice constants, or a cumulant method which uses only connected lattice constants.

1. Primitive method

Using elementary counting procedures of the type described in an older

TABLE VI. Zero field $\ln Z_0^I$ and susceptibility coefficients for general spin s . Numerical values of higher coefficients†
(eqns 2.35 and 2.36).

| | $s = \frac{1}{2}$ | exponent | $s = 1$ | exponent | $s = 2$ | exponent | $s = \infty$ | exponent |
|-----------------------------|-------------------|----------|--------------|----------|--------------|----------|--------------|----------|
| $\hat{a}_9^{(0)} X^9$ | 7.4379 55596 | 05 | 1.3742 68026 | 06 | 1.7558 13494 | 06 | 1.9816 56984 | 06 |
| $\hat{a}_{10}^{(0)} X^{10}$ | 1.7732 73314 | 07 | 3.4442 32438 | 07 | 4.5138 62124 | 07 | 5.1651 89143 | 07 |
| $\hat{a}_{11}^{(0)} X^{11}$ | 4.7971 63396 | 08 | 9.7793 89933 | 08 | 1.3127 49781 | 09 | 1.5219 07693 | 09 |
| $\hat{a}_{12}^{(0)} X^{12}$ | 1.4521 50455 | 10 | 3.1039 34098 | 10 | 4.2632 38586 | 10 | 5.0045 41198 | 10 |
| $\hat{a}_{13}^{(0)} X^{13}$ | 4.8638 13992 | 11 | 1.0893 57606 | 12 | 1.5297 42374 | 12 | 1.8174 67603 | 12 |
| $\hat{a}_7^{(2)} X^7$ | 7.0798 48629 | 03 | 8.7743 92785 | 03 | 9.5604 80884 | 03 | 9.9790 38801 | 03 |
| $\hat{a}_8^{(2)} X^8$ | 2.3830 28081 | 04 | 3.0788 31315 | 04 | 3.4130 88269 | 04 | 3.5938 59837 | 04 |
| $\hat{a}_9^{(2)} X^9$ | 7.9944 21405 | 04 | 1.0770 68335 | 05 | 1.2150 60583 | 05 | 1.2908 46666 | 05 |
| $\hat{a}_{10}^{(2)} X^{10}$ | 2.6747 48676 | 05 | 3.7587 25793 | 05 | 4.3157 76041 | 05 | 4.6264 00504 | 05 |
| $\hat{a}_{11}^{(2)} X^{11}$ | 8.9294 79072 | 05 | 1.3090 72204 | 06 | 1.5300 29812 | 06 | 1.6551 08838 | 06 |
| $\hat{a}_{12}^{(2)} X^{12}$ | 2.9755 92746 | 06 | 4.5514 82885 | 06 | 5.4198 12170 | 06 | 5.9121 71481 | 06 |

†(Private communication from Professor M. Wortis. The final entries may contain a small systematic error but this should not affect exponent and amplitude analysis.)



FIG. 12. Low-temperature configurations of three overturned spins.

review article (Domb, 1960; see also this volume Chapter 1, Section IV.A) we easily derive the following results for the first three terms in the expansion of Z_N^I for a torus in powers of y :

$$Z_N^I = y^{-N/2} z^{-qN/4} \left[1 + \sum_{r=1} y^r F_r(N, z) \right], \quad (2.39)$$

$$F_1(N, z) = Nz^q$$

$$F_2(N, z) = \frac{q}{2} N(z^{2q-2}) + \frac{N(N-q-1)}{2!} z^{2q}$$

$$\begin{aligned} F_3(N, z) &= NP_3 z^{3q-6} + N \left[\frac{q(q-1)}{2} - 3P_3 \right] z^{3q-4} \\ &\quad + N \left[\frac{Nq}{2} - q^2 + 3P_3 \right] z^{3q-2} \\ &\quad + N \left[\frac{q^2}{2} - P_3 - \frac{(N-1)q}{2} + \frac{(N-1)(N-2)}{3!} \right] z^{3q} \end{aligned} \quad (2.40)$$

Here P_3 is the strong lattice constant for a triangle ($= p_3$ the weak lattice constant). We have arranged the terms in (2.40) so that they can readily be identified with the appropriate configurations in Fig. 12.

Taking the coefficient of N in (2.40) in the standard manner to obtain $\ln Z^I$, we find that, for the expansion (1.43),

$$g_1(u) = u^{q/2}$$

$$g_2(u) = \frac{q}{2} u^{q-1} - \frac{q+1}{2} u^q$$

$$\begin{aligned} g_3(u) &= p_3 u^{3q/2-3} + \left[\frac{q(q-1)}{2} - 3p_3 \right] u^{3q/2-2} \\ &\quad + (3p_3 - q^2) u^{3q/2-1} + \left[\frac{q(q+1)}{2} - p_3 + \frac{1}{3} \right] u^{3q/2} \end{aligned} \quad (2.41)$$

We may note that, if we wish, we can take account of the energy configuration in which all spins point in the opposite direction. The complete partition function is in fact

$$Z_N^I = z^{-qN/4} \left[(y^{-N/2} + y^{N/2}) + \sum_{r=1} \left(y^{-N/2+r} + y^{N/2-r} \right) F_r(N, z) \right] \quad (2.42)$$

We easily see that when $y = 1$ the introduction of the second energy state of aligned spins multiplies Z_N^I by 2; when $y < 1$ it produces terms which are asymptotically negligible. The form (2.42) is useful for tracing in configurational terms how the discontinuity in spontaneous magnetization arises as $N \rightarrow \infty$ (Domb, 1960).

2. Relationship with high temperature expansions

By examining the behaviour of expansions (1.43), (2.41) near $u = 1$, Domb (1949) showed that they could be used to derive high temperature expansions. At the same time the form of the high temperature expansion enabled a good deal of configurational information about the lattice constants of disjoint clusters to be supplied automatically. To apply the method we first put $u = 1 - \zeta$ in (2.41) and examine the behaviour near $\zeta = 0$ as a power series in ζ .

Using expansion (1.40), the term independent of ζ is seen to be

$$y - \frac{y^2}{2} + \frac{y^3}{3} \dots \quad (2.43)$$

and we can reasonably conjecture that this sums to $\ln(1+y)$. The coefficient of ζ is

$$-\frac{q}{2} \left[y - 2y^2 + 3y^3 \dots \right], \quad (2.44)$$

which indicates a sum

$$-\frac{q}{2} \frac{y}{(1+y)^2}. \quad (2.45)$$

Proceeding similarly we are led to a general form as an expansion in

$$\ln Z^I = -\frac{1}{2} \ln y - \frac{q}{8} \ln u + \ln(1+y) + \sum_{r=1} \frac{\phi_r(y)^r}{(1+y)^{2r}}. \quad (2.46)$$

The symmetry of the model in regard to inversion of magnetic field enables the relation

$$\phi_r(y^{-1}) = y^{-2r} \phi_r(y) \quad (2.47)$$

to be deduced.

In fact this form (2.46) to which we have been led by conjecture can be readily derived from (1.39) if we replace τ by $(1-y)/(1+y)$ and w by $[1 - (1 - \zeta)^{\frac{1}{2}}] / [1 + (1 - \zeta)^{\frac{1}{2}}]$; the symmetry condition (2.47) corresponds to the configurational property in (2.5) that only even powers of τ occur. Thus the conjectured form is substantiated. However we see from (2.43) that we know exactly the value of $g_r(1)$ for all r and from (2.45) the value of $g_r'(1)$ for all r , and so on. Any information about $\psi_r(\tau)$ in (1.39) can be reflected back to $g_r(u)$ and vice-versa; for example in two dimensions knowledge of the exact coefficients $\psi_r(0)$ can help to extend the $g_r(u)$. We therefore have a useful device for exchanging configurational data between density and high temperature series.

The method has been generalized by Ferer (1970) to spin $s > \frac{1}{2}$ and to longer range interactions. This generalization is also contained in the thesis of M. F. Sykes (1956).

3. Relationship with the Mayer theory

It was pointed out in Section I.B4 that a lattice gas is equivalent to an Ising ferromagnet. For a lattice gas we can use the Mayer development described in Chapter 1 of this volume, Section III. Hence the Ising model expansions can also be cast into Mayer form, and the cluster integrals can be evaluated to quite a high order.

We start from a state of aligned spins and each overturned spin corresponds to a gas particle. Our first identifications from Chapter 1 eqn. (3.7) and (M.1) are

| <i>Mayer</i> | <i>Ising</i> | |
|----------------------------|---------------------|---------------------------|
| $\lambda' (= \lambda\eta)$ | yz^q | |
| N | N_- | (No. of overturned spins) |
| V | N | |
| $\Xi(\lambda, V, T)$ | $\Lambda_N^I(y, T)$ | (see 1.16) |

The variables describing the interaction are defined in Chapter 1 eqn. (3.3); for the specific case of a lattice gas we use Chapter 1 eqn. (4.43) with

$$h_i = 1 \quad \text{and} \quad f_{ij} = -\delta(\mathbf{r}_i - \mathbf{r}_j) + f \sum_{\mathbf{a}} \delta(\mathbf{r}_i - \mathbf{r}_j - \mathbf{a}), \quad (2.49)$$

$$1 + f = z^{-2} = u^{-1}, \quad (2.50)$$

\mathbf{a} being any unit vector of the lattice, and $\mathbf{r}_i, \mathbf{r}_j$ any two lattice sites.

The interaction (2.49) has only two non-zero values, and the evaluation of a contribution to a cluster integral from a connected graph of l lines is reduced to a sum of 2^l terms. In evaluating such a contribution directly it is convenient to follow the terminology of Temperley (1959) and refer to a “- 1”

interaction as a *pin* and an “*f*” interaction as a *link*. The summation over all lattice sites introduces lattice constants, and instead of cluster integrals we are led to *cluster sums* (Fuchs, 1942). Instead of (M.1) of Chapter 1 we have

$$\frac{1}{N} \ln \Lambda_N = \sum_p b_p(N, T) (yz^q)^p, \quad (2.51)$$

where $b_p(N, T)$ should tend to limit $b_p(T)$ as $N \rightarrow \infty$ following (M.1e) of Chapter 1. Comparing with (1.43) we find that

$$b_p(T) = u^{-pq/2} g_p(u). \quad (2.52)$$

We illustrate this relationship by calculating the first three terms of the series using (3.13) of Chapter 1.

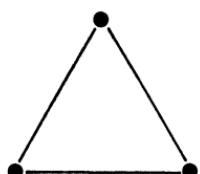
(i) Clearly

$$b_1(T) = 1. \quad (2.53)$$

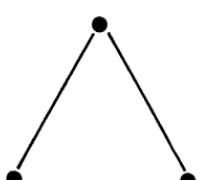
(ii) For $b_2(T)$ we must calculate . When the interaction is a link we obtain f , and when it is a pin we obtain -1 . There are $Nq/2$ links in the lattice (weak lattice constant of  each of which must be counted twice because of the interchange of sites for the two variables in the integral. We therefore have

$$b_2(T) = -\frac{1}{2} + \frac{q}{2}f. \quad (2.54)$$

(iii) There are two connected graphs contributing to $b_3(T)$ and we shall break down the contributions into the appropriate number of pins and links



| | |
|---------------|--|
| 3 pins | $-\frac{1}{6}$ |
| 1 pin 2 links | $-\frac{q}{2}f^2$ |
| 3 links | $p_3 f^3$ |
| 2 pins | $\frac{1}{2}$ |
| 1 pin 1 link | $-qf$ |
| 2 links | $\frac{q(q-1)}{2}f^2 + \frac{q}{2}f^2$ |



Hence

$$b_3(T) = \frac{1}{3} - qf + \frac{q(q-1)}{2}f^2 + p_3 f^3. \quad (2.55)$$

Using (2.52) and (2.50) it can readily be shown that (2.41) gives the same result as (2.53), (2.54), and (2.55), but the latter are much simpler in form.

An important feature of formula (M.1) is its applicability to finite volumes V . Correspondingly the Ising analogue is applicable to a finite net G but in the form (2.51) this would be valid only for a *homogeneous* net in which all vertices have the same co-ordination number q . For a more general net we must use the multinomial analogue (M.9) to give (taking two types of vertex as an example)

$$\frac{1}{N} \ln \Lambda_N = \sum_{p_1, p_2} b_{p_1 p_2}(N, T) (yz^{q_1})^{p_1} (yz^{q_2})^{p_2}. \quad (2.56)$$

We can transform (2.51) into a weak lattice constant expansion, which will lead to an analogue of the finite cluster expansion (2.19). In fact we need only group together in $b_p(N, T)$ all terms which use a particular link *at least once*, a particular pair of connected links *at least once*, and so on. For example, we could break down $b_3(T)$ into

$$b_3(T) = \frac{1}{3} (\bullet) - 2f (\bullet \text{---} \bullet) + f^2 \left(\begin{array}{c} \bullet \\ \bullet \backslash \diagup \bullet \\ \bullet \end{array} \right) + f^3 \left(\begin{array}{c} \bullet \\ \bullet \backslash \diagup \bullet \\ \bullet \end{array} \right) \quad (2.57)$$

Summing over all the $b_p(N, T)$ in (2.51) we obtain

$$\ln \Lambda(G) = \sum_i (c_i; G) \kappa_i(\lambda', T) \quad (\lambda' = yz^q) \quad (2.58)$$

for a homogeneous net, with an appropriate generalization in $\lambda'_1, \lambda'_2, \dots$ for an inhomogeneous net.

The weight functions $\kappa_i(\lambda', T)$ can be determined by evaluating $\Lambda(G)$ for finite clusters, and subgraph subtraction. However, a little care is necessary for inhomogeneous nets and we shall illustrate the evaluation by calculating the weight functions for the first few connected graphs

$$c_1 \quad c_2 \quad c_3 \quad c_4 \quad (2.59)$$

The partition function for a single isolated spin ($q = 0$) is

$$1 + y. \quad (2.60)$$

Hence we have

$$\kappa_1(\lambda', T) = \ln(1 + \lambda') = \lambda' - \frac{\lambda'^2}{2} + \frac{\lambda'^3}{3} - \frac{\lambda'^4}{4} \dots \quad (2.61)$$

The partition function for a pair of spins ($q = 1$) is

$$1 + 2yz + y^2. \quad (2.62)$$

Hence subtracting subgraphs

$$\begin{aligned} \kappa_2(\lambda', T) &= \ln [1 + 2\lambda' + \lambda'^2(1 + f)] - 2 \ln (1 + \lambda') \\ &= \ln [1 + f\lambda'^2/(1 + \lambda')^2] = \lambda'^2f - 2\lambda'^3f + \lambda'^4(3f + 2f^2) + \dots . \end{aligned} \quad (2.63)$$

For c_3 there are two types of point having $q_1 = 1, q_2 = 2$. The partition function is

$$\begin{aligned} 1 + (2y_1z + y_2z^2) + (y_1^2z^2 + 2y_1y_2z) + y_1^2y_2 \\ = 1 + (2\lambda'_1 + \lambda'_2) + [\lambda'^2_1 + 2\lambda'_1\lambda'_2(1 + f)] + \lambda'^2_1\lambda'_2(1 + f)^2. \end{aligned} \quad (2.64)$$

However, in the application in which we are interested all points are equivalent and we can put $\lambda'_1 = \lambda'_2 = \lambda'$. The differentiation between q_1 and q_2 is needed only in order to derive (2.64). (This may be seen more readily by considering a diagrammatic breakdown of contributions to $\kappa_2(\lambda', T)$). We therefore find

$$\begin{aligned} \kappa_3(\lambda', T) &= \ln [1 + 3\lambda' + (3\lambda'^2 + 2\lambda'^2f + \lambda'^3(1 + 2f + f^2))] \\ &\quad - 2\kappa_2(\lambda', T) - 3\kappa_1(\lambda', T) \\ &= \ln \left[1 + \frac{2f\lambda'^2}{(1 + \lambda')^2} \quad \frac{\lambda'^3f^2}{(1 + \lambda')^3} \right] - 2 \ln \left[1 + \frac{\lambda'^2f}{(1 + \lambda')^2} \right] \\ &= \lambda'^3f^2 - 4\lambda'^4f^2 + \dots . \end{aligned} \quad (2.65)$$

Finally, $\kappa_3(\lambda', T)$ is readily obtained from the partition function for a triangle

$$1 + 3\lambda' + 3\lambda'^2(1 + f) + \lambda'^3(1 + f)^3. \quad (2.66)$$

An example of particular interest is the weight function $\kappa(c_n; \lambda', T)$ for a simple chain c_n . We know from Chapter 1 eqn. (4.62) that this is given by

$$\ln \Lambda(c_n) = 2 \ln \Lambda(c_{n-1}) + \ln \Lambda(c_{n-2}). \quad (2.67)$$

The partition function of a linear Ising chain can easily be calculated in terms of the eigenvalues ξ_1, ξ_2 of a 2×2 matrix (Thompson Vol. 1, Chapter 5); and in our case these are given by $A \pm \sqrt{B}$ where

$$\left. \begin{aligned} A &= 1 + \lambda'(1 + f) = 1 + \lambda' z^{-2} \\ B &= (1 - \lambda' z^{-2})^2 + 4\lambda' \end{aligned} \right\}. \quad (2.68)$$

We shall see in Section III.B7 that (2.68) can be of help in elucidating the analytic behaviour of low temperature series (Domb and Guttman, 1970).

So far we have dealt only with the development in terms of reducible cluster integrals which has led to the expansion (2.58) in terms of connected lattice constants. We might expect that a transformation to the density ρ as an independent variable which gives rise to the Mayer irreducible cluster integrals would lead to an expansion in terms of star lattice constants. This is indeed the case, but the determination of the weight functions $\kappa_i(\rho, Y)$ needs special attention and we shall now consider this in more detail.

4. Star lattice constant expansion

The second stage in the Mayer theory development, Chapter 1, Section III.B, hinges on the relationship given by Chapter 1 eqn. (3.15) which for a normal continuum gas restricts the application to the thermodynamic limit $V \rightarrow \infty$. However, for the application to a lattice gas the relationship is satisfied for any homogeneous cluster, i.e. one in which all vertices are equivalent. We then have relations M4–M8 satisfied (Chapter 1), and the β_k can be calculated directly in the same way as the b_k . (In practice it is often more convenient to deal with the B_k given by (M6a), and the β_k are retained largely for historic reasons.) Following the method used for the b_k we find that

$$\left. \begin{aligned} B_2 &= \frac{\beta_1}{2} = \frac{q}{2} f - \frac{1}{2} \\ B_3 &= \frac{\beta_2}{3} = p_3 f^3 - \frac{q}{2} f^2 - \frac{1}{6}. \end{aligned} \right\} \quad (2.69)$$

Transforming (M5) into Ising model language by (2.48) we have

$$\frac{1}{N} \ln \Lambda_N^I(\rho, T) = \rho - \sum_{k=1}^{\infty} k B_{k+1}(T) \rho^{k+1} \quad (2.70)$$

where ρ is the density of overturned spins given from (1.30) by

$$\rho = \frac{y}{N} \frac{\partial}{\partial y} \ln \Lambda_N^I = \frac{\lambda'}{N} \frac{\partial}{\partial \lambda'} \ln \Lambda_N^I \quad (\lambda' = yz^q). \quad (2.71)$$

As before we can group the $B_k(T)$ into contributions which use every line of a particular lattice constant at least once, and hence obtain an expansion of the type (2.58). We now apply the important theorem of

Rushbrooke and Scoins (1955) that *the weight functions $\kappa_r(\rho, f)$ corresponding to any articulated lattice constant are zero*. This was proved by showing that all irreducible diagrams using the vertices of an articulated lattice constant cancel in pairs. The expansion analogous to (2.58) is then a star lattice constant expansion which is valid for any homogeneous graph G ,

$$\ln \Lambda^I(G) = \sum_r (s_r; G) \kappa_r(\rho, T), \quad (2.72)$$

the sum being taken over all star subgraphs s_r of G . It has already been noted in Chapter 1 that if we use a line grouping rather than a point grouping the saving in eliminating articulated graphs is very substantial. Hence the formula (2.72) can be of great help for series expansions if we can solve the problem of calculating the weights $\kappa_r(\rho, T)$.

For simple polygons this does not give rise to any particular difficulty, and formulae for calculating the weights were derived by Rushbrooke and Scoins (1955) as follows. For a single point (see 2.60)

$$\left. \begin{aligned} \Lambda^I &= 1 + y = 1 + \lambda' \\ \rho &= \lambda'/(1 + \lambda'). \end{aligned} \right\} \quad (2.73)$$

Hence transforming to ρ as variable we obtain

$$\kappa_1(\rho, T) = \ln(1 - \rho). \quad (2.74)$$

Using (2.70) we see that the single point contribution to $B_k(T)$ is $-1/k(k - 1)$.

For the graph  (see 2.62) we find that

$$\left. \begin{aligned} \ln \Lambda^I &= \ln [1 + 2\lambda' + \lambda'^2(1 + f)] \\ \rho &= \frac{\lambda' + \lambda'^2(1 + f)}{1 + 2\lambda' + \lambda'^2(1 + f)} \end{aligned} \right\} \quad (2.75)$$

From this we can derive the result

$$\begin{aligned} \kappa_2(\rho, T) &= \ln [1 - \rho + \frac{1}{2}(1 + f)^{-1}(2\rho - 1 + \xi)] \\ (\xi^2 &= 1 + 4\rho(1 - \rho)f). \end{aligned} \quad (2.76)$$

However, for practical calculation of the contribution to $B_k(T)$ it is usually more convenient to invert (2.75) obtaining λ' as a power series in ρ , and then use (M.4) (Chapter 1)

$$\ln \lambda' = \ln \rho - \sum_{k=1}^{\infty} \beta_k \rho^k. \quad (2.77)$$

It is worth noting that relation (2.77) is particularly useful in the magnetic context since it represents the magnetic equation of state $H(M, T)$. From the form of the equation we see that only star lattice constants enter, and it is not surprising that this turns out to provide the most convenient form of the equation of state for many practical purposes (see Section III.C). Series expansions use the variable ρ rather than M since they start from a configuration of aligned spins. The relation between the variables is

$$\frac{M}{Nm} = 1 - 2\rho. \quad (2.78)$$

For an n -gon the procedure is similar using

$$\ln \Lambda_n = \ln(\Lambda_1'' + \Lambda_2''), \quad (2.79)$$

$$\frac{\Lambda_1}{\Lambda_2} = \frac{1}{2}\{1 + y \pm \sqrt{[(1 - y)^2 + 4yz^2]}\}.$$

To obtain $\kappa_n(\rho, T)$ we must remember to subtract from $\ln \Lambda_n$ the subgraph contributions $n\kappa_2(\rho, T) + n\kappa_1(\rho, T)$.

We can, incidentally, show how the above developments enable us to solve a non-trivial configurational problem of evaluating the terms in (2.41) corresponding to a "Bethe lattice" (Domb, 1960, Fig. 13) which has no closed circuits. For such a lattice

$$\frac{1}{N} \ln \Lambda_N^I = \kappa_1(\rho, T) + \frac{q}{2} \kappa_2(\rho, T) \quad (2.80)$$

and the $\beta_k(T)$ are readily determined. Relation (M7) of Chapter 1 then enables the $b_p(T)$ to be calculated and hence $g_p(u)$ from (2.52).

However, the method fails for inhomogeneous clusters. The appropriate generalization, using multicomponent Mayer formulae, was suggested by Yvon (1945, 1948) and developed by Domb and Hiley (1962). (The method was applied by Fournet to a number of problems as a closed form approximation method, see Burley, Vol. 2 Chapter 9.).

Suppose we have a ferrimagnetic Ising model (Section I.B2). We can relate this to a two component lattice gas by a simple generalization of the procedure for a single component lattice gas. We have already made use of this idea in an elementary way in the previous section. In fact, the two components can differ from one another in magnetic moment and co-ordination number, and in this general case we write

$$\lambda_1' = \mu_+ y_+^{q_1}, \quad \lambda_2' = \mu_- y_-^{q_2}; \quad (2.81)$$

equation (2.56) remains valid. Let N_+ , N_- be the number of spins of each

type and let n_+ , n_- be the corresponding numbers overturned from the state of complete alignment, so that

$$\begin{aligned} n_+ &= N_+ - \sum_i \langle \sigma_{i+} \rangle = y_+ \frac{\partial}{\partial y_+} \ln \Lambda_N^I \\ n_- &= N_- - \sum_i \langle \sigma_{i-} \rangle = y_- \frac{\partial}{\partial y_-} \ln \Lambda_N^I. \end{aligned} \quad (2.82)$$

Define

$$a_1 = \frac{n_+}{N_+}, \quad a_2 = \frac{n_-}{N_-}, \quad \rho_1 = \frac{n_+}{N}, \quad \rho_2 = \frac{n_-}{N}. \quad (2.83)$$

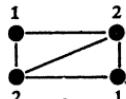
Then (M.15) of Chapter 1 gives

$$\frac{1}{N} \ln \Lambda_N^I(\rho_1, \rho_2, T) = \rho_1 + \rho_2 + \sum_{k_1, k_2} (k_1 + k_2 - 1) B_{k_1 k_2} \rho_1^{k_1} \rho_2^{k_2} \quad (k_1 + k_2 \geq 2), \quad (2.84)$$

and (M.13) and (M.14) remain unchanged,

$$\begin{aligned} \ln \lambda_1' &= \ln \rho_1 - \sum_{k_1, k_2} k_1 B_{k_1 k_2} \rho_1^{k_1-1} \rho_2^{k_2} \\ \ln \lambda_2' &= \ln \rho_2 - \sum_{k_1, k_2} k_2 B_{k_1 k_2} \rho_1^{k_1} \rho_2^{k_2-1}. \end{aligned} \quad (2.85)$$

Equations (2.83), (2.84) and (2.85) enable us to calculate the $B_{k_1 k_2}$ for inhomogeneous clusters. For example, if we take $(1,2,2)_\theta = p_{5a}$



the equations determining ρ_1, ρ_2 in terms of λ_1', λ_2' are

$$\begin{aligned} \Lambda^I(G) &= 1 + 2\lambda_1' + 2\lambda_2' + \lambda_1'^2 + z^{-2}\lambda_2'^2 + 4z^{-2}\lambda_1'\lambda_2' + 2z^{-4}\lambda_1'^2\lambda_2', \\ &\quad + 2z^{-6}\lambda_1'\lambda_2'^2 + z^{-10}\lambda_1'^2\lambda_2'^2 \end{aligned} \quad (2.86)$$

$$2\rho_1 = a_1 =$$

$$\frac{\lambda_1' + \lambda_1'^2 + 2z^{-2}\lambda_1'\lambda_2' + 2z^{-4}\lambda_1'^2\lambda_2' + z^{-6}\lambda_1'\lambda_2'^2 + z^{-10}\lambda_1'^2\lambda_2'^2}{\Lambda^I(G)}$$

$$2\rho_2 = a_2 =$$

$$\frac{\lambda_2' + z^{-2}\lambda_2'^2 + 2z^{-2}\lambda_1'\lambda_2' + 2z^{-6}\lambda_2'^2\lambda_1' + z^{-4}\lambda_2'\lambda_1'^2 + z^{-10}\lambda_1'^2\lambda_2'^2}{\Lambda^I(G)}$$

If these are inverted the $B_{k_1 k_2}$ can be read off from (2.85).

For many applications it is more convenient to use the variables a_1 and a_2 . The condition of homogeneity is

$$\begin{aligned} a_1 = a_2 &= \rho, \\ \rho_1 = \frac{N_+}{N} a_1, \quad \rho_2 = \frac{N_-}{N} a_2, \end{aligned} \tag{2.87}$$

and the condition of zero magnetic field even for a heterogeneous system is

$$a_1 = a_2 = \frac{1}{2}. \tag{2.88}$$

To obtain the $B_k(T)$ from the $B_{k_1 k_2}(T)$ for a homogeneous system, we use condition (2.87) and sum over all k_1 and k_2 satisfying $k_1 + k_2 = k$. Domb and Hiley (1962) calculated $B_k(\rho)$ for a general lattice for $k = 2$ to 6; these results are given in Table VII (taken from Hiley, 1963). We should also mention that Rushbrooke and Scoins (1962) used a direct method of calculation as in (2.69) to obtain β_k for loose packed lattices from $k = 1$ to 7. The results are not given in lattice constant form but as numerical tables for the s.q., s.c. and b.c.c. lattices.

Of particular importance are the applications of the method to high temperature series expansions for the susceptibility and its derivatives. Our discussion has shown that the equation of state

$$H = H(M, T) \tag{2.89}$$

contains only star lattice constants. From this we conclude that the high temperature expansions for

$$\left(\frac{\partial H}{\partial M} \right)_0, \left(\frac{\partial^3 H}{\partial M^3} \right)_0, \left(\frac{\partial^5 H}{\partial M^5} \right)_0 \dots$$

will contain only star lattice constants. Using the standard inversion formulae (Riordan, 1958, Chapter 2.8) we find that $1/\chi_0, \chi_0^{(2)}/\chi_0^4, \chi_0^{(4)}/\chi_0^6 - 10\chi_0^{(2)2}/\chi_0^7, \dots$ should have star lattice constant expansions. (Here $\chi_0^{(s)} = d^s \chi_0 / dH^s$.)

We consider particularly the susceptibility, χ_0 , and write it in the form

$$\frac{2m^2}{kT\chi_0} = \frac{2}{\chi_0(w)} = 2 - \frac{2qw}{1+w} + p_3\xi_3(w) + p_4\xi_4(w) + p_{5a}\xi_{5a}(w) + \dots \tag{2.90}$$

(we have chosen the form of the expansion (2.90) to conform with Domb and Hiley, 1962). The term corresponding to \bullet — \bullet has been evaluated by the

TABLE VII. Irreducible cluster sums for the f.c.c. lattice (eqns. 2.69 and 2.70)

| | | | | |
|--|---|---|---|---|
| $B_2 = \frac{\beta_1}{2} = -\frac{1}{2} + \frac{q}{2}f$ | $B_3 = \frac{\beta_2}{3} = -\frac{1}{6} - \frac{q}{2}f^2 + p_3 f^3$ | $B_4 = \frac{\beta_3}{4} = -\frac{1}{12} + \frac{q}{12}(10f^3 + 3f^2) - 3p_3(2f^4 + f^3) + p_4 f^4 + p_{5a} f^5 + p_{6a} f^6$ | $B_5 = \frac{\beta_4}{5} = -\frac{1}{20} - \frac{q}{4}(7f^4 + 4f^3) - \frac{3p_3}{2}(f^6 - 18f^5 - 16f^4 - 2f^3) - 4p_4(2f^5 + f^4) - 4p_{5a}(3f^6 + 2f^5) - 12p_{6a}(f^7 + f^6) + p_5 f^5 + \sum_{l=6}^8 p_{lx} f^l$ | $B_6 = \frac{\beta_5}{6} = -\frac{1}{30} + \frac{q}{30}(126f^5 + 105f^4 + 10f^3) + 3p_3\left(7f^7 - \frac{97}{3}f^6 - 45f^5 - 12f^4 - \frac{1}{3}f^3\right) + 4p_4\left(11f^6 + 10f^5 + \frac{3}{2}f^4\right) + p_{5a}(-6f^8 + 85f^7 + 107f^6 + 26f^5) + 2p_{6a}(31f^6 + 75f^7 + 27f^8 - 6f^9) - 5p_5(f^5 + 2f^6) - 3p_{6a}(3f^6 + 4f^7) - p_{6b}(9f^6 + 14f^7) - p_{7c}(13f^7 + 18f^8) - p_{7g}(17f^7 + 20f^8) - p_{7h}(13f^7 + 14f^9) - 16p_{8u}(f^8 + f^9) + p_6 f^6 + \sum_{l=7}^{12} p_{lx} f^l$ |
| $p_1 \equiv (l)_p; \quad p_{5a} \equiv (1,2,2)_q; \quad p_{6a} \equiv (1,1;1,1;1,1)_x; \quad p_{6b} \equiv (2,2,2)_\theta; \quad p_{7c} \equiv (1,2,3)_\theta; \quad p_{7g} \equiv (1,2;1,2;1)_v; \quad p_{7h} \equiv (1,2,2,2)_\delta;$ | $p_{7h} \equiv (1,1;1,1;1,2)_x; \quad p_{8q} \equiv (1,1;1,1;1,2)_j; \quad p_{8u} \equiv (1,1,1;1,1,1)_F$ | | | |
| F graph | For convenience we also list the graphs in terms of homeomorphic classification (Chapter 1, eqn. 2.10): | | | |

Here the $\sum p_{lx}$ in B_k refers to star graphs with l lines and k vertices. The notation follows Domb (1960) except for p_{8u} which is the

F graph

method of homogeneous clusters, and for a polygen it is easy to show that

$$\xi_n(w) = \frac{4nw^n(1-w)}{(1+w)(1-w^n)}. \quad (2.91)$$

We wish to show how to obtain the $\xi_{nx}(w)$ for non-homogeneous clusters.

Consider a cluster with N_1 points of type 1, N_2 points of type 2, ... N_r points of type r . The contribution of this cluster to $2/\chi_0(w)$ is given by

$$\frac{\partial}{\partial \rho} [\ln \Lambda_G(\rho_1, \rho_2, \dots, \rho_r)]_{\alpha_1=\alpha_2, \dots} = \rho = \frac{1}{2} = \sum_{i=1}^r \frac{N_i}{N} \frac{\partial}{\partial \rho_i} [\ln \Lambda_G]_{\alpha_i=\frac{1}{2}}. \quad (2.92)$$

The $(\partial/\partial \rho_i) [\ln \Lambda_G]$ in (2.92) must be determined in terms of the $(\partial/\partial \lambda'_i) [\ln \Lambda_G]$ from the transformation of variables

$$\lambda'_i \frac{\partial}{\partial \lambda'_i} [\ln \Lambda_G] = \rho_i. \quad (2.93)$$

Following the standard methods of Jacobians it is a straightforward matter to establish the following procedure. Define a determinant χ_{ij} with elements

$$\begin{aligned} \chi_{ii} &= \frac{1}{2} N_i + \frac{\partial^2}{\partial \lambda_i'^2} (\ln \Lambda_G) \\ \chi_{ij} &= \frac{\partial^2}{\partial \lambda_i' \partial \lambda_j'} (\ln \Lambda_G) \quad (i \neq j). \end{aligned} \quad (2.94)$$

Here χ_{ii} and χ_{ij} can be regarded as partial susceptibilities

$$\begin{aligned} \chi_{ii} &= \sum d_l^{(ii)} w^l / Y_G^I \\ \chi_{ij} &= \frac{1}{2} \sum d_l^{(ij)} w^l / Y_G^I \quad (i \neq j) \end{aligned} \quad (2.95)$$

where the $d_l^{(ij)}$ are magnetic graphs (see Section II.A1) with two odd vertices at points of type (i,j) and Y_G^I is the partition function of the cluster without the $2^N(\cosh K)^L$ term. Let Δ represent the determinant $|\chi_{ij}|$. Then (2.92) is given by

$$\frac{1}{N\Delta} \sum_{i,j=1}^r N_i N_j \partial \Delta / \partial \chi_{ij}. \quad (2.96)$$

This method has been successfully used by D. C. Rapaport (1973) to add an additional term to the high temperature expansion for χ_0 for the f.c.c. lattice. Work is currently in progress at King's College to extend the applications further.

C. Density and low temperature expansions. Shadow lattice and code method

The primitive approach described in Section II.B1,2 was used during the early period to derive polynomials $g_s(u)$ for a number of standard two- and three-dimensional lattices. Thus for example Domb and Sykes (1956) gave numerical values for the following s :-

$$\text{s.q. } s \leq 8, \text{ p.t. } s \leq 6, \text{ s.c. } s \leq 8, \text{ b.c.c. } s \leq 6, \text{ f.c.c. } s \leq 5.$$

In principle the star lattice constant expansion of Section II.B4 should have led to considerable further progress, but in practice the calculation of weights proved extremely difficult. An effective method of tackling this problem has only recently begun to emerge.

Instead an idea put forward by Sykes *et al.* in 1965 has led to a substantial extension of the earlier data. The method was initially concerned with the general ferrimagnetic problem on "even" lattices like the s.q., h.c., s.c., b.c.c., and d. Subsequently relationships developed between the h.c. and p.t. lattices and between the d. and f.c.c. lattices enabled the method to be put to practical use for the close-packed lattices.

To introduce the method we start with formula (1.54) for a ferrimagnet, and taking out the zero energy terms we write

$$\ln \Lambda = \sum_{s,t=1}^{\infty} y_+^s y_-^t g_{st}(u). \quad (2.97)$$

The combinatorial problem to be solved in deriving polynomials $g_{st}(u)$ is the number of ways of choosing $s + t$ sites with r first-neighbour bonds between them. This number will be a polynomial in N and we denote the coefficient of N by $[s, t; r]$. We then have

$$g_{st}(u) = \sum_{s,t,r} [s,t;r] u^{\frac{1}{4}qs + \frac{1}{4}qt - r}. \quad (2.98)$$

It is convenient to define a generating function

$$G(X, Y, b) = \sum_{s,t,r} [s,t;r] X^s Y^t b^r, \quad (2.99)$$

and a knowledge of G would be equivalent to a complete solution of the problem. We introduce partial generating functions which are equivalent to the solution of the problem when the number of overturned spins on one sublattice is held constant. Owing to the symmetric equivalence of the two sublattices a knowledge of the first n partial generating functions

enables the values of all $[s,t;r]$ with $s+t \leq 2n+1$ to be derived. Explicitly we write

$$G(X, Y, b) = \sum_n Y^n G_n(X, b), \quad (2.100)$$

$$G_n(X, b) = \sum_{s,r} [s,n;r] X^s b^r. \quad (2.101)$$

Let us take the s.q. lattice as a simple example. The first partial generating function, G_0 , corresponds to configurations for which all the sites are on the + sublattice. Such sites cannot be neighbours of one another and therefore $r = 0$ always. We may choose s + sites on a torus of $2N$ sites in $\binom{N}{s}$ ways. $[s,o;o]$ is therefore the coefficient of N in

$$N(N-1)(N-2)\dots(N-s+1)/s! \quad (2.102)$$

or $(-1)^{s+1}/s!$ Hence the function G_0 is simply

$$G_0(X, b) = \ln(1 + X) \quad (2.103)$$

To calculate $G_1(X, b)$ we consider configurations in which there is one - site and the remainder are +. We first choose the - site in N ways and observe that it casts a "shadow" on the four neighbouring + sites in the sense that if any one of these is now selected a nearest-neighbour bond will be formed. If we choose α + sites from the four sites in the "shadow" and β + sites from the remaining $(N-4)$ sites, we shall obtain α bonds in

$$\binom{4}{\alpha} \binom{N-4}{\beta} \quad (2.104)$$

ways. Taking the coefficient of N , this gives rise to a term in $G_1(X, b)$ equal to

$$(Xb)^\alpha X^\beta \binom{4}{\alpha} \binom{-4}{\beta}, \quad (2.105)$$

and summing over all α, β we obtain

$$G_1(X, b) = (1 + bX)^4 (1 + X)^{-4}. \quad (2.106)$$

To derive $G_2(X, b)$ we consider configurations with two - sites and the remainder + sites, but we note that each - site casts its own shadow and these shadows may overlap. There are three distinct cases as shown in (a), (b) and (c) of Fig. 13. In case (a) the two squares have two sites in common so that only six + sites are shaded by the - sites. Of these six sites the two on the common edge will create two bonds if chosen, and the

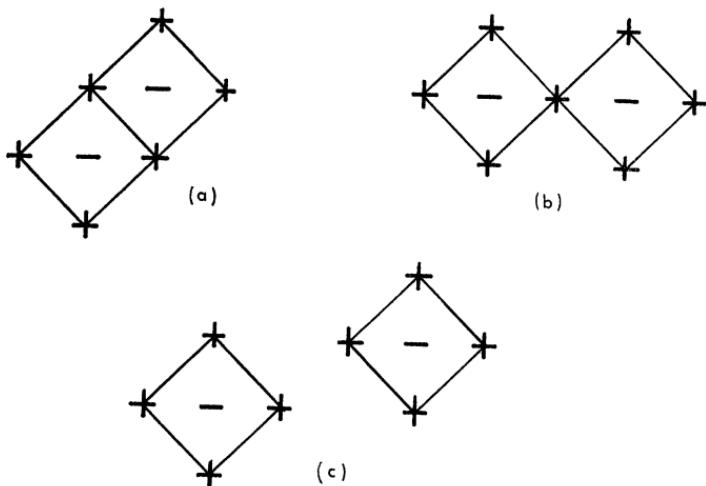


FIG. 13. Shadows cast by two overturned spins in the s.q. lattice.

remaining four will create one bond. Hence it is easy to show that this case gives a contribution

$$2(1 + bX)^4 (1 + b^2X)^2 (1 + X)^{-6} \quad (2.107)$$

to $G_2(X, b)$. Dealing similarly with cases (b) and (c) we find that

$$\begin{aligned} G_2(X, b) = & 2(1 + bX)^4 (1 + b^2X)^2 (1 + X)^{-6} \\ & + 2(1 + bX)^6 (1 + b^2X) (1 + X)^{-7} \\ & - 4\frac{1}{2} (1 + bX)^8 (1 + X)^{-8} \end{aligned} \quad (2.108)$$

Expressions like (2.108) are cumbersome and it is convenient to use a shorthand notation. We observe that the general term is of the form

$$(1 + bX)^\alpha (1 + b^2X)^\beta (1 + b^3X)^\gamma \dots (1 + X)^{-\alpha-\beta-\gamma} \dots \quad (2.109)$$

and this will be denoted by

$$(\lambda, \alpha, \beta, \gamma \dots), \quad \lambda = \alpha + \beta + \gamma + \dots, \quad (2.110)$$

which serves as a convenient "code" for supplying data of this kind to a computer.

As a second more complicated example we take the b.c.c. lattice for which we readily find that

$$G_1(X, b) = 1(8, 8); \quad (2.111)$$

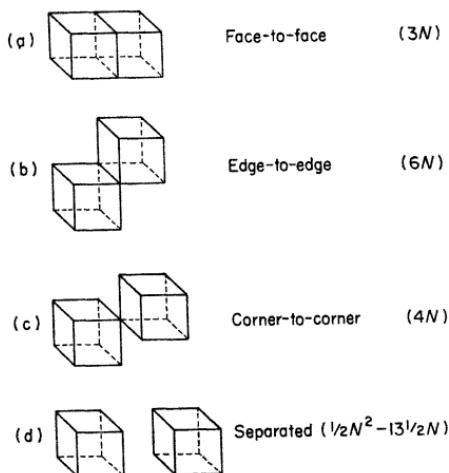


FIG. 14. Shadows cast by two overturned spins in the b.c.c. lattice (from Sykes *et al.*, 1965, p. 287).

from the breakdown given in Fig. 14 it is easy to see that

$$G_2(X, b) = 3(12, 8, 4) + 6(14, 12, 2) + 4(15, 14, 1) - 13\frac{1}{2}(16, 16). \quad (2.112)$$

We also see that the problem we are considering is naturally associated with an isomorphic problem on a "shadow lattice". For the s.q. lattice the shadow lattice is an s.q. lattice with first- and second-neighbour interactions. For the b.c.c. lattice the shadow lattice is an s.c. lattice with first-, second-, and third-neighbour interactions. The method can be applied to any loose-packed lattice, and the appropriate shadow lattices are listed as follows:

| Lattice | Shadow | Shadow lattice |
|---------|-------------|---|
| h.c. | Triangle | p.t. |
| s.q. | Square | s.q. with 1st and 2nd neighbours |
| d. | Tetrahedron | f.c.c. |
| s.c. | Octahedron | f.c.c. with 1st and 2nd neighbours |
| b.c.c. | Cube | f.c.c. with 1st, 2nd and 3rd neighbours |

However, the isomorphic problem is *not* a simple Ising model on the shadow lattice and we shall now define it in more detail for particular cases.

1. Code Specification

The following discussion is based on a recent publication by Sykes *et al.* (1973a). If a code $(\lambda, \alpha, \beta, \gamma \dots)$ occurs in G_s , we call s the *order* of the code. The complete s th code is then the total of all codes of order s and is appropriate for the derivation of density series. For the low-temperature series an important property is the highest power of b that occurs in the coefficient of X^n in the expansion of

$$(\lambda, \alpha, \beta, \gamma \dots) = (1 + bX)^\alpha (1 + b^2X)^\beta (1 + b^3X)^\gamma \dots (1 + X)^{-\lambda}, \quad (2.113)$$

and this will be called the *n-th rank* of the code. Finally, for any code $(\lambda, \alpha, \beta, \gamma, \delta, \varepsilon \dots)$ the quantity

$$\gamma + 2\delta + 3\varepsilon + \dots \quad (2.114)$$

is termed the *class* of the code.

We first consider the honeycomb lattice with $q = 3$. The complete shadow system is illustrated in Fig. 15(a) and the corresponding shadow lattice in Fig. 15(b). Each triangular shadow can touch another only at a vertex

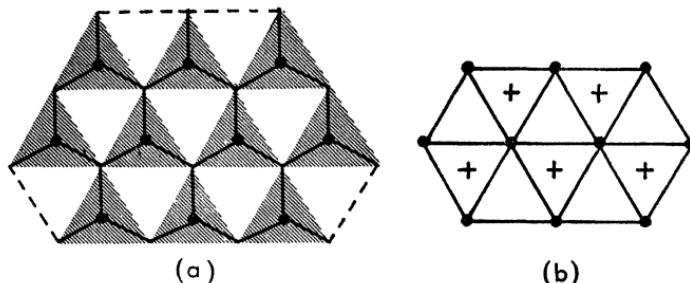


FIG. 15. (a) Honeycomb lattice and its complete shadow system; the full circles represent the B-sites (overturned B-spins). (b) Corresponding shadow lattice. This is a triangular lattice with the original B-sites as vertices. The triangles have alternate parity; those marked with a cross are of significant parity and correspond to three shadows that meet at one point. (From Sykes *et al.*, 1973.)

and never along an edge, and no more than three shadows can meet at any point. Thus the codes involve at most four parameters, α , β , and γ representing the number of + spins which lie in 1, 2 or 3 shadows respectively. If s is the number of - spins (the *order* of the code) then since each - spin casts a shadow on 3 + spins,

$$3s = \alpha + 2\beta + 3\gamma. \quad (2.115)$$

A typical example with $s = 5$ is shown in Fig. 16(a) giving rise to the code $(10, 6, 3, 1)$.

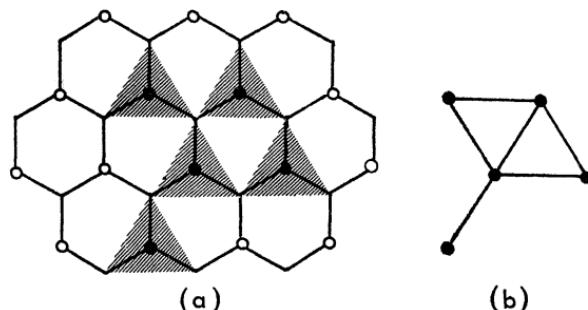


FIG. 16. (a) Honeycomb with 5 spins overturned on the B sub-lattice. The five shadows correspond to the code $(10, 6, 3, 1)$. (b) Corresponding shadow graph. \circ B-spins, \bullet overturned B-spins (From Sykes *et al.*, 1973.)

It should be noted that the shadow lattice is not the triangular lattice formed by connecting the $-$ spins; we must distinguish between the parity of the triangles as in Fig. 15(b), and the parameter γ , which arises from triplets of triangles with a vertex in common, corresponds to the set of triangles with a $+$ inside. These will be said to have *significant parity* (see Fig. 17). The parameter β arises from pairs of triangles with a vertex in

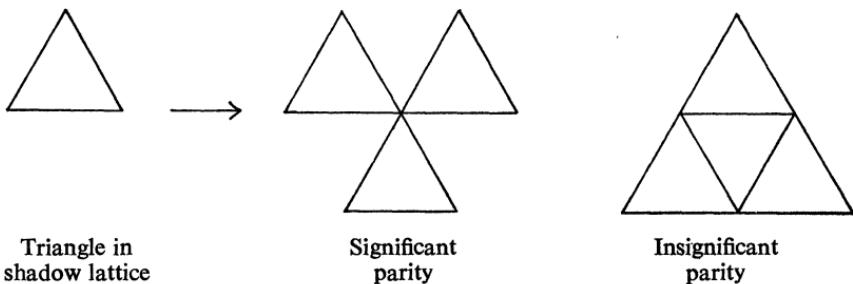


FIGURE 17.

common on the honeycomb lattice, and each of these implies a nearest-neighbour bond in the corresponding graph on the shadow lattice (the *shadow graph*, see Fig. 16(b)).

We see that the code $(\lambda, \alpha, \beta, \gamma)$ can be specified equally well by $-$ configurations of s overturned $-$ spins on the h.c. lattice or the configurations of s overturned spins on the ferromagnetic p.t. lattice. Hence we can refer to the honeycomb-triangular code system.

From the above discussion it is easy to see that the ferromagnetic polynomials $g_s(u)$ for the triangular lattice can be determined from the codes.

Regarding the shadow graph as a strong embedding, the total number of bonds is

$$r = \beta + 3\gamma \quad (2.116)$$

because each bond corresponds to the contact of two shadows unless it lies in a triangle of significant parity; and each triangle of significant parity has three bonds but contributes only once to γ . The class of each code is determined by γ . From the discussion in Section II.B it is clear that a configuration of s overturned spins on the p.t. lattice with r connecting bonds gives rise to a term

$$\gamma^s u^{3s-r}. \quad (2.117)$$

Hence the substitution into the codes of

$$(\lambda, \alpha, \beta, \gamma) \rightarrow \gamma^s u^{\alpha+\beta} \quad (2.118)$$

will give the $g_s(u)$ [using (2.115) and (2.116)]. It can be then shown that the transformation (2.118) leads to the well-known star-triangle relation between the honeycomb and triangular lattices (see Syozi, Vol. 1, Chapter 7).

Proceeding to the diamond lattice with $q = 4$ the shadows are tetrahedra and the shadow lattice is the f.c.c. lattice. The code now contains five parameters $\lambda, \alpha, \beta, \gamma, \delta$, γ representing triangles and δ tetrahedra of significant parity. The relations (2.115) and (2.116) generalize to

$$4s = \alpha + 2\beta + 3\gamma + 4\delta, \quad (2.119)$$

$$r = \beta + 3\gamma + 6\delta. \quad (2.120)$$

We can refer to the diamond-f.c.c. code system and the substitution

$$(\lambda, \alpha, \beta, \gamma, \delta) \rightarrow \gamma^s u^{3\alpha+4\beta+3\gamma+4\delta} \quad (2.121)$$

enables us to derive the $g_s(u)$ for the f.c.c. lattice. The class of each code is now $\gamma + 2\delta$.

It is interesting to pursue the generalization of the star-triangle transformation to the diamond-f.c.c. system and (2.121) leads to

$$2 \ln \Lambda_d(z) = \ln(1+z^4) + \ln \Lambda_{f.c.c.}(w_1, w_2) \quad (2.122)$$

$$w_1^3 = z(1+z^2)/(1+z^4) \quad w_2^4 = 2z^2/(1+z^4)$$

This is the three-dimensional star-tetrahedron substitution but because of the need to distinguish between w_1 and w_2 it is of little practical use.

For the s.q. lattice the shadow lattice is an s.q. lattice with first and

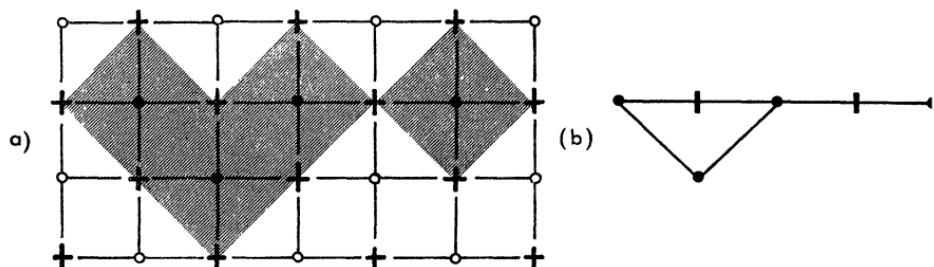


FIG. 18. (a) Simple quadratic with 4 spins overturned. (b) Corresponding shadow graph. \circ , B-spins; \bullet — \bullet , 1st neighbour bond; \bullet , overturned B-spins; \bullet —■— \bullet , 2nd neighbour bond. (From Sykes *et al.*, 1973.)

second neighbour bonds, and a particular situation is illustrated in Fig. 18(a) and the corresponding shadow graph in Fig. 18(b). Since $q = 4$ the general code has 4 parameters. If r_1 and r_2 denote the number of first and second neighbour bonds in the shadow graph corresponding to $(\lambda, \alpha, \beta, \gamma, \delta)$ we find the relations (analogous to (2.119) and (2.120))

$$\begin{aligned} 4s &= \alpha + 2\beta + 3\gamma + 4\delta. \\ 2r_1 + r_2 &= \beta + 3\gamma + 6\delta \end{aligned} \quad (2.123)$$

Thus the s.q. codes can be used to derive the solution for the s.q. lattice with second neighbour interactions if the first energy is twice the second.

Analogous relations can be derived for the s.c. and b.c.c. lattices. However the need to introduce second and higher neighbour bonds greatly complicates the treatment.

2. Numerical results. Series expansions

Although the initial codes can be determined in an elementary way, complications rapidly increase and sophisticated techniques have been introduced to make further progress. These are described in more detail in a series of publications (Sykes *et al.*, 1973b, c, d, e); a computer programme for determining codes has been developed by Elliott (1969). We shall here confine our attention to a brief account of some of the important features.

In the first place we note that since the sub-lattices are symmetrical we must have

$$g_{st}(u) = g_{ts}(u). \quad (2.124)$$

Thus any new code G_n must reproduce the sub-lattice polynomials g_{mn} correctly for all $m < n$. This principle of complete code-balance provides a check on the correctness of each new complete code as it is added. It implies a set of constraints on each complete code or partial generating function.

We have seen in the previous section that the codes depend on a limited number of parameters. Giving these parameters all possible numerical values we obtain the *algebraic* code system. However not all of these codes can be realized on the shadow lattice and it is convenient to distinguish between a *graphical* code which can be realized and a *non-graphical* code which cannot. To take a practical example for the h.c.-p.t. code β and γ are independent parameters and λ and α are then determined by (2.110) and (2.115). β and γ will be limited by the condition $\alpha \geq 0$ which gives

$$2\beta + 3\gamma \leq 3s. \quad (2.125)$$

The number of distinct graphical codes in a complete code increases fairly slowly with s , and data from high temperature series expansions for the specific heat and susceptibility can be used to place constraints on these codes, using the transformation described in Section II.B2. By adding these to the symmetry constraints (2.124) it is possible to reduce very substantially the number of configurations to be counted. In practice a few extra configurations are counted to serve as a check.

TABLE VIII. Ferromagnetic polynomials $g_r(u)$ in a density expansion (eqn. 1.43).

| | <i>p.t. lattice</i> |
|--|---------------------|
| $g_1 = u^3$, | |
| $g_2 = 3u^5 - 3\frac{1}{2}u^6$, | |
| $g_3 = 2u^6 + 9u^7 - 30u^8 + 19\frac{1}{3}u^9$, | |
| $g_4 = 3u^7 + 12u^8 + 5u^9 - 178\frac{1}{2}u^{10} + 288u^{11} - 129\frac{3}{4}u^{12}$, | |
| $g_5 = 6u^8 + 21u^9 + 18u^{10} - 177u^{11} - 680u^{12} + 2637u^{13} - 2796u^{14} + 971\frac{1}{5}u^{15}$, | |
| $g_6 = 14u^9 + 42u^{10} + 33u^{11} - 278u^{12} - 1320u^{13} - 136\frac{1}{2}u^{14} + 16807u^{15} - 34920u^{16} + 27555u^{17} - 7796\frac{2}{3}u^{18}$, | |
| $g_7 = u^9 + 30u^{10} + 105u^{11} + 24u^{12} - 564u^{13} - 2682u^{14} - 3007u^{15} + 21168u^{16} + 63870u^{17} - 307476u^{18} + 437997u^{19} - 275184u^{20} + 65718\frac{1}{4}u^{21}$, | |
| $g_8 = 6u^{10} + 69u^{11} + 227u^{12} + 120u^{13} - 1822\frac{1}{2}u^{14} - 5313u^{15} - 8859u^{16} + 30825u^{17} + 165894\frac{1}{2}u^{18} - 58668u^{19} - 1907846\frac{1}{4}u^{20} + 4905025u^{21} - 5324130u^{22} + 2778678u^{23} - 5742057u^{24}$. | |
| $g_9 = 27u^{11} + 160u^{12} + 483u^{13} + 228u^{14} - 4181u^{15} - 16704u^{16} - 11109u^{17} + 43868\frac{3}{2}u^{18} + 375483u^{19} + 408072u^{20} - 3019394u^{21} - 6438150u^{22} + 40681902u^{23} - 72302016u^{24} + 63438876u^{25} - 28314960u^{26} + 5157414\frac{4}{5}u^{27}$ | |
| $g_{10} = 3u^{11} + 86u^{12} + 432u^{13} + 837u^{14} + 449u^{15} - 10353u^{16} - 42315u^{17} - 48618\frac{1}{2}u^{18} + 205386u^{19} + 663288u^{20} + 1680030u^{21} - 4347964\frac{1}{2}u^{22} - 22703382u^{23} + 20150487u^{24} + 236013501\frac{3}{5}u^{25} - 741600943\frac{1}{2}u^{26} + 1012339456u^{27} - 745686690u^{28} + 290732760u^{29} - 47346449\frac{1}{5}u^{30}$ | |

TABLE VIII *cont.**s.q. lattice*

$$\begin{aligned}
g_1 &= u^2, \\
g_2 &= 2u^3 - 2\frac{1}{2}u^4, \\
g_3 &= 6u^4 - 16u^5 + 10\frac{1}{3}u^6, \\
g_4 &= u^4 + 18u^5 - 85u^6 + 118u^7 - 52\frac{1}{4}u^8, \\
g_5 &= 8u^5 + 43u^6 - 400u^7 + 926u^8 - 872u^9 + 295\frac{1}{3}u^{10}, \\
g_6 &= 2u^5 + 40u^6 + 30u^7 - 1651u^8 + 5992\frac{2}{3}u^9 - 9144u^{10} + 6520u^{11} - 1789\frac{5}{6}u^{12}, \\
g_7 &= 22u^6 + 136u^7 - 486u^8 - 5664u^9 + 33609u^{10} - 75640u^{11} + 85954u^{12} \\
&\quad - 49328u^{13} + 11397\frac{1}{4}u^{14}, \\
g_8 &= 6u^6 + 134u^7 + 194\frac{1}{2}u^8 - 3986u^9 - 13323u^{10} + 164790u^{11} - 532196\frac{1}{2}u^{12} \\
&\quad + 867670u^{13} - 785091u^{14} + 377040u^{15} - 75238\frac{1}{8}u^{16}, \\
g_9 &= u^6 + 72u^7 + 540u^8 - 1420u^9 - 19786u^{10} + 5112u^{11} + 691734u^{12} \\
&\quad - 3282328u^{13} + 7330033u^{14} - 9367653\frac{1}{3}u^{15} + 7040042u^{16} \\
&\quad - 2906956u^{17} + 510609\frac{4}{9}u^{18}, \\
g_{10} &= 30u^7 + 461u^8 + 1144u^9 - 15480u^{10} - 66020u^{11} + 300885\frac{1}{2}u^{12} \\
&\quad + 2300266u^{13} - 17888832u^{14} + 53980742\frac{2}{5}u^{15} - 92320336u^{16} \\
&\quad + 97010462u^{17} - 62337864u^{18} + 22576512u^{19} - 3541971u^{20}, \\
g_{11} &= 8u^7 + 310u^8 + 1864u^9 - 3373u^{10} - 91688u^{11} - 69358u^{12} + 2204652u^{13} \\
&\quad + 4259359u^{14} - 85259912u^{15} + 353290460u^{16} - 787713256u^{17} \\
&\quad + 1092475985u^{18} - 974679560u^{19} + 547000294u^{20} - 176425772u^{21} \\
&\quad + 25009987\frac{1}{1}u^{22}, \\
g_{12} &= 2u^7 + 151u^8 + 1894u^9 + 3315u^{10} - 53428u^{11} - 383706\frac{2}{3}u^{12} + 1032758u^{13} \\
&\quad + 10552273u^{14} - 14665400u^{15} - 341367843\frac{1}{2}u^{16} + 2067415954u^{17} \\
&\quad - 5967607048\frac{1}{4}u^{18} + 10581976596u^{19} - 12347150173u^{20} \\
&\quad + 9570815133\frac{1}{3}u^{21} - 4767367976u^{22} + 1386008952u^{23} \\
&\quad - 179211452\frac{1}{2}u^{24}, \\
g_{13} &= 68u^8 + 1340u^9 + 7389u^{10} - 20332u^{11} - 350828u^{12} - 965172u^{13} \\
&\quad + 10420351u^{14} + 32176924u^{15} - 210691538u^{16} - 1007111904u^{17} \\
&\quad + 10753093949u^{18} + 40670308548u^{19} + 90746211502u^{20} \\
&\quad - 133748320084u^{21} + 134710804372u^{22} - 92310171884u^{23} \\
&\quad + 41333506670u^{24} - 10938421828u^{25} + 1300139553\frac{1}{3}u^{26}, \\
g_{14} &= 22u^8 + 864u^9 + 7372u^{10} + 11536u^{11} - 257378u^{12} - 1557816u^{13} \\
&\quad + 1314978u^{14} + 62452942u^{15} - 2072348u^{16} - 1354656284u^{17} \\
&\quad - 785938734u^{18} + 48542073472u^{19} - 250471809911\frac{1}{2}u^{20} \\
&\quad + 700726407966\frac{2}{7}u^{21} - 1278321358994u^{22} + 1613014033334u^{23} \\
&\quad - 1429269896596u^{24} + 877614310184u^{25} - 356891308190u^{26} \\
&\quad + 86670538138u^{27} - 9532294556\frac{6}{7}u^{28}, \\
g_{15} &= 6u^8 + 456u^9 + 6404u^{10} + 24436u^{11} - 94888u^{12} - 1677728u^{13} \\
&\quad - 3997457u^{14} + 34493510\frac{2}{3}u^{15} + 267958908u^{16} - 885175436u^{17} \\
&\quad - 5903060870\frac{2}{3}u^{18} + 16408972700u^{19} + 177977336689\frac{1}{4}u^{20} \\
&\quad - 1388708571629\frac{1}{3}u^{21} + 4917742574549u^{22} - 10990712090268u^{23} \\
&\quad + 16983610970872\frac{2}{3}u^{24} - 18741629318887\frac{1}{4}u^{25}
\end{aligned}$$

TABLE VIII *cont.**s.q. lattice cont.*

$$+ 14\ 825\ 042\ 097\ 211u^{26} - 8\ 245\ 969\ 418\ 426\frac{2}{3}u^{27} \\ + 3\ 071\ 337\ 551\ 762u^{28} - 689\ 136\ 584\ 016u^{29} + 70\ 528\ 002\ 102\frac{2}{3}u^{30}.$$

f.c.c. lattice

$$g_1 = u^6, \\ g_2 = 6u^{11} - 6\frac{1}{2}u^{12}, \\ g_3 = 8u^{15} + 42u^{16} - 120u^{17} + 70\frac{1}{3}u^{18}, \\ g_4 = 2u^{18} + 24u^{19} + 123u^{20} + 126u^{21} - 1653u^{22} + 2322u^{23} - 944\frac{1}{4}u^{24}, \\ g_5 = 30u^{22} + 96u^{23} + 448u^{24} + 792u^{25} - 2871u^{26} - 16296u^{27} + 49290u^{28} \\ - 45792u^{29} + 14303\frac{1}{2}u^{30}, \\ g_6 = u^{24} + 30u^{25} + 168u^{26} + 776u^{27} + 1212u^{28} + 3930u^{29} - 6904u^{30} - 65070u^{31} \\ - 64224u^{32} + 771272u^{33} - 1329240u^{34} + 922152u^{35} - 234103\frac{1}{6}u^{36}, \\ g_7 = 8u^{27} + 36u^{28} + 336u^{29} + 1\ 350u^{30} + 3\ 528u^{31} + 9\ 036u^{32} - 1160u^{33} \\ + 1\ 038u^{34} - 281\ 400u^{35} - 622\ 498u^{36} + 1\ 503\ 912u^{37} \\ + 8\ 356\ 041u^{38} - 28\ 260\ 664u^{39} + 34\ 148\ 478u^{40} - 18\ 902\ 160u^{41} \\ + 4\ 044\ 119\frac{1}{4}u^{42}, \\ g_8 = 28u^{30} + 96u^{31} + 786u^{32} + 2\ 432u^{33} + 9\ 804u^{34} + 19\ 314u^{35} + 29\ 146u^{36} \\ + 20\ 550u^{37} - 322\ 950u^{38} - 474\ 806u^{39} - 4\ 371\ 355\frac{1}{2}u^{40} + 1\ 944\ 846u^{41} \\ + 40\ 271\ 875u^{42} + 32\ 438\ 508u^{43} - 452\ 857\ 765\frac{1}{2}u^{44} + 916\ 579\ 240u^{45} \\ - 853\ 695\ 741u^{46} + 393\ 105\ 420u^{47} - 72\ 699\ 427\frac{1}{3}u^{48}.$$

b.c.c. lattice

$$g_1 = u^4, \\ g_2 = 4u^7 - 4\frac{1}{2}u^8, \\ g_3 = 28u^{10} - 64u^{11} + 36\frac{1}{3}u^{12}, \\ g_4 = 12u^{12} + 204u^{13} - 798u^{14} + 948u^{15} - 366\frac{1}{4}u^{16}, \\ g_5 = 12u^{14} + 216u^{15} + 1262u^{16} - 9072u^{17} + 17592u^{18} - 14184u^{19} + 4174\frac{1}{5}u^{20}, \\ g_6 = 27u^{16} + 312u^{17} + 2368u^{18} + 4312u^{19} - 92992u^{20} + 275021\frac{1}{3}u^{21} \\ - 353640u^{22} + 216036u^{23} - 51444\frac{1}{2}u^{24}, \\ g_7 = 72u^{18} + 704u^{19} + 4404u^{20} + 17616u^{21} - 36348u^{22} - 833064u^{23} \\ + 3795726u^{24} - 7072736u^{25} + 6798900u^{26} - 3344712u^{27} \\ + 669438\frac{1}{4}u^{28}, \\ g_8 = 4u^{19} + 198u^{20} + 2016u^{21} + 10300u^{22} + 41352u^{23} + 55536u^{24} - 989076u^{25} \\ - 6007194u^{26} + 46866408u^{27} - 122039509u^{28} + 166096620u^{29} \\ - 127471458u^{30} + 52501716u^{31} - 9066913\frac{1}{8}u^{32}, \\ g_9 = 24u^{21} + 692u^{22} + 5816u^{23} + 30714u^{24} + 99648u^{25} + 226692u^{26} \\ - 887688u^{27} - 13103579u^{28} - 24522136u^{29} + 514861877\frac{1}{3}u^{30} \\ - 1874111776u^{31} + 3435605052u^{32} - 3684304933\frac{1}{3}u^{33} \\ + 2353070344u^{34} - 833603008u^{35} + 126632261\frac{1}{8}u^{36},$$

TABLE VIII *cont.**b.c.c. lattice cont.*

$$\begin{aligned}
 g_{10} = & 156u^{23} + 2418u^{24} + 19568u^{25} + 89832u^{26} + 312984u^{27} + 534960u^{28} \\
 & - 582528u^{29} - 21524820u^{30} - 122555960u^{31} + 184704162u^{32} \\
 & + 4891550184u^{33} - 25940728064u^{34} + 62669293900\frac{1}{3}u^{35} \\
 & - 88827538116u^{36} + 78607759128u^{37} - 42991931004u^{38} \\
 & + 13362730248u^{39} - 1812137048\frac{9}{10}u^{40}, \\
 g_{11} = & 12u^{24} + 800u^{25} + 9720u^{26} + 65112u^{27} + 302497u^{28} + 897848u^{29} \\
 & + 1976484u^{30} - 2366032u^{31} - 34701994u^{32} - 284193600u^{33} \\
 & - 704476488u^{34} + 6025344368u^{35} + 36918882951u^{36} \\
 & - 323871127432u^{37} + 1029543128536u^{38} - 1871827463448u^{39} \\
 & + 2164621975492u^{40} - 1630783111424u^{41} + 779883805680u^{42} \\
 & - 215938102896u^{43} + 26449153814\frac{1}{11}u^{44}.
 \end{aligned}$$

s.c. lattice

$$\begin{aligned}
 g_1 = & u^3, \\
 g_2 = & 3u^5 - 3\frac{1}{2}u^6, \\
 g_3 = & 15u^7 - 36u^8 + 21\frac{1}{3}u^9, \\
 g_4 = & 3u^8 + 83u^9 - 328\frac{1}{2}u^{10} + 405u^{11} - 162\frac{3}{4}u^{12}, \\
 g_5 = & 48u^{10} + 426u^{11} - 2804u^{12} + 5532u^{13} - 4608u^{14} + 1406\frac{1}{5}u^{15}, \\
 g_6 = & 18u^{11} + 496u^{12} + 1575u^{13} - 22144\frac{1}{2}u^{14} + 64574u^{15} - 84738u^{16} + \\
 & + 53370u^{17} - 13150\frac{3}{2}u^{18}, \\
 g_7 = & 8u^{12} + 378u^{13} + 3888u^{14} - 1360u^{15} - 157380u^{16} + 674652u^{17} \\
 & - 1261904u^{18} + 1240035u^{19} - 628236u^{20} + 129919\frac{1}{4}u^{21}, \\
 g_8 = & u^{12} + 306u^{14} + 4622u^{15} + 22396\frac{1}{2}u^{16} - 106113u^{17} - 947582\frac{1}{2}u^{18} \\
 & + 6392769u^{19} - 16362155\frac{1}{4}u^{20} + 22521935u^{21} - 17686675\frac{1}{2}u^{22} \\
 & + 7496787u^{23} - 1336290\frac{3}{2}u^{24}, \\
 g_9 = & 24u^{14} + 127u^{15} + 5544u^{16} + 40050u^{17} + 60804u^{18} - 1368954u^{19} \\
 & - 3978300u^{20} + 54753064u^{21} - 190517760u^{22} + 348702921u^{23} \\
 & - 379686836u^{24} + 248294610u^{25} - 90480828u^{26} + 14175534\frac{1}{2}u^{27}, \\
 g_{10} = & 24u^{15} + 396u^{16} + 4131u^{17} + 67267u^{18} + 236808u^{19} - 614784u^{20} \\
 & - 12412763u^{21} + 2839656u^{22} + 414942978u^{23} - 2018275270u^{24} \\
 & + 4793140380\frac{3}{5}u^{25} - 6835882485u^{26} + 6156900766u^{27} \\
 & - 3449297064u^{28} + 1102444428u^{29} - 154094468\frac{7}{10}u^{30}, \\
 g_{11} = & 24u^{16} + 660u^{17} + 6656u^{18} + 70275u^{19} + 602928u^{20} + 423644u^{21} \\
 & - 12635748u^{22} - 86214999u^{23} + 306005260u^{24} + 2620578876u^{25} \\
 & - 19491928200u^{26} + 59739201959u^{27} - 108143883564u^{28} \\
 & + 126406988784u^{29} - 97076564452u^{30} + 47569139712u^{31} \\
 & - 13540389348u^{32} + 1708597533\frac{1}{11}u^{33}, \\
 g_{12} = & 3u^{16} + 1080u^{18} + 11562u^{19} + 101685u^{20} + 814709u^{21} + 3894597u^{22} \\
 & - 12171177u^{23} - 135740953u^{24} - 397387542u^{25} + 4338189541\frac{1}{2}u^{26}
 \end{aligned}$$

TABLE VIII *cont.**s.c. lattice cont.*

$$\begin{aligned}
 & + 11093270424\frac{2}{3}u^{27} - 170115111953\frac{1}{4}u^{28} + 682270008351u^{29} \\
 & - 1542754484221u^{30} + 2260372621941u^{31} - 2238908395410u^{32} \\
 & + 1498634619771u^{33} - 652575075531u^{34} + 167442968667u^{35} \\
 & - 19258135545u^{36} \\
 g_{13} = & 96u^{18} + 732u^{19} + 23976u^{20} + 163820u^{21} + 1256172u^{22} + 6874170u^{23} \\
 & + 12343160u^{24} - 220608330u^{25} - 1032194100u^{26} \\
 & + 226958615u^{27} + 43210929384u^{28} - 18514105314u^{29} \\
 & - 1306808581968u^{30} + 7163363995983u^{31} - 20147356102164u^{32} \\
 & + 36242844825794u^{33} - 44637329262900u^{34} + 38365757618721u^{35} \\
 & - 22758644334336u^{36} + 8917222503222u^{37} - 2082822677172u^{38} \\
 & + 220080372439\frac{1}{3}u^{39}.
 \end{aligned}$$

As a result codes have been calculated for the following values of s and are tabulated in the publications referred to above (Sykes *et al.*, 1965, 1973b,d): h.c. ($s \leq 10$), s.q. ($s \leq 7$), d ($s \leq 8$), s.c. ($s \leq 6$), b.c.c. ($s \leq 5$). From these codes the general ferrimagnetic polynomials $g_{st}(u)$ can readily be obtained using (2.98) and (2.99); putting y_+ equal to y_- and summing for $s+t=m$ the ferromagnetic polynomials $g_m(u)$ are derived. Since they represent an important body of numerical data for the Ising model we reproduce the results for the p.t., s.q., f.c.c., b.c.c. and s.c. lattices in Table VIII. For other lattices data are available as follows: h.c. ($m \leq 21$), d. ($m \leq 17$).

If the expansion (2.97) is rearranged as a series in u , we can obtain the low temperature polynomials $f_r^{(a)}(y_+, y_-)$ of (1.55) for a ferrimagnet, and when $y_+ = y_-$ the polynomials $f_r(y)$ of (1.52) for a ferromagnet. However it is possible to extend these series by enumerating a limited number of *partial* codes for larger values of s . It is the class of a code and its successive ranks which are significant in these u -series. As a result of the calculations of Sykes *et al.* (1973 c, e) the following terms are available:

h.c. ($r \leq 16$), s.q. ($r \leq 11$), p.t. ($r \leq 16$), d. ($r \leq 15$), s.c. ($r \leq 20$),
b.c.c. ($r \leq 28$), f.c.c. ($r \leq 40$).

We reproduce in Tables IX–XII the coefficients in the expansion of $\ln Z_0^I$ in zero field, the spontaneous magnetization M_0 , and the initial ferromagnetic and antiferromagnetic susceptibilities χ_0 , $\chi_0^{(a)}$ as follows:

$$\ln Z_0^I = -\frac{q}{8} \ln u + u^{q/2} \sum_{r=0}^{\infty} b_r^{(0)} u^r \quad (2.126)$$

$$M_0/m = 1 - 2u^{q/2} - u^{q-1} \sum_{r=1}^{\infty} b_r^{(1)} u^r \quad (2.127)$$

$$\chi_0 = 4\beta m^2 u^{q/2} \sum_{r=0}^{\infty} b_r^{(2)} u^r \quad (2.128)$$

$$\chi_0^{(a)} = 4\beta m^2 u^{q/2} \sum_{r=0}^{\infty} b_{ra}^{(2)} u^r. \quad (2.129)$$

.3 Spin $s > \frac{1}{2}$

The configurational problems which arise in deriving density or low temperature series expansions for spin $s > \frac{1}{2}$ are basically the same as those for $s = \frac{1}{2}$. Using the Hamiltonian (1.3), a ground state with all spins aligned in a magnetic field H , the ground state having energy

$$- N(\frac{1}{2}qJ + mH). \quad (2.130)$$

This is identical with the ground state energy for $s = \frac{1}{2}$, and results from the normalization we have chosen in (1.3) for which the maximum interaction between two parallel spins and the maximum interaction with an external field are independent of s .

We then consider excited states of overturned spins; however there is no longer a single state of an overturned spin but there are $2s$ such states, and for any configuration of excited states the state of each spin must be specified. The problem parallels a many component fluid. By analogy with (1.16) and (1.17) we can write

$$kT \ln Z_N^I = \frac{1}{2}qJ + mH + kT \ln \Lambda_N^I(y, u) \quad (2.131)$$

where now

$$y = \exp - (\beta mH/s), \quad u = \exp - (\beta J/s^2). \quad (2.132)$$

We can also develop series expansions for $\ln \Lambda^I(s)$ analogous to (1.43),

$$\ln \Lambda^I(s) = \sum_{r=1}^{\infty} y^r g_r(u), \quad (2.133)$$

where $g_r(u)$ is a polynomial in u whose highest power is u^{rs} .

The primitive method for obtaining $g_r(u)$ was used by Sykes (1956) but was not taken very far because of the complexity of the resulting series and the difficulty of assessing critical behaviour. With the advent of more sophisticated methods of analysis (Gaunt and Guttman, this volume,

TABLE IX. *Zero field coefficients $b_r^{(0)}$ of $\ln Z^I$ (eqn. 2.126).

| Lattice | d. | s.c. | b.c.c. | f.c.c. |
|---------|----------|--------------|---------------|-------------|
| r = 0 | 1 | 1 | 1 | 1 |
| 1 | 2 | 0 | 0 | 0 |
| 2 | 3½ | 3 | 0 | 0 |
| 3 | 6 | - 3½ | 4 | 0 |
| 4 | 12½ | 15 | - 4½ | 0 |
| 5 | 30 | - 33 | 0 | 6 |
| 6 | 83¾ | 104½ | 28 | - 6½ |
| 7 | 250²₃ | - 280½ | - 64 | 0 |
| 8 | 768½ | 849 | 48½ | 0 |
| 9 | 2442 | - 2461¾ | 204 | 8 |
| 10 | 8009½ | 7485 | - 786 | 42 |
| 11 | 26956 | - 22534½ | 1164 | - 120 |
| 12 | 93140²₅ | 69393½ | 922¾ | 72½ |
| 13 | 3 29258½ | - 2 13754½ | - 8760 | 24 |
| 14 | | 6 66750 | 20032 | 123 |
| 15 | | - 20 86734½ | - 9164 | 126 |
| 16 | | 65 83341 | - 84215½ | - 1623 |
| 17 | | - 208 52363½ | 2 94677½ | 2418 |
| 18 | | | - 3 78996 | - 495½ |
| 19 | | | - 5 69704 | 822 |
| 20 | | | 38 32961½ | - 2703 |
| 21 | | | - 79 41796 | - 15512 |
| 22 | | | 11 18118 | 50538 |
| 23 | | | 430 16052 | - 41526 |
| 24 | | | - 1335 95088½ | 8777½ |
| 25 | | | | - 61446 |
| 26 | | | | - 54402 |
| 27 | | | | 7 72624 |
| 28 | | | | - 13 17960 |
| 29 | | | | 6 61848 |
| 30 | | | | - 8 20665½ |
| 31 | | | | 15 49408 |
| 32 | | | | 80 84382 |
| 33 | | | | - 285 89452 |
| 34 | | | | 298 89394½ |

* Values of $b_r^{(0)}$ for the h.c., s.q. and p.t. lattices in two dimensions can be derived from the high temperature coefficients in Table IV by a suitable transformation (Domb 1960; Syozi Vol. 1 Chapter 7).

TABLE X. Spontaneous magnetization coefficients $b_r^{(1)}$ (eqn. 2.12).

| Lattice | h.c.* | s.q. | p.t. |
|---------|-------------|--------------|---------------|
| $r = 0$ | 6 | 8 | 12 |
| 1 | 18 | 34 | - 2 |
| 2 | 54 | 152 | 78 |
| 3 | 168 | 714 | - 24 |
| 4 | 534 | 3472 | 548 |
| 5 | 1732 | 17318 | - 228 |
| 6 | 5706 | 88048 | 4050 |
| 7 | 19038 | 4 54378 | - 2030 |
| 8 | 64176 | 23 73048 | 30960 |
| 9 | 2 18190 | 125 15634 | - 17670 |
| 10 | 7 47180 | 665 51016 | 2 42402 |
| 11 | 25 74488 | 3563 45666 | - 1 52520 |
| 12 | 89 18070 | 19194 53984 | 19 32000 |
| 13 | 310 36560 | 103927 92766 | - 13 12844 |
| 14 | 1084 57488 | 565272 00992 | 156 12150 |
| 15 | 3803 90574 | | - 112 97052 |
| 16 | 13384 95492 | | |
| Lattice | d. | s.c. | b.c.c. |
| $r = 0$ | 8 | 12 | 16 |
| 1 | 26 | - 14 | - 18 |
| 2 | 80 | 90 | 0 |
| 3 | 268 | - 192 | 168 |
| 4 | 944 | 792 | - 384 |
| 5 | 3474 | - 2148 | 314 |
| 6 | 13072 | 7716 | 1632 |
| 7 | 49672 | - 23262 | - 6264 |
| 8 | 1 91272 | 79512 | 9744 |
| 9 | 7 44500 | - 2 52054 | 10014 |
| 10 | 29 24680 | 8 46628 | - 86976 |
| 11 | 115 96284 | - 27 53520 | 2 05344 |
| 12 | 463 64456 | 92 05800 | - 80176 |
| 13 | | - 303 71124 | - 10 09338 |
| 14 | | 1015 85544 | 35 79568 |
| 15 | | - 3380 95596 | - 45 75296 |
| 16 | | | - 83 01024 |
| 17 | | | 540 12882 |
| 18 | | | - 1126 40896 |
| 19 | | | 51 64464 |
| 20 | | | 6948 45120 |
| 21 | | | - 21607 81086 |
| 22 | | | 92 79376 |
| 23 | | | - 157 71600 |
| 24 | | | - 4 67336 |
| 25 | | | - 109 35114 |
| 26 | | | 218 35524 |
| 27 | | | 1127 52684 |
| 28 | | | - 4005 76168 |
| 29 | | | 4102 87368 |

* Expansion Variable $z = u^{1/2}$

The following recurrence relations may be noted (Sykes, private communication)

$$\text{h.c. } (n+4)b_n^{(1)} = 4(n+3)b_{n-1}^{(1)} - (n+2)b_{n-2}^{(1)} - 6b_{n-3}^{(1)} + nb_{n-4}^{(1)} - 4(n-1)b_{n-5}^{(1)}$$

$$+ (n-2)b_{n-6}^{(1)}$$

$$\text{s.q. } (n+3)b_n^{(1)} = 6(n+2)b_{n-1}^{(1)} - 4b_{n-2}^{(1)} - 6nb_{n-3}^{(1)} + (n-1)b_{n-4}^{(1)}$$

$$+ (n-1)b_{n-5}^{(1)} = 10(n-3)b_{n-1}^{(1)} - (b_{n-1}^{(1)})^2 - 9(n+1)b_{n-4}^{(1)}$$

TABLE II. THEORETIC SUSCEPTIBILITY COEFFICIENTS FOR THE ISING MODEL

| Lattice | $h.c.*$ | s.q. | p.t. | d. | s.c. | b.c.c. | f.c.c. |
|---------|------------|-----------|------------|--------------|--------------|--------------|--------|
| $r = 0$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 1 | 6 | 8 | 0 | 8 | 0 | 0 | 0 |
| 2 | 27 | 60 | 12 | 44 | 12 | 0 | 0 |
| 3 | 122 | 416 | 4 | 208 | -14 | 16 | 0 |
| 4 | 516 | 2791 | 129 | 984 | 135 | -18 | 0 |
| 5 | 2148 | 18296 | 122 | 4584 | -276 | 0 | 24 |
| 6 | 8792 | 1 18016 | 1332 | 21314 | 1520 | 252 | -26 |
| 7 | 35622 | 7 52008 | 960 | 98292 | -4056 | -576 | 0 |
| 8 | 1 43079 | 47 46341 | 10919 | 4 48850 | 17778 | 519 | 0 |
| 9 | 5 70830 | 297 27472 | 11372 | 20 38968 | -54392 | 3264 | 72 |
| 10 | 22 64649 | | 1 32900 | 92 20346 | 2 13522 | -12468 | 378 |
| 11 | 89 42436 | | 1 26396 | 415 45564 | -7 00362 | 20568 | -1080 |
| 12 | 351 69616 | 12 99851 | 1867 96388 | 26 01674 | 26662 | 665 | |
| 13 | 1378 39308 | 13 49784 | 8286 23100 | -88 36812 | -2 15568 | 384 | |
| 14 | | | | 319 25046 | 5 28576 | 1968 | |
| 15 | | | | -1103 23056 | -1 64616 | 2016 | |
| 16 | | | | 3930 08712 | -30 14889 | -25698 | |
| 17 | | | | -13695 33048 | 108 94920 | 39552 | |
| 18 | | | | | -137 96840 | -3872 | |
| 19 | | | | | -299 09616 | 20880 | |
| 20 | | | | | 1904 23962 | -65727 | |
| 21 | | | | | -3997 39840 | -3 79072 | |
| 22 | | | | | -227 68752 | 12 77646 | |
| 23 | | | | | 28034 02560 | -9 86856 | |
| 24 | | | | | -87430 64909 | 1 76978 | |
| 25 | | | | | | -21 63504 | |
| 26 | | | | | | -18 18996 | |
| 27 | | | | | | 278 71080 | |
| 28 | | | | | | -471 38844 | |
| 29 | | | | | | 207 89424 | |
| 30 | | | | | | -365 09652 | |
| 31 | | | | | | 770 55330 | |
| 32 | | | | | | 3930 46656 | |
| 33 | | | | | | -14029 34816 | |
| 34 | | | | | | -14038 43388 | |

TABLE XII. Low temperature antiferromagnetic susceptibility coefficients $b_{ra}^{(2)}$ (eqn. 2.129).

| Lattice | *h.c. | s.q. | d. | s.c. | b.c.c. |
|---------|---------|-------|---------|------------|-------------|
| $r = 0$ | 1 | 1 | 1 | 1 | 1 |
| 1 | 0 | 0 | 0 | 0 | 0 |
| 1 | 3 | 4 | 4 | 0 | 0 |
| 3 | 2 | 8 | 0 | -2 | 0 |
| 4 | 12 | 39 | 16 | 15 | -2 |
| 5 | 24 | 152 | 24 | -36 | 0 |
| 6 | 80 | 672 | 122 | 104 | 28 |
| 7 | 222 | 3016 | 348 | -312 | -64 |
| 8 | 687 | 13989 | 1266 | 1050 | 39 |
| 9 | 2096 | 66664 | 4464 | -3312 | 224 |
| 10 | 6585 | | 16394 | 10734 | -884 |
| 11 | 20892 | | 57932 | -34518 | 1368 |
| 12 | 67216 | | 2 15916 | 1 13210 | 1350 |
| 13 | 2 18412 | | 8 28348 | -3 70236 | -12272 |
| 14 | | | | 12 20922 | 28752 |
| 15 | | | | -40 28696 | -11944 |
| 16 | | | | 133 64424 | -1 38873 |
| 17 | | | | -444 09312 | 4 94184 |
| 18 | | | | | -6 40856 |
| 19 | | | | | -11 11568 |
| 20 | | | | | 73 63194 |
| 21 | | | | | -154 88224 |
| 22 | | | | | 11 98848 |
| 23 | | | | | 935 06112 |
| 24 | | | | | -2934 73869 |

* Expansion variable $z = u^{1/2}$

Chapter 4) interest in the problem revived. The shadow lattice method can be generalized (Sykes and Gaunt, 1973) and the following tabulations have now been made for a number of two- and three-dimensional lattices (Fox and Gaunt, 1972):

$s = 1$

h.c. ($r \leq 12$); s.q. ($r \leq 10$); p.t. ($r \leq 7$); d. ($r \leq 12$);

s.c. ($r \leq 10$); b.c.c. ($r \leq 10$); f.c.c. ($r \leq 7$)

$s = 3/2$

p.t. ($r \leq 7$); f.c.c. ($r \leq 7$).

III. Critical Behaviour

In the previous sections we have been concerned with deriving power series expansions for various thermodynamic properties of Ising systems. The coefficients in these expansions are exact but they are limited in number. We first quote a few general properties of power series.

Consider a function $f(z)$ defined by (Dienes, 1931)

$$f(z) = \sum_{n=0}^{\infty} a_n z^n. \quad (3.1)$$

Then if

$$\lim_{n \rightarrow \infty} |a_n|^{1/n} \quad (3.2)$$

exists and is equal to $1/z_c$ the series converges for $|z| < z_c$. We can then write

$$|a_n| \sim f(n)/z_c^n, \quad (3.3)$$

where

$$\lim_{n \rightarrow \infty} [f(n)]^{1/n} = 1 \quad (3.4)$$

There is always a singularity on the circle $z = z_c$. If all of the a_n are consistent in sign, then the dominant singularity lies on the positive real axis. (For example the series in Tables I and II.) Replacing z by $-z$ we see that if the a_n alternate regularly the dominant singularity lies on the negative real axis (e.g. Table X p.t. and s.c.). More irregular alternations indicate dominant singularities in the complex plane (e.g. Table X b.c.c. and f.c.c.). If a_n is real these must occur in complex pairs $(1/z_c) \exp \pm (i\sigma)$. For a single pair we should expect

$$a_n \sim \frac{f(n)}{z_c^n} \cos n\sigma. \quad (3.5)$$

If σ is a simple fraction, this gives rise to cyclic behaviour, otherwise it is more random.

If all the a_n are known *exactly* we can (in principle) continue the function analytically across the whole plane. Asymptotic values of a_n determine the behaviour near to the dominant singularity. Hence we see that series of terms consistent in sign are particularly useful since a numerical analysis of the a_n provides direct information about the singularity of physical interest, which must be on the positive real axis to correspond to a positive temperature. When the terms are not consistent in sign there is a dominant unphysical singularity which masks the behaviour of the singularity of physical interest. We may then use a transformation in the complex plane which

brings the physical singularity into the dominant position, or some alternative procedure for by-passing the non-physical singularities and focussing attention on the physical singularity.

These points are well illustrated by the coefficients in the spontaneous magnetization series for the s.q. and p.t. lattices in Table X. The former are all positive and regular and the dominant singularity corresponds to $u_c = 3 - 2\sqrt{2}$; they represent the expansion of the function

$$\left[1 - \frac{16u^2}{(1-u)^4}\right]^{1/8} = (1-6u+u^2)^{1/8}(1+u)^{1/4}(1-u)^{-1/2} \quad (3.6)$$

The latter alternate in sign and are extremely irregular; they represent the expansion of the function

$$\left[1 - \frac{16u^3}{(1+3u)(1-u)^3}\right]^{1/8} = (1+3u)^{-1/8}(1-3u)^{1/8}(1-u)^{-3/8}(1+u)^{3/8}, \quad (3.7)$$

and the dominant singularity corresponds to the unphysical value $u_c = -1/3$. The singularity of physical interest corresponds to $u_c = 1/3$. It is interesting that in terms of T/T_c as variable the functions represented by (3.6) and (3.7) differ little in magnitude over the whole range of physical interest from 0 to 1 even though they differ considerably in analytic form.

During the past two decades a good deal of attention has been focussed on manipulating finite numbers of terms of series expansions so as to obtain estimates of critical behaviour. From the mathematical point of view no rigorous results can be derived from a *finite* number of terms; hence such estimates depend on some *a priori* assumption. However, physical insight into the nature of the model together with a knowledge of the behaviour of exact solutions for specific models provide a clear indication of the type of assumption which can reasonably be made. The first assumption made by Domb and Sykes in 1957 in investigating the high temperature susceptibility was a branch point singularity of the form

$$f(z) \sim A(z - z_c)^{-\gamma}, \quad (3.8)$$

γ defining the *critical exponent* and A the *critical amplitude*. This assumption served well in the investigation of other exponents, but when more lengthy series became available it became advisable to refine the assumption to take account of correction terms. Following a suggestion of Ninham (1963) Domb and Sykes adopted the Darboux form

$$f(z) \sim (z - z_c)^{-\gamma} A(z) + B(z) \quad (3.9)$$

where $A(z)$ and $B(z)$ are analytic at z_c (Domb, 1970a).

Once assumptions like (3.8) and (3.9) have been made, we are no longer faced with a problem of extrapolation but of fitting parameters to numerical data. The methods which have been most effectively used are described by Gaunt and Guttman in Chapter 4 of this volume. Most of their illustrative examples have been drawn from Ising model series, and we shall refer to them in due course. In the present section we shall not provide any details of numerical analysis on which estimates of critical behaviour are based. We aim, rather, to assemble the results which have been put forward in a coherent form with some assessment of their reliability. We shall usually take our results from the latest papers, but we shall give reference to the papers containing earlier estimates. This should enable any reader who is interested to trace the historical development and numerical details for himself.

A. Critical parameters

1. Critical temperature

The value of T_c , the critical temperature, is known exactly for many two-dimensional lattices, and very accurately for the common three-dimensional lattices. It was found quite early on that high temperature series were better behaved, and provided more accurate estimates than their low temperature counterparts (Domb and Sykes, 1956, 1957a). The high accuracy is important since estimates of critical parameters and other aspects of critical behaviour are very sensitive to the choice of T_c . The best series for estimating T_c is usually the high temperature susceptibility, but the high temperature series for $\ln Z_0^I$ usually provides a useful check. It is worth noting that the series become smoother with increasing co-ordination number q .

We quote the values of $1/w_c$ since these are obtained directly from analysis of the series. Corresponding values of kT_c can be obtained from

TABLE XIII. Critical parameters for the $J(\frac{1}{2})$ model.

| Lattice | q | kT_c/qJ | S_c/k | $(S_\infty - S_c)/k$ | $(U_c - U_0)/kT_c$ | $-U_c/kT_c$ |
|--------------|----------|-----------|---------|----------------------|--------------------|-------------|
| Linear Chain | 2 | 0 | 0 | 0.69315 | 0 | ∞ |
| h.c. | 3 | 0.50621 | 0.26471 | 0.42844 | 0.22737 | 0.76035 |
| s.q. | 4 | 0.56730 | 0.30647 | 0.38668 | 0.25814 | 0.62323 |
| p.t. | 6 | 0.60683 | 0.33028 | 0.36287 | 0.27465 | 0.54931 |
| d. | 4 | 0.6761 | 0.510 | 0.183 | 0.417 | 0.323 |
| s.c. | 6 | 0.75180 | 0.5579 | 0.1352 | 0.4451 | 0.2200 |
| b.c.c. | 8 | 0.79416 | 0.5820 | 0.1111 | 0.4576 | 0.1720 |
| f.c.c. | 12 | 0.81627 | 0.5902 | 0.1029 | 0.4609 | 0.1516 |
| Mean Field | ∞ | 1.0 | 0.69315 | 0 | 0.5 | 0 |

Table XIII. For the two-dimensional lattices the exact values are as follows (e.g. Domb, 1960):

$$\begin{aligned} \text{h.c.} \quad \sqrt{3} &= 1.7320508 \\ \text{s.q.} \quad 1 + \sqrt{2} &= 2.4142136 \\ \text{p.t.} \quad 2 + \sqrt{3} &= 3.7320508. \end{aligned} \quad (3.10)$$

For the s.c., b.c.c. and f.c.c. the latest estimates are given in Sykes *et al.* (1972b):

$$\begin{aligned} \text{s.c.} \quad 4.6844 &\pm 0.0002 \\ \text{b.c.c.} \quad 6.4055 &\pm 0.0010 \\ \text{f.c.c.} \quad 9.8290 &\pm 0.0005 \end{aligned} \quad (3.11)$$

For earlier estimates see Domb (1960), Fisher (1963, 1967a); it will be found that even the earliest estimates achieved quite a high standard of accuracy. Latest estimates for the diamond lattice are given in Gaunt and Sykes (1973):

$$\text{d.} \quad 2.82641 \pm 0.00010. \quad (3.12)$$

For earlier estimates see Essam and Sykes (1963). The confidence intervals in (3.11) and (3.12) are of the order of one part in 10^4 .

For $s > \frac{1}{2}$ the latest estimates are due to Wortis and collaborators. We quote values of kT_c/J for the f.c.c. lattice (private communication); these values together with those for the s.c. and b.c.c. lattices are being prepared for publication.

$$\begin{aligned} s = 1 &: 6.8211 \pm 0.0002 \\ s = 3/2 &: 5.7582 \pm 0.0003 \\ s = 2 &: 5.2117 \pm 0.0008 \\ s = 5/2 &: 4.8789 \pm 0.0004 \\ s = \infty &: 3.5080 \pm 0.0002. \end{aligned} \quad (3.13)$$

Earlier estimates are given in Domb and Sykes (1962) and Domb and Miedema (1964).

2. Thermodynamic functions

We shall deal shortly with estimates of the high temperature specific heat exponent α . Any such estimate automatically involves an asymptotic fit

of the coefficients a_n which can then be used to sum the series and calculate $\ln Z$ and the internal energy U at T_c . The resultant values are not too sensitive to the choice of α .

For the two-dimensional lattices the values of U_c are known exactly as follows (e.g. Domb, 1960):

$$\begin{aligned} - U_c/J &= \text{h.c. } 2/\sqrt{3} = 1.547005 \\ \text{s.q. } &\quad \sqrt{2} = 1.4142136 \\ \text{p.t. } &\quad 2.0 \end{aligned} \quad (3.14)$$

The value of S_c for the s.q. lattice involves Catalan's constant, whilst those for the h.c. and p.t. lattice involve the evaluation of a definite integral

$$\begin{aligned} S_c/k &= \text{h.c. } 0.26471 \\ \text{s.q. } &\quad 0.30647 \\ \text{p.t. } &\quad 0.33028. \end{aligned} \quad (3.15)$$

For three-dimensional lattices the latest estimates for the s.c., b.c.c., and f.c.c. lattices (Sykes *et al.*, 1972a) are as follows:

$$\begin{aligned} - U_c/J &0.99218 \pm 0.00015 \quad 1.0928 \pm 0.0006 \quad 1.4845 \pm 0.0003 \\ S_c/k &0.55793 \pm 0.00003 \quad 0.58203 \pm 0.00010 \quad 0.59023 \pm 0.00003 \end{aligned}$$

For the diamond lattice (Hunter, 1967)

$$\begin{aligned} - U_c/J &\simeq 0.874 \pm 0.005 \\ S_c/k &\simeq 0.5103 \pm 0.0018. \end{aligned} \quad (3.16)$$

3. Dependence of critical parameters on dimension and lattice structure

One of the earliest important conclusions drawn from series expansions for the Ising model was that dimension rather than lattice structure is the decisive influence on critical behaviour (Domb, 1960). This is already reflected in the critical parameters. If we look at the values of S_c/k in Table XIII we see clearly the transition which occurs in passing from two to three dimensions; for all two-dimensional lattices more than 50% of the entropy change occurs above T_c , but even for the diamond lattice ($q = 4$) in three dimensions this is no longer true.

In order to assess the dependence of the specific heat anomaly on lattice

structure and dimension it is convenient to take T_c as a unit of temperature and consider c_M as a function of τ ($= T/T_c$). Then

$$S_c = \int_0^1 \frac{c_M}{\tau} d\tau \quad (3.17)$$

$$S_\infty - S_c = \int_1^\infty \frac{c_M}{\tau} d\tau,$$

so that a tabulation of S_c and $S_\infty - S_c$ enables us to compare the magnitude of the specific heat curves below and above T_c . The sum of the two terms, S_∞ , is the same for all models with $s = \frac{1}{2}$, and is equal to $k \ln 2$ ($= 0.693147k$).

It is useful similarly to tabulate

$$(U_c - U_0)/kT_c = \frac{1}{k} \int_0^1 c_M d\tau, \quad (3.18)$$

$$- U_c/kT_c = 1/k \int_1^\infty c_M d\tau,$$

which represent directly the areas under the specific heat curve below and above T_c . The sum of these two terms, $- U_0/kT_c$, is no longer constant, but decreases from ∞ to a limiting value of $\frac{1}{2}$ as $q \rightarrow \infty$.

On studying the values of the parameters (3.17) and (3.18) in Table XIII we note that the "tail" of the specific heat curve is much reduced in three dimensions.

If we now wish to study the effect of spin on the specific heat curve, we can tabulate the same parameters for a given lattice for varying s , but we must now remember that the total entropy change is $k \ln(2s + 1)$. Table XIV shows these critical parameters for the f.c.c. lattice, and a striking feature is the insensitiveness to s of the portion *above* T_c ; nearly all of the increase in entropy takes place below T_c .

To appreciate the dependence of T_c on lattice structure and dimension it is convenient to compare the values of kT_c/qJ which takes the value 1 in the mean-field approximation (this approximation should be correct as $q \rightarrow \infty$, see Domb (1960)). Again we see clearly the separation into groups of lattices in two and three dimensions. For spin s the corresponding quantity is kT_c/qJ ($3s/s + 1$) which is presented in Table XIV; this varies little as s passes from $\frac{1}{2}$ to ∞ .

TABLE XIV. Critical parameters for the $I(s)$ model (f.c.c. lattice) (from Domb and Miedema, 1964).

| S | $3kT_c s/qJ(s+1)$ | S_c/k | $(S_\infty - S_c)/k$ | $(U_c - U_0)/kT_c$ | $-U_{cl}/kT_c$ |
|---------------|-------------------|----------|----------------------|--------------------|----------------|
| $\frac{1}{2}$ | 0.816 | 0.590 | 0.103 | 0.461 | 0.152 |
| 1 | 0.851 | 0.983 | 0.116 | 0.721 | 0.160 |
| 2 | 0.864 | 1.486 | 0.123 | 0.990 | 0.167 |
| ∞ | 0.874 | ∞ | 0.131 | 1.541 | 0.175 |

B. Critical exponents and amplitudes

We shall use the notation of Fisher (1967a) for critical exponents which has become widely accepted.

1. High temperature susceptibility γ

This is the oldest and best established critical exponent. For the s.q. and p.t. lattices Domb and Sykes (1957a) suggested that $\gamma = 7/4$. A theoretical justification for this value was first given by Fisher (1959a), and the argument has subsequently been made completely rigorous (Ryazanov, 1965; Kadanoff, 1966a; Wu, 1966; Cheng and Wu, 1967; Abraham, 1973). For the three-dimensional lattices Domb and Sykes initially suggested $\gamma = 1.250$ for the s.c. and f.c.c. lattices and 1.244 for the b.c.c. lattice. However, they later (1961a) made the conjecture that $\gamma = 5/4$ for all three-dimensional lattices, and this constituted an important step towards the so-called *universality hypothesis* (e.g. Kadanoff, 1971; Stanley this volume, Chapter 7). Numerical evidence supporting this value of $5/4$ has accumulated steadily (for details see Gaunt and Guttman this volume Chapter 4), and the latest error bounds are of the order 10^{-3} .

Once a numerical value for the critical exponent has been adopted, Domb and Sykes (1957a) suggested a practical procedure for constructing mimic function to χ_0 over the whole range of interest of the form

$$\chi_0 \sim A(1 - t')^{-\gamma} + \Phi(t'), \quad (t' = T_c/T) \quad (3.19)$$

where $\Phi(t')$ is a polynomial containing the deviations of the initial terms from the asymptotic value given by the first term. In fact the fit (3.19) is usually insensitive to the estimate of γ except in the region very close to T_c .

In this latter region the extension of series expansions in the past few years necessitated the provision of a more refined approximation, and as we have already mentioned the Darboux form (3.9) was adopted. Naturally the first application of this form was to two-dimensional lattices for which the critical

temperatures and exponent γ are known exactly. The present author (Domb, 1970b) has pointed out that a study of the form of the correlations at T_c suggests that the susceptibility is not precisely of Darboux form (3.9), but contains residual singularities of the form

$$(1 - t')^m [\ln(1 - t')]^n \quad (m, n > 0). \quad (3.20)$$

However, these singularities give a smaller contribution than the first three Darboux terms, and they can therefore be neglected in numerical analysis of the terms currently available.

For the p.t. lattice Sykes *et al.* (1972a) obtained the following numerical estimates:

$$\begin{aligned} kT\chi_0/m^2 \simeq & 0.847086 (1 - \theta)^{-7/4} + 0.1756 (1 - \theta)^{-3/4} \\ & + 0.0287 (1 - \theta)^{1/4} + \Psi_{\text{p.t.}}(\theta) \quad (3.21) \\ & (\theta = w/w_c). \end{aligned}$$

$\Psi_{\text{p.t.}}(\theta)$ is a small residual polynomial whose value in the critical region is about -0.272 . The first coefficient in (3.21) representing the amplitude A_+ is the most accurately determined, and Sykes *et al.* suggest that

$$A_+(\text{p.t.}) = 0.84709 \pm 0.00002. \quad (3.22)$$

For the s.q. lattice the antiferromagnetic singularity must be taken into account, and Fisher (1959a) suggested it should have the same form as the internal energy. (We shall discuss the antiferromagnetic aspect in more detail in Section III.D). Sykes *et al.* (1972a) put forward the following numerical estimates:

$$\begin{aligned} kT\chi_0/m^2 = & 0.771742(1 - \theta)^{-7/4} + 0.3472(1 - \theta)^{-3/4} \\ & - 0.2003(1 + \theta) \ln(1 + \theta) + \Psi_{\text{s.q.}}(\theta) \quad (3.23) \end{aligned}$$

Again $\Psi_{\text{s.q.}}(\theta)$ is a small residual polynomial whose critical value is -0.073 . The error limits for the amplitude A_+ are as follows:

$$A_+(\text{s.q.}) = 0.77174 \pm 0.00002. \quad (3.24)$$

For the h.c. lattice Sykes *et al.* (1972a) experienced much greater difficulty in fitting the series expansions because of the presence of a pair of disturbing singularities in the complex plane at $w = \pm i/\sqrt{3}$. They were able to obtain a direct estimate of A_+ of 0.6478 , but they suggested that a more accurate estimate could be obtained by transformation from the

p.t. lattice. (Fisher, 1959b; Syozi, Vol. 1 Chapter 7):

$$A_+(\text{h.c.}) = 2 \cdot 3^{-7/8} A_+(\text{p.t.}) = 0.64786 \pm 0.00002. \quad (3.25)$$

In terms of the temperature variable t' the corresponding amplitudes are as follows:

$$kT\chi_0/m^2 \sim A'_+(1-t')^{-7/4} \quad (t' = T_c/T)$$

where

$$A'_+(\text{p.t.}) = 0.92421 \pm 0.00003$$

$$A'_+(\text{s.q.}) = 0.96259 \pm 0.00003 \quad (3.26)$$

$$A'_+(\text{h.c.}) = 1.04642 \pm 0.00003.$$

Earlier estimates for the planar lattices can be found in Sykes and Fisher (1962).

For the three dimensional lattices Sykes *et al.* (1972b) accept the conjecture that $\gamma = 5/4$ and again use the Darboux form for a more refined analysis. For the f.c.c. lattice this analysis leads to the following numerical estimates:

$$\frac{kT\chi_0}{m^2} \simeq 0.9634(1-\theta)^{-5/4} + 0.1965(1-\theta)^{-1/4} \\ + 0.4993(1-\theta)^{3/4} + \psi_{\text{f.c.c.}}(\theta). \quad (3.27)$$

However, only the leading amplitude is reasonably well defined

$$A_+(\text{f.c.c.}) = 0.963 \pm 0.002. \quad (3.28)$$

For the s.c. and b.c.c. lattices it is necessary to take account of the antiferromagnetic singularity, and Fisher's argument leads to a Darboux form as follows:

$$\frac{kT\chi_0}{m^2} = (1-\theta)^{-\gamma} \phi_f(\theta) + (1+\theta)^{-\alpha+1} \phi_a(\theta) + \psi_f(\theta). \quad (3.29)$$

We shall see shortly that there is good numerical support for the conjecture $\alpha = 1/8$, and this was the value adopted by Sykes *et al.* (1972b). They then found for the s.c. lattice,

$$\frac{kT\chi_0}{m^2} \simeq 1.0161(1-\theta)^{-5/4} + 0.0590(1-\theta)^{-1/4} + 0.5610(1+\theta)^{7/8} \\ + \psi_{\text{s.c.}}(\theta); \quad (3.30)$$

and for the b.c.c. lattice

$$\frac{kT\chi_0}{m^2} \simeq 0.9660(1-\theta)^{-5/4} + 0.1826(1-\theta)^{-1/4} + 0.5359(1+\theta)^{7/8} \\ + \psi_{\text{b.c.c.}}(\theta). \quad (3.31)$$

The error bounds in the amplitude estimates are as follows:

$$\left. \begin{aligned} A'_+(s.c.) &= 1.0160 \pm 0.0010 \\ A'_+(\text{b.c.c.}) &= 0.965 \pm 0.003 \end{aligned} \right\} \quad (3.32)$$

In terms of the temperature variable t' in (3.26)

$$\left. \begin{aligned} A'_+(\text{f.c.c.}) &= 0.971 \pm 0.002 \\ A'_+(\text{b.c.c.}) &= 0.985 \pm 0.003 \\ A'_+(\text{s.c.}) &= 1.0582 \pm 0.0010 \\ A'_+(\text{d.}) &= 1.172 \pm 0.001 \dagger \end{aligned} \right\} \quad (3.33)$$

Ferer and Wortis (1972) give as corresponding estimates for the first three lattices 0.9750 ± 0.0003 , 0.9904 ± 0.0004 , 1.0615 ± 0.0010 . Since these are based on fewer terms in the expansion and a less refined analysis the error bounds are probably unduly optimistic. The general agreement is quite satisfactory. Earlier estimates for the three dimensional lattices can be found in Fisher and Sykes (1962).

For general spin s fewer terms are available and it has not been possible so far to undertake such a refined analysis. Domb and Sykes in 1962 suggested that γ is independent of spin, and this provided a second step towards the universality hypothesis. The more extensive expansions of Wortis and his group have confirmed this view, but when $s > \frac{1}{2}$ there seems to be a non-Darboux singularity which complicates the analysis (Ferer *et al.*, 1971). However, in an analysis of the p.t. lattice for varying s Moore and Trainin (1972) have expressed some reservations. They say that, whilst the data are not inconsistent with a spin-independent γ , the evidence is inconclusive.

For the f.c.c. lattice the following amplitudes were obtained for $s > \frac{1}{2}$ (Wortis, private communication)

$$\begin{aligned} A'_+(s=1) &= 0.565 \pm 0.003 \\ A'_+(s=3/2) &= 0.452 \pm 0.002 \\ A'_+(s=2) &= 0.401 \pm 0.003 \\ A'_+(s=\infty) &= 0.256 \pm 0.002 \end{aligned} \quad (3.34)$$

[†]This value is taken from Essam and Hunter (1968).

2. Spontaneous magnetization β

For a number of two dimensional lattices closed form solutions are available for the spontaneous magnetization and $\beta = 1/8$ (see e.g. Domb, 1960). For the s.q. lattice, terms in the series expansion are all consistent in sign, and if the exact solution were not available there would have been little difficulty in estimating the exponent from these terms (Domb, 1949). However, for the s.c. lattice the terms alternate in sign and there is a masking unphysical singularity, whilst for the b.c.c. and f.c.c. lattices the coefficients behave in a very irregular fashion (Table X).

It was in connection with these series that the Padé approximant registered its first notable success, and as a result Baker (1961) suggested that for these three dimensional lattices $\beta \approx 0.30$. Subsequently Essam and Fisher (1963) modified this value slightly, giving the bounds

$$0.303 \leq \beta \leq 0.318 \quad (3.35)$$

but conjectured that β is exactly equal to $5/16$. Essam and Sykes (1963) developed series expansions for the diamond lattice which are all consistent in sign; applying the ratio method they suggested that it might be possible to decrease the error interval to $\beta = 0.312 \pm 0.002$. However, more extensive series expansions developed recently (Gaunt and Sykes, 1973) show that there are irregularities in behaviour characteristic of low temperature series and extend the error bounds to 0.312 ± 0.005 ; certainly there is still a good case for accepting $\beta = 5/16$. For detailed numerical treatment of the above and corresponding references see Gaunt and Guttman, this volume Chapter 4.

We have mentioned the development of low temperature series expansions when $s > \frac{1}{2}$. The cases $s = 1, 3/2$ have been subjected to detailed analysis, and the results are consistent with the same value of β , $1/8$, in two dimensions and $5/16$ in three dimensions (Fox and Guttman, 1973; Guttman *et al.*, 1971). This supports the universality hypothesis that critical exponents are independent of spin.

It is interesting to see how the spontaneous magnetization changes with s for a given lattice; Fig. 19 taken from Fox and Guttman (1973) shows that the variation is in fact quite small, and of the same order as the change with lattice structure in a given dimension.

The amplitudes have been estimated as

$$\frac{M_0}{m} \sim B(1 - t)^\beta \quad (3.36)$$

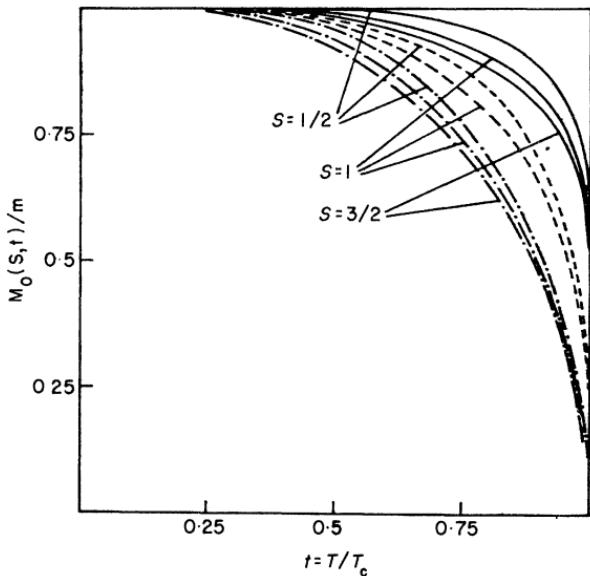


FIG. 19. Variation of the spontaneous magnetization of the Ising model on the p.t. and b.c.c. lattices with spin s and relative temperature $t = T/T_c$. Molecular field theory results are also shown. —, p.t. lattice; - - -, b.c.c. lattice; - · - · -, molecular field theory. (From Fox and Guttman, 1973.)

with the following values of B :

| Lattice | $s = \frac{1}{2}$ | $s = 1$ | $s = \frac{3}{2}$ |
|---------|-------------------|-------------------|-------------------|
| h.c. | 1.253178 | 1.180 ± 0.003 | — |
| s.q. | 1.222410 | 1.137 ± 0.003 | — |
| p.t. | 1.203270 | 1.112 ± 0.002 | 1.074 ± 0.008 |
| d. | 1.666 ± 0.004 | 1.509 ± 0.001 | — |
| s.c. | 1.569 ± 0.003 | 1.433 ± 0.001 | — |
| b.c.c. | 1.506 ± 0.002 | 1.378 ± 0.001 | — |
| f.c.c. | 1.487 ± 0.002 | 1.361 ± 0.001 | 1.31 ± 0.04 |

(3.37)

3. Critical isotherm δ

The series expansion (1.46) taken at the critical temperature u_c defines the $M-H$ relationship along the critical isotherm. The terms are all consistent in sign, the dominant singularity corresponding to $y=1$ or $H=0$; hence the critical exponent δ is determined by the asymptotic value of the coefficients $g_r(u_c)$. The first attempt to estimate δ in this way was made by Gaunt *et al.* (1964) and yielded the values

$$\delta = 15.00 \pm 0.08 \quad (\text{two dimensions})$$

$$\delta = 5.20 \pm 0.15 \quad (\text{three dimensions}). \quad (3.38)$$

It was suggested that the two dimensional value might be exactly 15 since this would satisfy certain exponent relations which had been derived for the droplet model (Essam and Fisher, 1963).

Shortly afterwards Domb and Hunter (1965) proposed an equation of state in the critical region in which all critical exponents depended on only two parameters. In addition to δ being 15 in two dimensions the currently accepted values of γ and β in three dimensions led to the conclusion that δ is exactly 5 in three dimensions. This proposal led Gaunt (1967) to re-examine the series expansions mentioned above, and using an alternative analysis he was indeed led to the exact integral values. The latest investigation by Gaunt and Sykes (1972) makes use of several additional terms in the expansion (see Sykes *et al.* 1973d). The result confirms $\delta = 15$ in two dimensions to within $\frac{1}{2}\%$ and $\delta = 5$ in three dimensions to within 1% ($\delta = 5.00 \pm 0.05$). Incidentally, certain patterns of oscillation in the coefficients $g(u_c)$ are traced to the presence of spurious unphysical singularities just outside the circle of convergence. Also the singularity is not expected to be of Darboux form (see Section III.D).

For $s = 1$ the error bounds are larger, and Fox and Gaunt (1972) estimate

$$\begin{aligned} \delta &= 15.0 \pm 1.0 && \text{(two dimensions)} \\ \delta &= 5.05 \pm 0.15 && \text{(three dimensions).} \end{aligned} \quad (3.39)$$

For $s = 3/2$ it is more difficult to make definite estimates but the results are consistent with the $s = \frac{1}{2}$ values. Hence again there is moderate evidence that δ is independent of s .

Near the critical point ($H = 0$) writing

$$1 - y \simeq 2\beta mH \simeq DM^\delta \quad (3.40)$$

the estimates for amplitude D are as follows (Gaunt and Sykes, 1972; Fox and Gaunt, 1972):

| Lattice | $s = \frac{1}{2}$ | $s = 1$ | $s = 3/2$ |
|---------|-------------------|-----------------|-----------------|
| h.c. | 0.550 ± 0.004 | 1.09 ± 0.04 | — |
| s.q. | 0.847 ± 0.004 | 2.0 ± 0.15 | — |
| p.t. | 1.100 ± 0.005 | 2.8 ± 0.5 | 3.4 ± 0.4 |
| d. | 0.390 ± 0.015 | 0.57 ± 0.09 | — |
| s.c. | 0.535 ± 0.015 | 0.66 ± 0.02 | — |
| b.c.c. | 0.66 ± 0.02 | 0.79 ± 0.03 | — |
| f.c.c. | 0.715 ± 0.015 | 0.84 ± 0.15 | 0.87 ± 0.15 |

(3.41)

4. Gap exponent Δ

In their investigation of the critical equation of state Domb and Hunter

(1965) started by considering the high temperature critical exponents of the field derivatives of the susceptibility. Numerical analysis of the first few derivatives indicated that they were of the form

$$\frac{d^{2r}\bar{\chi}_0}{d\bar{H}^{2r}} = C_{2r}^+ (1 - t')^{-\gamma - 2r\Delta}, \quad (\bar{\chi}_0 = kT\chi_0/m^2, \bar{H} = \beta mH) \quad (3.42)$$

where $2\Delta \approx 3\frac{3}{4}$ in two dimensions and $3\frac{1}{2}$ in three dimensions. Domb and Hunter conjectured that (3.42) was generally valid and they termed 2Δ the *gap exponent*.

A detailed numerical treatment of the available data was subsequently provided by Essam and Hunter (1968), using both the ratio and PA methods. The conjecture (3.42) and the numerical values of Domb and Hunter were confirmed, the error bounds for the PA analysis being

$$\Delta = 1.87 \pm 0.01 \quad (\text{two dimensions})$$

$$\Delta = 1.563 \pm 0.003 \quad (\text{three dimensions}). \quad (3.43)$$

The amplitude estimates $C_{2r}^+/(2r + 2)!$ are reproduced in Table XV. (The notation differs from Essam and Hunter, 1968).

5. High temperature specific heat α

The high temperature series for $\ln Z$ take considerably longer to settle down to their asymptotic behaviour than those for χ_0 . This is particularly true for "even" lattices like the s.c. and b.c.c. where all odd coefficients vanish, but even for the f.c.c. lattice the convergence is slow. The earliest estimate of α by Domb and Sykes (1957b) from the terms then available for the f.c.c. lattice suggested a small positive power $< \frac{1}{4}$.

The critical equation of state proposed by Domb and Hunter (1965) led to the conjecture $\alpha = 1/8$ (taking $\gamma = 5/4$, $\beta = 5/16$). This conjecture stimulated Sykes and his collaborators to add several new terms to the expansion for the f.c.c. lattice and they were able to provide remarkable evidence to support it. Their "ratio-plot" for the susceptibility and specific heat is reproduced in Fig. 20. Subsequently they extended the calculations to the s.c., and b.c.c. lattices and obtained the same value of α .

Detailed numerical results are given in two papers by Sykes *et al.* (1967) and (1972c); as for χ_0 the approximation to C_H consists of an asymptotic

TABLE XV. Critical amplitudes of derivatives of susceptibility (eqn. 3.42). (Data from Essam and Hunter, 1968)

| | s.q. | p.t. | d. | s.c. | b.c.c. | f.c.c. |
|--------------|---------------|---------------|---------------|---------------|---------------|-----------------|
| $C_2/4!$ | -0.182 ± .002 | -0.167 ± .002 | -0.184 ± .001 | -0.153 ± .001 | -0.138 ± .002 | -0.1334 ± .0001 |
| $C_4/6!$ | 0.176 ± .003 | 0.154 ± .003 | 0.180 ± .004 | 0.137 ± .001 | 0.117 ± .001 | 0.1130 ± .0006 |
| $C_6/8!$ | -0.24 ± .02 | -0.21 ± .01 | -0.26 ± .02 | -0.172 ± .002 | -0.140 ± .002 | -0.136 ± .004 |
| $C_8/10!$ | 0.34 ± .06 | 0.32 ± .01 | 0.39 ± .05 | 0.26 ± .01 | 0.202 ± .007 | 0.20 ± .02 |
| $C_{10}/12!$ | -0.7 ± .1 | -0.6 ± .1 | -0.7 ± .1 | -0.5 ± .1 | -0.33 ± .03 | -0.24 ± .03 |

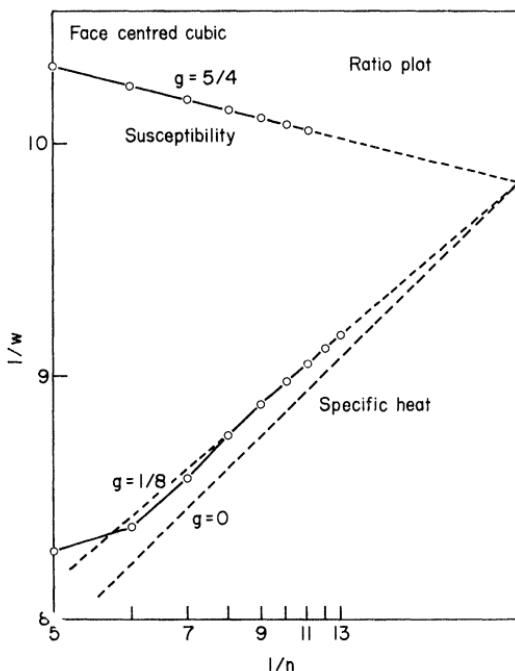


FIG. 20. Ratio plot of a_n/a_{n-1} versus $1/n$ for the susceptibility and specific heat of the f.c.c. lattice; g represents the exponent. (After Sykes.)

term and a correction polynomial. In the critical region the approximation proposed is

$$\frac{C_H}{R} \simeq E_+ (1 - t')^{-1/8} + e_+ \quad (3.44)$$

with the following values of E_+ , e_+ :

$$\begin{aligned} E_+(\text{f.c.c.}) &\simeq 1.089, & e_+ &\simeq -1.241, \\ E_+(\text{b.c.c.}) &\simeq 1.106, & e_+ &\simeq -1.248, \\ E_+(\text{s.c.}) &\simeq 1.136, & e_+ &\simeq -1.242. \end{aligned} \quad (3.45)$$

For the diamond lattice corresponding results are given by Hunter (1967)

$$E_+(\text{diamond}) \simeq 1.17, \quad e_+ \simeq -1.23. \quad (3.46)$$

Hunter (1969) has suggested that the constant e_+ and the weakness of the singularity explain why PA analyses do not give very satisfactory results

for C_H . He finds that d^2C_H/dT^2 is a much better function for a PA analysis.

The form of the specific heat is insensitive to lattice structure as is well illustrated by Fig. 6 in Chapter 4 of this volume (Gaunt and Guttman), taken from Hunter (1967).

For spin s the data of Domb and Sykes (1962) were insufficient for an estimate of the critical exponent. The most lengthy series currently available are due to Wortis and his collaborators (Wortis *et al.*, 1973) but no detailed analysis has yet been published.

6. High temperature correlation exponents

In the present review we are basically concerned with series expansions for thermodynamic properties. Corresponding expansions for correlation functions will be discussed in Vol. 4 of the present publication by Fisher and Jasnow. However, because of certain relations between thermodynamic and correlation exponents we summarize the numerical data currently available for the Ising model.

In 1967 Fisher and Burford published a definitive paper on correlation functions for the Ising model. They introduced two primary exponents which characterize correlation functions; the first, ν , represents the rate of divergence of the "coherence length" as $T \rightarrow T_c$,

$$L \sim (1 - t')^{-\nu}; \quad (3.47)$$

the second, η , represents the decay of correlations with distance at the critical temperature

$$\Gamma(r) \sim 1/r^{d-2+\eta}. \quad (3.48)$$

More fully the asymptotic behaviour of the pair correlation function in the critical region is given by

$$\Gamma(r) \sim \frac{1}{r^{d-2+\eta}} P(\kappa r), \quad (3.49)$$

where

$$\kappa(\nu) \sim (1 - t')^\nu, \quad (3.50)$$

$P(0)$ is non zero, and $P(x)$ has an exponential decay for large x . ν and η are related by Fisher's relation (1964)

$$\gamma = \nu(2 - \eta). \quad (3.51)$$

For the three dimensional $I(\frac{1}{2})$ model Fisher and Burford estimated

$$\begin{aligned} \nu &\simeq 0.6430 \pm 0.0025, \\ \eta &\simeq 0.056 \pm 0.008. \end{aligned} \quad (3.52)$$

Subsequent extended calculations by Moore *et al.* (1969) modified these estimates only slightly to

$$\begin{aligned} \nu &= 0.638^{+0.002}_{-0.001} \\ \eta &= 0.041^{+0.006}_{-0.003}. \end{aligned} \quad (3.53)$$

Finally, for $I(s)$ strong evidence has been adduced to suggest that the exponents are independent of s (Ferer *et al.*, 1971).

7. Low temperature exponents γ' , α' and Δ'

It was recognized quite early that low temperature series are often inconsistent in sign and therefore harder to deal with than their high temperature counterparts (Wakefield, 1951; Domb, 1952). For the spontaneous magnetization we have seen in a previous section that these difficulties were overcome when the Padé approximant was introduced. However, PA analysis was less satisfactory when applied to α' and γ' . For the s.q. lattice Essam and Fisher (1963) suggested that $\gamma' \simeq 1.75 \pm 0.01$ which is sufficiently close to γ to suggest symmetry of the exponents below and above T_c . For the s.c., b.c.c. and f.c.c. lattices they still suggested symmetry ($\gamma' \simeq 1.25^{+0.07}_{-0.02}$) although the error bars were considerably larger.

For a heuristic model (the droplet model Section IV.E) Essam and Fisher found that the relation

$$\alpha' + 2\beta + \gamma' = 2 \quad (3.54)$$

was satisfied exactly. They pointed out that this relation was also satisfied for the two dimensional Ising model, and suggested that it might be satisfied for the three dimensional model in which case $\alpha' \sim 1/8$. However, direct PA analysis of the s.c., b.c.c. and f.c.c. lattices gave $\alpha' \simeq 0$ (Baker, 1963), and for the diamond lattice for which all terms are positive, Essam and Sykes (1963) showed that the ratio method also led to $\alpha' \simeq 0$.

Rushbrooke (1963) then made the important observation that thermodynamics alone enabled one to derive an inequality,

$$\alpha' + 2\beta + \gamma' \geq 2,$$

which was violated if $\alpha' \simeq 0$, $\beta \simeq 5/16$ and $\gamma' \simeq 5/4$. It was clear therefore that some of the exponents needed modification. Gaunt and Essam (1964)

undertook a careful examination of the series expansions for α' for the diamond lattice but were unable to increase its value significantly above 0.

In 1965 a new proposal was advanced of a particular form of equation of state (the *scaling form*) for the Ising model in the critical region (see Section III.C) and this required (at least in its simplest form) symmetry of critical exponents below and above T_c . A number of authors suggested that whilst a simple form of equation of state was adequate for the two-dimensional model, a more sophisticated form of equation of state which allowed asymmetry might be needed for the three-dimensional model. Thus, for example, Baker and Gaunt (1967) analysed C_M/C_H and suggested that $\alpha' \approx 1/16$, $\beta\beta \approx 5/16$, $\gamma' \approx 1 - \frac{5}{T_6}$, and Essam and Hunter (1968) were in favour of $\Delta' \neq \Delta$ (see also Fisher 1967; Guttmann and Thompson, 1969).

An alternative proposal maintained symmetry in the critical exponents, but suggested that the low temperature series converge only slowly, and that the current estimates did not represent the true exponents (Domb, 1966, 1967, 1970a; Gaunt, 1967; Gaunt and Domb, 1968). This latter view has gained support recently as more theoretical and experimental evidence has accrued in favour of the simple scaling form for the equation of state. Indirect support for $\alpha' \approx 1/8$, $\gamma' \approx 5/4$ has also come from Garelick and Essam (1968) from the Syozi model (see Essam, Vol. 2, Chapter 6) who concluded that $0.117 < \alpha' < 0.178$.

However, the question has not yet been resolved satisfactorily even by the addition recently of several more terms to the diamond and f.c.c. lattices. The latest discussion by Gaunt and Sykes (1973) points out that whilst the data are not inconsistent with $\gamma' = \gamma$, the rate of convergence is too slow for precise conclusions to be drawn. Analysis for spin s leads to the conclusion that the exponents do not depend noticeably on s (Fox and Guttmann, 1970, 1973; Guttmann *et al.*, 1971).

For this reason we have not quoted low temperature amplitudes since their reliability is in question. However, for the susceptibility of the two dimensional lattices the position is better, and, as mentioned above, Essam and Fisher (1963) using a PA analysis concluded that $\gamma' = \gamma$, a conclusion which was borne out subsequently by rigorous analysis (see references in Section III.B1). They then estimated the following amplitudes:

$$\begin{aligned}\bar{\chi}_0 &\sim A'_-(1-t)^{-7/4}, \\ A'_-(\text{h.c.}) &= 0.0281 \pm 0.0006 \\ A'_-(\text{s.q.}) &= 0.0262 \pm 0.0006 \\ A'_-(\text{p.t.}) &= 0.0248 \pm 0.0006.\end{aligned}\tag{3.55}$$

Essam and Fisher drew the important physical conclusion that there is a

large asymmetry in the amplitudes, A'_+/A'_- being about 37; they estimated the corresponding asymmetry in three dimensions to be about 5.

In an attempt to obtain a better understanding of the structure of low temperature series Guttmann (1969) used the method of N -point fits (see Gaunt and Guttmann, this volume Chapter 4, Section IV) to locate the unphysical singularities for various lattices. For the s.c. lattice he found that there is one such singularity on the negative real axis, for the b.c.c. lattice there is a complex pair, and for the f.c.c. lattice there are two complex pairs. These singularities lie closer to the origin than the physical singularity thus masking the critical behaviour. We have seen that for the spontaneous magnetization the PA method enables the spurious singularities to be by-passed and attention to be focussed on the physical singularity. However, it seems that the degree of success with which this can be done depends on the relative strengths of the physical and unphysical singularities. For the spontaneous magnetization this is favourable, less so for the susceptibility and worst for the specific heat (Guttmann, 1969; Thompson *et al.*, 1969).

Domb and Guttmann (1970) have initiated a configurational analysis of terms of the low temperature series which shows how the spurious singularities arise. Starting from the empirical observation that Cayley-tree embeddings are far more numerous than those of any other group of connected graphs, they estimate the Cayley-tree contribution to the low temperature series to be

$$\sum (v\xi)^n n^{-h}$$

where v is a constant depending on lattice structure, and ξ is a low temperature variable (analogous to $\tanh \beta J$ at high temperatures) given by

$$\xi = \frac{4u^{q/2}(u^{-1}-1)}{\{1+u^{q/2-1}+\sqrt{[(1-u^{q/2-1})^2+4u^{q/2}]}\}}. \quad (3.56)$$

The singularities correspond to $\xi = 1/v$, and a first approximation, from (3.56) gives

$$u_c^{q/2-1} = 1/4v. \quad (3.57)$$

For $q = 4$ there is only one solution; for $q = 6$ there are two at $\pm 2^{-1}v^{-1/2}$; for $q = 8$ there are three at $2^{-2/3}v^{-1/3} \exp 2s\pi i/3$; and for $q = 12$ there are five at $2^{-2/5}v^{-1/5} \exp 2s\pi i/5$. In this approximation the spurious singularities all lie on the circle $u = u_c$. Higher order approximations move the spurious singularities in nearer to the origin, and give results reasonably close to the numerical calculations (Fig. 21).

For the diamond lattice there are no spurious singularities within $u = u_c$ and one might expect rapid convergence. Unfortunately, there seems here

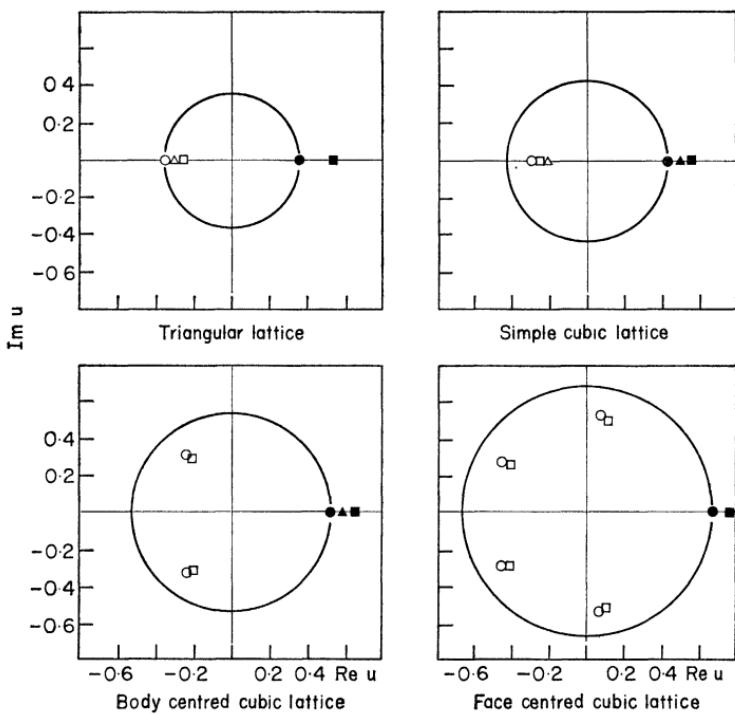


FIG. 21. Distribution of singularities in the complex u plane for various lattices. ●○, obtained from series expansions; ▲■, approximations (physical singularity); △□, approximations (non-physical singularities). (Domb and Guttman, 1969.)

to be a conjugate pair of spurious singularities on or very close to the circle of convergence and the imaginary axis, and these slow down the convergence (Gaunt and Sykes, 1973).

We should finally mention an attempt by Gaunt and Domb (1968) to construct a low temperature specific heat curve assuming that $\alpha' = \alpha$. Taking a Darboux correction term, they were led to the expression

$$\frac{C_H}{R(\ln z)^2} \simeq 3.1(1 - \theta')^{-1/8} - 39.68(1 - \theta')^{7/8} + \phi(\theta'), \quad (\theta' = u/u_c) \quad (3.58)$$

where $\phi(\theta')$ is a correction polynomial. The large amplitude of the correction term could account for slowness of convergence, and Gaunt and Domb showed that it led to a region in the range $(t - 1) > 10^{-4}$ where C_H was virtually logarithmic. In the critical region they suggested the approximation

$$C_H \sim 0.20(1 - t)^{-1/8} + 0.13, \quad (3.59)$$

but it was later pointed out by Hohenberg and Barmatz (1972) that this formula, taken in conjunction with (3.46), is inconsistent with the scaling form of equation of state since the constant term should be the same above and below T_c . This point requires further investigation.

C. Equation of state in the critical region

One of the most important recent developments in the theory of critical behaviour took place in 1965 with the proposal of an equation of state for a ferromagnet (or fluid) in the critical region. The same equation of state was postulated independently and almost simultaneously in three different papers, Widom (1965), Domb and Hunter (1965) and Patashinskii and Pokrovskii (1966). Widom attempted to find a generalization for a fluid of the van der Waals equation which would allow non-classical values for critical exponents; he was thereby led to a "homogeneous" form of equation of state. Patashinskii and Pokrovskii, using the physical picture of a critical region consisting of large blocks of coherent spins in opposite directions, conjectured a form for the multiple-correlation functions between spins. Domb and Hunter followed up the consequences of the existence of a "gap" exponent for the high temperature derivatives of the susceptibility of a ferromagnet. All three were led to the same form of thermodynamic equation of state. Subsequently, in a remarkable interpretive paper Kadanoff (1966b) suggested a scaling hypothesis from which this equation of state could be derived, and for this reason it has often been described subsequently as a *scaling equation of state*.

The discussion in Section III.B has dealt with critical exponents in isolation from one another, but in Section II.B7 mention was made of suggestions that there might be relations between these exponents. The scaling equation of state leads to many such relations (called *scaling laws*) and to the conclusion that two independent parameters suffice to derive all *thermodynamic* critical exponents. However, Kadanoff's ideas (and likewise those of Patashinskii and Pokrovskii) lead to additional relations involving correlation exponents. To differentiate between the two groups of relations the former are usually referred to as *thermodynamic scaling* and the latter as *length scaling*. Our own concern is mainly with thermodynamic scaling, but we shall refer briefly to numerical evidence for length scaling since this is a problem of great current interest.

Since we are dealing with the Ising model we shall follow the approach of Domb and Hunter, and this leads naturally to the use of critical amplitudes to obtain a numerical estimate of the equation of state.

1. M-H relation in the critical region

We have already introduced the gap exponent Δ in Section II.B4, and if

we follow the Domb-Hunter conjecture (3.42), we can obtain the following expansion for M as a function of H :

$$\begin{aligned} \bar{M} &\simeq \bar{H} C_0^+ \tau^{-\gamma} + \frac{\bar{H}^3}{3!} C_2^+ \tau^{-\gamma-2\Delta} + \frac{\bar{H}^5}{5!} C_4^+ \tau^{-\gamma-4\Delta} \\ &+ \frac{\bar{H}^7}{7!} C_6^+ \tau^{-\gamma-6\Delta} + \dots \\ &= \bar{H} \tau^{-\gamma} (C_0^+ + \frac{1}{3!} C_2^+ \bar{H}^2 \tau^{-2\Delta} + \frac{1}{5!} C_4^+ \bar{H}^2 \tau^{-4\Delta} + \dots) \quad (3.60) \\ &= \bar{H} \tau^{-\gamma} Y^+(\bar{H} \tau^{-\Delta}) \quad (\bar{M} = M/m, \bar{H} = \beta m H) \end{aligned}$$

Here

$$\tau = (T/T_c - 1), \quad (3.61)$$

and should not be confused with the magnetic field variable defined in (1.34). Domb and Hunter also assumed that the function defined by the expansion in (3.60) is analytic, and that the series expansion can therefore be manipulated in the normal manner of power series.

Some guidance on the nature of this function was obtained from the mean field equation of state (see e.g. Domb, (1960); Burley, Vol. 2 Chapter 9)

$$\bar{M} = \tanh(t' \bar{M} + \beta m \bar{H}), \quad (t' = T_c/T), \quad (3.62)$$

which can readily be inverted to give,

$$\begin{aligned} \beta m \bar{H} &= \tanh^{-1} \bar{M} - t' \bar{M} \\ &= \bar{M}(1 - t') + \frac{1}{3} \bar{M}^3 + \frac{1}{5} \bar{M}^5 + \dots \end{aligned} \quad (3.63)$$

It is clear that (3.63) is much easier to handle as an expression of critical behaviour than (3.60). Domb and Hunter therefore inverted (3.60) to obtain

$$\bar{H} = \bar{M} D_0^+ \tau^\gamma + \bar{M}^3 D_2^+ \tau^{3\gamma-2\Delta} + \bar{M}^5 D_4^+ \tau^{5\gamma-4\Delta} + \dots \quad (3.64)$$

or

$$\bar{H} \tau^{-\Delta} = X^+(\bar{M} \tau^{\gamma-\Delta}), \quad (3.65)$$

where

$$X^+(u) = D_0^+ u + D_2^+ u^3 + D_4^+ u^5 + \dots \quad (3.66)$$

The coefficients D_0^+ , D_2^+ , D_4^+ ... can readily be derived from C_0^+ , C_2^+ , C_4^+ . In the case of the mean field equation (3.63) only D_0^+ and D_2^+ in (3.66) are non-zero to the order of approximation with which we are presently concerned.

Equation (3.65) is an equation of state depending on two parameters γ and Δ , and a single function X^+ ; therefore we might expect all critical exponents to be expressible in terms of γ and Δ . However, the expansion (3.66) covers only a portion of the critical region, say

$$u = \bar{M} \tau^{\gamma - \Delta} < A; \quad (3.67)$$

since $(\Delta - \gamma)$ is always positive (we shall see shortly that it is equal to the spontaneous magnetization exponent β) expansion (3.66) cannot be used near $\tau = 0$ for finite \bar{M} . We need an analytic continuation of the series. But we have another source of information which enables us to determine the form of an alternative expansion which constitutes such an analytic continuation; rigorous theorems have established that the M - H relation is analytic as long as $H \neq 0$ (see Griffiths, Vol. 1 Chapter 2). This means that we can write

$$\bar{H} = K_0(\bar{M}) + \tau K_1(\bar{M}) + \tau^2 K_2(\bar{M}) + \dots \quad (3.68)$$

where the $K_r(\bar{M})$ are analytic as long as $\bar{M} \neq 0$. The critical exponent δ has already been defined when $\tau = 0$ by (3.40), so that

$$K_0(\bar{M}) \simeq k_0 \bar{M}^\delta. \quad (3.69)$$

Comparing (3.68) with (3.65) we can readily see that they are compatible only if

$$\left. \begin{aligned} \Delta - \delta\beta &= 0 \\ K_r(\bar{M}) &\simeq k_r \bar{M}^{\delta - r/\beta} \end{aligned} \right\} \quad (3.70)$$

where we have anticipated by writing $\beta = (\Delta - \gamma)$ for convenience. The alternative expansion (3.68) then corresponds to

$$X^+(u) = u^{\delta\beta} [k_0 + k_1 u^{-1/\beta} + k_2 u^{-2/\beta} \dots + k_r u^{-r/\beta} \dots], \quad (3.71)$$

which should be valid in a region complementary to (3.67)

$$u^{-1/\beta} < B, \quad \bar{M}\tau^{-\beta} > B'. \quad (3.72)$$

However, using (3.68) and (3.70) we are in a position (following Griffiths, 1967) to rewrite (3.65) in the simpler alternative form

$$\bar{H} = \bar{M}^\beta h(x), \quad (x = \tau \bar{M}^{-1/\beta}) \quad (3.73)$$

where the function $h(x)$ can be expanded in a manner analogous to (3.66) and (3.71) as follows. The large x expansion corresponds to the high

temperature side of the critical point, and is obtained from (3.66),

$$h(x) = x^\Delta (D_0^+ x^{-\beta} + D_2^+ x^{-3\beta} + D_4^+ x^{-5\beta} + \dots). \quad (3.74)$$

The small x expansion corresponds to the critical isotherm region, and is obtained from (3.71),

$$h(x) = k_0 + k_1 x + k_2 x^2 + \dots. \quad (3.75)$$

The low temperature side of the critical point corresponds to negative x ; a spontaneous magnetization can arise only if there is a solution $H = 0$, $M \neq 0$, i.e. if there is a value $-x_0$ satisfying

$$h(-x_0) = 0. \quad (3.76)$$

We then have

$$\bar{M}_0 \simeq (x_0)^\beta |\tau|^\beta, \quad (3.77)$$

so that β as defined above $= (\Delta - \gamma)$, is indeed the critical exponent of the spontaneous magnetization; x_0 is related to the amplitude B in (3.36).

TABLE XVI. Scaling relations between critical exponents

| Thermodynamic quantity | Exponent | [2] Ising | [3] Ising | Mean field |
|---------------------------------|-------------------------------------|--------------|--------------|---------------|
| High temperature susceptibility | γ | 7/4 | 5/4 | 1 |
| High temperature gap | 2Δ | 15/4 | 25/8 | 3 |
| High temperature specific heat | $\alpha = 2 + \gamma - 2\Delta$ | 0 | 1/8 | 0 |
| Low temperature specific heat | $\alpha' = \alpha$ | 0 | 1/8 | 0 |
| Spontaneous magnetization | $\beta = \Delta - \gamma$ | 1/8 | 5/16 | $\frac{1}{2}$ |
| Magnetization vs field at T_c | $\delta = \Delta/(\Delta - \gamma)$ | 15 | 5 | 3 |
| Low temperature susceptibility | $\gamma' = \gamma$ | 7/4 | 5/4 | 1 |
| Low temperature gap | $\Delta' = \Delta$ | 15/8 | 25/16 | 3/2 |

Equation (3.73) can be integrated to obtain an expression for the free energy in terms of $h(x)$ as was shown by Griffiths (1967). Critical exponents for all thermodynamic quantities can thus readily be expressed in terms of two parameters as illustrated in Table XVI (adapted from Domb, 1966). It is usually assumed that the function $h(x)$ is analytic for $-x_0 \leq x < \infty$. The mean field equation of state (3.62) leads to a simple linear form for $h(x)$.

The general problem of constructing functions having the requisite analytic properties and expansions of the form (3.74) and (3.75) was solved independently by Josephson (1969) and Schofield (1969). (For further details see Vicentini-Missoni, Vol. 2 Chapter 2.)

2. Numerical estimate for the Ising model

It was suggested by Domb (1968b) that the knowledge of $h(x)$ as $x \rightarrow \infty$, near $x = 0$, and near $x = -x_0$ should be sufficient to provide a reasonable estimate of $h(x)$ over the whole range $-x_0 \leq x < \infty$. The coefficients D_{2r}^+ in (3.74) are known from the calculations of Essam and Hunter (1968). The coefficient k_0 in (3.75) is known from the amplitude D of the critical isotherm in (3.40); and $k_1, k_2 \dots$ can be obtained from the critical amplitudes of $\partial \bar{M}/\partial T, \partial^2 \bar{M}/\partial T^2 \dots$ as functions of \bar{H} [†]. The value x_0 is determined from the amplitude of the spontaneous magnetization B in (3.36); and provided that the susceptibility χ_0 and its derivatives exist on the low temperature side of T_c it is easy to show that

$$h(x) = j_1(x + x_0) + j_2(x + x_0) + \dots \quad (3.78)$$

as $x \rightarrow -x_0 +$, where the coefficients j_r are determined by the low temperature amplitudes C_r^- given by

$$d^r \bar{\chi}_0 / d\bar{H}^r \sim C_r^- \tau^{-r-\Delta} \quad (\bar{\chi}_0 = kT \chi_0/m^2). \quad (3.79)$$

Gaunt and Domb (1970) used numerical data for the s.q. and b.c.c. lattices to estimate $h(x)$ for these lattices. They suggested the following interpolation formulae:

$$(\varepsilon = x + x_0)$$

s.q. lattice

$$h(x) = \frac{1.4588\varepsilon + 17.1079\varepsilon^2}{1 + 8.1857\varepsilon} \quad (-x_0 \leq x < -0.12)$$

$$(x_0 = 0.200569)$$

$$h(x) = 0.4255 + 2.6280x + 1.9780 \quad (-0.12 \leq x \leq 0.1)$$

$$h(x) = \frac{0.4255 + 2.7073x + 2.4677x^2}{1 + 0.1863x} \quad (0.1 < x \leq 3.160493)$$

$$\frac{h(x)}{x^2} = \frac{1.0387y - 10.2746y^2 - 5.6371y^3}{1 - 10.7081y + 2.5925y^2 + 4.9557y^3} \quad (3.160493 < x < \infty) \quad (y = x^{-1/4}) \quad (3.80)$$

[†] A comprehensive analysis of the critical exponents and amplitudes of these derivatives has recently been undertaken by Betts and Filipow (1972) for the h.c., s.q. and p.t. lattices.

b.c.c. lattice

$$(x_0 = 0.269979)$$

$$h(x) = \frac{1.1528\varepsilon}{1 - 0.4089\varepsilon + 1.4697\varepsilon^2} \quad (-x_0 \leq x < -0.16)$$

$$h(x) = \frac{0.3450 + 1.3212x}{1 - 0.1821x} \quad (-0.16 < x \leq 0)$$

$$h(x) = \frac{0.3450 + 7.3421x + 24.1535x^2}{1 + 17.2698x} \quad (0 \leq x \leq 0.15)$$

$$h(x) = \frac{0.3450 + 13.3440x + 47.1377x^2}{1 + 34.6666x - 3.1676x^2} \quad (0.15 \leq x \leq 1)$$

$$\frac{h(x)}{x^{15/8}} = \frac{1.0097y + 1.0196y^2 + 0.4950y^3 + 0.1700y^4}{1 + 0.4396y} \quad (1 \leq x < \infty) \quad (y = x^{-5/8}). \quad (3.81)$$

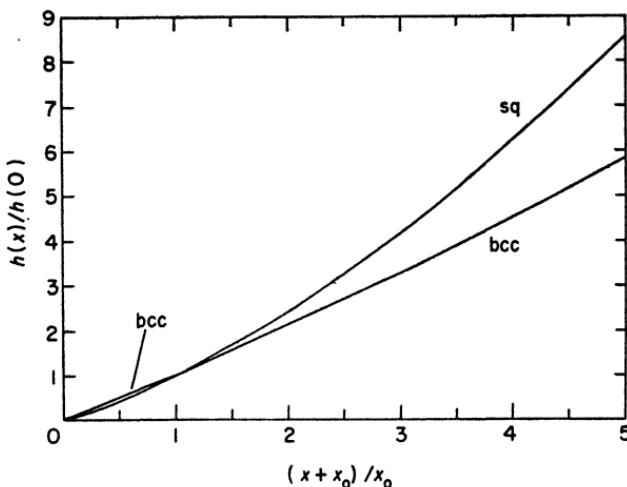


FIG. 22. Plots of $h(x)/h(0)$ against $(x + x_0)/x_0$ for the s.q. and b.c.c. lattices for $(x + x_0)/x_0 \leq 5$ (Gaunt and Domb, 1970).

The resulting $h(x)$ curves are shown in Fig. 22. It is seen that they are smooth and well behaved, the three-dimensional curve being much closer to linear (mean-field) than the two-dimensional curve.

3. Lattice-lattice scaling and a generalized law of corresponding states

One of the important conjectures of our numerical investigations has been that critical exponents are determined by dimension and are independent of lattice structure in a given dimension. Watson (1969a,b) made the important suggestion that $h(x)/h(1)$ might likewise be dependent on dimension only and not on lattice structure. It should then be possible to construct certain functions of the amplitudes which should be *invariant*, i.e. independent of lattice structure in a given dimension. Examples of such invariants are

$$E_+/E_-, \quad C^+_{2r}/C^-_{2r}, \quad E_+ A'_+/B^2. \quad (3.82)$$

The last example is particularly useful in two dimensions since E_+ and B are known exactly, and A'_+ very accurately from series expansions, and hence this could serve as a test of the conjecture. Watson (1969b) found the *same* value 0.3186 to four figures for the h.c., s.q. and p.t. lattices and this provides remarkably good support. With the improved estimates that we have quoted in (3.26) we find the *same* value 0.31857 to five figures!

Betts *et al.* (1971) put forward an alternative hypothesis paralleling the law of corresponding states of van der Waals, which leads to a more general formulation of critical amplitude relations. They suggested that for any model there is a universal function $\bar{M}(\tau, \bar{H})$, representing the equation of state in the critical region, and moving from one lattice to another merely changes the scale of τ and \bar{H} . More specifically for any lattice X two parameters n_X, g_X are defined, and in the critical region two lattices X and Y satisfy the relation

$$\bar{M}_X(\tau_X, \bar{H}_X) = \bar{M}_Y(\tau_Y, \bar{H}_Y) = \bar{M}(\tau, \bar{H}), \quad (3.83)$$

where

$$\left. \begin{aligned} n_X \bar{H}_X &= n_Y \bar{H}_Y = \bar{H} \\ g_X \tau_X &= g_Y \tau_Y = \tau \end{aligned} \right\}. \quad (3.84)$$

This implies a similar relationship for the most singular part of the free energy per site $f(\tau, H)$,

$$n_X f_X(\tau_X, \bar{H}_X) = n_Y f_Y(\tau_Y, \bar{H}_Y) = f(\tau, \bar{H}). \quad (3.85)$$

Betts *et al.* noted that when $\bar{H} = 0$ relations (3.83) and (3.85) can be derived exactly for the h.c. and p.t. lattices from the star-triangle transformation (see Syozi, Vol. 1 Chapter 7). For the mean-field approximation $n_X = g_X = 1$, and for the spherical model $g_X = 1$ and n_X can readily be calculated.

If we now apply (3.83) to the critical form of spontaneous magnetization (3.36) we find that

$$\begin{aligned} m_X &= B_X |\tau_X|^\beta \\ m_Y &= B_Y |\tau_Y|^\beta \end{aligned} \quad (3.86)$$

Hence using (3.84) we deduce that

$$\frac{g_X}{g_Y} = \left(\frac{B_X}{B_Y} \right)^{1/\beta}. \quad (3.87)$$

Similarly from the critical isotherm (3.40) we deduce that

$$\frac{n_X}{n_Y} = \frac{D_Y}{D_X}; \quad (3.88)$$

and for the specific heat amplitudes by differentiating (3.85)

$$\frac{E_X^+}{E_Y^+} = \frac{n_Y}{n_X} \left(\frac{g_X}{g_Y} \right)^{2-\alpha}, \quad (3.89)$$

$$\frac{E_X^-}{E_Y^-} = \frac{n_Y}{n_X} \left(\frac{g_X}{g_Y} \right)^{2-\alpha'}. \quad (3.90)$$

From these relations it is clear that g_X , n_X can be calculated exactly for standard two dimensional lattices.

We see how Watson's critical invariants arise when the scaling laws between exponents are satisfied. Thus if $\alpha = \alpha'$ it is clear from (3.89) and (3.90) that

$$\frac{E_X^+}{E_X^-} = \frac{E_Y^+}{E_Y^-}; \quad (3.91)$$

and likewise

$$\frac{E_X^+ A_{X'}^+ B_X^{-2}}{E_Y^+ A_{Y'}^+ B_Y^{-2}} = \left(\frac{g_X}{g_Y} \right)^{2-\alpha-2\beta-\gamma} \quad (3.92)$$

equals 1 if the scaling law

$$\alpha + 2\beta + \gamma = 2 \quad (3.93)$$

is satisfied. These examples show that the corresponding states hypothesis is more general than the equation of state (3.73), and amplitude relations could be derived for models which do not satisfy the exponent relations in Table XV.

From their numerical estimates Betts *et al.* make the important conjecture that the field parameter n_X is a lattice property independent of model. Hence n_X can be determined exactly from the spherical model amplitudes (Joyce,

Vol.2 Chapter 10), and the only parameter to be estimated numerically is g_x ; for this purpose the accurate susceptibility amplitudes A_+ in (3.33) can be used. Betts *et al.* then use these g_x values to estimate the specific heat amplitudes E_+ for s.c., b.c.c. and d. lattices assuming the f.c.c. value; they find good agreement with the values in (3.45) and (3.46). This provides good evidence in support of the above hypotheses for the three dimensional Ising model.

Agreement for other amplitudes like C_{2r}^+ , C_r^- is less satisfactory, but this is probably due to the larger errors in the estimation of these quantities. Values of $s \neq \frac{1}{2}$ are also considered, and there is modest support for the idea that g_x is independent of s . More accurate amplitude estimates are needed for a searching test.

If the above conjectures are correct, accurate estimates of a particular amplitude need be undertaken for one lattice only in a given dimension; the amplitudes for the remaining lattices can be obtained immediately on multiplying by the appropriate scaling factor.

4. Definition of the critical region. Correction terms

The scaling equation of state (3.73) applies "in the critical region". To define more clearly this region of applicability we must take account of correction terms and estimate where they become significant. A procedure suggested by Domb (1971c) was to assume a Darboux form at this singularity for the susceptibility and its higher derivatives as follows:

$$\begin{aligned}\bar{\chi}_0 &= \phi_1(\tau) + \tau^{-\gamma}\psi_1(\tau) \\ \frac{d^2\bar{\chi}_0}{dH^2} &= \phi_3(\tau) + \tau^{-\gamma-2\Delta}\psi_3(\tau) \\ \frac{d^4\bar{\chi}_0}{dH^4} &= \phi_5(\tau) + \tau^{-4-4\Delta}\psi_5(\tau) \\ &\dots\end{aligned}\tag{3.94}$$

Following the procedure described in Section III.D.1 we then obtain

$$\begin{aligned}\bar{H} &= \bar{M}^\delta h(x) + \bar{M}^{\delta+1/\beta}h_1(x) + \bar{M}^{\delta+2/\beta}h_2(x) + \dots \\ &\quad + \bar{M}^{\delta+\gamma/\beta}k_1(x) + \bar{M}^{\delta+(\gamma+1)/\beta}k_2(x) + \dots \\ &\quad + \bar{M}^{\delta+2\gamma/\beta}l_1(x) + \dots\end{aligned}\tag{3.95}$$

The functions $h_1(x)$, $h_2(x) \dots k_1(x) \dots l_1(x) \dots$ are all expected to be analytic because of the analyticity of the $\bar{M} - \bar{H}$ relationships when $\bar{H} \neq 0$. From (3.95) we should expect that on the critical isotherm

$$\bar{H} = g_0 \bar{M}^\delta + g_1 \bar{M}^{\delta+1/\beta} + g_2 \bar{M}^{\delta+2/\beta} + \dots j_1 \bar{M}^{\delta+\gamma/\beta} + \dots \quad (3.96)$$

so that this relationship is no longer of Darboux form.

Numerical estimates of the first order correction function $h_1(x)$ for $I(\frac{1}{2})$ can be made in a rather similar manner to that for $h(x)$ in Section III.D2; the errors are much larger, but provide a reliable order of magnitude estimate (see Domb and Gaunt, 1970).

D. Critical behaviour of an antiferromagnet

1. Historical review

Series expansions were first applied to an Ising antiferromagnet by Brooks and Domb (1951). These authors were able to give a general account of critical behaviour for the s.q. lattice, locating the critical curve (Fig. 3), and relating their results to order-disorder transitions. It was clear that the expansions were less well behaved and more difficult to handle than those of a ferromagnet. For the antiferromagnetic susceptibility, $\chi^{(a)}$, they estimated a maximum at the Néel temperature T_c accompanied by a discontinuity of slope which is in qualitative agreement with mean-field theory.

The true nature of the antiferromagnetic susceptibility in the critical region was first demonstrated by Sykes and Fisher (1958, 1962), Fisher and Sykes (1962), Fisher (1959a, 1962), Sykes (1961). These authors first made use of the Sykes' susceptibility theorem (see 2.12):

$$\frac{\chi_0}{\beta m^2} = \bar{\chi}_0 = (1 - \sigma w)^{-2} \{1 - (\sigma - 1)w + w^2 - 2wU(w) + G(w)\},$$

where $\sigma = q - 1$, $U(w)$ is the reduced energy, and $G(w)$ the residual correlation function. Numerical investigation showed that for an antiferromagnet the residual correlation function contributed only a few percent to the susceptibility $\chi^{(a)}$ near the critical point. If $G(w)$ is ignored, an approximation to $\chi^{(a)}$ is obtained which was termed the *energetic approximation*. In this approximation $\chi^{(a)}$ has a vertical tangent at T_c like the energy; and since it must eventually go to zero as $T \rightarrow \infty$ it is clear that it must pass through a maximum for some value of $T_m > T_c$.

Theoretical support for this behaviour was provided by Fisher (1959a) from a study of the correlations, using relation (1.12). Whereas for a ferromagnet the correlations all add to give a large exponent γ , for an antiferromagnet the alterations in sign cause cancellations, and the residual

singularity corresponds to the nearest neighbour correlation, which is effectively identical with the energy.

Detailed numerical analyses of $\chi^{(a)}$ for the s.q. and h.c. lattices in two dimensions were given by Sykes and Fisher (1962) and for the s.c. and b.c.c. lattices by Fisher and Sykes (1962). The form of $\chi^{(a)}$ for two dimensional lattices is reproduced in Fig. 23. The temperature of the maximum T_m was found to be significantly larger than T_c in two dimensions ($T_m \sim 1.5T_c$) but much less so in three dimensions ($T_m \sim 1.08T_c$).

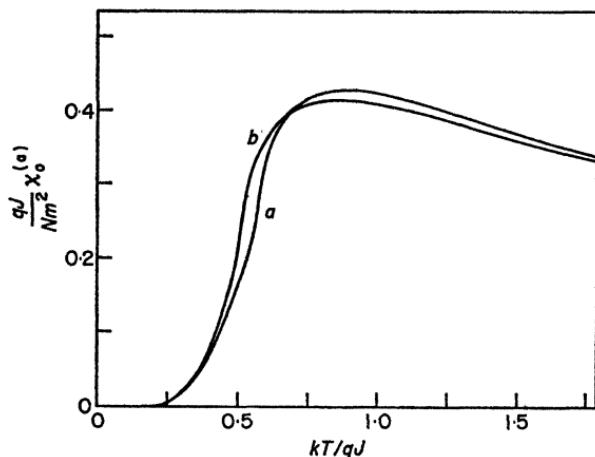


FIG. 23. Antiferromagnetic susceptibility of (a) the s.q. and (b) the h.c. lattice (after Sykes and Fisher, 1962).

However, a number of features of the 1962 analyses were unsatisfactory and have been modified in a later treatment (Sykes *et al.*, 1972a,b). Firstly it was assumed that the dominant ferromagnetic singularity could be removed by division, whereas a Darboux form implies that such a division will not remove the singularity. Secondly in three dimensions it was assumed that the specific heat had a logarithmic singularity at T_c (as in two dimensions) whereas strong evidence was forthcoming subsequently that $\alpha \approx 1/8$ (See Section III. B5).

In non-zero field Fisher (1960) derived an exact solution for a two-dimensional "super-exchange" model by applying an appropriate transformation to Onsager's solution. Two features of this solution were of particular interest; the specific heat retained the same singularity when $H \neq 0$, and the magnetic susceptibility when $H \neq 0$ contained a term which was logarithmically infinite like the specific heat. However, it was not clear whether these properties arose from the special character of the

model, or whether they were general properties which would also be present in the Ising model and possibly in other models.

Bienenstock and Lewis (1967) undertook a PA analysis of high temperature series expansions for an $I(\frac{1}{2})$ antiferromagnet in non-zero field; their results were also applied to order-disorder transitions of varying composition. The high temperature series was derived from the low-temperature codes using a generalized low \rightarrow high temperature transformation (Section II. B2). To locate the critical temperature they used the *staggered susceptibility* χ_s (Rushbrooke and Wood, 1963; see Rushbrooke *et al.*, this volume Chapter 5) corresponding to a field which is alternately positive and negative on odd and even lattice sites; this susceptibility has a strong singularity at T_c and enables T_c to be located with considerably greater accuracy than $\chi^{(a)}$. However, they did not obtain any detailed information on critical behaviour when $H \neq 0$.

The formulation by Griffiths (1970, 1971) of the *smoothness postulate*[†] opened the way to a more comprehensive treatment of series expansions. Griffiths suggested that on the boundary between the antiferromagnetic and paramagnetic phases (Fig. 3) there is no *a priori* reason to single out the particular point corresponding to zero field, and it is reasonable to assume that the singularity in free energy does not change its basic character along this boundary. If this postulate is accepted, Griffiths showed that features analogous to those of Fisher's model are reproduced quite generally.

In order to assess the validity of this postulate Rapaport and Domb (1971) developed more extensive series expansions for $I(\frac{1}{2})$ and formulated a number of tests which could be applied. They found good evidence to support the postulate. We shall now proceed to discuss in more detail the numerical results obtained in the above papers.

2. Antiferromagnetic susceptibility in zero field

We have already referred to the Darboux form of approximation to the susceptibility of an even lattice,

$$\tilde{\chi}_0 = \Phi_f(\theta)(1 - \theta)^{-\gamma} + \Phi_a(\theta)(1 + \theta)^{-\alpha+1} - \Upsilon(\theta) \quad (\theta = w/w_c) \quad (3.97)$$

in connection with the ferromagnetic behaviour in the critical region. For the antiferromagnetic critical behaviour of the two-dimensional lattices near the Néel temperature T_c this leads to the approximation

$$\tilde{\chi}_0^{(a)} \simeq \chi_a - a \pm \ln |1 + \theta| \quad (3.98)$$

Sykes *et al.* (1972a) estimated the following numerical values for the s.q.

[†] A similar hypothesis had been advanced by Pippard (1956).

lattice from high temperature series:

$$\chi_a = 0.1594 \pm 0.0010, \quad \gamma_+ = 0.22 \pm 0.01. \quad (3.99)$$

Below T_c they used the low temperature series in Table XII to estimate

$$\chi_a = 0.1589 \pm 0.0005, \quad a_- = 0.222 \pm 0.002. \quad (3.100)$$

The values of χ_a in (3.99) and (3.100) are consistent with each other, and the values of a_+ and a_- suggest the relation

$$a_+ = a_- \quad (3.101)$$

which is in accord with the Griffiths smoothness postulate. Sykes *et al.* noted that the energetic approximation which can be calculated exactly for this lattice gives values very close to those in (3.100),

$$\chi_a^E = 0.1647, \quad a_+^E = a_-^E = 0.2097. \quad (3.102)$$

The high temperature series for the h.c. lattice is more difficult to deal with because of the presence of a pair of singularities in the complex plane at $w = \pm i/\sqrt{3}$. Sykes *et al.* stated that they were unable to find a method of analysis which is completely satisfactory, but they estimated

$$\chi_a = 0.1230 \pm 0.0010, \quad a_+ \approx 0.23. \quad (3.103)$$

The corresponding estimates from low temperature series were

$$\chi_a = 0.1224 \pm 0.0003, \quad a_- = 0.240 \pm 0.001, \quad (3.104)$$

and again it was reasonable to assume that relation (3.101) is satisfied. The energetic approximation gave

$$\chi_a^E = 0.1244, \quad a_+^E = a_-^E = 0.2375 \quad (3.105)$$

which is again very close to the estimates in (3.104).

The close-packed p.t. lattice does not order antiferromagnetically, and its susceptibility can be related to that of the h.c. lattice by the transformation (Fisher, 1959b; see Syozi Vol. I, Chapter 7.)

$$\begin{aligned} \chi_T(w) &= \frac{1}{2} [\chi_H(w^*) + \chi_H(-w^*)] \\ w^{*2} &= w(1+w)/(1+w^2). \end{aligned} \quad (3.106)$$

As w varies from 0 to -1 , w^{*2} varies from 0 to $-\frac{1}{3}$ and within this range $\chi_H(w^*)$ converges; this lattice was first investigated by Sykes and Zucker (1961) who therefore concluded that $\chi_T(w)$ had no singularity for any finite

temperature. However, the behaviour as $T \rightarrow 0$ ($w \rightarrow -1$, $w^{*2} \rightarrow -\frac{1}{3}$) will be singular.

In their analysis of the problem Sykes and Zucker attempted to divide out the dominant ferromagnetic singularity, and sum the residual series to calculate χ_a as $w \rightarrow -1$; their treatment was in accord with the energetic approximation. However, the subsequent more detailed analysis by Sykes *et al.* (1972a) indicated that the energetic approximation

$$\chi^E \simeq \frac{1}{9} - \frac{\sqrt{3}}{18\pi} (1+w)^2 \ln(1+w) \quad (w \rightarrow -1) \quad (3.107)$$

is not a good one for the p.t. lattice near $w = -1$. These authors suggested instead a wider range in the estimate for χ_a

$$0.141 < \chi_a < 0.150 \quad (3.108)$$

with the upper limit uncertain because of the possibility of a stronger singularity than (3.107).

For three-dimensional lattices the analyses of $\chi_0^{(a)}$ currently available are less complete because of the difficulty of handling the low temperature series. Instead of (3.98) the high temperature portion is now of the form

$$\bar{\chi}_0^{(a)} \simeq \chi_a + a_+ (1 + w/w_c)^{7/8}, \quad (3.109)$$

with the following numerical estimates for χ_a , a_+ (Sykes *et al.* 1972b):

$$\left. \begin{aligned} \chi_a &= 0.3394, & a_+ &= 0.630 \text{ (s.c.)} \\ \chi_a &= 0.3693, & a_+ &= 0.622 \text{ (b.c.c.)} \end{aligned} \right\} \quad (3.110)$$

These amplitudes are within a few per cent of the independent estimates of the energetic approximation.

In terms of the temperature variable $t' = T_c/T$, the estimates for $\bar{\chi}_0^{(a)}$ in two dimensions are

$$\bar{\chi}_0^{(a)} \simeq \chi_a - a_{\pm}' \ln|1-t'| \quad (3.111)$$

with

$$\left. \begin{aligned} a_{\pm}' &= 0.196 \pm 0.002 \text{ (s.q.)} \\ a_{\pm}' &= 0.182 \pm 0.001 \text{ (h.c.)} \end{aligned} \right\} \quad (3.112)$$

In three dimensions they are

$$\bar{\chi}_0^{(a)} = \chi_a + a_{\pm}' (1-t')^{7/8} \quad (3.113)$$

with

$$\left. \begin{aligned} a_+ &= 0.612 \text{ (s.c.)} \\ a_+ &= 0.613 \text{ (b.c.c.)} \end{aligned} \right\} \quad (3.114)$$

Finally, for the close-packed f.c.c. lattice Danielian (1961) showed that the lowest energy state differs from that of the p.t. lattice in not having a finite entropy at $T = 0$. He was able to classify the lowest energy states systematically, and to indicate that they possessed a two dimensional order. The problem of deriving low temperature series is very complex, but Danielian (1964) was able to derive a few terms of the series and estimate the Néel temperature T_N to be $2.4J/k$ (much less than T_c and comparable with T_N for the s.q. lattice). Subsequently Betts and Elliott (1965) derived a series for the long range order which, they claimed, gave a better estimate of T_N as $(1.81 \pm 0.05) J/k$. The conjectured curve of critical points in Fig. 5 makes qualitative use of these results.

3. Critical behaviour in non-zero field.

In I.C2 we mentioned a method due to Sykes of passing from low temperature to high temperature expansions for ferromagnets and antiferromagnets. This leads to a generalization of (2.46) of the form

$$\begin{aligned} \ln Z^I &= -\frac{1}{4} \ln y_+ - \frac{1}{4} \ln y_- - q/8 \ln u + \frac{1}{2} \ln [(1+y_+)(1+y_-)] \\ &\quad + \sum_{r=1}^{\infty} \frac{\phi_r(y_+, y_-)\zeta^r}{[(1+y_+)(1+y_-)]^r} \quad (\zeta = 1-u) \end{aligned} \quad (3.115)$$

where the $\phi_r(y_+, y_-)$ can be calculated from the $g_{st}(u)$ in (2.97). Numerical calculations of the $\phi_r(y_+, y_-)$ polynomials from available data of $g_{st}(u)$ were first undertaken by Bienenstock and Lewis (1967) and were later extended by Rapaport and Domb (1971).

The series for an antiferromagnet is derived by putting $y_+ = y, y_- = y^{-1}$. However, the susceptibility of an antiferromagnet is only weakly singular and is not very suitable for the location of $T_c(H)$. Instead Bienenstock and Lewis used the staggered susceptibility χ_s which is obtained by writing

$$\left. \begin{aligned} H_+ &= H + h \\ H_- &= H - h \end{aligned} \right\} \quad (3.116)$$

and calculating

$$\chi_s = kT \frac{\partial^2}{\partial h^2} \left[(\ln Z^I) \right]_{h=0} \quad (3.117)$$

In zero field χ_s is identical with the susceptibility of a *ferromagnet* which is strongly singular, and the strong singularity remains when $H \neq 0$.

Bienenstock and Lewis took $H = cJ/m$ for varying values of c and used a PA analysis to locate $T_c(H)$. This becomes increasingly difficult as H approaches the critical field $H_c = qJ/m$, and the results are therefore not reliable near $H = H_c$. The estimates for the s.q., s.c. and b.c.c. lattices are summarized by the formula

$$\begin{aligned} T_c(H)/T_c(0) &= [1 - (H/H_c)^2]^\xi, \\ \xi &= 0.87 \quad \text{s.q.} \\ \xi &= 0.36 \quad \text{s.c., b.c.c.} \end{aligned} \quad (3.118)$$

and the ranges of reliability are given by

$$\left. \begin{aligned} |H/H_c| &\leq 0.7 && \text{s.q., s.c.} \\ |H/H_c| &\leq 0.9 && \text{b.c.c.} \end{aligned} \right\}. \quad (3.119)$$

Rapaport and Domb (1971) concentrated on the region near $H = 0$ where much greater accuracy can be achieved. Following the smoothness postulate of Griffiths (1970) they suggested the following form of free energy near the phase boundary:

$$F(H, T) = F_0(H, T) + \phi(H)f\{\theta(H)[T - T_c(H)]\}. \quad (3.120)$$

Here F_0 , ϕ , θ and T_c are smooth functions of their respective arguments, ϕ and θ being defined to be unity at $H = 0$. This means that the singular part of F is proportional to a function of a single variable $f(u)$ where for a given H , u is the distance of T from the appropriate critical temperature. The "unit" in which this temperature difference is measured is scaled with respect to its value in zero field by the function $\theta(H)$.

Since F is invariant under the change $H \rightarrow -H$, $T_c(H)$ can be expanded for small H as

$$T_c(H) = T_c + \frac{1}{2!} T_c^{(2)} H^2 + \frac{1}{4!} T_c^{(4)} H^4 + \dots \quad (3.121)$$

The specific heat and temperature derivative of the susceptibility in zero field can be deduced from (3.120),

$$T^{-1} C_H = -\frac{\partial^2 F_0}{\partial T^2} - \frac{d^2}{dT^2} f(T - T_c), \quad (3.122)$$

$$\frac{d\chi}{dT} = \chi' = T_c^{(2)} \frac{d^2}{dT^2} f(T - T_c). \quad (3.123)$$

Thus the ratio of the amplitudes of the singularities of χ' and C_H is $-T_c^{(2)}/T_c$. In non-zero field one can readily show from (3.120) that the singular parts of χ and C are proportional, which is also a characteristic of the exact calculation by Fisher (1960) of a superexchange model. The behaviour in zero field is unusual because the curve $T_c(H)$ is then parallel to the H axis.

In zero field the critical behaviour of the staggered susceptibility is given by (Section III.B1)

$$\frac{\chi_s}{\beta m^2} = \bar{\chi}_s = A_+ ' \left(\frac{T}{T_c} - 1 \right)^{-\gamma}. \quad (3.124)$$

The smoothness postulate suggests that for $H \neq 0$,

$$\bar{\chi}_s(H) = A_+ '(H) \left[\frac{T}{T_c(H)} - 1 \right]^{-\gamma}, \quad (3.125)$$

where $A_+ '(H)$ is a smooth function. Expanding $A_+ '(H)$ as

$$A_+ '(H) = A_+ ' + \frac{1}{2!} A_+ ''^{(2)} H^2 + \frac{1}{4!} A_+ ''^{(4)} H^4 + \dots \quad (3.126)$$

and substituting in (3.125) it is easy to establish the following pattern of critical behaviour of the derivatives of $\bar{\chi}_s$:

$$\left. \begin{aligned} \frac{d^{2r} \bar{\chi}_s}{dH^{2r}} &= \bar{\chi}_s^{(2r)} \sim G_{2r} (1 - t')^{-\gamma_{2r}} \\ \gamma^{(2r)} &= \gamma + r \end{aligned} \right\} \quad (3.127)$$

with the amplitudes satisfying

$$\frac{G_{2r+2}}{G_{2r}} = (2r+1)(r+\gamma) \frac{T_c^{(2)}}{T_c}. \quad (3.128)$$

We may summarize the predictions of the smoothness postulate as follows: (i) the exponent γ is independent of H ; (ii) at $H = 0$ the ratio of the amplitudes of χ' and C_H is proportional to $T_c^{(2)}$; (iii) $\bar{\chi}_s$ and all its even field derivatives diverge at T_c for $H = 0$ the exponent of $\bar{\chi}_s^{(2r)}$ being $\gamma + r$; (iv) the ratios of the amplitudes of successive $\bar{\chi}_s^{(2r)}$ are given by (3.128).

Rapaport and Domb found satisfactory agreement on all these points with numerical estimates for the s.q. and s.c. lattices, and they therefore

concluded that there was good evidence to support the smoothness postulate. Near $H = 0$ they found

$$T_c(H)/T_c = \begin{cases} 1 - 0.380(m/J)^2 H^2 + O(H^4) & \text{s.q.} \\ 1 - 0.115(m/J)^2 H^2 + O(H^4) & \text{s.c.} \end{cases} \quad (3.129)$$

The value for the s.q. lattice differs appreciably from the estimate (3.118) of Bienenstock and Lewis; Rapaport and Domb suggested that this might have arisen from fitting the parameter ξ in (3.118) over a wide range of H values which sacrificed accuracy near $H = 0$.

We finally mention a peculiar feature of closed-form approximations to $T_c(H)$ near $H = H_c$ for three dimensional lattices which predict that the curve approaches the H axis with a *positive* slope; this would mean that there exists a range of values of H just above H_c in which there are *two* transition points. Ziman (1951) who first noticed this effect rejected the result on physical grounds, and he was supported by Bienenstock (1966) whose estimate of the $T_c(H)$ curve, (3.118), cuts the axis horizontally. Also in support of this view are the calculations of Burley (Vol.1, Chapter 9) which show that the magnitude of the positive slope decreases as the approximation improves. However, recent Monte Carlo work of Shirley (1972) has claimed support for a positive slope for the b.c.c. lattice, and since the series estimates are unreliable near $H = H_c$ the matter is not yet resolved.

IV. Miscellaneous Topics

A. Special lattices

We have so far been concerned with calculations for standard lattices, the h.c., s.q. and p.t. lattices in two dimensions and the d., s.c., b.c.c. and f.c.c. lattices in three dimensions. However, calculations have been undertaken for more specialized lattices which have provided additional information of interest. We shall not quote numerical data on series expansions for these lattices, but will summarize the main conclusions.

In two dimensions the kagomé lattice (Domb, 1960; Syozi, Vol. I Chapter 7) is related to the decorated honeycomb lattice by means of a star-triangle transformation. It has co-ordination number $q = 4$, and a comparison of its critical parameters with those of the s.q. lattice illustrates the degree of variation between two lattices with the same q . The antiferromagnetic susceptibility of the kagomé lattice has been investigated by Sykes and Zucker (1961).

A three dimensional lattice with $q = 3$, the hydrogen peroxide (h.p.) lattice, was studied by Leu *et al.* (1969). By means of a star-triangle trans-

formation this can be related to a lattice with $q = 6$, the hypertriangular lattice (h.t.), and by means of a decoration and star-triangle transformation to a lattice with $q = 4$, the hyperkagomé (h.k.) lattice. Leu *et al.* found that the critical exponents had the standard three dimensional values, and they obtained the following estimates of other critical parameters:

| | h.p. | h.t. | h.k. | cristobalite | |
|-------------|---------|----------|----------|--------------|-------|
| w_c | 0.51841 | 0.222087 | 0.394384 | 0.233 | |
| S_c/k | 0.451 | 0.558 | — | 0.548 | |
| $-U_c/kT_c$ | 0.480 | 0.228 | — | 0.268 | |
| A_+' | 1.354 | 1.085 | — | 1.100 | (4.1) |

The two-layer quadratic lattice with $q = 5$ has been studied by Ballentine (1964). As expected the high temperature susceptibility exponent has two-dimensional value $7/4$; critical parameters are $kT_c/qJ = 0.643$, $S_c/k = 0.373$.

The standard lattices which we have considered are all *regular* (Domb, 1960) in the sense that all lattice points and nearest neighbour bonds are equivalent. However, the h.c. and d. lattices are not Bravais lattices, i.e. they have more than one atom per unit cell. Another example of a regular non-Bravais lattice with $q = 6$ is the cristobalite lattice, and high temperature series expansions have been developed for $\ln Z^I$ and χ_0 by Betts and Ditzian (1968). The critical parameters are given in the last column of (4.1).

An example of a non-regular lattice is the hexagonal close-packed (h.c.p.). Lattice constant data are very similar to those of the f.c.c. lattice (Domb, 1960) and the critical parameters for these lattices differ only slightly from one another.

High temperature series expansions of χ_0 for a spinel lattice were developed by Jasnow and Moore (1968). On the basis of 6 terms of the expansion previous authors (Baltzer *et al.*, 1966; Stanley and Kaplan, 1967) had surmised that the exponent for this lattice differed from the standard three dimensional value. Jasnow and Moore showed that six terms were inadequate for an assessment of the critical exponent; when more terms were taken into account the exponent moved towards the standard value.

B. Distant neighbour interactions

Series expansions for the s.q. lattice with first and second neighbour interactions were developed by Domb and Potts (1951). They were used to estimate the dependence of T_c on the ratio of the two interactions, and particularly to locate the ordered regions when the two interactions were opposite in sign (this aspect has recently been investigated more comprehensively by Stephenson 1970).

It is quite difficult to process data for such a two parameter system, and taking further neighbours into account would seriously increase the complication. Domb and Dalton (1966) therefore introduced the *equivalent neighbour model* in which the interactions between a spin and a certain finite number of its neighbours are equal, and the remaining interactions are all zero. When the interactions extend to r shells they described the model as *equivalent neighbour of order r* . For any r the series depend one on parameter only, and by considering different lattices in two and three dimensions a variety of effective co-ordination numbers q could be covered. Hence conclusions could also be drawn about asymptotic behaviour for large q .

Domb and Dalton took $r = 1, 2, 3$ for the s.q., p.t., s.c., b.c.c. and f.c.c. lattices. Their first conclusion was that critical exponents were unchanged by the distant neighbour interactions, but as the range increased more terms were needed to establish the true critical exponent.

Regarding asymptotic behaviour and the manner in which the mean field solution is approached as $q \rightarrow \infty$ Domb and Dalton found that as q increases lattice structure ceases to be significant in a given dimension, and the critical parameters depend on q only. They derived the following estimates for critical parameters in three dimensions:

$$\left. \begin{aligned} q K_c &= 1 + 3.5/q \\ \frac{S_\infty - S_c}{k} &= 1.4/q \\ - U_c/kT_c &= 1.9/q \end{aligned} \right\} \quad (4.2)$$

In two dimensions they found that the correction term to the mean field solution is no longer of order $1/q$ and they suggested instead A/q^γ where $0 < \gamma < 1$.

In a subsequent paper, Dalton and Domb (1966) put forward a theoretical justification for the pattern of critical behaviour represented by (4.2). They related the various types of lattice constant to the virial coefficients of a hard sphere gas, and showed that the dominant terms in the series expansion coefficients for $\ln Z^I$ correspond to simple polygons. Taking account of polygons alone gave numerical results close to (4.2).

Additional support for this pattern of behaviour was provided by Thouless (1969) who investigated a modified version of the Ising model by diagrammatic methods. Thouless found that the correction term to the mean field solution was of the form

$$aq^{-1} + bq^{-2} \ln q \quad (4.3)$$

in three dimensions, and

$$q^{-1} \ln q \quad (4.4)$$

in two dimensions. He suggested that the calculations of Domb and Dalton in three dimensions had not gone far enough to require the second term in (4.3).

A further investigation of the equivalent neighbour model was undertaken by Dalton and Wood (1969) who in addition developed low temperature series expansions. They confirmed the conclusion of Domb and Dalton (1966) that the critical exponents are unchanged for $r = 2, 3$. (For a recent confirmation see Paul and Stanley, 1972.) Dalton and Wood also performed extensive calculations for a model with first and second neighbour interactions of strength J_1 and J_2 respectively, where the ratio $\rho = J_2/J_1$ lies between 0 and 1. Estimates were given of critical parameters as a function of ρ for the s.q., p.t., s.c., b.c.c., and f.c.c. lattices. For the critical temperatures they suggested the simple formula

$$T_c(\rho) = T_c(0)(1 + c\rho) \quad (4.5)$$

the values of c being 1.45, 1.35, 2.47, 0.85, 0.61 for the above lattices respectively. For the f.c.c. lattice more extensive calculations were undertaken by Philhours, J. (1971) which include first, second and third neighbour interactions.

For longer range forces of the form $1/R^{d+\sigma}$, high temperature expansions developed by Joyce showed that for a sufficiently small σ the critical exponents changed from their values for short range forces (a typical result for $\sigma = 1$ in two dimensions is given in Domb *et al.*, 1964). More recently these calculations have been extended by Joyce and Webb, and we quote the following expansions for $d = 1$, $\sigma = 1$ which is a critical case (Dyson, 1971).

$$\begin{aligned} \bar{\chi}_0 = 1 &+ \left(\frac{\pi^2}{3}\right)K + \left(\frac{4\pi^4}{45}\right)K^2 + \left(\frac{61\pi^6}{2835}\right)K^3 \\ &+ \left(\frac{208\pi^8}{42525}\right)K^4 + \left(\frac{166\pi^{10}}{155925}\right)K^5 + \left(\frac{6445576\pi^{12}}{28733079375}\right)K^6 + \dots \end{aligned} \quad (4.6)$$

Here the Hamiltonian is

$$\mathcal{H} = - \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j - mH \sum_i \sigma_i \quad (J_{ij} = J/n^2).$$

C. Anisotropic systems. Crossover exponent†

Onsager's solution of the two dimensional $I(\frac{1}{2})$ model (1944) extended to the anisotropic rectangular lattice with different interactions J, J' in the two principal lattice directions; likewise the spontaneous magnetization could be generalized to the anisotropic lattice (see Domb, 1960; Chapter 3,

† See also Stanley, this Volume, Chapter 7, Section VI.

eqn. (111)). For these exact solutions critical exponents remain unchanged as long as the lattice is two dimensional, i.e. as long as $J' \neq 0$.

The smoothness postulate (Griffiths, 1970, 1971) generalizes this result to any isotropic system in d dimensions. For example, if we consider a set of parallel s.q. lattices with internal interactions J coupled to one another with interaction J' , we should expect the system to display three dimensional critical exponents as long as $J' > 0$, and to revert to two dimensional exponents only when $J' = 0$.

Let us consider the transition from two to three dimensional behaviour at $J' = 0$ in terms of the parameter $\eta = J'/J$. We could write, for example, for the magnetic susceptibility

$$\bar{\chi}(\eta) = \bar{\chi}_{02} + \eta \chi_{02}^{(1)} + \frac{\eta^2}{2!} \chi_{02}^{(2)} + \dots \quad (4.7)$$

where χ_{02} is the two dimensional susceptibility with critical behaviour

$$\chi_{02} \sim A_+ (1 - t_2')^{-\gamma_2}, \quad t_2' = T_{c2}/T \quad (4.8)$$

and $\chi_{02}^{(r)}$ is the r th derivative of $\bar{\chi}(\eta)$ w.r.t. η . Following the ideas of Domb and Hunter (1965) in connection with the derivatives w.r.t. magnetic field H (see Section III.B3) we might reasonably conjecture the existence of a "gap" exponent ϕ satisfying

$$\chi_0^{(r)} \sim A_{+r} (1 - t_2)^{-\gamma_2 - r\phi}. \quad (4.9)$$

We should then find by analogy with (3.60) a relation for $\bar{\chi}(\eta)$ of the form

$$\bar{\chi}(\eta) \sim \tau_2^{-\gamma_2} F(\eta \tau_2^{-\phi}) \quad (\tau_2 = 1 - t_2) \quad (4.10)$$

which should be valid in the "critical region" for τ_2, η .

A relation of the form (4.10) was first suggested by Riedel and Wegner (1969) who termed ϕ the *crossover exponent*. The same pattern of behaviour would be expected in any transition from one set of critical exponents to another at a specific value of a parameter at which the change takes place (from *one universality class to another* in the terminology of Kadanoff, 1971). Alternative arguments leading to (4.10) have been advanced by Abe (1970) and Suzuki (1971) who used heuristic arguments to suggest that $\phi = \gamma_2$ and by Coniglio (1972). More recently Hankey and Stanley (1972) have developed scaling equations of state on the basis of a *generalized homogeneity postulate*, that

$$G(\lambda^{a_\tau} \tau, \lambda^{a_H} H, \lambda^{a_\eta} \eta) = \lambda G(\tau, H, \eta), \quad (4.11)$$

where G is the singular part of the Gibbs potential, and λ is an arbitrary parameter.

Relation (4.10) means that the critical temperature $T_c(\eta)$ near $\eta = 0$ satisfies the relation

$$T_c(\eta) - T_{c2} \sim C\eta^{1/\phi}. \quad (4.12)$$

The transition from two dimensional to three dimensional behaviour takes place in a region of temperature satisfying

$$C_1\eta^{1/\phi} < T < C_2\eta^{1/\phi} \quad (4.13)$$

where C_1 and C_2 depend on arbitrary levels of significance.

Oitmaa and Enting (1971, 1972) developed series expansions for $\bar{\chi}_0(\eta)$ for the above model of the anisotropic s.c. lattice. Writing

$$\bar{\chi}_0(\eta) = 1 + 2 \sum_{r=1}^{\infty} H_r(\eta) w^r \quad (4.14)$$

they evaluated the first eleven polynomials $H_r(\eta)$. Using ratio and P.A. analysis of the coefficients $H_r(\eta)$ for different η they found a continuous variation of the critical exponent γ with η which, they claimed, conflicted with the smoothness postulate prediction of a sharp change at $\eta = 0$.

Rapaport (1971) pointed out that such a continuous variation must be expected from a *finite* number of terms in (4.14); as η approaches zero more and more terms are required to indicate the true character of the critical exponent. Using an alternative analysis which attempted to estimate the critical exponent of $\chi_{02}^{(r)}$ in (4.7), Rapaport showed that the data were consistent with (4.9) with $\phi = \gamma_2$. He therefore concluded that the data did not conflict with universality and smoothness. Similar conclusions were drawn by Paul and Stanley (1971) who had independently developed high temperature expansions for the anisotropic s.c. and f.c.c. lattices. Rapaport's conclusions were challenged by Enting and Oitmaa (1971) who estimated a value for ϕ differing from γ_2 , and suggested that scaling theory was not obeyed.

The controversy was resolved when Liu and Stanley (1972) and Cittleur and Kasteleyn (1972a) showed rigorously that $\phi = \gamma_2$, and Harbus and Stanley (1973) developed series for the specific heat, susceptibility and second correlation moment for the anisotropic s.c. and f.c.c. lattices; these were subsequently analysed by Krasnow *et al.* (1973) who found good evidence in support of scaling.

The problem of an anisotropic d -dimensional lattice with one interaction J_1 much stronger than all the remainder has been investigated by Cittleur and Kasteleyn in a recent series of publications. Paper I (1972b) deals with

the s.q. lattice, and it is shown that to leading order the susceptibility can be represented by the high temperature expansion

$$\bar{\chi}_0 \simeq (1 - w_1)^{-1} \sum_{n=0}^{\infty} b_{n0} w_2^n (1 - w_1)^{-n} \quad (w_i = \tanh \beta J_i); \quad (4.15)$$

here the b_{n0} are constants which are calculated for $n \leq 5$. Numerical evidence suggests the critical behaviour

$$\bar{\chi}_0 \simeq [1 - bw_2(1 - w_1)^{-1}]^{-p} \quad (4.16)$$

with $b = 2.02 \pm 0.03$ and $p = 1.77 \pm 0.03$. It is known from the critical temperature that the true value of b must be 2, and it is conjectured that $p = 7/4$.

Paper II (Citteur, 1973a) generalizes the treatment to the s.c. lattice for which

$$\bar{\chi}_0 \simeq (1 - w_1)^{-1} \sum_{m,n=0}^{\infty} b_{mn0} w_2^m w_3^n (1 - w_1)^{-(m+n)}. \quad (4.17)$$

Taking $w_2 = aw_3$, the critical behaviour can be represented by

$$[1 - b(a) w_2(1 - w_1)^{-1}]^{-5/4}$$

with $b(a)$ having the values 6.10 ± 0.02 , $4.48^5 \pm 0.02$, 3.54 ± 0.02 , 3.19 ± 0.02 , 2.99 ± 0.02 for $a = 1, 2, 4, 6, 8$ respectively. The form of the critical surface in w_1, w_2, w_3 space is discussed.

In paper III (Citteur, 1973b), the Sykes' susceptibility theorem (2.12) is used to simplify the graphical problems associated with the derivation of the expansions, and two new terms are added to the s.q. expansion (4.15). Paper IV (Citteur and Kasteleyn, 1973a) is concerned with antiferromagnetism (dominant interaction $J_1 < 0$). The approximation to $\bar{\chi}_0^{(a)}$ in three dimensions now takes the form

$$\bar{\chi}_0^{(a)} = (1 + w_1) \sum_{m,n=0}^{\infty} c_{mn0} w_2^m w_3^n (1 + w_1)^{-(m+n)} \quad (4.18)$$

with an appropriate generalization to d dimensions. In the critical region this behaves as the nearest neighbour correlation function in the direction of the dominant interaction.

Paper V (Citteur and Kasteleyn, 1973b) derives some rigorous relations for the functions $\chi_{02}^{(r)}$ in a d -dimensional anisotropic system which are analogous to relations derived by Liu and Stanley (1972), and which provide a theoretical basis for a crossover exponent ϕ equal to γ_{d-1} .

In three dimensions the following equation is proposed for the surface of critical points:

$$[1 - 2w_2(1 - w_1)^{-1}]^{7/4} + [1 - 2w_3(1 - w_1)^{-1}]^{7/4} = 1. \quad (4.19)$$

D. Hypercubical lattices in d dimensions

In 1964 Fisher and Gaunt developed high temperature expansions for $\ln Z^I$ and χ_0 for a general hypercubical lattice in d dimensions. By arranging the coefficients as polynomials in decreasing powers of q ($q = 2d$) and examining their general form, they were able to derive an expansion for the critical temperature in powers of q^{-1} as follows:

$$\begin{aligned} kT_c/qJ = & 1 - q^{-1} - 1\frac{1}{3}q^{-2} - 4\frac{1}{3}q^{-3} \\ & - 21\frac{3}{4}\frac{4}{5}q^{-4} - 133\frac{1}{1}\frac{4}{5}q^{-5} - \dots \end{aligned} \quad (4.20)$$

Mean field theory gives the first term, the Bethe approximation (see Burley, Vol. 2 Chapter 9) agrees as far as the second term, and higher order approximations would agree with more terms. Fisher and Gaunt suggested that this series might be asymptotic, and by stopping at the smallest term they obtained reasonable approximations to T_c even when $d = 2, 3$ (errors $\sim 6\%, 1\%$ respectively). For higher d the estimates are probably much more accurate.

Confining attention to $d = 4, 5, 6$ Fisher and Gaunt obtained numerical estimates of the susceptibility exponent $\gamma(d)$ which they assumed to go steadily and continuously to its mean field value of 1 as d increases through these values. For $d = 4$ subsequent calculations by Moore (1970) suggested $\gamma = 1.065 \pm 0.003$, $\nu = 0.536 \pm 0.003$, $\alpha = -0.12 \pm 0.03$. Abe (1972) attempted to use the diagrammatic methods described by Wortis in this volume, Chapter 3, to show that in high dimensions

$$\gamma(d) \sim 1 + \exp - Bd. \quad (4.21)$$

However powerful theoretical evidence has accumulated in recent years to support the view that critical exponents achieve their mean field values (with the exception of logarithmic factors) when $d = 4$. First this is the behaviour of the spherical model (Joyce, Vol. 2 Chapter 10) whose critical exponents always deviate more from mean field than those of $I(\frac{1}{2})$. The renormalization group approach of Wilson (1971) also leads to this conclusion; and Wegner and Riedel (1973) following an earlier treatment by Larkin and Khmelnitski

(1969) used renormalization group methods to calculate the logarithmic factors in four dimensions as follows:

$$\begin{aligned}\chi_0 &\sim \tau^{-1} |\ln \tau|^{1/3} \\ C_H &\sim |\ln \tau|^{1/3}.\end{aligned}\tag{4.22}$$

It is not surprising to find that a limited number of terms of a series expansion can mistake the logarithmic factors in (4.22) for a small power.

E. Droplet model

We have seen in Section II.B that it is difficult to derive exact density expansions for $I(\frac{1}{2})$ beyond a limited number of terms. However, for larger terms we might hope to select configurations which dominate asymptotically, and hence to assess the singularities of the partition function and the critical behaviour. With this aim in view the droplet model was introduced by Essam and Fisher (1963) and later developed by Fisher (1967b). (The model was first used by Bijl (1938), Frenkel (1939) and Band (1939) in connection with the condensation of a gas.)

In the expansion (2.39) the coefficient $F_n(N, z)$ of y^n arises from overturned connected clusters of various sizes and shapes containing $n_1, n_2 \dots n_r$ spins where $n_1 + n_2 + \dots + n_r = n$. If interactions between these clusters are ignored (i.e. attractive forces between adjacent clusters and volume exclusion of hard sphere type which prevent two spins from occupying the same site) it is easy to show that $g_n(u)$ in expansion (1.43) consists of the sum of independent clusters,

$$g_n(u) = \sum_s w(n, s) u^s. \tag{4.23}$$

Here the sum is taken over all different connected clusters of n spins, s is the surface area of the cluster, and $w(n, s)$ is a weight or entropy term representing the number of clusters with a given n, s . For any cluster we must have

$$s = An^\sigma \tag{4.24}$$

where the maximum value of σ , 1, corresponds to linear configurations and the minimum value ($\frac{1}{2}$ in two dimensions, $\frac{2}{3}$ in three dimensions) corresponds to a circle or sphere. Following standard procedure in statistical mechanics, the sum (4.23) could be replaced by its maximum term corresponding to \bar{s} equal to $An^{\bar{\sigma}}$ where it was assumed that $\bar{\sigma} < 1$.

Exact enumerations for loops in two dimensions (Hiley and Sykes, 1961) provided evidence for the assumption that

$$w(n, \bar{s}) = \frac{\lambda^{\bar{s}}}{(\bar{s})^\tau} = \frac{\lambda^{n\bar{\sigma}}}{n^{\bar{\sigma}\tau}} \quad (4.25)$$

where λ is a constant characteristic of the lattice, and τ an exponent characteristic of dimension. This led to the "mimic" partition function

$$\ln Z^I \simeq \sum y^n u^{n\bar{\sigma}} \lambda^{n\bar{\sigma}} n^{-\bar{\sigma}\tau}. \quad (4.26)$$

The function has the following properties:

- (i) The power series in y always has radius of convergence 1 corresponding to a singularity on the phase boundary.
- (ii) Putting $y = 1$, the power series in u has radius of convergence λ^{-1} and this value corresponds to the critical point.
- (iii) All the derivatives w.r.t. y of the function converge at $y = 1$, so that the function has an essential singularity at $y = 1$.
- (iv) Critical behaviour depends on two parameters $\bar{\sigma}$ and τ ; this was the first model to suggest such a dependence and was historically the precursor of the scaling law developments.

There have been a number of criticisms of the above treatment (see e.g. Gaunt and Baker, 1970; Domb and Guttmann, 1970; Fisher, 1971; Domb, 1973).

- (a) Ignoring the interactions between droplets means that the model can only be valid at low densities and not in the critical region. Thus the numerical estimate of $\bar{\sigma}$ obtained in three dimensions of 0.640 is geometrically impossible. The model must therefore be regarded as empirical in the critical region.
- (b) Gaunt and Baker point out that the partition function (4.26) has a line of singularities *above* T_c .
- (c) The terms of (4.26) do not mimic the true expansions. For example, putting $y = 1$, the terms of (4.26) are positive for all lattices whereas the actual term structure is complex and lattice dependent (see Table IX).

However, it seems likely that the conclusion regarding the essential singularity at $y = 1$ is valid since it also applies at low temperatures, and is supported by a rigorous theorem of Lanford and Ruelle (1969). These authors showed that if the *stable* thermodynamic state is not analytic at a given point (as is the case in a first order phase transition) then the

multiple correlation functions cannot all be analytic at this point. We should then expect a singularity in one of the multiple correlation functions to be reflected by a singularity in the partition function.

To obtain a proper representation of behaviour in the critical region we must endeavour to take account of interactions between clusters. This can be done in principle by the method of Section II.B3, and we can write instead of (4.23).

$$g_n(u) = \sum_s p_x(n, s) \theta_x(n, s, u). \quad (4.27)$$

Here $p_x(n, s)$ is the lattice constant of a given type of cluster with n spins and s surface bonds, and $\theta_x(n, s, u)$ is the function which must replace u^s constructed by subtraction of sub-clusters in the manner described in Section II.B3. For linear configurations, which have the largest entropy, this procedure was adopted by Domb and Guttmann (1970) who found that they obtained a good representation of all the singularities of the low temperature series (Section III.B7).

However, in the critical region it is essential to take account of non-linear configurations and this poses great practical difficulties. Currently (with the collaboration of K. Binder) the above authors are attempting numerical calculations for small clusters.

Because of the dominance of linear configurations it is better to interpret the partition function (4.26) with $\bar{\sigma} < 1$ as corresponding to nuclei of the new phase rather than as mimicking the total partition function of the assembly. This is in accord with standard nucleation theory, and enables a coherent account to be given of metastable states (Domb, 1973).

F. Self-avoiding walks

A self-avoiding walk (SAW) on a lattice is a random walk which is not allowed to occupy any site more than once. A self-avoiding polygonal closure is a SAW which is allowed to return to the origin at the last step. The parallelism between the total number of SAW's of n steps c_n and the high temperature $I(\frac{1}{2})$ susceptibility coefficients $a_n^{(2)}$, and between the total number of SAW polygonal closures u_n and the $\ln Z^I$ coefficients $a_n^{(0)}$ has been known for many years (see e.g. Fisher and Sykes, 1959) but recently considerable additional light has been cast on the relationship between SAW's and the $I(\frac{1}{2})$ model.

For a general review of the properties of SAW's see Domb (1969). Evidence is there assembled to support the asymptotic behaviour

$$\left. \begin{aligned} c_n &\sim \mu^n n^g \\ u_n &\sim \mu^n n^{-h} \end{aligned} \right\}, \quad (4.28)$$

where μ is a constant associated with each lattice known as the *connective constant*. Numerical estimates of g and h (which are independent of lattice structure in a given dimension) are $\frac{1}{2}$ and $\frac{3}{2}$ respectively in two dimensions, and $\frac{1}{6}$ and $\frac{7}{4}$ in three dimensions. The approximation in which $a_n^{(2)}$ is replaced by c_n and $a_n^{(0)}$ by u_n/n , so that

$$\begin{aligned}\bar{\chi}_0 &= \sum c_n w^n \simeq \sum \mu^n n^g w^n \sim (1 - \mu w)^{-g-1} \\ \ln Z^I &= \sum n^{-1} u_n w^n \simeq \sum \mu^n n^{-h-1} w^n \sim (1 - \mu w)^h\end{aligned}\quad (4.29)$$

has been termed the SAW approximation (Domb, 1970b). In this approximation therefore the critical Ising temperature and exponents corresponding to (4.28) are

$$w_c = \mu^{-1}, \quad \gamma = g + 1, \quad \alpha = 2 - h, \quad (4.30)$$

The SAW provides us with a geometric interpretation of the other high temperature exponents. For example, Domb (1970b, 1971a) noted that the exponent v is related to $\langle R_n^2 \rangle$ the mean square end to end length of an SAW, and Δ to the interaction between two disjoint SAW's. It is also possible to give a geometric interpretation to scaling in terms of SAW's, and this approach has been developed by Brout (1970, 1971, 1972a, b, 1973).

The properties of the $I(\frac{1}{2})$ model can be expressed more precisely in terms of the statistics of near and distant neighbour contacts on an SAW (Domb, 1972a). The terms neglected in the SAW approximation corresponding to star graph contributions with cyclomatic number $c = 2, 3, 4 \dots$ (IIA3) can be arranged in terms of an SAW polygon and various types of bridge across of increasing complication. Hence it is possible to derive a series expansion giving μ in terms of w_c :

$$\ln \mu = \ln \left(\frac{1}{w_c} \right) + A_2 w_c^2 + A_3 w_c^3 + A_4 w_c^4 + \dots, \quad (4.31)$$

with

$$\begin{aligned}A_2 &= k(1) \\ A_3 &= 2k(1, 2; \delta) \\ A_4 &= k(2) + 2k(1, 3; \delta) + 2k(2, 2; \delta) - k(1, 1) + k(1, 1; \alpha)\end{aligned}\quad (4.32)$$

The $k(r, s; \theta)$ in (4.31) are cumulants of the statistics of the various types of bridge across the polygon. Substituting the numerical values of μ and the

$k(r, s; \theta)$ in (4.31) and (4.32) gives an estimate of $1/w_c$ less than 1% different from its true value.

Taking account of the higher order star graph contributions one can usefully describe the coefficients in high temperature $I(\frac{1}{2})$ expansions as *Ising walks*, which consist of SAW's with a particular type of interaction between neighbours whose properties closely parallel those of an SAW.

More recently the renormalization group approach has been applied by Wilson (1972) and Wilson and Fisher (1972) to obtain expansions for critical exponents of the classical vector model with n spin dimensions. $I(\frac{1}{2})$ corresponds to $n = 1$, and de Gennes (1972) noted that the SAW approximation corresponds to $n = 0$. This is in accord with the treatment by Domb (1972b) of the same n -spin vector model as a star graph expansion since all stars other than the polygon have weights containing a factor n . The transition from the SAW to $I(\frac{1}{2})$ described above can therefore be regarded as a transition from the $n = 0$ to $n = 1$ universality class (Kadanoff, 1971).

G. Dilute magnets

Consider an Ising ferromagnet which is diluted by introducing non-magnetic atoms. As the concentration p of non-magnetic atoms increases the magnetic behaviour weakens and one might expect that for sufficiently high concentrations the ferromagnetism will disappear even at $T = 0$. The exploration of critical behaviour as a function of p is a problem of interest and importance.

In 1959 Brout pointed out that there are two distinct problems which must not be confused; the *equilibrium problem* in which the impurities are allowed to move around freely, and the *frozen in or quenched problem* in which the impurities are locked in position in a particular random arrangement. The former problem is obtained by averaging the partition function Z^I over all possible arrangements; it corresponds to a normal three component solution and is best handled by constructing a grand partition function and fixing the number of impurity atoms in the standard manner. The latter problem is obtained by averaging $\ln Z^I$ over all possible arrangements. If the suffix s denotes spin average, and the suffix c configurational average the free energies of the two problems are obtained from $\ln \langle Z \rangle_{s,c}$ and $\langle \ln Z_s \rangle_c$, respectively.

High temperature series expansions for the susceptibility of a frozen-in dilute magnet were developed independently by Rushbrooke and Morgan (1961) and Elliott and Heap (1962). Both groups noted that there was a critical concentration p_c below which no magnetic ordering was possible (Elliott *et al.*, 1960). It was pointed out by Domb and Sykes (1961b)

that p_c was precisely the critical probability for a site percolation process (see Essam, Vol. 2 Chapter 6). It may be noted that the finite cluster method (Section II.A3) is particularly convenient for dealing with this model; expansions like (2.21) can be immediately adapted by multiplying the lattice constant of a connected cluster of r spins by p^r (see also Rushbrooke, 1964).

Unfortunately, for $p_c < p < 1$ the expansions are not well behaved and despite considerable efforts to derive additional terms and apply new techniques of series analysis no clear pattern of critical behaviour has emerged (for a review of the current situation see Rushbrooke, 1971; Rushbrooke *et al.*, 1972; Rapaport, 1972). It has been possible to estimate $T_c(p)$ quite accurately, but little reliable information has been obtained on critical exponents.

In regard to the equilibrium problem the position is much better because of the introduction of a particular soluble model, the Syozi model (Syozi, 1965; Syozi and Miyazima, 1966). This model applies to a lattice which can be divided into A and B sub-lattices; the A sub-lattice is occupied by magnetic atoms and the B sub-lattice is occupied randomly by magnetic and non-magnetic atoms. Syozi and Miyazima showed that the two dimensional model for $H = 0$ could be transformed into a standard $I(\frac{1}{2})$ model, and hence its behaviour could be determined as a function of T , p and p_c could be calculated exactly; Essam and Garellick (1967) extended the treatment to three dimensions and non-zero field. The most important conclusion was that the exponents α^* , β^* , γ^* of the Syozi model were related to the standard exponents in the same dimension as follows:

$$\begin{aligned}\alpha^* &= -\alpha/(1-\alpha) \\ \beta^* &= \beta/(1-\alpha) \\ \gamma^* &= \gamma/(1-\alpha)\end{aligned}\quad (4.33)$$

with corresponding relations for low temperature and other exponents. Scaling relations satisfied by the standard exponents were also satisfied by the starred exponents.

Fisher (1968) suggested that relations (4.33) were not specific to the Syozi model, but would be satisfied by any equilibrium model; he introduced the term *renormalized critical exponents* to describe them and this has gained wide acceptance. Rapaport (1972) introduced a model of random bond impurities which he was able to transform in a similar way to the Syozi model. He demonstrated that by series expansions it would be very difficult to determine the renormalized exponent values since the renormalization occurs only very close to T_c .

For the frozen-in problem the following points which have been made recently are worth recording. Griffiths (1969) showed rigorously that the

magnetization is a non-analytic function of field H at $H = 0$ for a range of temperature extending as far as the critical temperature $T_c(1)$ of the pure system. Watson (1970) suggested the possibility of a "spectrum" of critical points, properties like spontaneous magnetization, susceptibility, etc. diverging at a different critical temperature.

The SAW approximation to this problem was discussed by Domb (1972a). The critical temperature is given by

$$w_c = (p\mu)^{-1}, \quad J/kT_c = \ln \left(\frac{p\mu - 1}{p\mu + 1} \right), \quad (4.34)$$

but this is inaccurate near $p = p_c$. The more refined analysis which takes higher order star lattice constants into account gives, instead of (4.31)

$$\ln(p\mu) = \ln 1/w_c + A_2(p)w_c^2 + A_3(p)w_c^3 + A_4(p)w_c^4 \quad (4.35)$$

where

$$\begin{aligned} A_2(p) &= k(1) \\ A_3(p) &= 2pk(1, 2; \delta) \\ A_4(p) &= pk(2) + p^2k(1, 3; \delta) + 2p^2k(2, 2; \delta) - k(1, 1) + k(1, 1; \alpha). \end{aligned} \quad (4.36)$$

This then leads to the relation for the slope at $p = 1$

$$\frac{dw_c}{dp} = w_c \frac{[1 - \sum r A'_r(1) w_c^r]}{[1 + \sum r A_r(1) w_c^r]}. \quad (4.37)$$

The portion in square brackets differs only slightly from 1, and hence approximately

$$\frac{dw_c}{dp} \simeq w_c \quad (4.38)$$

a relation noted empirically by Rushbrooke and Morgan (1961).

Regarding the critical exponent, in the SAW approximation it is independent of p . Domb gave heuristic arguments for thinking that this property is not changed by taking into account higher order stars. The "interaction" which converts a SAW into an Ising walk is not changed in character, but weakened, by impurity dilution.

Low temperature series expansions could be of help in investigating the critical region. They are difficult to derive because of the complexity of the lowest energy state for $p \neq 1$, but Domb (1971b) has shown how to derive such expansions using the finite cluster technique (Section II.A3).

V. Conclusions

In surveying the conclusions which have been drawn from the analysis of series expansions for the Ising model we can legitimately claim that they have played a major role in unravelling the nature of critical behaviour. We have pointed out, however, that caution must be exercised in using the method if wrong conclusions are to be avoided; physical insight into the nature of the expected solution should be invoked wherever possible, and it can be of great help in providing consistency checks; also methods of series analyses should be tested wherever possible on exact closed form solutions.

The most reliable results have been obtained with high temperature expansions whose convergence is usually rapid. A remarkable confirmation of the accuracy which can be attained by proper analysis of such data was provided very recently when an exact calculation by Barouch *et al.* (1973) made available susceptibility amplitudes for the s.q. lattice. We have noted the estimates of Sykes *et al.* (1972a) in (3.23) which, converted to the temperature variable, give

$$\bar{\chi}_0 \simeq A'_+(1-t')^{-7/4} + A'_{+1}(1-t')^{-3/4}, \quad (5.1)$$

$$A'_+ = 0.96259 \pm 0.00003, \quad A'_{+1} \simeq 0.0742.$$

The values calculated by the above authors were

$$A'_+ = 0.9625817322 \dots, \quad A'_{+1} = 0.0749881538 \dots \quad (5.2)$$

Thus the confidence limits in the estimates of Sykes *et al.* were completely vindicated. In fact the critical data which have been estimated on the high temperature side of T_c are adequate for any comparison with experiment.

On the low temperature side the position is reasonably satisfactory for two dimensional lattices. Instead of (5.1) one has

$$\bar{\chi}_0 \simeq A'_-(1-t)^{-7/4}; \quad (5.3)$$

we have seen that Essam and Fisher (1963) obtained the estimate of 0.0262 ± 0.0006 for A'_- for the s.q. lattice and this was modified to 0.0256 ± 0.0001 by Guttman (private communication). Barouch *et al.* calculated

$$A'_- = 0.0255369719 \dots \quad (5.4)$$

However, the position is less satisfactory for three dimensional lattices for which the series converge more slowly; further information is needed to provide direct estimates of critical exponents and amplitudes which can

be considered as adequate. The reason for slow convergence may perhaps be understood by reference to the droplet model (IV.E). On the low temperature side three dimensional nuclei make a significant contribution to critical behaviour, and they are not properly developed in the terms currently available.

Probably the most important results to have emerged are the conjectures for general patterns of behaviour in the critical region. The first, thermodynamic scaling, has been discussed in Section III.C; the high temperature exponents fit in well with the conjecture, and the low temperature behaviour can at least be regarded as consistent with it. Results for other models are discussed in other chapters of this volume, and the experimental situation is reviewed in the article by Vicentini-Missoni in Vol. 2, Chapter 2.

We have also referred in Section III.C to length scaling introduced originally by Kadanoff (1966b) and developed considerably by Wilson (1971). Length scaling enables the correlation exponents ν and η to be expressed in terms of the same critical exponents which suffice for thermodynamic scaling. However, there are significant discrepancies in numerical values. These are well illustrated by the formula for η ,

$$2 - \eta = d \frac{\delta - 1}{\delta + 1}; \quad (5.5)$$

if we take $\delta = 5$ as has been estimated for $I(\frac{1}{2})$ in three dimensions, we find that $\eta = 0$. But direct numerical analysis gives $\eta \approx 1/18$ (3.52), and this is consistent with the result of renormalization group expansions (Wilson, 1972). If we substitute $\eta \approx 1/18$ into (5.5) we obtain $\delta \approx 4.7$, which is well outside the confidence limits in the analyses quoted in Section III.B3. This must be regarded as a serious inconsistency.

Regarding the actual values of critical exponents, we know that in two dimensions they are all simple integers and fractions. Numerical data given in Table XVI suggest a similar result in three dimensions. It would be difficult to support any such conclusions from a renormalization group treatment. Nevertheless, the possibility is appealing, and hints that there may be simplifying features of the three dimensional Ising model which remain to be discovered. For example, δ may be exactly 5 as suggested by numerical analysis; recent investigations initiated by Brout (1973) have endeavoured to find a basis for such a striking result.

Other important ideas which have drawn on series expansions for the Ising model are generalized scaling (Section IV.C) and the hypotheses of universality (Kadanoff, 1971) and smoothness (Griffiths, 1970, 1971). The last two ideas (as their authors point out) represent a crystallization of results derived from exact solutions and conjectured from series expansions

for a variety of models; they are also discussed in connection with different models in other chapters of this volume, and particularly in Chapter 7 by Stanley. Limitations on the validity of the hypotheses have been demonstrated by Baxter's exact solution of a special model (1971, 1972) in two dimensions, and series expansions have been used to draw similar conclusions in three dimensions (Ditzian, 1972a). Kadanoff and Wegner (1971) have put forward an explanation for the special atypical character of the Baxter model; in fact once many body forces are introduced one can expect complications in critical behaviour (Ditzian, 1972b; Griffiths and Wood, 1973).

However, for the simpler models with which theoretical physicists have been concerned in the past few decades the above hypotheses lead to a ready grasp of a mass of theoretical and experimental data related to critical behaviour. Because of this it is very desirable to subject the hypotheses to further tests wherever possible.

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7. D-Vector Model or "Universality Hamiltonian": Properties of Isotropically-Interacting D-Dimensional Classical Spins*

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I. Introduction

"Which features of a microscopic interparticle interaction are important for determining critical properties and which are not?" This is a fundamental question to which we pay much attention in this chapter; in particular, we shall organise much of our discussion around the concept of a universal class, defined as follows: All systems belonging to the same universal class have the same set of critical point exponents. We shall see that series expansions provide us with considerable insight in our effort to determine the full set of universal classes, and that series expansions combined with a suitable generalisation of the scaling hypothesis provide us with information about what happens when a system is made, by varying some appropriately-chosen parameter, to "cross over" from one universal class to another.

II. Definition of the Universality Hamiltonian

A. The model Hamiltonian

Consider the simple model Hamiltonian

$$\mathcal{H}_U(D, d) = -J \sum_{\langle ij \rangle} \sum_{\alpha=1}^D S_i^\alpha S_j^\alpha \quad (2.1a)$$

$$= -J \sum_{\langle ij \rangle} \mathbf{s}_i \cdot \mathbf{s}_j. \quad (2.1b)$$

Here the summation is over all pairs of nearest-neighbour sites $\langle i,j \rangle$ in a d -dimensional regular lattice, and the quantities s_i are isotropically-interacting D -dimensional classical spins of length $\sqrt{\mathcal{N}}$ (with $\mathcal{N} = 1$ or D generally),

$$\mathbf{s}_i = (S_i^1, S_i^2, \dots, S_i^D), \quad (2.2)$$

where

$$\sum_{\alpha=1}^D (S_i^\alpha)^2 = \mathcal{N}, \quad (2.3)$$

and $-J$ is the energy of a neighbouring pair of spins that are parallel. The Hamiltonian (2.1) was first proposed, to the best of our knowledge, by Stanley (1968b); it has come to be called the D-vector model.[†]

B. Four special cases

The model Hamiltonian (2.1) reduces for four special cases to four commonly-studied models (cf. Fig. 2.1 and Table 2.1).

$$\mathcal{H}(D, d) = -\sum_{ij} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j$$

$S = D$ -dimensional classical spins



Examples:

$D = 1$ (Ising model)



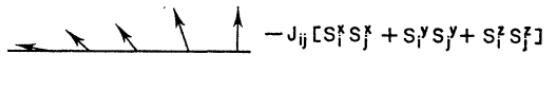
$$-J_{ij} \mathbf{s}_i^z \mathbf{s}_j^z$$

$D = 2$ (Planar model)



$$-J_{ij} [s_i^x s_j^x + s_i^y s_j^y]$$

$D = 3$ (Heisenberg model)



$$-J_{ij} [s_i^x s_j^x + s_i^y s_j^y + s_i^z s_j^z]$$

⋮

$D = \infty$ (Spherical model)

Fig. 2.1. Schematic illustration of the special cases of the Hamiltonian (2.1) for $D = 1, 2, 3$ and ∞ .

[†]Some authors replace the symbol D by the symbol n , in which case the model Hamiltonian (2.1) is called the "n-vector model".

TABLE 2.1. Special cases of the model Hamiltonian (2.1)

| <i>D</i> | Hamiltonian | Name | System |
|----------|---|--|--|
| 1 | $\mathcal{H} = -J \sum_{\langle ij \rangle} S_i^x S_j^x$ | Ising model | One-component fluid, binary alloy, mixture |
| 2 | $\mathcal{H} = -J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y)$ | Plane rotator model ("Vaks-Larkin" model) | λ -transition in a Bose fluid displacive transition (SrTiO_3)? |
| 3 | $\mathcal{H} = -J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z)$ | Classical Heisenberg model | Ferrromagnet; antiferromagnet |
| ∞ | $\mathcal{H} = -J \sum_{\langle ij \rangle} (\sum_{\alpha=1}^{\infty} S_i^{\alpha} S_j^{\alpha})$ | Spherical model | None |

(i) For $D = 1$, the spins are simply one-dimensional "sticks", capable of assuming the two discrete orientations +1 (up) and -1 (down); thus (2.1) reduces for $D = 1$ to the simple spin half Ising model, denoted by $I(1/2)$ (Ising, 1925).

(ii) For $D = 2$, the Hamiltonian (2.1) describes a system of isotropically interacting two-dimensional unit vectors and is called the plane rotator model, denoted $P(\infty)$ (Vaks and Larkin, 1966; Bowers and Joyce, 1967; Stanley, 1968a).

(iii) For $D = 3$ (2.1) describes the "classical Heisenberg model", denoted $H(\infty)$ (Heller and Kramers, 1934; Brown and Luttinger, 1955; Stanley and Kaplan, 1966a; Joyce and Bowers, 1966a, b; Wood and Rushbrooke, 1966).

(iv) For $D > 3$, (2.1) continues to describe a well-defined system, although it becomes rather difficult to draw a picture of the spins. Moreover, no physical system has been put forward to date that corresponds to, say, four-dimensional spins. Nevertheless, when the Hamiltonian (2.1) was first considered (Stanley, 1968b), the author was led to investigate whether any simplifications occurred in the limit $D \rightarrow \infty$ that might render the system soluble for lattices of dimensionality $d > 1$. He found (Stanley, 1968c, 1969c) that the model of infinite-dimensional spins was in fact quite simple to solve—even for a three-dimensional lattice. The solution was recognised as being essentially equivalent to that of the Berlin-Kac spherical model (Berlin and Kac, 1952; Joyce, Vol. 2, Chapter 10).

We shall review below the evidence that claims to justify the term "universality Hamiltonian" for (2.1) by demonstrating that all systems with the same values of D and d belong to the same universal class, and that the simple generalisations of (2.1) in which one allows for (A) anisotropic spin-spin interactions, (B) directional lattice anisotropy, and (C) second neighbour interactions do not give rise to any new universal classes so that consideration of (2.1) is sufficient to obtain all universal classes for systems with short-range interactions. [Extremely long-range interactions, in which the potential between two spins a distance r apart falls off as some power of r , present a special case—see, e.g. the very recent work of Fisher, Ma and Nickel (1972) and the earlier work of Joyce (1966), Nagle and Bonner (1970), Hiley and Joyce (1965), and Gunton and Buckingham (1968b).]

C. Exactly-soluble limits of the universality Hamiltonian

The model Hamiltonian (2.1) is exactly soluble, at least for certain properties, in various special limits (cf. Table 2.2).

TABLE 2.2. Some of the cases in which the model Hamiltonian (2.1) is exactly soluble. Here the notation "n.n." stands for "nearest neighbour interactions only", and H denotes the magnetic field. A blank indicates that the system has not yet been solved.

| D | $d = 1$ | $d = 2$ | $d = 3$ | $d > 3$ |
|----------|---|--|--|--|
| 1 | All H ; both n.n. and $1/r^{d+x}$ | $H = 0$; n.n. | — | — |
| 2 | $H = 0$; n.n. | — | — | — |
| 3 | $H = 0$; n.n. | — | — | — |
| • | • | • | • | • |
| ∞ | All H ; both n.n. and $1/r^{d+x}$ | All H ; both n.n. and $1/r^{d+x}$ | All H ; both n.n. and $1/r^{d+x}$ | Only critical point exponents are known exactly. |

(1) As mentioned in Section II.B, in the limit of infinite spin dimensionality, $D \rightarrow \infty$, the partition function can be exactly calculated for all lattice dimensionality d and the solution is essentially equivalent (Stanley, 1968c) to the spherical model (cf. Fig. 2.2). This result will be discussed below in Section XIII.

Example: $N=2$

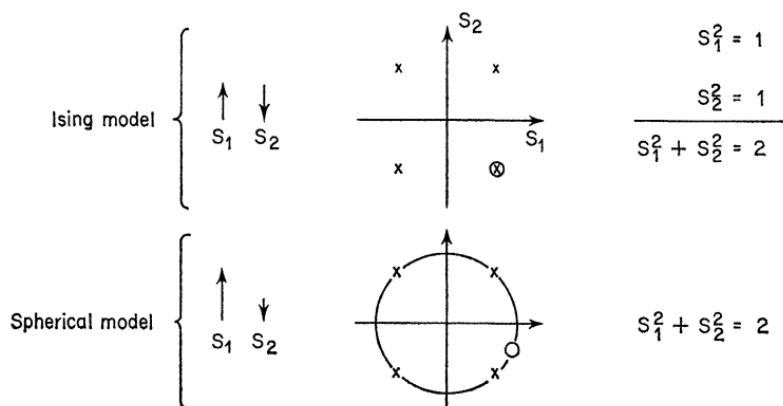


FIG. 2.2. The spherical model was originally defined by Kac as a “continuum modification of the Ising model” in which the one-dimensional spins s_i are no longer restricted to the discrete values $+1$ and -1 , but instead are allowed to assume any values whatsoever, so long as the sum of their squares is equal to the total number of spins in the system. In this figure, we show the case $N = 2$, and represent the $2^N = 4$ allowed states of the Ising system by the corners of an N -dimensional “hypercube.” The spherical model replaces this *discrete* set of allowed states with a *continuum* of states, by replacing the N -dimensional hypercube with an N -dimensional “hypersphere.” Note that the spins are still one-dimensional scalar quantities; all that we have done is to replace the “strong” constraints that *each* spin be of unit magnitude by the “weak” constraint that the sum of the squares of all the N spins in the system add up to N . The circle indicates the particular state shown; thus for the Ising model, the state shown has $s_1 = 1$ and $s_2 = -1$, while for the spherical model the state has $s_1 = \sqrt{3}/2$ and $s_2 = -1/2$ (so that the constraint $s_1^2 + s_2^2 = 2$ is satisfied).

(2) For a linear chain lattice ($d = 1$), one can solve for the partition function and two-spin correlation function for all spin dimensionalities D (Stanley, 1969c, d). The solution reveals that many properties—in particular the two-spin correlation function—are monotonic functions of D (cf. Fig. 2.3). As one might expect intuitively, for fixed T the spin correlation function decreases with increasing D , since the higher-dimensional spins have more phase space available in which they can move (Milošević, Matsuno and Stanley, 1970).

(3) In the limit of infinite lattice dimensionality, $d \rightarrow \infty$, the high-temperature series become equivalent to these of the mean field theory.

In fact, as regards most critical point exponents, the mean field values are reached long before $d = \infty$, with $d = 4$ being the dividing line (Wilson, 1971a, b; Wilson and Kogut, 1974) between the so-called classical (mean field) behaviour and the non-classical behaviour. See Fig. 2.4.

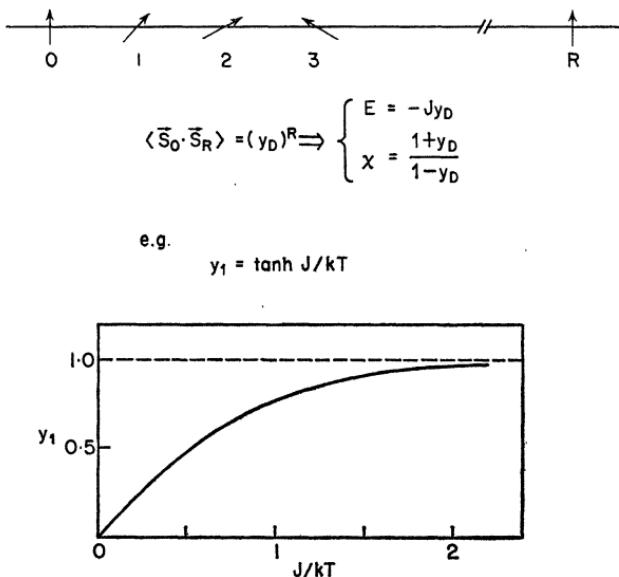


FIG. 2.3. Illustration of the solution for $d = 1$; notice that the thermodynamic quantities have the same form for all D , the only difference being the function y_D , which in general is given by the expression $y_D = I_{D/2}(J)/I_{D/2-1}(J)$, where the $I(x)$ are Bessel functions, and $y_1 = \tanh(J/kT)$. Plots for other values of D are in Stanley, 1969d.

(4) For the case of a $d = 2$ lattice, only certain functions are known in zero magnetic field. (See Temperley Vol. 1, Chapter 6.) Kramers and Wannier (1941a, b) located the critical temperature T_c , Onsager (1944), Kaufman (1949), and Kaufman and Onsager (1949) have obtained the zero field Gibbs potential and certain properties of the correlation functions. Yang (1952) published a derivation of the zero field magnetisation and, most recently, Wu (1966), Cheng and Wu (1967), and McCoy and Wu (1967a, b) have studied the spin correlations in some detail. (See Vol. 4.)

III. Generalizations of the Universality Hamiltonian

A study of the critical properties of the universality Hamiltonian (2.1) for *all* spin dimensionality D and lattice dimensionality d will be carried out below using the method of high-temperature series expansions.

However, we should take care to point out explicitly that there are several assumptions which (2.1) makes for all D and d which are probably not realistic assumptions for most physical systems in nature. These assumptions are made largely in order that the mathematical problem of obtaining critical point predictions remains one of manageable complexity, and fortunately there exists much recent evidence that certain of these assumptions, which we treat under subsections A-C below, do not affect the critical point exponents in the limit $T \rightarrow T_c$.

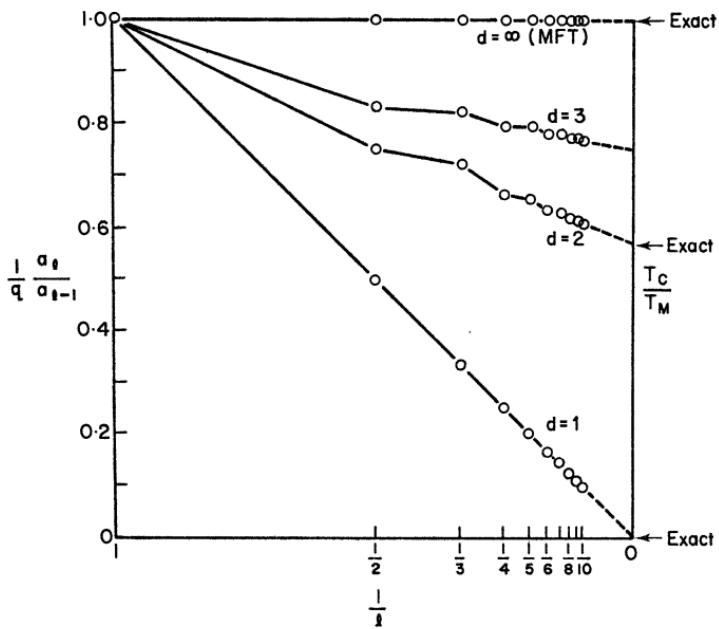


FIG. 2.4. Dependence upon inverse order $1/l$ of the ratio of successive coefficients in the high-temperature series (8.3) for the reduced susceptibility χ for the Ising model ($D = 1$) for selected lattice dimensionalities $d = 1, 2, 3$, and ∞ (for $d = \infty$, the series coefficients are identical to those of the mean field theory). Note that the critical temperatures $T_c(D = 1, d)$ appear to be monotonically increasing functions of d (contrast the behaviour of Fig. 11.2, for which $T_c(D = 1, d)$ appears to be a monotonically decreasing function of D). The ratios are divided by the lattice coordination number q in order that they approach T_c/T_M in the limit $l \rightarrow \infty$. Although $T_c/T_M \rightarrow 1$ "slowly" as $d \rightarrow \infty$, the critical point exponent $\gamma(D = 1, d) = \gamma(D = 1, d = \infty)$ for all $d > 4$ [the limiting slope is proportional to $\gamma - 1$]. See Milošević and Stanley, (1971).

A. Different exchange interactions in different lattice directions

In many real materials, the interactions in one lattice direction are different from those in another lattice direction, and $\mathcal{H}_v(D, d)$ of (2.1) must

be replaced by the corresponding Hamiltonian with "lattice anisotropy",

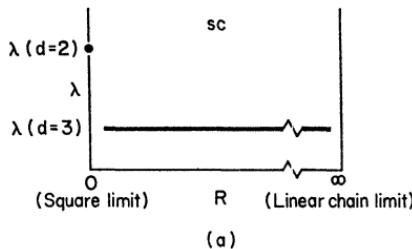
$$\mathcal{H}_{\text{l anis.}}(D, d) \equiv - \sum_{\langle ij \rangle} J_{ij} s_i s_j, \quad (3.1)$$

where J_{ij} in general depends upon the direction of the site separation vector $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$.

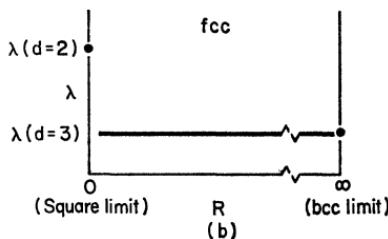
In particular, Paul and Stanley (1971c, 1972a) studied extensively for the s.c. and f.c.c. lattices the special case $D = 1$ of (3.1),

$$\begin{aligned} \mathcal{H}_{\text{l anis.}} &\equiv -J_{xy} \sum_{\langle ij \rangle}^{xy} s_i s_j - J_z \sum_{\langle ij \rangle}^z s_i s_j \\ &= -J_{xy} \left\{ \sum_{\langle ij \rangle}^{xy} s_i s_j + R \sum_{\langle ij \rangle}^z s_i s_j \right\}, \end{aligned} \quad (3.2)$$

where $R \equiv J_z/J_{xy}$ is the anisotropy parameter. Here the first summation is over all pairs of nearest-neighbour sites whose relative displacement vector r_{ij} has no z component, while the second summation is over all other pairs of nearest-neighbour sites. Hence for $R = 0$, both the s.c. and f.c.c. lattices reduce to "stacks" of two-dimensional square lattices, while in the limit $R \rightarrow \infty$, the s.c. lattice becomes a set of one-dimensional linear chains and the f.c.c. becomes two non-interacting three-dimensional b.c.c. lattices.



(a)



(b)

FIG. 3.1. Predictions of the universality hypothesis for $\mathcal{H}_{\text{l anis.}}$ for (a) s.c. and (b) f.c.c. lattices. The exponent γ is predicted to change discontinuously at $R = 0$ (s.c., f.c.c.) and at $R = \infty$ (s.c.).

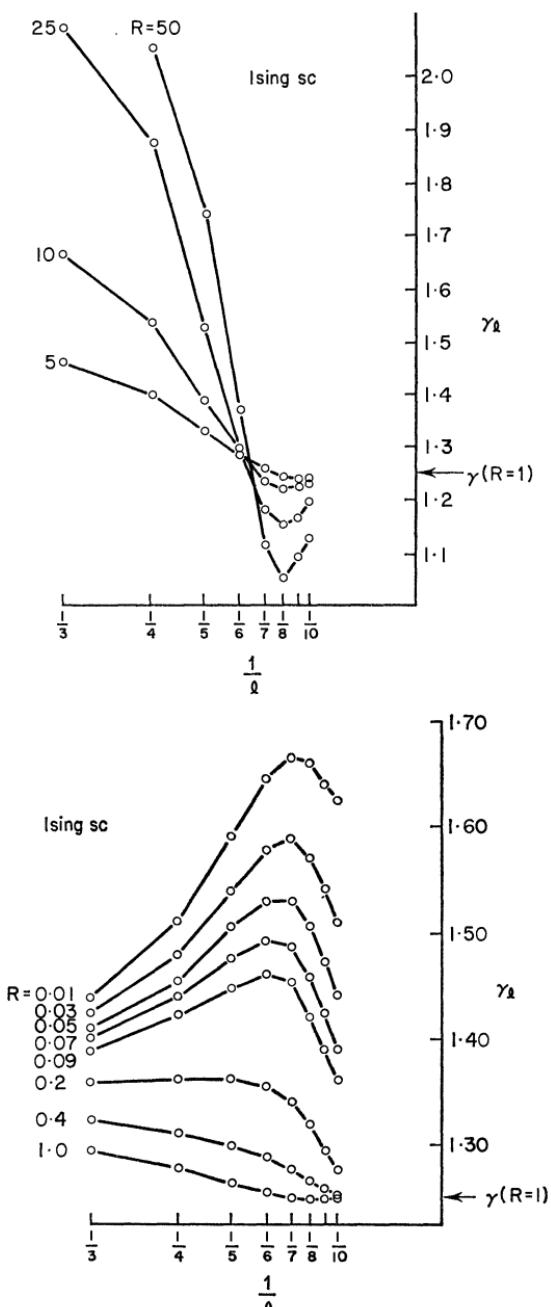


FIG. 3.2. Estimates for γ for the s.c. Ising lattice from Park's method applied to series which have been transformed to reduce the effects of antiferromagnetic singularities. The transformation has eliminated all trace of the oscillations present in the estimates from the untransformed series. The absence of the oscillations allows one to clearly observe the marked curvature in the estimates for exponents when $R \ll 1$ and $R \gg 1$. After Paul and Stanley (1972b).

Paul and Stanley (1971a, 1972a) calculated series for the two-spin correlation function,

$$C_2(\mathbf{r}) = \langle \mathbf{s}_0 \mathbf{s}_r \rangle - \langle \mathbf{s}_0 \rangle \langle \mathbf{s}_r \rangle, \quad (3.3)$$

through tenth order for a wide variety of values of the anisotropy parameter R , from which they could then obtain series of corresponding lengths for the specific heat, susceptibility, and second moment. Analysis of these series yield the following results: when $R = 0$, $d = 2$ critical point exponents are obtained, but for any positive value of R the susceptibility exponent γ and the correlation length exponent ν were found to change discontinuously to their $d = 3$ values (cf. Fig. 3.1 and 3.2).

A somewhat more restricted calculation was carried out for the susceptibility of the s.c. lattice only by Oitmaa and Enting (Oitmaa and Enting, 1971; Enting and Oitmaa, 1972; Oitmaa and Enting, 1972). These authors concluded that the susceptibility exponent γ varied continuously from its $d = 2$ value of 1.75 for $R = 0$ to somewhat smaller values for positive R . These claims were challenged by Rapaport (1971) and Harbus, Krasnow, Liu, and Stanley (1972), who believe that the Oitmaa-Enting results were artifacts due to the shortness of the series used. Specifically, for small values of the anisotropy parameter R , the region near T of three-dimensional behaviour shrinks. This will be discussed extensively below in Section VI.

Very recently, Lambeth and Stanley (1973) (see also Harbus *et al.*, 1972) have calculated the analogous expansions for $D = 2$ and 3 (the classical planar and classical Heisenberg models). Their results will be discussed in Section XI in connection with the question of whether $T_c = 0$ for the limit $R = 0$.

It is perhaps worth pointing out that for $R < 0$, the Hamiltonian of (3.2) can simulate a metamagnet. This system is interesting because it should display a *tricritical point* (where three lines of critical points intersect). Very recently Harbus and Stanley (1972, 1973 b, c, d) have carried out expansions for (3.2) for $D = 1$ in the presence of a magnetic field, and located the phase boundary in the HT plane and the tricritical point to an accuracy of a few percent (cf. Fig. 3.3).

B. Next-nearest neighbour interactions

In essentially all real materials, interactions extend beyond nearest neighbour only in range, and hence $\mathcal{H}_U(D, d)$ of (2.1) must be replaced by a more general interaction range Hamiltonian of the form

$$\mathcal{H}(D, d) \equiv - \sum_{\langle ij \rangle} J_{ij} \mathbf{s}_i \mathbf{s}_j, \quad (3.4)$$

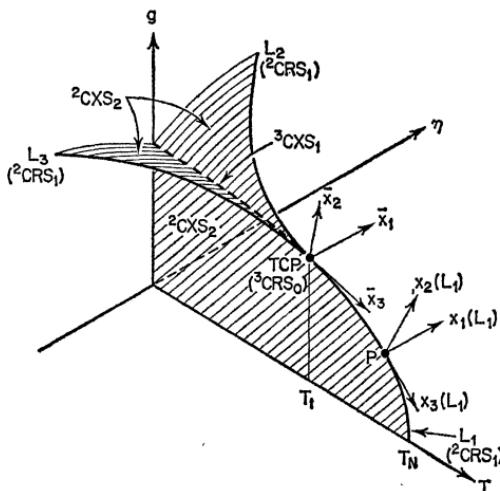


FIG. 3.3. Phase diagram in the three-dimensional space of field variables T , $g(=H)$, and $\eta(=H_{\text{staggered}})$ for the Hamiltonian (3.2) with a fixed negative value of R . We note that there are three lines of ordinary critical points, L_1 , L_2 , and L_3 . These three lines, denoted by ${}^2\text{CRS}_1$ (${}^o\text{CRS}_d$, where o is the order of a critical point), intersect at a so-called "tricritical point," denoted by TCP and ${}^3\text{CRS}_o$. The critical surfaces (CRS) bound coexistence surfaces (CXS) denoted by ${}^p\text{CXS}_d$, where p is the number of phases coexisting at the surface. Note that $o + d = n$, while $p + d = n + 1$, where n is the number of field variables. The properties of such phase diagrams are a subject of much current study; qualitatively new features are found at the "higher order" critical points (such as the ${}^3\text{CRS}_o$). If one treats the parameter R as a fourth field variable ($n = 4$), then one obtains four lines of tricritical points which intersect at a ${}^4\text{CRS}_o$, a critical point of fourth order, at $[T = T_c(D = 1, d = 2), H = 0, H_{\text{staggered}} = 0, R = 0]$. (Harbus, Hankey, Stanley, and Chang, 1973). See also Hankey, Stanley, and Chang, 1972; Chang, Hankey, and Stanley, 1973a, b; Hankey, Chang, and Stanley, 1973; and Hankey, Chang, and Stanley, 1974.

where now we do not assume that $J_{ij} = 0$ for all pairs of lattice sites i and j that are not nearest neighbours of each other. Many authors have studied the critical point exponents of model Hamiltonians that include more than nearest-neighbour interactions, and among the most interesting results are those of Fisher, Ma and Nickel (1972) who confirm the suspicion (cf. Joyce, 1966) that for long-range interactions of the form $J_{ij} = r^{-\sigma}$, exponents do in fact depend upon σ . However, for reasonably short-range interactions, there has been steadily accumulating evidence that exponents are independent of interaction range. The effect of range was first studied by Domb and Dalton (1966) using the "equivalent neighbour model" (a model in which the first r shells of neighbours interact with the same force constant). From studies of the s.q. and p.t. lattices in two dimensions and the s.c., b.c.c., and f.c.c. lattices in three dimensions with $r = 2, 3$, Domb and Dalton concluded that the critical exponents

were unchanged. Until recently the most thorough study of first and second neighbour interactions was that of Dalton and Wood (1969) (but see also Menyuk, Dwight and Reed, 1971; Pirnie, Wood and Eve, 1966; Bowers and Woolf, 1969; and Philhours, 1971).

Recently, Paul and Stanley (1971b, 1972b) studied one important case of (3.4) in great detail,

$$\begin{aligned}\mathcal{H}_{\text{nnn}}(D, d) &\equiv -J_1 \sum_{\langle ij \rangle}^{\text{nn}} \mathbf{s}_i \mathbf{s}_j - J_2 \sum_{\langle ij \rangle}^{\text{nnn}} \mathbf{s}_i \mathbf{s}_j \\ &\equiv -J_1 \left\{ \sum_{\langle ij \rangle}^{\text{nn}} \mathbf{s}_i \mathbf{s}_j + R' \sum_{\langle ij \rangle}^{\text{nnn}} \mathbf{s}_i \mathbf{s}_j \right\},\end{aligned}\quad (3.5)$$

where $R' \equiv J_2/J_1$. Here the first and second sums are over pairs of nearest-neighbour (nn) and next nearest-neighbour (nnn) sites. The two-spin correlation function, $C_2(\mathbf{r})$, was calculated to tenth, ninth, eighth and twentieth order in $1/T$ for the cases $D = 1, 2, 3$ and ∞ , respectively (for the f.c.c., b.c.c. and s.c. lattices). These represented the first series expansions of the spin correlation function for nnn interactions. Analysis of the series and detailed comparison (cf. Fig. 3.4) with the exactly soluble spherical model ($D = \infty$) [for which exponents are rigorously independent of R'] suggest that γ and ν may be independent of R' .

C. Anisotropic spin–spin interactions

In some real materials (e.g., FeF_2) the spin–spin interactions are not purely isotropic, i.e. $\mathcal{H}_v(D, d)$ of (2.1) should be replaced by the more general interaction Hamiltonian

$$\mathcal{H}_{\text{spin anis.}}(D, d) \equiv - \sum_{\langle ij \rangle} \sum_{\alpha=1}^D J_\alpha S_i^\alpha S_j^\alpha,\quad (3.6)$$

where S_i^α denotes the α th Cartesian coordinate of \mathbf{s}_i [cf. eqn (2.2)]. Again, the best indication of the effect of this modification of (2.1) comes from numerical studies. For example, Jasnow and Wortis (1968) have considered the anisotropic classical Heisenberg model ($D = 3$). In particular, they claim to find that the exponents are the conventional $D = 3$ exponents *only* if $J_\alpha = J$ for $\alpha = 1 - 3$. If there is a slight favouring of one axis, (e.g., $J_1 > J_2 = J_3$), then the exponents are those of a pure $D = 1$ system, while if there is a planar anisotropy (e.g., $J_1 = J_2 > J_3$) then the exponents are those of a $D = 2$ system.

D. Quantum-mechanical effects

By restricting our attention to the purely classical Hamiltonian (2.1), we

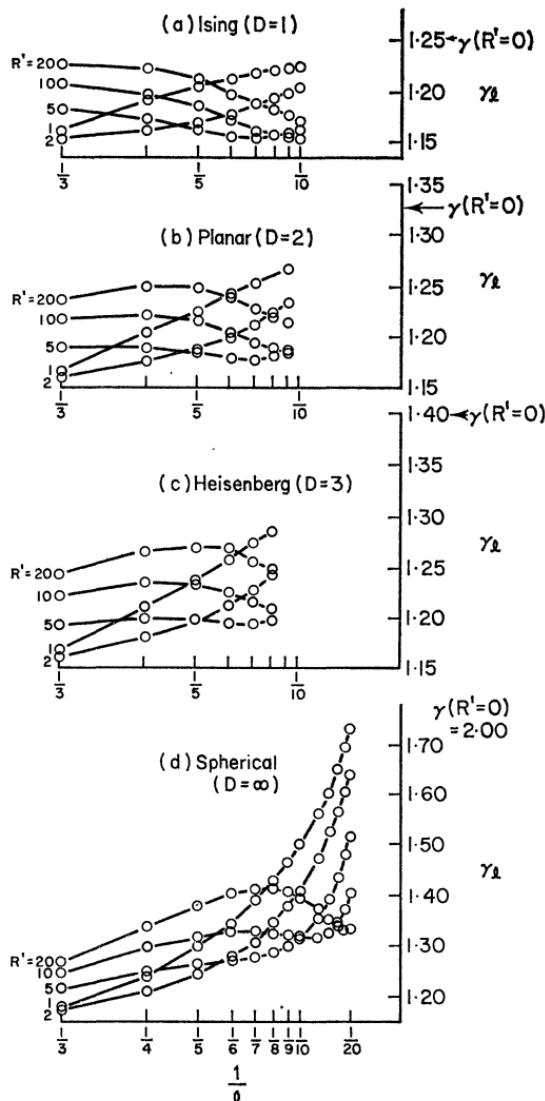


FIG. 3.4. Estimates for γ from Park's method for the (a) Ising [$\gamma(R' = 0) \cong 1.25$], (b) classical-planar [$\gamma(R' = 0) \cong 1.33$], (c) classical-Heisenberg [$\gamma(R' = 0) \cong 1.40$], and (d) spherical [$\gamma(R' = 0) = 2.00$] models on the s.c. lattice. We note the similar behaviour for all four models. The reader should note that later terms of the series for $R' = 1, 2$, and 5 indicate a "turning up" to larger values of γ . Moreover, this bending occurs at larger order l for larger values of R' , suggesting that perhaps a similar turning up might occur for very large R' ($R' = 20$, for example) if a sufficiently large number of terms in the series were available. This must occur in the spherical model, for which γ is rigorously independent of R' . After Paul and Stanley (1972b).

are ignoring quantum-mechanical effects which are known to be crucial to determining the properties of systems in the limit $T \rightarrow 0$. It is becoming widely believed that near the critical point, these quantum-mechanical properties have no effect on critical point exponents, or at least if there exists any effect, it is sufficiently small to be within the experimental error. Actually, most claimed effects are now being believed to be artifacts of the extrapolation process.

Thus, e.g. Jasnow and Wortis (1968) claimed that for $D = 1$, γ decreased slightly from its value of 1.25 to a somewhat smaller value for $s = \infty$; however, Saul and Wortis (1973) have interpreted this result in terms of confluent singularities.

For the case $D = 2$, it is tempting to compare with the $s = \frac{1}{2}XY$ model, but actually this model (see Betts, this volume, Chapter 8) is kinematically different in that the spins are true three-dimensional objects interacting with a highly-anisotropic exchange interaction which has zero z-component. Nevertheless, the critical-point exponents of the $s = \frac{1}{2}XY$ model are apparently identical to those of the $s = \infty$ planar model [the case $D = 2$ of (2.1)].

Finally, we come to the case of the Heisenberg model. Originally workers proposed that the susceptibility exponent γ had the value $\frac{4}{3}$ for all values of the spin quantum number (Domb and Sykes, 1962; Gammel, Marshall, and Morgan, 1963). In fact, Baker (1964) attempted to place an upper bound on γ using certain assumed properties of the susceptibility function. Apparently the susceptibility did not possess these properties, for two years later Baker, Gilbert, Eve and Rushbrooke (1966, 1967) extended the series for $s = \frac{1}{2}$ by several terms and claimed that $\gamma = 1.43 \pm 0.01$. This meant that either γ varied with s or that $\gamma(s)$ estimates for larger s were much too low. Most workers at the time inclined to the former viewpoint, and heuristic arguments were presented by many workers favouring a discontinuous change of exponent from its high value at 1.43 for $s = \frac{1}{2}$ to a lower value for $s > \frac{1}{2}$. Still other arguments favoured $\gamma(s) = 1.43$ for all finite s with a discontinuous change at $s = \infty$. Stanley and Kaplan (1967b) proposed a continuous variation $\gamma(s) = 1.33 + 0.05/s$ which also proved to be erroneous, and with the extension of the series for $s = \infty$ (Wood and Rushbrooke, 1966; Joyce and Bowers 1966b; Stanley, 1967b) and for general s (Stephenson, Pirnie, Wood and Eve, 1968), and, perhaps more importantly, with refined methods of analysis (Lee and Stanley, 1971 and references contained therein), it is coming to be widely believed that the critical point exponent for the susceptibility is independent of s , with the value being somewhere between 1.38 and 1.40 (Ritchie and Fisher, 1972; Ferer, Moore and Wortis, 1971; Lee and Stanley, 1971).

E. The universality hypothesis

One of the most important general suggestions to have emerged in the theory of critical behaviour is the hypothesis that critical behaviour for short-range forces can be specified by the two numbers D and d and does not depend on any other details of the lattice structure or the Hamiltonian. This suggestion resulted from the efforts of several different research groups. Older "closed form" approximations (e.g. Bethe, quasichemical; see Burley, Vol. 2, Chapter 9) focussed attention on the co-ordination number of the lattice as the key parameter in describing critical behaviour. However, once series expansions came into prominence they demonstrated clearly that dimension d is the primary factor and lattice structure in a given dimension is of secondary importance (see, e.g. Domb, 1960). This naturally led to the idea that critical exponents for a given model depend on dimension only and are independent of lattice structure, a suggestion which received strong support from exact solutions and numerical calculations for a variety of lattices (see, e.g. Fisher, 1963).

Next to be investigated was the dependence of critical behaviour on spin value for a given model. Domb and Sykes (1962) found strong indications that the susceptibility of the Ising model of spin s is independent of s . A few years later Jasnow and Wortis (1968) put forward the more general proposal that critical exponents depend only on the symmetry of the ordered state. This means (i) that for a given Hamiltonian critical exponents depend on the symmetry of the Hamiltonian (e.g. Ising or Heisenberg) but not on the spin s ; (ii) for a Hamiltonian which is anisotropic in spin interactions, e.g. $a(S_i^{(x)}S_j^{(x)} + S_i^{(y)}S_j^{(y)}) + bS_i^{(z)}S_j^{(z)}$, they depend on whether $a < b$, $a = b$, or $a > b$ (this relation determines the lowest energy ordered state). This proposal was formulated more coherently by Griffiths (1970, 1971) in his *smoothness postulate* that critical exponents change only at certain discrete values of parameters in the Hamiltonian (e.g., $a/b = 1$, in the above example).

Finally it was suggested by Watson (1969a, b) that the scaling function describing the equation of state in the critical region (see Section V) is also independent of spin and lattice structure (see also Fisk and Widom, 1969). This suggestion has been confirmed by numerical studies (Gaunt and Domb, 1970; Milošević and Stanley, 1972c).

These suggestions have been integrated into a general formulation of behaviour in the critical region by a number of authors (Domb, 1971; Kadanoff, 1971; Griffiths, 1970, 1971; Betts, Guttman and Joyce, 1971), which has been termed by Kadanoff the "universality hypothesis". If this hypothesis is valid the Hamiltonian (2.1) is capable of describing the critical behaviour of all systems with "short-range" interactions, and we therefore call it the "universality Hamiltonian".

IV. Physical Systems described by the Universality Hamiltonian

A. $D = 1$ systems

From what has been said in the previous section, it should be clear that any system with an ordered state characterised by an order parameter that has essentially one degree of freedom should be described by the universality Hamiltonian (2.1) with $D = 1$ and with d appropriate to the dimensionality of the system. Thus, e.g., to $D = 1$ should correspond a spin system with anisotropic spin coupling favouring a particular axis, a simple fluid (cf. the lattice gas models described elsewhere in this treatise; see Domb this volume, Chapter 6), a binary alloy, a binary mixture, and so forth. Most of these $D = 1$ systems belong to the universal class with $d = 3$, even though in some systems the interactions in the third direction are sufficiently weak that they are "quasi-two-dimensional". A detailed discussion of this situation is given below in Section VI.

B. $D = 2$ systems

For $D = 2$, the Hamiltonian (2.1) describes a system of isotropically-interacting two-dimensional classical spins. It has been called the Vaks-Larkin model because Vaks and Larkin (1966) have showed it to be a good model for the superfluid transition in liquid helium. The intuitive reasoning behind this claim is that the order parameter of helium is described by a phase and an amplitude and hence is representable by a two-dimensional vector. Indeed, the critical point exponents of the $D = 2$ system correspond quite closely to those measured for helium near its superfluid transition (e.g., $\alpha \cong 0$, $2\beta \cong 2/3$, $\nu \cong 2/3$, etc.).

Strontium titanate (SrTiO_3) undergoes a displacive type of transition in which octahedra of oxygen atoms rotate through a small angle, and the order parameter (the angle) varies with temperature near the ordering temperature (about 105°K) as $(T_c - T)^\beta$ with $\beta \cong 1/3$ (Müller and Berlinger, 1971). These observations led Stanley to suggest at the 1971 NATO Spring School on *Structural Phase Transitions and Soft Modes* that perhaps the $D = 2$ case of (2.1) is not an altogether inappropriate model with which to describe SrTiO_3 near its transition (Stanley, 1971b).

Finally, it is worth mentioning that there exist magnetic systems with an easy plane of magnetisation [see Betts and Lee (1968), Wielinga, Lubbers and Huiskamp (1967), and references contained therein, as well as Chapter 8 of this volume]. These systems should have critical point exponents given by the $D = 2$ case of (2.1), providing spin-dependence is insignificant.

C. $D = 3$ systems

For the case of three-dimensional spins, (2.1) reduces to the classical

Heisenberg model, which we argued above in Section IIID should have the same critical point exponents as the quantum-mechanical Heisenberg model (see Rushbrooke *et al.*, this volume, Chapter 5). This is fortunate, for when the classical Heisenberg model was first introduced (Heller and Kramers, 1934) it was found to produce drastically different behaviour in the spin wave region. The importance of the classical Heisenberg model in studying the critical region (both for its drastic simplicity of calculation and for its relative accuracy) was pointed out independently by three groups of workers: Stanley and Kaplan (1966a), Joyce and Bowers (1966a, b), and Wood and Rushbrooke (1966). It is important to stress, however, that even the quantum-mechanical Heisenberg model is not valid for a very wide range of real magnetic materials, as it makes the rather stringent assumptions of (a) well-localised spins and (b) complete isotropy of interaction. Most magnetic materials in nature fail in one or the other of these two assumptions. For example, the $3d$ transition metals probably do not satisfy assumption (a) while most of the rare-earth elements do not satisfy assumption (b). Fortunately, certain materials have been discovered in recent years which satisfy both assumptions to a fair extent (e.g., EuO and EuS). Also, it should be pointed out that the same exponents are expected to describe the analogous "staggered" quantities of an antiferromagnet (e.g., $\chi_{\text{st}} \equiv \partial M_{\text{st}} / \partial H_{\text{st}}$, where the subscript "st" refers to a quantity varying through the lattice such that it is positive on one sublattice and negative on the other). Thus the case $D = 3$ is also germane to isotropic antiferromagnets such as RbMnF₃.

D. $D > 3$ systems

For $D > 3$, the Hamiltonian (2.1) continues to describe a well-defined mathematical model, and some authors have tentatively proposed (in an effort to explain, e.g., unusually large values of the susceptibility exponent γ observed in certain materials) that certain forms of spin-spin interaction might correspond to the Hamiltonian (2.1) for $D > 3$.

V. Scaling Functions for Certain Universal Classes*

To date most experimental data taken in the critical region cannot be compared with microscopic theory since they do not pertain to the two paths along which critical exponents are defined (for a magnet, these are the axes $H = 0$ and $\tau \equiv T - T_c = 0$). Nevertheless these data serve to support the hypothesis, originally put forth independently by Widom (1965a, b) and by Domb and Hunter (1965), that the Gibbs potential is a generalised homogeneous function; for a simple magnet, this says that we can find

* See also Vicentini-Missoni, Volume 2, Chapter 2

two numbers, a_τ and a_H , such that for all positive values of the parameter L ,

$$G(L^{a_\tau} \tau, L^{a_H} H) = LG(\tau, H). \quad (5.1)$$

From (5.1) it follows by differentiation that the magnetisation,

$$M(T, H) = \left(\frac{\partial G}{\partial H} \right)_T, \quad (5.2)$$

obeys the functional equation

$$M(L^{a_\tau} \tau, L^{a_H} H) = L^{1-a_H} M(\tau, H). \quad (5.3)$$

Since (5.3) is valid for all positive L , it must be valid for the choice $L \equiv 1/|H|^{1/a_H}$, whence (5.3) becomes

$$\frac{M(\tau, H)}{|H|^{(1-a_H)/a_H}} = M\left(\frac{\tau}{|H|^{a_\tau/a_H}}, 1\right). \quad (5.4)$$

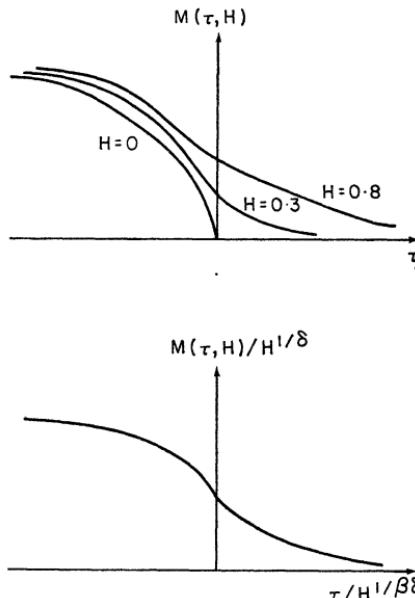


FIG. 5.1. Schematic illustration of the "data collapsing" predicted by the scaling hypothesis (5.1) [cf. eqn (5.4)]. Data which fall in part (a) on a family of curves for each value of H are predicted to fall upon a single curve (a so-called MHT scaling function) when the variables M and T are scaled by appropriate powers of H . Here τ denotes $T - T_c$. Another MHT scaling function can be constructed by scaling with respect to τ , but this results in a scaling function with two separate branches (see Ho and Litster, 1970).

Equation (5.4) says that if we "scale" the magnetisation by dividing it by a power of the magnetic field, and if we scale the temperature by dividing it by another power of the field, then although $M(\tau, H)$ data fall on a family of curves when plotted on the axes τ and H , scaled M vs scaled τ data will "collapse" onto a single curve (cf. Fig. 5.1). This single curve is called a MHT scaling function, and the dramatic collapsing of data from two dimensions to one dimension is shown for CrBr_3 (Ho and Litster, 1970) in Fig. 5.2. The two scaling powers appearing in (5.4) may be re-expressed in terms of any two directly-measurable critical point exponents one finds that $(1 - a_H)/a_H = 1/\delta$ by setting $\tau = 0$ in (5.4); similarly, one finds $a_\tau/a_H = 1/\beta\delta$ by returning to (5.3), choosing $L \equiv 1/|\tau|^{1/a_\tau}$, and then setting $H = 0$. This straightforward approach has been applied to static and dynamic scaling of thermodynamic potentials and correlation functions, as well as to scaling with a parameter, in Hankey and Stanley (1972).

Clearly it would be desirable to extend the question asked in the first sentence of this chapter to include "On what features of an interaction Hamiltonian does the *scaling function* depend?" The search for a definitive answer to this question is still underway. It began with the calculation of the MHT scaling function by Gaunt and Domb (1970) for the case $D = 1$; their method is not generalisable to the case of larger D because it relies upon

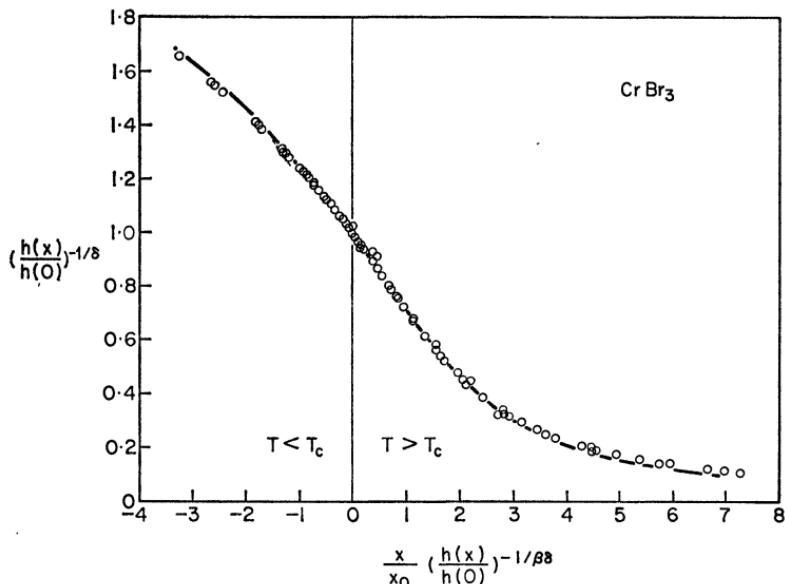


FIG. 5.2. Plot of the experimental data of Ho and Litster (1970) according to the prescription of eqn (5.4). The fact that the data fall upon a single smooth curve shows that the scaling hypothesis (5.1) is valid for this material [cf. Stanley, 1971a, for the proof that (5.4) implies (5.1)]. The solid curve shown is the scaling function calculated for the spin $\frac{1}{2}$ Heisenberg model by Milošević and Stanley (1972a, b, c).

the use of low-temperature expansions as well as high-temperature expansions, and these are not known for $D > 1$. Recently Milošević and Stanley (1972a, b, c, 1973) and Milošević, Karo, Krasnow, and Stanley (1973) have calculated the $D = 3$ scaling function for all three $d = 3$ lattices (f.c.c., b.c.c., and s.c.) and for both $s = \frac{1}{2}$ and $s = \infty$; perhaps not surprisingly, the differences between the suitably normalised scaling functions are within the error of the numerical extrapolation procedures. The comparison (cf. Fig. 5.2) of their $D = 3$ scaling function with the data on the insulating ferromagnet CrBr_3 (for which there exists considerable lattice anisotropy) and on EuO (for which there exist non-negligible next-nearest-neighbour interactions) suggests the further conjecture that the scaling function might be independent of these features of the interaction. By contrast, the change in the scaling function on going from Ising coupling ($D = 1$) to Heisenberg coupling ($D = 3$) was quite substantial (cf. Fig. 5.3) as was the change observed on going to the spherical model ($D = \infty$). The planar ($D = 2$) scaling function was not calculated, because the Milošević-Stanley

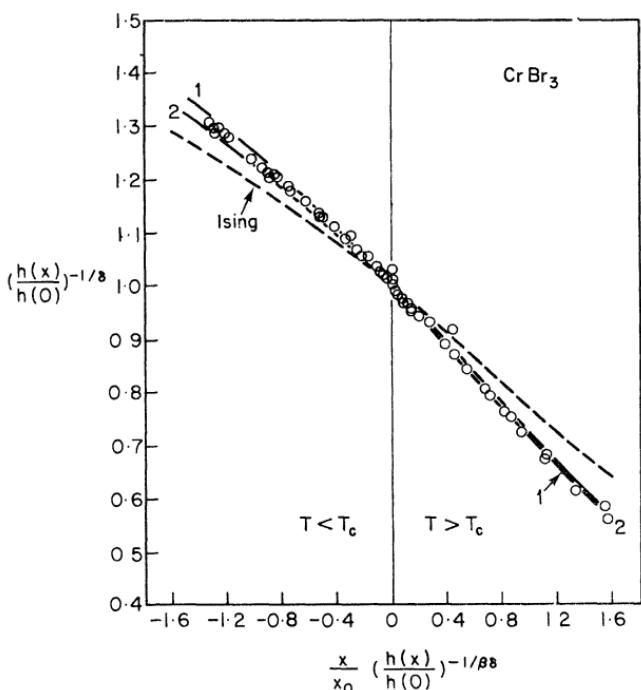


FIG. 5.3. Enlarged portion of Fig. 5.2. The curve labelled 1 is the same curve as that in the previous figure, i.e. it corresponds to the spin $\frac{1}{2}$ Heisenberg model with $\beta = 0.385$ and $\delta = 4.71$; the curve numbered 2 corresponds to the same model but the estimates $\beta = 0.35$ and $\delta = 5$ were used in its construction. The broken curve corresponds to the Ising model scaling function (Gaunt and Domb, 1970).

method requires the use of series for the Gibbs potential in magnetic field, and these have not been calculated (to the best of our knowledge) for $D = 2$.

Gaunt and Domb (1970) also observed a marked change in the $D = 1$ MHT scaling function on going from the $d = 3$ to the $d = 2$ Ising model, so that the scaling function evidently depends on d also. Thus the evidence to date from series expansions suggests that the universal classes for the scaling function are the same as those for the critical point exponents—and that $\mathcal{H}_U(D, d)$ of (2.1) is sufficient to describe a very large class of physical systems.

Very recently additional evidence supporting the universality hypothesis for MHT scaling functions has arisen from Monte Carlo calculations of Binder and Müller-Krumbhaar (1973), and from the calculations of the CHT and CMT scaling functions for the specific heats $C_H(H, T)$ and $C_M(M, T)$ for $D = 1, 3$ and their comparison with Ni data (Krasnow and Stanley, 1973).

Also very recently Brézin, Wallace, and Wilson (1972, 1973) have calculated the MHT scaling function using the Wilson-Fisher method of expanding in powers of $\epsilon \equiv (4 - d)$ [Wilson and Fisher, 1972].

Finally, we should mention that data near *tricritical* points also appear to “collapse” onto a single curve (Tuthill, Harbus, and Stanley 1973), and that the Wilson-Fisher expansion can also be generalized to arbitrary order \mathcal{O} (Chang, Tuthill, and Stanley, 1974), with expansion parameter $\epsilon_{\mathcal{O}} \equiv 2\mathcal{O}/(\mathcal{O} - 1) - d$; here $\mathcal{O} = 2$ is an ordinary critical point, $\mathcal{O} = 3$ a tricritical point, and so forth.

VI. Crossing Over from One Universal Class to Another

In this section we describe what happens as $T \rightarrow T_c$ in a system which is not clearly in one universal class or another. Consider, for the sake of simplicity, a quasi-two-dimensional system with, say, $D = 3$. This system, sketched in Fig. 6.1, has interactions of strength J within the plane and RJ between planes, with $R \ll 1$. A most dramatic finding of the earliest detailed neutron scattering experiments [e.g., those of Birgeneau, Guggenheim, and Shirane (1969) on K_2NiF_4] was that well above the critical temperature $T_c = T_c(R)$, the system displays behaviour that is essentially two-dimensional. This is intuitively plausible, since well above $T_c(R)$, the correlations between the moments are governed by the stronger interactions J so that the magnetic order will begin to appear in these directions first. Only as one gets close to $T_c(R)$ will the correlations arising from the weaker interactions RJ (in the remaining lattice direction) begin to manifest themselves, and accordingly the system will “cross over” from two-dimensional to three-dimensional behaviour as $T \rightarrow T_c(R)^+$.

This crossing over is of course not infinitely sharp, and hence the frequently-used term “crossover temperature” $T_x(R)$ is somewhat of a

TABLE 6.1a. Rigorous results referred to in the text of Section VI, for crossing over from a quasi d -dimensional lattice to a true 3-dimensional lattice. The lattice coefficients are defined in Table 6.1b. S denotes the structure factor.

| Physical Quantity | Lower Bound | Upper Bound | Range of (T, H) |
|--|---|-------------|------------------------|
| 1. $\left[\frac{\partial}{\partial R} G(T, H, R) \right]_{R=0}$ | $\frac{1}{2} N g_1 J \bar{M}_d^2$ | | Arbitrary |
| 2. $\left[\frac{\partial}{\partial R} C_H(T, H, R) \right]_{R=0}$ | $-\frac{1}{2} N g_1 J T \frac{\partial^2}{\partial T^2} [\bar{M}_d^2]$ | | Arbitrary |
| 3. $\left[\frac{\partial}{\partial R} \bar{M}(T, H, R) \right]_{R=0}$ | $g_1 \mathcal{J} \bar{M}_d \bar{x}_d$ | | Arbitrary |
| 4. $\left[\frac{\partial}{\partial R} \mu_2(T, H, R) \right]_{R=0}$ | $g_1 \mathcal{J} \bar{M}_d \frac{\partial}{\partial h} \mu_2(0) + g_1 \mathcal{J} \bar{x}_d [\bar{x}_d + 2\mu_2(0)]$ | | Arbitrary |
| 5. $\left[\frac{\partial}{\partial R} S(T, H, \mathbf{q}, R) \right]_{R=0}$ | $g_1 \mathcal{J} \bar{M}_d \frac{\partial S_d(q)}{\partial h} + g_1 \mathcal{J} \cos(\mathbf{q} \cdot \mathbf{z}) S_d(\mathbf{q}) S_d(-\mathbf{q})$ | | Arbitrary |
| 5a. $\left[\frac{\partial}{\partial R} \bar{x}(T, H, R) \right]_{R=0}$ | $g_1 \mathcal{J} \bar{M}_d \frac{\partial}{\partial h} \bar{x}_d + g_1 \mathcal{J} \bar{x}_d^2$ | | Arbitrary |

$$6. \quad \left[\frac{\partial^2}{\partial R^2} \bar{M}(T, H, R) \right]_{R=0} \quad 2g_{21}\mathcal{J}^2 \bar{M}_d \tilde{x}_d^2 + (g_{21} + g_{22}) \quad (g_{21} + g_{22}) \mathcal{J}^2 \left[2\bar{M}_d \tilde{x}_d^2 + \bar{M}_d^2 \frac{\partial \tilde{x}_d}{\partial h} \right] \quad \text{Arbitrary}$$

$$\times \bar{M}_d^2 \mathcal{J}^2 \frac{\partial \tilde{x}_d}{\partial h}$$

$$7. \quad \left[\frac{\partial^2}{\partial R^2} \bar{x}(T, H = 0, R) \right]_{R=0} \quad 2g_{21} \mathcal{J}^2 \tilde{x}_d^3$$

$$2(g_{21} + g_{22}) \mathcal{J}^2 \tilde{x}_d^3$$

$$T > T_c, H = 0$$

$$8. \quad \left[\frac{\partial^2}{\partial R^2} \mu_2(T, H = 0, R) \right]_{R=0} \quad 2g_{21} \mathcal{J}^2 [3\mu_2(0) + 4\tilde{x}_d] \tilde{x}_d^2$$

$$2(g_{21} + g_{22}) \mathcal{J}^2 [3\mu_2(0) \tilde{x}_d^2]$$

$$T > T_c, H = 0$$

$$+ 8g_{21} \mathcal{J}^2 \tilde{x}_d^3$$

$$9. \quad \left[\frac{\partial^3}{\partial R^3} \bar{x}(T, H = 0, R) \right]_{R=0} \quad (6g_{31} - 2g_{33}) \mathcal{J}^3 \tilde{x}_d^4$$

$$(6g_{31} + 12g_{32} + 6g_{33}) \mathcal{J}^3 \tilde{x}_d^4$$

$$T > T_c, H = 0$$

$$10. \quad \left[\frac{\partial^3}{\partial R^3} \mu_2(T, H = 0, R) \right]_{R=0} \quad (6g_{31} - 2g_{33}) 4 \mathcal{J}^3 \tilde{x}_d^3 \mu_2(0)$$

$$(6g_{31} + 12g_{32} + 6g_{33}) 4 \mathcal{J}^3 \tilde{x}_d^3 \mu_2(0)$$

$$T > T_c, H = 0$$

$$+ (54g_{31} - 2g_{33}) \mathcal{J}^3 \tilde{x}_d^4 \\ + (54g_{31} + 12g_{32} + 6g_{33}) \mathcal{J}^3 \tilde{x}_d^4$$

TABLE 6.1b. Lattice coefficients used in Table 6.1a.

| g | s.q. \rightarrow s.c. | s.q. \rightarrow f.c.c. | l.c. \rightarrow s.c. | l.c. \rightarrow s.q. |
|----------|-------------------------|---------------------------|-------------------------|-------------------------|
| g_1 | 2 | 8 | 4 | 2 |
| g_{21} | 2 | 32 | 12 | 2 |
| g_{22} | 2 | 32 | 4 | 2 |
| g_{31} | 2 | 128 | 36 | 2 |
| g_{32} | 2 | 128 | 12 | 2 |
| g_{33} | 2 | 128 | 4 | 2 |

misnomer. In fact, the crossing over from two-dimensional to three-dimensional behaviour begins, literally, at infinite temperature and is not complete until $T = T_c(R)$. However, Liu and Stanley (1972a, b, 1973) have shown that it makes sense to speak of a crossover region, $T_A(R) \geq T \geq T_B(R)$, defined such that within it "most of the crossing over" takes place.

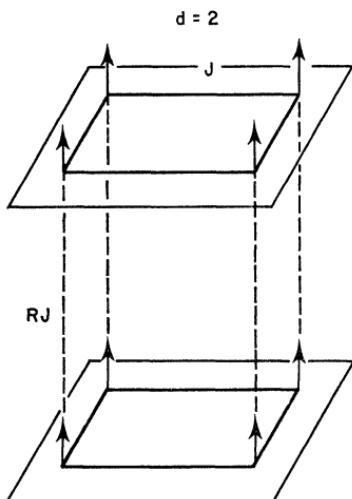


FIG. 6.1. Schematic representations of quasi-two-dimensional lattice. Here the solid lines indicate interaction bonds of strength J , while the dashed lines indicate bonds of strength RJ with $R \ll 1$.

Apart from scaling-type arguments, little has been done to attempt to understand this crossover effect, and in fact the crossover region has never been defined precisely. Liu and Stanley (1972a, b, 1973) have succeeded in establishing numerous rigorous relations for derivatives of thermodynamic functions and moments of correlation functions with respect to R , and using these they can actually predict the temperature at which a p -percent

deviation from two-dimensional behaviour should occur. Their rigorous relations are summarised in Table 6.1.

These relations, plus extensive series expansion analysis of Harbus, Krasnow, Liu, and Stanley (1972), Harbus and Stanley (1973a), and Krasnow, Harbus, Liu, and Stanley (1973) have confirmed many of the exponent predictions of the generalised scaling hypothesis (Riedel and Wegner, 1969; Abe, 1970; Suzuki, 1971; Coniglio, 1972; Hankey and Stanley, 1972), in which one assumes that the parameter R also scales; i.e. (5.1) is replaced by

$$G(L^{a\tau}, L^{aH} H, L^{aR} R) = LG(\tau, H, R) \quad (6.1)$$

[cf. Section VI of Hankey and Stanley (1972) and references contained therein].

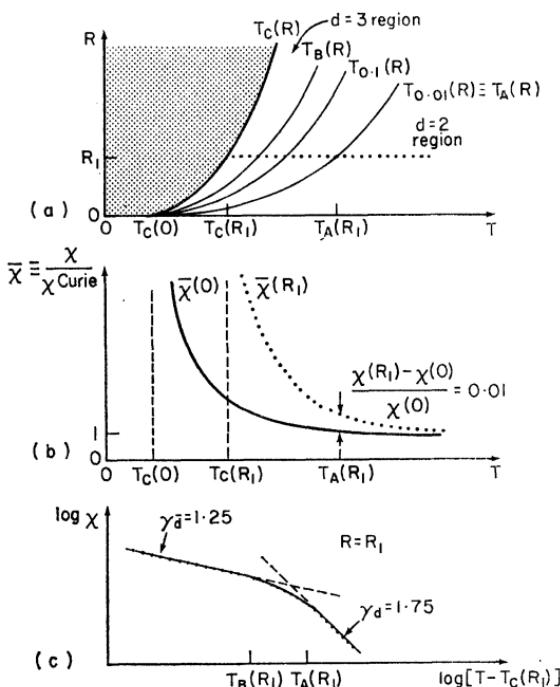


FIG. 6.2. Schematic diagram of the crossover behaviour. (a) The crossover region (shaded area) is bounded by $T_A(R)$ and $T_B(R)$. [$T_A(R) = T_{0.01}(R)$ is the temperature at which the system differs appreciably (1%) from being two dimensional.] $T_c(R)$ is the critical temperature. The generalised scaling hypothesis predicts that all curves should approach $T_c(0)$ via the power law $R^{1/\phi}$. (b) Dependence of reduced susceptibility \bar{X} upon T for $R = 0$ and for $R = R_1$, indicating the definition of $T_A(R)$. Note that this drawing is not to scale. (c) Sketch of hypothetical experimental data, plotted in the conventional log-log plot, for a system which is described by the Hamiltonian with $R = R_1$. After Liu and Stanley (1972b).

Thus the conclusion is that the Hamiltonian (2.1) suffices to understand behaviour in the limit $T = T_c$ (such as critical point exponents), and also crossover effects arising when one approaches $T_c(R)$ along a path of constant R (cf. Fig. 6.2).

We may finally draw attention to a recent paper by Rapaport (1972) which uses exact analytical results to describe the transition of the spherical model from four to three dimensions.

VII. Formalism for Deriving Arbitrary- D Expressions for the Zero-Field Gibbs Potential and the Two-Spin Correlation Function

In this section we present the formalism utilised to obtain the general- D high-temperature series expansions; the reader not interested in the particular formalism used in this work but only in the results is urged to skip to Sections VIII and IX.

A. Basic idea of high-temperature series expansions

The basic idea of the high-temperature expansion method is that one expands the exponential $\exp(-\beta\mathcal{H})$ as a power series in its argument $\beta\mathcal{H}$, where here $\beta \equiv 1/kT$. The motivation for this expansion is that this exponential occurs in two quantities of immediate interest, the Gibbs potential

$$G(T, H) = -kT \ln Z = -kT \ln (Tr e^{-\beta\mathcal{H}}) \quad (7.1a)$$

and the pair correlation function

$$\Gamma_{fg}(T, H) = \langle \mathbf{s}_f \cdot \mathbf{s}_g \rangle = \frac{Tr \mathbf{s}_f \cdot \mathbf{s}_g e^{-\beta\mathcal{H}}}{Tr e^{-\beta\mathcal{H}}}. \quad (7.1b)$$

Here the notation “ Tr ” denotes a trace for quantum mechanical systems, but for the classical systems of interest here it denotes a configurational integral over the surface of a D -dimensional hypersphere; for an arbitrary function of the N spin variables, $f(\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_N)$, we have

$$Tr f(\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_N) = \frac{\int d\Omega_1 d\Omega_2 \dots d\Omega_N f(\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_N)}{\int d\Omega_1 d\Omega_2 \dots d\Omega_N}. \quad (7.2)$$

When a series expansion is valid, we can write

$$\ln Z = -\beta G(T, H) = \sum_{l=0}^{\infty} \frac{\lambda_l \beta^l}{l!} \quad (7.3a)$$

and

$$\Gamma_{fg}(T, H) = \sum_{l=0}^{\infty} \frac{\alpha_l(f, g) \beta^l}{l!}. \quad (7.3b)$$

It is our goal to calculate the coefficients λ_l and $\alpha_l(f, g)$; these are given, by the Taylor theorem, as

$$\lambda_l = \frac{\partial^l}{\partial \beta^l} \ln (Tr e^{-\beta H}) \Big|_{\beta=0} \quad (7.4a)$$

and

$$\alpha_l(f, g) = \frac{\partial^l}{\partial \beta^l} \left. \frac{Tr(s_f s_g e^{-\beta H})}{Tr e^{-\beta H}} \right|_{\beta=0}. \quad (7.4b)$$

In regard to practical computation of series expansions there are several alternative methods (see Domb, this volume, Chapter 1, Section IV.B). We shall here use the method of Stanley and Kaplan (1966a) and Stanley (1967a, b); the method of Wood and Rushbrooke (1966) is described in Chapter 5 of this volume. The method of Joyce and Bowers (1966a, b) uses a star lattice constant expansion for finite clusters and is discussed by Domb in Chapter 1. It draws heavily on the work of Joyce (1967), which expresses the partition function for star clusters in terms of $3j$ and $6j$ symbols. This method has recently been extended by Domb (1972) to the D -dimensional vector model, and he has formulated an alternative method of calculating the weights of finite clusters.

B. Two theorems

We begin by proving two theorems for $H = 0$ which have the combined effect of requiring only one basic calculation for both the λ_l and the $\alpha_l(f, g)$, and of reducing the number of configurational integrals ("traces") needed for the present calculation from 298 to 15. Before stating the two theorems, we observe that one can write (7.4a) formally as

$$\lambda_l = \frac{J^l}{\beta^l} \left(\sum_{ij} \frac{\partial}{\partial J_{ij}} \right)^l \ln (Tr e^{-\beta H}) \Big|_{\{J_{ij}\}=0}. \quad (7.5)$$

On using the multinomial theorem, (7.5) becomes

$$\lambda_l = \frac{J^l}{\beta^l} \sum'_{\{l\}} \frac{l!}{l_{12}! l_{13}! \dots} \left[\left(\frac{\partial}{\partial J_{12}} \right)^{l_{12}} \left(\frac{\partial}{\partial J_{13}} \right)^{l_{13}} \dots \ln (Tr e^{-\beta H}) \right]_{\{J_{ij}\}=0}, \quad (7.6)$$

where the summation symbol $\sum'_{\{l\}}$ in (7.6) denotes a summation over all values of the set $\{l\}$ of integers l_{ij} such that $\sum_{ij} l_{ij} = l$. In the present work we set $J_{ij} = J$ and limit the summation to the case for which i, j are nearest-neighbour sites. Thus we can write for λ_l the simple formula

$$\lambda_l = \sum'_{\{l\}} \lambda\{l\}, \quad (7.7a)$$

where

$$\lambda\{l\} = \frac{J^l}{\beta^l} \frac{l!}{l_{12}! l_{13}! \dots} \left(\frac{\partial}{\partial J_{12}} \right)^{l_{12}} \left(\frac{\partial}{\partial J_{13}} \right)^{l_{13}} \dots \ln (Tr e^{-\beta \mathcal{H}}) \Big|_{\{J_{ij}\}=0}. \quad (7.7b)$$

Similarly, for the correlation function coefficients $\alpha_l(f, g)$ we have

$$\alpha_l(f, g) = \sum'_{\{l\}} \alpha_{fg}\{l\}, \quad (7.8a)$$

where

$$\alpha_{fg}\{l\} = \frac{J^l}{\beta^l} \frac{l!}{l_{12}! l_{13}! \dots} \left(\frac{\partial}{\partial J_{12}} \right)^{l_{12}} \left(\frac{\partial}{\partial J_{13}} \right)^{l_{13}} \dots \frac{Tr s_f \cdot s_g e^{-\beta \mathcal{H}}}{Tr e^{-\beta \mathcal{H}}} \Big|_{\{J_{ij}\}=0}. \quad (7.8b)$$

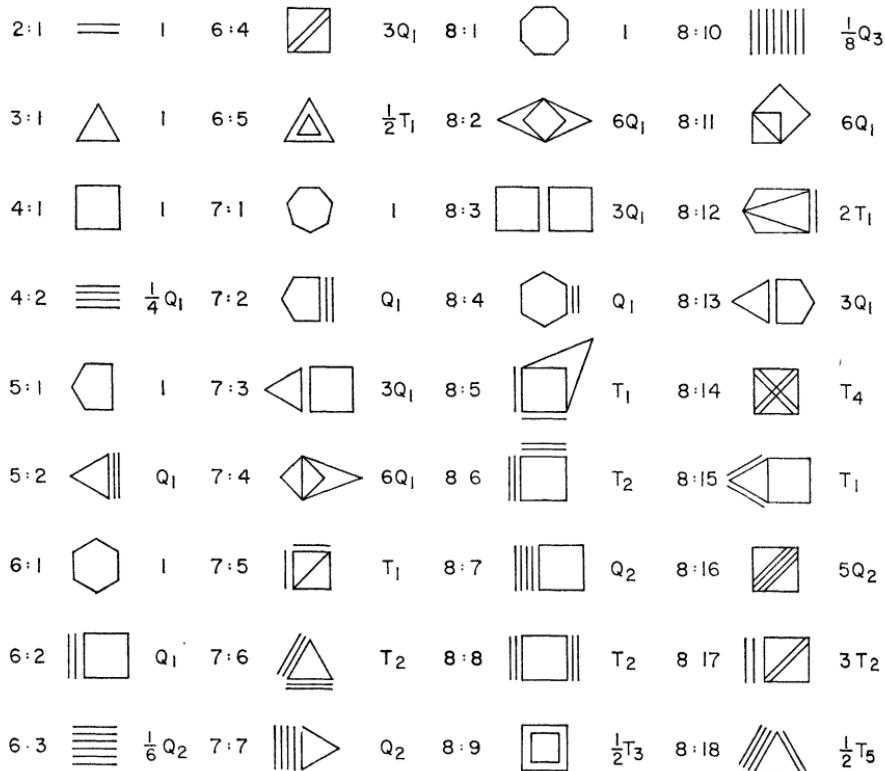


FIG. 7.1. The diagram $\mathcal{D}_\lambda = (l:t)$ contributing to the expansion (7.7a) of the coefficient λ_l in (7.3a) for the Gibbs potential. Shown are the diagrams through order $l = 8$. The numbers shown are defined in eqn (7.20a).

Next we associate a diagram with every $\lambda\{l\}$ and $\alpha_{fg}\{l\}$ by drawing l_{12} straight lines between vertices 1 and 2, l_{13} lines between vertices 1 and 3, and so forth. Thus, each diagram contributing to λ_l or $\alpha_l(f, g)$ has precisely l straight lines. In addition, we join by a wavy "correlation line" the sites f and g of all diagrams corresponding to $\alpha_{fg}\{l\}$. These diagrams have been discussed extensively for the case $D = 3$ elsewhere (Stanley, 1967a, b); for the present general- D calculation, no change in the diagrams is necessary. Fortunately it turns out that for the classical problem, large classes of diagrams do not contribute and need not be considered in (7.7a) or (7.8a). We denote a diagram contributing to λ_l of (7.7a) by the symbol \mathcal{D}_λ and a diagram contributing to $\alpha_l(f, g)$ of (7.8a) by the symbol \mathcal{D}_α . The 93 diagrams \mathcal{D}_λ which have a non-zero contribution to λ_l (through the orders considered in this work) are displayed in Figs. 7.1–7.3. There are a corresponding 298 diagrams \mathcal{D}_α making a non-zero contribution to $\alpha_l(f, g)$; since we can relate the contribution from the diagrams \mathcal{D}_α to those of the diagrams \mathcal{D}_λ (see Theorem 1 below), we need not display all 298

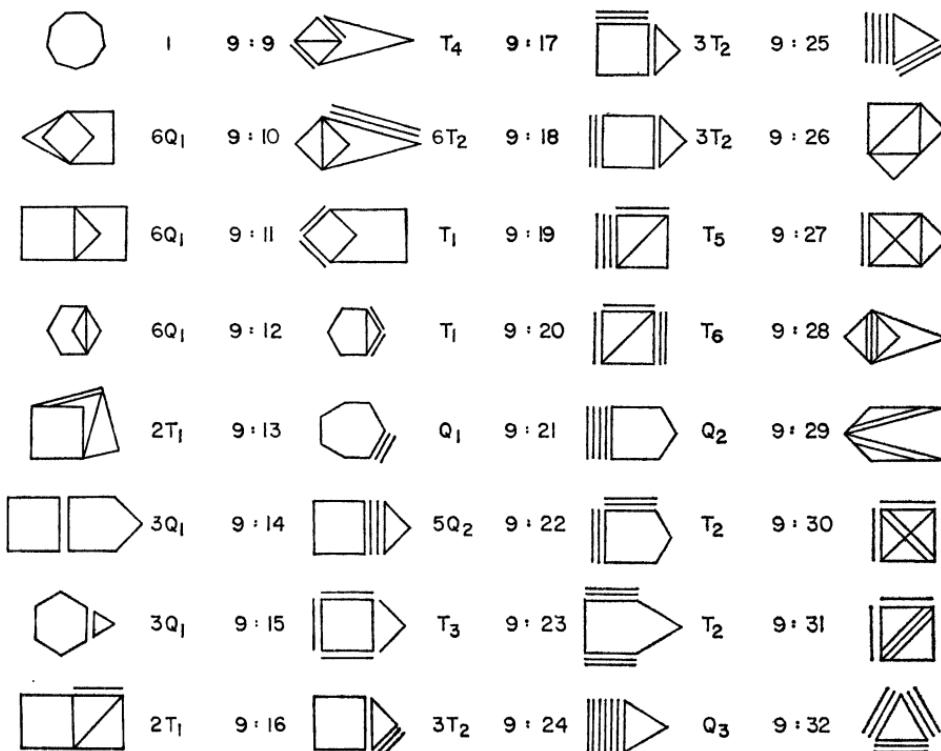


FIG. 7.2. Additional diagrams $\mathcal{D}_\lambda = (l:t)$ needed for order $l = 9$.

diagrams; Fig. 7.4 lists the 33 diagrams \mathcal{D}_α needed through order $l = 6$. The reader can generate the remaining 265 diagrams from Figs. 7.2–7.3 by simply forming as many topologically distinct diagrams as one can by successively replacing each of the lines l_{12}, l_{13}, \dots by a wavy correlation line (all 298 diagrams are tabulated in Stanley, 1967a).

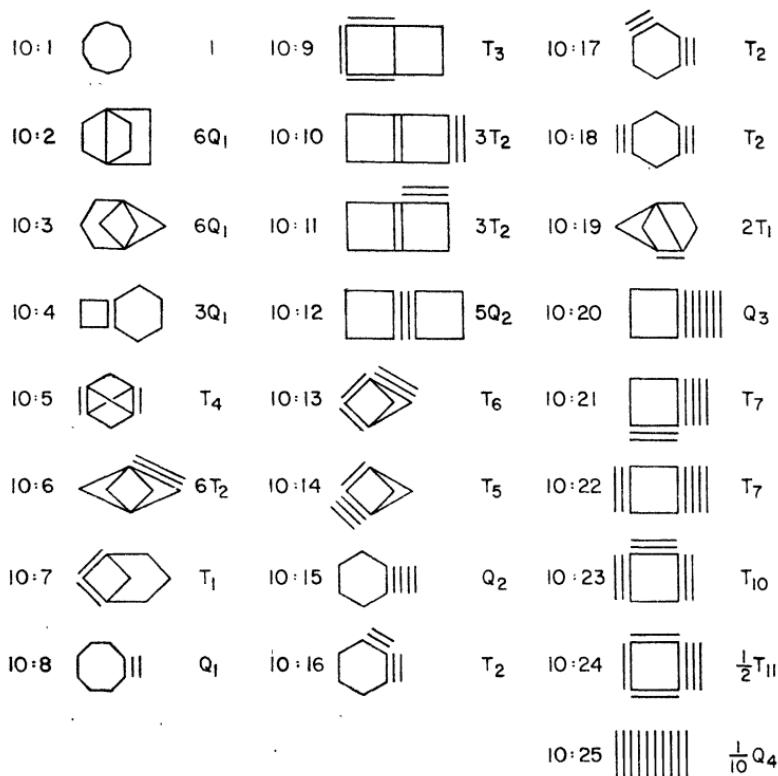


FIG. 7.3. Diagrams $\mathcal{D}_\lambda = (l:l)$ for only the loose-packed lattices for order $l = 10$. Many more diagrams would be needed for close-packed lattices.

In Stanley (1967a) we derived the coefficients in the spin correlation function series from a recursion relation; here we have both used the recursion relation and a second, simpler, method. Since the results of both methods agree, and since the reader can easily generalise the recursion relation method of Stanley (1967a) to general spin dimensionality D , we present only the simpler method here. We present our results in the form of two theorems (Paul and Stanley, 1971a). Theorem 1 permits one to write down immediately the contribution to $\alpha_l(f, g)$ from a particular diagram \mathcal{D}_α immediately, given the knowledge of the contribution to λ_l from another

"corresponding" \mathcal{D}_λ diagram, thus obviating the need for any complicated calculations once the 93 diagrams \mathcal{D}_λ contributing to λ_l are all evaluated; Theorem 2 simplifies the calculation of the 93 diagrams contributing to λ_l by relating most (but not all) complex diagrams to simpler diagrams. The net effect of utilising the two theorems is that of the 298 diagrams \mathcal{D}_α needed for the correlation function, *the contribution of all but 15 is trivial!*

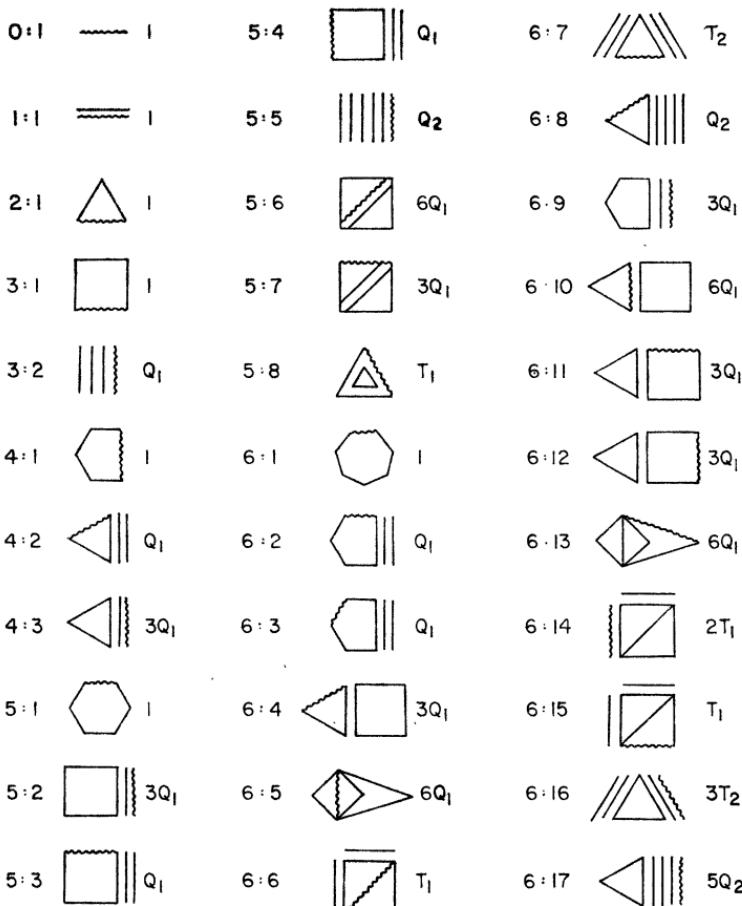


FIG. 7.4. Diagrams $\mathcal{D}_\alpha = (l:i)$ contributing to (7.7b) for the coefficients $\alpha_i(f, g)$ of the series expansion (7.3) of the two-spin correlation function. Shown are the diagrams through order $l = 6$. Higher order diagrams can be obtained from Figs 7.1-7.3 using Theorem 1 [eqn (7.9)]. The numbers shown are defined in (7.20b).

THEOREM 1. Consider an arbitrary diagram \mathcal{D}_α and its contribution $\alpha_{fg}(l_{12}, l_{13}, \dots, l_{fg}, \dots)$ to $\alpha_l(f, g)$ of (7.8a), and consider a corresponding diagram \mathcal{D}_λ contributing to λ_{l+1} in which we have replaced the wavy “correlation line” joining sites f and g by a straight line. Then

$$\alpha_{fg}(l_{12}, \dots, l_{fg}, \dots) = \frac{l_{fg} + 1}{(l + 1)J} \lambda(l_{12}, \dots, l_{fg} + 1, \dots). \quad (7.9)$$

Proof. From (7.7b), we have

$$\begin{aligned} \lambda(l_{12}, \dots, l_{fg} + 1, \dots) &= \frac{J^{l+1}}{\beta^{l+1}} \frac{(l+1)!}{l_{12}! \dots (l_{fg} + 1)! \dots} \\ &\times \left[\left(\frac{\partial}{\partial J_{12}} \right)^{l_{12}} \dots \left(\frac{\partial}{\partial J_{fg}} \right)^{l_{fg}+1} \dots \ln (Tr e^{-\beta \mathcal{H}}) \right]_{\{J_{ij}\}=0}. \end{aligned} \quad (7.10)$$

If we carry out one of the $l_{fg} + 1$ derivatives with respect to J_{fg} that are indicated in (7.10), we obtain

$$\begin{aligned} \lambda(l_{12}, \dots, l_{fg} + 1, \dots) &= \frac{J^l}{\beta^l} \frac{J(l+1)}{\beta(l_{fg} + 1)} \frac{l!}{l_{12}! \dots l_{fg}! \dots} \\ &\times \left[\left(\frac{\partial}{\partial J_{12}} \right)^{l_{12}} \dots \left(\frac{\partial}{\partial J_{fg}} \right)^{l_{fg}} \dots \frac{Tr(\beta s_f \cdot s_g e^{-\beta \mathcal{H}})}{Tr e^{-\beta \mathcal{H}}} \right]_{\{J_{ij}\}=0}. \end{aligned} \quad (7.11)$$

Equation (7.9) follows directly from (7.11) and (7.8b), and Theorem 1 is proved.

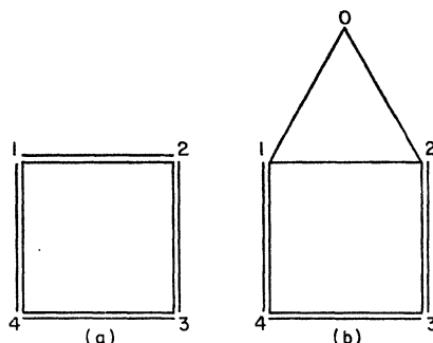


FIG. 7.5. Example of two diagrams related by the insertion of a vertex of valence two. Diagram (b) is obtained from diagram (a) by the insertion of a vertex of valence two between vertices 1 and 2. Note that (a) is diagram (8:9) of Fig. 7.1, whereas (b) is diagram (9:15) of Fig. 7.2, so that Theorem 2 holds.

THEOREM 2. Consider an arbitrary diagram \mathcal{D}'_λ of $l+1$ lines which is obtained from a diagram \mathcal{D}_λ of l lines by the insertion of a vertex of valence two (cf. Fig. 7.5). That is \mathcal{D}'_λ contains a point k such that the only lines emanating from k are l_{ki} and l_{kj} , with $i \neq j$. Then the cumulant for \mathcal{D}'_λ is related to the cumulant of \mathcal{D}_λ by the expression

$$\lambda(\mathcal{D}'_\lambda) = \frac{J}{D} (l+1) l_{ij} \lambda(\mathcal{D}_\lambda), \quad (7.12)$$

where l_{ij} is the number of lines joining vertices i and j in the diagram \mathcal{D}_λ .

Proof. For the sake of convenience it is helpful to be more explicit about i , j , and k . Without loss of generality, we label the vertices so that $k = 0$, $i = 1$, and $j = 2$, whence (7.12) becomes (cf. Fig. 7.5)

$$\lambda(l_{10} = 1, l_{02} = 1, l_{12} - 1, \dots) = \frac{J}{D} (l+1) l_{12} \lambda(0, 0, l_{12}, \dots). \quad (7.13)$$

By definition

$$\begin{aligned} \lambda(\mathcal{D}'_\lambda) &= \frac{J^{l+1}}{\beta^{l+1}} \frac{(l+1)!}{(l_{12}-1)! l_{13}! \dots} \left(\frac{\partial}{\partial J_{10}} \right) \left(\frac{\partial}{\partial J_{02}} \right) \\ &\quad \times \left. \left(\frac{\partial}{\partial J_{12}} \right)^{l_{12}-1} \dots \ln (Tr e^{-\beta \mathcal{H}}) \right|_{\{J_{ij}\}=0}. \end{aligned} \quad (7.14)$$

Carrying out the derivatives $\partial/\partial J_{10}$ and $\partial/\partial J_{02}$ explicitly, we have

$$\begin{aligned} \lambda(\mathcal{D}'_\lambda) &= \frac{J^{l+1}}{\beta^{l+1}} \frac{(l+1)!}{(l_{12}-1)! \dots} \left(\frac{\partial}{\partial J_{12}} \right)^{l_{12}-1} \\ &\quad \times \left[\frac{Tr(s_1 \cdot s_0)(s_0 \cdot s_2) e^{-\beta \mathcal{H}}}{Tr e^{-\beta \mathcal{H}}} - \frac{(Tr s_1 \cdot s_0 e^{-\beta \mathcal{H}})(Tr s_0 \cdot s_2 e^{-\beta \mathcal{H}})}{(Tr e^{-\beta \mathcal{H}})^2} \right]_{\{J_{ij}\}=0} \end{aligned} \quad (7.15)$$

Because there are no further derivatives involving lines that end at vertex 0, we can set all $J_{i0} = J_{0i} = 0$ and perform the trace integration of ds_0 . Using the facts that

$$Tr S_0^\alpha S_0^\beta = \frac{1}{D} \delta_{\alpha\beta} \quad (7.16a)$$

and

$$Tr S_0^\alpha = 0, \quad (7.16b)$$

we have that

$$\lambda(\mathcal{D}'_\lambda) = \frac{1}{D} \frac{J^{l+1}}{\beta^{l-1}} \frac{(l+1)!}{(l_{12}-1)! \dots} \left(\frac{\partial}{\partial J_{12}} \right)^{l_{12}-1} \dots \left. \frac{\text{Tr } s_1 \cdot s_2 e^{-\beta \mathcal{H}}}{\text{Tr } e^{-\beta \mathcal{H}}} \right|_{(J_{ij})=0} \quad (7.17)$$

On carrying out one of the differentiations with respect to J_{12} , in

$$\lambda(\mathcal{D}'_\lambda) = \frac{1}{D} \frac{J^{l+1}}{\beta^l} \frac{(l+1)!}{(l_{12}-1)! \dots} \left(\frac{\partial}{\partial J_{12}} \right)^{l_{12}} \dots \ln \left. (\text{Tr } e^{-\beta \mathcal{H}}) \right|_{(J_{ij})=0} \quad (7.18)$$

it is clear that (7.18) reduces to (7.17), and hence

$$\lambda(\mathcal{D}'_\lambda) = \frac{J}{D} (l+1) l_{12} \lambda(\mathcal{D}_\lambda) \quad (7.19)$$

and Theorem 2 is proved.

TABLE 7.1. General- D expressions for the quantities Q_j and T_j appearing in Figs. 7.1-7.4.

| |
|---|
| $Q_1 = -D/(D+2)$ |
| $Q_2 = 2D^2/[(D+2)(D+4)]$ |
| $Q_3 = -D^3(5D+12)/[(D+6)(D+4)(D+2)^2]$ |
| $Q_4 = 2D^4(7D+24)/[(D+6)(D+4)(D+2)^2]$ |
| $T_1 = -D(5D+4)/(D+2)^2$ |
| $T_2 = D^2/(D+2)^2$ |
| $T_3 = -D(7D^2+12D+8)/(D+2)^3$ |
| $T_4 = -D(9D^2+10D+8)/(D+2)^3$ |
| $T_5 = 2D^2(7D+8)/[(D+4)(D+2)^2]$ |
| $T_6 = D^2(5D+4)/(D+2)^3$ |
| $T_7 = -2D^3/[(D+4)(D+2)^2]$ |
| $T_8 = 2D^2(13D+14)/(D+2)^3$ |
| $T_9 = 8D^2(5D^2+12D+8)/[(D+2)^2(D+4)^2]$ |
| $T_{10} = -D^3/(D+2)^3$ |
| $T_{11} = 2D^2(9D^2+20D+16)/[(D+4)(D+2)^3]$ |

C. Calculation of traces through ninth order for loose-packed and through eighth order for close-packed lattices

Using Theorems 1 and 2, we need evaluate only the requisite traces of 15 diagrams and the rest can be evaluated by inspection. The 15 diagrams whose traces need evaluation are obtained by methods described in Stanley

(1967a) for the special case $D = 3$, and they are given the notation $Q_1 - Q_4$ and $T_1 - T_{11}$; these symbols are listed for general D in Table 7.1. Accordingly, we show in Figs 7.1-7.3 the 93 diagrams contributing to λ_l through order $l = 10$ for loose-packed lattices and through order $l = 9$ for close-packed lattices. The diagrams have been indexed with the notation $(l:t)$, when l is the number of straight lines and t is the topological type of the diagram. The number to the right of the diagram, $\lambda(l:t)$, is defined by

$$\lambda(l:t) \equiv Dl! \left(\frac{J}{D}\right)^l \bar{\lambda}(l:t). \quad (7.20a)$$

From the 93 diagrams contributing to λ_l one can use Theorem 1 to obtain the corresponding traces for the 298 diagrams contributing to $\alpha_l(f,g)$ through order $l = 9$ for loose-packed lattices and through order $l = 8$ for close-packed lattices. The diagrams contributing through order $l = 6$ are shown in Fig. 7.4 and the remaining diagrams are given in Figs 2-5 of Stanley (1967a) for the case $D = 3$. The number to the right of each diagram in Fig. 7.4, $\bar{\alpha}(l:t)$, is defined by

$$\alpha(l:t) \equiv l! \left(\frac{J}{D}\right)^l \bar{\alpha}(l:t). \quad (7.20b)$$

VIII. Calculation of the Coefficients in the Zero Field Susceptibility Series

A. General- D , general-lattice expressions

To calculate the zero-field susceptibility series, we multiply each diagram by the appropriate lattice occurrence factor. These are listed in Tables A and B of Appendix II of Domb (1960) for all cases considered in this work, except the hypercubical lattices (cf. Table 8.1.). Thus we obtain general- D series for any desired lattice.

Rather than list the series in the original variable $\mathcal{J} \equiv J/kT$, where k is the Boltzmann constant, it is convenient to expand in the variable

$$y_D \equiv \frac{1}{\mathcal{N}} \frac{\partial}{\partial \mathcal{J}} \ln [\mathcal{J}^{1-D/2} I_{D/2-1}(\mathcal{N}\mathcal{J})], \quad (8.1)$$

where $I_v(x)$ is the modified Bessel function of the first kind of order v ; y_D is the two-spin correlation function for a linear chain lattice (Stanley,

1969a) of classical spins of length $\mathcal{N}^{1/2}$. This function is plotted for $\mathcal{N} = D$ in Fig. 8.1; for $D = 1, 2, 3$, and ∞ we have

$$y_1 = \tanh(\mathcal{N}\mathcal{J}), \quad (8.2a)$$

$$y_2 = I_1(\mathcal{N}\mathcal{J})/I_0(\mathcal{N}\mathcal{J}), \quad (8.2b)$$

$$y_3 = \mathcal{L}(\mathcal{N}\mathcal{J}) = \coth(\mathcal{N}\mathcal{J}) - 1/(\mathcal{N}\mathcal{J}), \quad (8.2c)$$

and

$$y_\infty = \frac{2\mathcal{J}}{1 + [1 + (2\mathcal{J})^2]^{1/2}}. \quad (8.2d)$$

TABLE 8.1. Lattice constants p_{kx} for d -dimensional “hypercubical lattices” (linear chain, s.q., s.c., . . .). All constants p_{kx} in Tables 8.3 and 9.1 other than those shown here are zero for loose-packed lattices. The notation f_j denotes the binomial coefficient $d!/[j!(d-j)!]$. These numbers were first obtained by Fisher and Gaunt (1964).

| |
|---|
| $q = 2d$ |
| $p_4 = f_2$ |
| $p_6 = 2f_2 + 16f_3$ |
| $p_{7a} = 2f_2 + 12f_3$ |
| $p_8 = 7f_2 + 186f_3 + 648f_4$ |
| $p_{8c} = 24f_3$ |
| $p_{8h} = 2f_2 + 24f_3 + 48f_4$ |
| $p_{9j} = 8f_2 + 168f_3 + 576f_4 + 480f_5$ |
| $p_{9k} = 12f_2 + 288f_3 + 768f_4$ |
| $p_{9l} = 20f_3 + 32f_4$ |
| $p_{10} = 28f_2 + 2,328f_3 + 2,3136f_4 + 47,616f_5$ |
| $p_{10b} = 12f_3 + 32f_4$ |

The recursion formulae for obtaining the coefficients a_l in the original variable \mathcal{J} ,

$$\bar{\chi} \equiv \chi/\chi_{\text{Curie}} = 1 + \sum_{l=1}^{\infty} a_l \mathcal{J}^l, \quad (8.3)$$

from the coefficients A_l in the new variable $y_D = f(\mathcal{J})$,

$$\bar{\chi} = 1 + \sum_{l=1}^{\infty} A_l(y_D)^l, \quad (8.4)$$

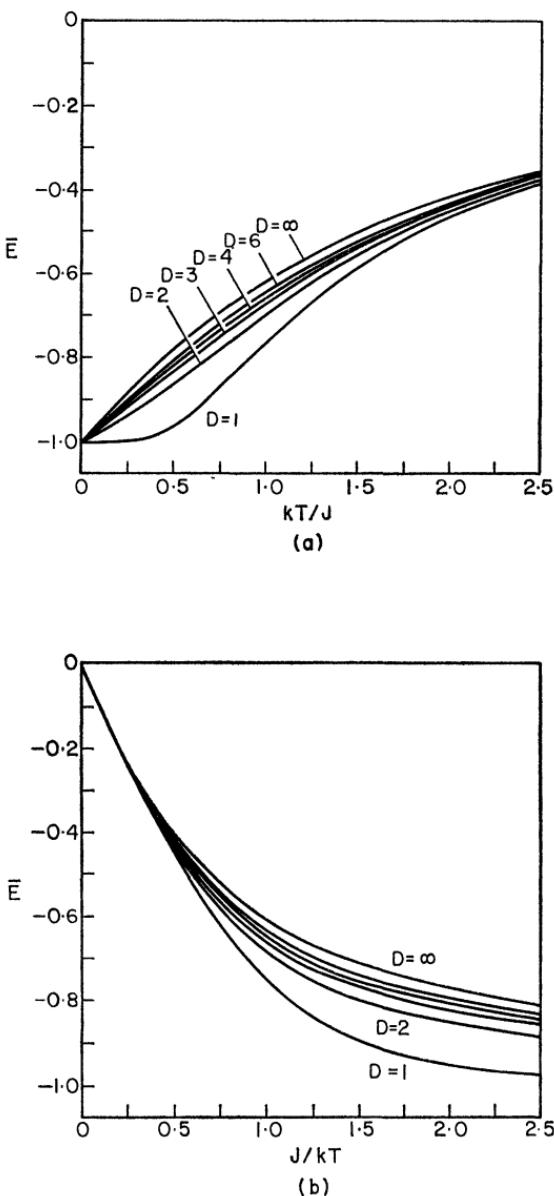


FIG. 8.1. Dependence of the reduced enthalpy upon $1/\mathcal{J}$ and \mathcal{J} for various values of D for the linear chain lattice. Since E is proportional to the nearest-neighbour correlation function and the arbitrary- r correlation function is just r th power of the nearest-neighbour correlation function, we see here graphically the fact (Milošević *et al.*, 1970) that the correlation function is monotonic decreasing in D for fixed T .

are listed in Table 8.2. Generally the series coefficients A_l in the expansion (8.4) are smoother as a function of order l than the expansion coefficients a_l in (8.3), as first noted for $D = 3$ by Stanley (1967c). However, this is not necessarily always the case, and the prospective worker is urged to utilise both sets of coefficients in an effort to ascertain some measure of confidence limits.

TABLE 8.2. Reversion formula for obtaining the coefficients a_l in

$$\bar{\chi} = 1 + \sum_{l=1}^{\infty} a_l J^l$$

given the coefficients A_l in

$$\bar{\chi} = 1 + \sum_{l=1}^{\infty} A_l [f(J)]^l,$$

where here $f(J) = y_D = 1 + Q_1 J^2 + Q_2 J^4 + Q_3 J^6 + Q_4 J^8 + \dots$ and the Q_j are defined in Table 7.1.

$$a_1 = A_1$$

$$a_2 = A_2$$

$$a_3 = A_3 + Q_1 A_1$$

$$a_4 = A_4 + 2Q_1 A_2$$

$$a_5 = A_5 + 3Q_1 A_3 + Q_2 A_1$$

$$a_6 = A_6 + 4Q_1 A_4 + (Q_1^2 + 2Q_2) A_2$$

$$a_7 = A_7 + 5Q_1 A_5 + (3Q_1^2 + 3Q_2) A_3 + Q_3 A_1$$

$$a_8 = A_8 + 6Q_1 A_6 + (6Q_1^2 + 4Q_2) A_4 + (2Q_1 Q_2 + Q_3) A_2$$

$$a_9 = A_9 + 7Q_1 A_7 + (10Q_1^2 + 5Q_2) A_5 + (3Q_3 + 6Q_1 Q_2 + Q_1^3) A_3 + Q_4 A_1$$

In particular, the fluctuation-dissipation relation requires that the isothermal susceptibility $\bar{\chi}$ be related to the two-spin correlation function $C_2(\mathbf{r})$,

$$\bar{\chi} \propto \sum_{\mathbf{r}} C_2(\mathbf{r}). \quad (8.5)$$

For a linear chain lattice, $C_2(\mathbf{r}) \propto (y_D)^r$ (Stanley, 1969d), and hence the coefficients A_l in (8.4) are all constant. This suggests expanding the susceptibility for a given lattice in terms of the nearest-neighbour correlation function of that particular lattice; this procedure is currently being tested in an effort to obtain smoother series.

Also worthy of mention are those methods in which series are re-expanded in a variable $f(\mathcal{J})$, where $f(\mathcal{J})$, is of the form

$$f(\mathcal{J}) \equiv \frac{A}{1 + B\mathcal{J}}. \quad (8.6)$$

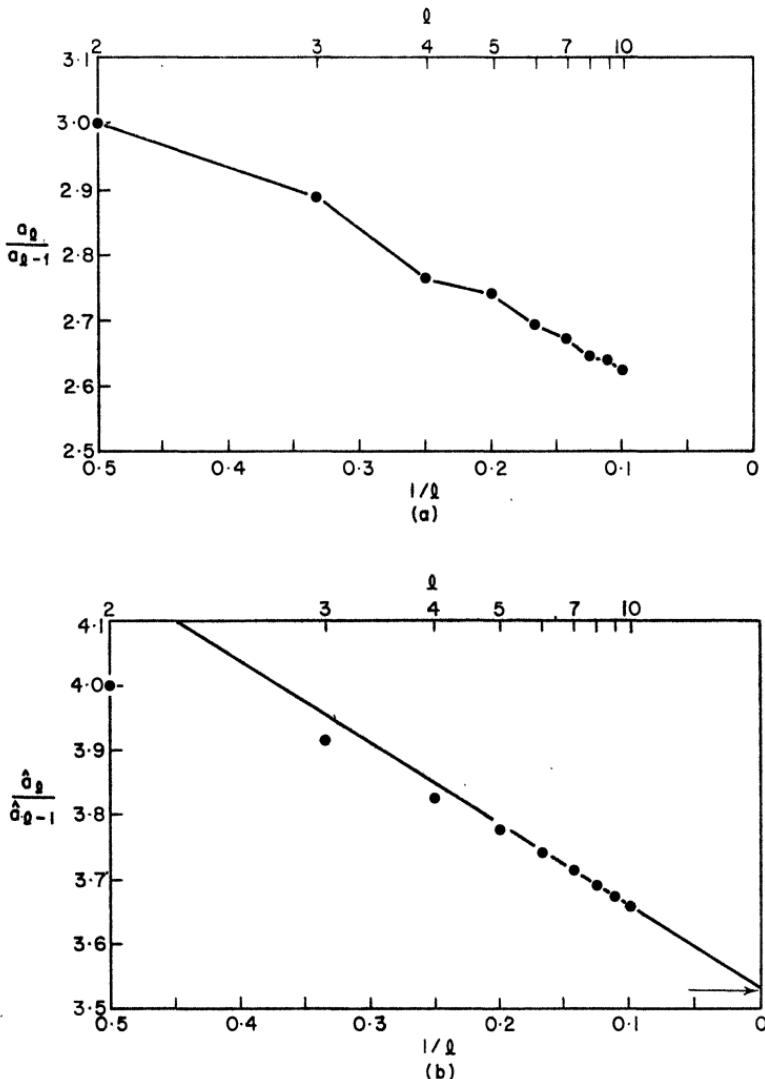


FIG. 8.2. Effect upon ratio plots for the series coefficients of the spin $\frac{1}{2}$ Heisenberg model (b.c.c. lattice) of using the transformation (8.6). Part (a) shows the original susceptibility series coefficients of (8.3), while part (b) shows the coefficients \hat{a}_l when χ is re-expanded in the variable $f(\mathcal{J})$ of (8.6).

Such "Euler transformations" can be chosen in order that the singularities *near* the physical singularity (the singularity on the real $\mathcal{J} \equiv J/kT$ axis closest to the origin $\mathcal{J} = 0$) are moved further away in order that the ratio method [cf. Fig. 8.2] and other methods which are ineffective when two singularities are close together will work (see Guttman, 1969; Lee and Stanley, 1971; Betts, Elliott, and Ditzian, 1971; Stanley, Hankey, and Lee, 1971; the original work of Danielian and Stevens, 1957; Gaunt and Guttman, this volume, Chapter 4).

TABLE 8.3. Coefficients in the series of eqn (8.7) for the susceptibility for general-*D* and general lattice. The symbols used are defined in Tables 8.4. \tilde{A}_9 is for loose-packed lattices only. These expressions generalise those of eqn (13) of Sykes (1961) to all *D* and to higher order.

$$\begin{aligned}\tilde{A}_3 &= -6p_3 \\ \tilde{A}_4 &= -8p_4 - \chi_1 p_3 \\ \tilde{A}_5 &= -10p_5 - (\frac{4}{3})\chi_1 p_4 + \chi_2 p_3 + \chi_3 p_{5a} \\ \tilde{A}_6 &= -12p_6 - (\frac{5}{3})\chi_1 p_5 + \chi_4 p_4 + \chi_5 p_3 + \chi_3(p_{6a} + p_{6b}) \\ &\quad + 8p_{6c} + \chi_6 p_{5a} \\ \tilde{A}_7 &= -14p_7 - 2\chi_1 p_6 + \chi_3(p_{7a} + p_{7b} - p_{7f}) + 8(p_{7d} + p_{7e}) \\ &\quad + (2\chi_4 - \chi_2)p_5 + \chi_7 p_4 + \chi_8 p_3 + \chi_9 p_{7c} + \chi_{10} p_{7g} \\ &\quad + \chi_{11} p_{6a} + \chi_{12} p_{6b} + \chi_{13} p_{6c} + \chi_{14} p_{6d} + \chi_{15} p_{5a} \\ \tilde{A}_8 &= -16p_8 - (\frac{7}{3})\chi_1 p_7 + (3\chi_4 - 2\chi_2)p_6 + \chi_{16} p_5 + \chi_{17} p_4 \\ &\quad + \chi_{18} p_3 + \chi_3(p_{8a} + p_{8b} + p_{8c} + p_{8d}) + \chi_9(p_{8e} + p_{8f} + p_{8g}) \\ &\quad + 8(p_{8g} + p_{8h} + p_{8j} + p_{8k}) + \chi_{19} p_{8l} + \chi_{20} p_{8q} \\ &\quad + \chi_{21}(p_{8r} + p_{8s}) + \chi_{22}(p_{7a} + p_{7b}) + \chi_{23} p_{7c} \\ &\quad + \chi_{24}(p_{7d} + p_{7e}) + \chi_{25} p_{7f} + \chi_{26} p_{7q} + \chi_{27} p_{7h} \\ &\quad + \chi_{28} p_{6a} + \chi_{29} p_{6b} + \chi_{30} p_{6c} + \chi_{31} p_{6d} + \chi_{32} p_{5a} \\ \tilde{A}_9 &= -(\frac{8}{3})\chi_1 p_8 + \chi_{38} p_6 + \chi_{33} p_4 + \chi_3(p_{9k} + p_{9l}) + 8p_{9j} \\ &\quad + \chi_9 p_{9m} + \chi_{25} p_{8c} + \chi_{24} p_{8h} + \chi_{34} p_{8r} \\ &\quad + \chi_{35} p_{8t} + \chi_{36} p_{7a} + \chi_{37} p_{6a}\end{aligned}$$

We could tabulate the general-*D*, general-lattice expressions for the A_i , but the expressions become considerably less cumbersome if we instead tabulate (cf. Tables 8.3–8.4) the coefficients \tilde{A}_i obtained as the coefficients in the series (Sykes, 1961)

$$\chi = (1 - \sigma y_D)^{-2} \left[1 - (\sigma - 1)y_D - \sigma y_D^2 + \sum_{i=3}^{\infty} \tilde{A}_i y_D^i \right], \quad (8.7)$$

where here $\sigma \equiv q - 1$, where *q* is the lattice coordination number. The

TABLE 8.4. Coefficients utilised in Table 8.3 (cf. Fig. 8.2)

| | | |
|--|---|---|
| $\chi_1 = 6[1 + 3Q_1]$ | $\chi_{17} = 8[-10Q_2 + 42Q_1 - 6T_1Q_1^2 + T_1 - 30T_2 - 2T_3 + 2T_5 + 2T_6]$ | $\chi_{32} = 4[T_8 + 14T_6 + 26T_5 - 2T_4 - 2T_3 - 198T_2 + 17T_1 - 75Q_2] - 6Q_1\chi_6$ |
| $\chi_2 = 6[T_1 - 6Q_1]$ | $\chi_{18} = 6[9Q_2 + 7Q_3 + 18T_2 - 8T_5 - 2T_6 + 16T_7 + T_9] - 6Q_1\chi_5 + \chi_1[6Q_1^2 + 4Q_2]$ | $\chi_{33} = 8[10Q_2 + 7Q_3 + 25T_2 + T_3 - 4T_5 - 6T_6 + 24T_7 + 9T_{10} + 5T_{11}] - 7Q_1\chi_7 + (20/3)\chi_1$ |
| $\chi_3 = 12[1 + Q_1]$ | $\chi_{19} = -24Q_1$ | $\chi_{34} = 96[3Q_1 - T_1 + 3T_2] \times [2Q_1^2 + Q_2]$ |
| $\chi_4 = 8[T_1 - 6Q_1]$ | $\chi_{20} = 8[9Q_1 - 4T_1 + T_4]$ | $\chi_{35} = 16[9Q_1 - 4T_1 + T_4]$ |
| $\chi_5 = 6[3Q_1(1 - 4Q_1) + 5Q_2 - 2T_1 + 6T_2]$ | $\chi_{21} = -144Q_1$ | $\chi_{36} = 4[39Q_1 - 21Q_1^2 + 10Q_2 - 18T_1 + 45T_2 + 6T_3 + T_4]$ |
| $\chi_6 = 4[4T_1 - 33Q_1]$ | $\chi_{22} = 16[T_1 - 9Q_1]$ | $\chi_{37} = 24[35Q_1^2 - 7Q_1T_1 - 5Q_2 + 4T_1 - 29T_2 - T_3 - T_4 + 3T_5 + 7T_6]$ |
| $\chi_7 = 8[3Q_1(1 - 5Q_1) + 5Q_2 - 2T_1 + 9T_2 + T_3]$ | $\chi_{23} = 8[24Q_1 - 12T_1 + 9T_2 + T_4]$ | $\chi_{38} = 12[3Q_1 - 21Q_1^2 + 5Q_2 - 2T_1 + 15T_2 + T_3]$ |
| $\chi_8 = 6[Q_1(33Q_1 - 5T_1) - 10Q_2 + T_1]$ | $\chi_{24} = -48Q_1$ | |
| $\chi_9 = 8[T_1 - 6Q_1]$ | $\chi_{25} = 24[T_1 - 5Q_1]$ | |
| $\chi_{10} = -132Q_1$ | $\chi_{26} = 24[13Q_1 + 5Q_2 - 3T_1 + 9T_2]$ | |
| $\chi_{11} = 24[T_1 - 5Q_1]$ | $\chi_{27} = 2.5\chi_{20}$ | |
| $\chi_{12} = 2[8T_1 - 69Q_1]$ | $\chi_{28} = 12[10Q_1 - 6Q_1^2 - 9T_1 + 6T_2 + T_4]$ | |
| $\chi_{13} = -48Q_1$ | $\chi_{29} = 2[75Q_1 - 36Q_1^2 + 20Q_2 - 38T_1 + 75T_2 + 6T_3 + 2T_4]$ | |
| $\chi_{14} = 8[27Q_1 - 12T_1 + 3T_4]$ | $\chi_{30} = 8[6Q_1 - 2T_1 + 9T_2]$ | |
| $\chi_{15} = 4[3Q_1(12 - 5Q_1) + 10Q_2 - 19T_1 + 30T_2 + T_4]$ | $\chi_{31} = 48[5T_1 - 9T_2 - 3T_4 + T_8]$ | |

reader will observe that the new coefficients \tilde{A}_l are related to the old coefficients A_l by means of the simple recursion relation

$$\tilde{A}_l = A_l - 2\sigma A_{l-1} + \sigma^2 A_{l-2}. \quad (8.8)$$

From Table 8.3, we see that for a Bethe lattice (a lattice with constant coordination number q but with no polygons), $\tilde{A}_l = 0$ for $l \geq 3$ and eqn (8.8) reduces to the result of the Bethe-Peierls approximation (Bethe, 1935; Peierls, 1936),

$$\bar{\chi}^{BP} = \frac{1 + y_D}{1 - \sigma y_D}. \quad (8.9)$$

Thus the Bethe-Peierls "approximation" (8.9) is exact for lattices with no closed circuits, though real multiply-connected crystal structures contain many closed circuits and the coefficients \tilde{A}_l are by no means zero. Including terms in the high-temperature expansion (8.7) beyond order $l = 2$ therefore corresponds in some sense to taking account of the multiple connectivity of the lattice, and one might intuitively expect that extrapolations based upon high-temperature expansions carried beyond second order to be more realistic than the Bethe-Peierls approximation.

For the convenience of the reader, we have summarised the process of obtaining the general- D , general lattice expressions in Fig. 8.3.

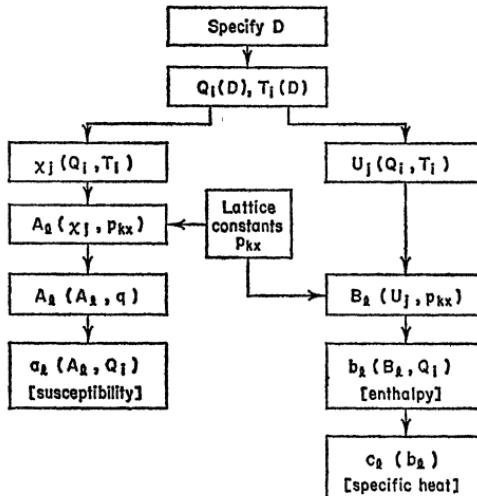


FIG. 8.3. Simple "flow chart" to illustrate the method of obtaining general- D and general- d coefficients in the susceptibility series (8.3), the enthalpy series (9.5b), and the specific heat series (9.9).

TABLE 8.5. The susceptibility coefficients $a_l(D)$ in the high-temperature series expansion (8.3) for $D = 1, 2, 3, 4, 5, 8, 10$, and ∞ for $l = 1, 2, 3, \dots, 8$, for an f.c.c. lattice. The coefficient $a_0(D) = 1$ for all D . Accuracy is to at least 10 significant figures. The coefficients for $D = \infty$ are all integers.

| l | $D = 1$ | $D = 2$ | $D = 3$ | $D = 4$ | $D = 5$ | $D = 8$ | $D = 10$ | $D = \infty$ |
|-----|----------------|----------------|----------------|----------------|----------------|----------------|----------------|--------------|
| 1 | 12·0000 | 12·0000 | 12·0000 | 12·0000 | 12·0000 | 12·0000 | 12·0000 | 12 |
| 2 | 132·0000 | 132·0000 | 132·0000 | 132·0000 | 132·0000 | 132·0000 | 132·0000 | 132 |
| 3 | 1400·0000 | 1393·0000 | 1396·8000 | 1396·0000 | 1395·4286 | 1394·4000 | 1394·0000 | 1392 |
| 4 | 14564·0000 | 14496·0000 | 14455·2000 | 14428·000 | 14408·5714 | 14373·6000 | 14360·0000 | 14292 |
| 5 | 149713·6000 | 148294·0000 | 147439·1314 | 146868·0000 | 146459·4830 | 145723·0400 | 145436·2857 | 144000 |
| 6 | 1526845·8667 | 1503063·0000 | 1488691·2000 | 1479070·6667 | 1472180·8930 | 1459744·8000 | 1454897·6667 | 1430592 |
| 7 | 15483628·9524 | 15132379·2500 | 14919610·8617 | 14777003·4667 | 14674800·8934 | 14490203·7349 | 14418224·9345 | 14057280 |
| 8 | 156350472·4190 | 151568185·1725 | 148668067·0064 | 146723406·6784 | 145329514·7610 | 142811981·2020 | 141830361·3561 | 136914804 |

TABLE 8.6. The susceptibility coefficients $a_l(D)$ in the expansion (8.3) for $l = 1, 2, 3, \dots, 9$ for a b.c.c. lattice. Here $a_0(D) = 1$ for all D .

| l | $D = 1$ | $D = 2$ | $D = 3$ | $D = 4$ | $D = 5$ | $D = 8$ | $D = 10$ | $D = \infty$ |
|-----|------------|---------------|---------------|----------------|---------------|---------------|---------------|--------------|
| 1 | 8·0000 | 8·0000 | 8·0000 | 8·0000 | 8·0000 | 8·0000 | 8·0000 | 8 |
| 2 | 56·0000 | 56·0000 | 56·0000 | 56·0000 | 56·0000 | 56·0000 | 56·0000 | 56 |
| 3 | 389·3333 | 388·0000 | 387·2000 | 386·6667 | 386·2857 | 385·6000 | 385·3333 | 384 |
| 4 | 2610·6667 | 2592·0000 | 2580·8000 | 2573·3333 | 2568·0000 | 2558·4000 | 2554·6667 | 2536 |
| 5 | 17473·0667 | 17230·6667 | 17085·7143 | 16989·3333 | 16920·6349 | 16797·3333 | 16749·5238 | 16512 |
| 6 | 15250·4889 | 112843·3333 | 111399·6800 | 110438·2222 | 109752·2358 | 108519·7867 | 108041·5556 | 105664 |
| 7 | 59545·7016 | 736900·1667 | 723335·8263 | 714311·6444 | 707878·7634 | 696336·1859 | 691863·3849 | 669696 |
| 8 | 66694·5778 | 4773834·3333 | 4658268·0046 | 4581382·5778 | 4526582·3918 | 4228289·2587 | 4390219·3254 | 4201832 |
| 9 | 58605·2120 | 30866012·1052 | 29914360·3665 | 292282502·1141 | 28832837·3041 | 28027927·8499 | 27716812·5397 | 26183808 |

The coefficients A_l were first given for $D = 1$ (to lower order) as eqn (13) of Sykes (1961); subsequently they were published to the present order for $D = 3$ (Table I of Stanley, 1967c), for $D = 2$ (Table I of Stanley, 1968a), and for $D = \infty$ (Table I of Stanley, 1969c).

B. Numerical values for the f.c.c. and b.c.c. lattices

In Tables 8.5 and 8.6 we list the numerical coefficients a_l of eqn (8.3) for the f.c.c. and b.c.c. lattices, respectively. We give the values for $D = 1, 2, 3, 4, 5, 8, 10, \infty$; the reader should note that the coefficients vary monotonically with D . An analysis of these series shows that the susceptibility exponent γ is independent of lattice, and varies with spin dimensionality D in a smooth and monotonic fashion conveniently summarised by the handy mnemonic formula (Stanley and Betts, 1973)

$$\gamma(D, d=3) \cong \frac{8+2D}{7+D}. \quad (8.10)$$

We can write this as

$$\gamma(D) = \gamma(\infty)R_\gamma(D), \quad (8.11a)$$

where $\gamma(\infty) = 2$, the spherical model value, and the “renormalisation function” $R_\gamma(D)$ is

$$R_\gamma(D) \cong \frac{4+D}{7+D}. \quad (8.11b)$$

IX. Calculation of the Coefficients in the Zero Field Enthalpy and Specific Heat Series

A. General- D , general-lattice expressions

In this section we consider the zero-field specific heat, which is related to the entropy S , the magnetic enthalpy E , and the Gibbs potential G by the relation [cf. eqn (2.48) of Stanley (1971a)]

$$C_H(T, H) = T \left(\frac{\partial S}{\partial T} \right)_H = \left(\frac{\partial E}{\partial T} \right)_H = -T \left(\frac{\partial^2 G}{\partial T^2} \right)_H. \quad (9.1)$$

Combining (9.1) with (7.1a), we have

$$E(T, H=0) = -\frac{\partial}{\partial \beta} \{\ln Z(T, H=0)\}. \quad (9.2)$$

Finally, on using (7.3a),

$$E(T, H=0) = -\sum_{l=1}^{\infty} \frac{l \lambda_l \beta^{l-1}}{l!}. \quad (9.3)$$

Thus one can obtain the coefficients in the enthalpy series and hence, by differentiation [cf. (9.1)], in the specific heat series.

As with the susceptibility series, it is convenient to expand in the variable y_D , the nearest-neighbour correlation function of a linear chain ($D = 1$) lattice, for which the enthalpy is simply

$$E(T, H = 0) = -Jy_D. \quad (9.4)$$

Consequently we have used the recursion relation of Table 8.2 together with our general lattice expressions for the enthalpy to obtain the simpler coefficients B_l in the expansion

$$E(T, H = 0) = \frac{-J}{2y_0} \sum_{l=2}^{\infty} B_l y_D^l. \quad (9.5a)$$

These coefficients B_l are listed in Tables 9.1 and 9.2. Note that the expressions in Table 9.1 generalise from $D = 1$ to all D and to higher order eqn (14) of Sykes (1961), who defines $U(\tanh \mathcal{J})$ to be the enthalpy divided by $-J$, $v \equiv \mathcal{J} = y_1$, so that (9.5) takes the form $(2y_1)U(y_1) = \sum_l B_l y_1^l$, with $U(T = 0) = q/2$. Thus an immediate partial check on Table 9.1 is

TABLE 9.1. Coefficients in eqn (9.5a) for the internal energy. Here q is the lattice coordination number, and the rest of the symbols are defined in Tables 8.1–8.4. and 9.2. B_{10} is for loose-packed lattices only. These expressions generalise those of eqn (14) of Sykes (1961) to all D and to higher order.

| |
|---|
| $B_2 = q$ |
| $B_3 = 6p_3$ |
| $B_4 = 8p_4$ |
| $B_5 = 10p_5 + 18Q_1p_3$ |
| $B_6 = 12p_6 + 24Q_1p_4 + 6T_1p_3 + 36Q_1p_{5a}$ |
| $B_7 = 14p_7 + 30Q_1p_5 + U_1p_3 + 84Q_1p_{7g} + 42Q_1p_{6b} + 28T_1p_{5a}$ |
| $B_8 = 16p_8 + 36Q_1p_6 + U_2p_4 + U_3p_3 + 96Q_1(p_{8r} + p_{8s})$ |
| $+ 48Q_1(p_{7a} + p_{7b}) + 32T_1p_{7c} + 48T_4p_{6d}$ |
| $+ 16T_1(3p_{6a} + p_{6b}) + U_4p_{5a}$ |
| $B_9 = 18p_9 + U_5p_7 + U_6p_5 + U_7p_3 + U_8(p_{9e} + p_{9f} + p_{9h})$ |
| $+ U_9p_{9g} + U_{10}(p_{8a} + p_{8b}) + U_{11}(p_{8e} + p_{8p} + p_{7f})$ |
| $+ U_{12}(p_{8q} + p_{7h}) + U_{13}p_{7b} + U_{14}p_{7c} + U_{15}p_{7g}$ |
| $+ U_{16}p_{6b} + U_{17}p_{6d} + U_{18}p_{5a}$ |
| $B_{10} = 20p_{10} + U_{19}p_8 + U_{20}p_6 + U_{21}p_4 + U_{22}(p_{10b} + p_{10c})$ |
| $+ U_{23}p_{9k} + U_{24}(p_{9m} + p_{8c}) + U_{25}p_{8t}$ |
| $+ U_{26}p_{8r} + U_{27}p_{7a} + U_{28}p_{6a}$ |

TABLE 9.2. The quantities U_j utilised in Table 9.1 (cf. the flow chart of Fig. 8.3.).

| | |
|---|---|
| $U_1 = 6[5Q_2 + 7T_2 - 13Q_1^2]$ | $U_{15} = 72[9T_2 + 5Q_2 - 7Q_1^2]$ |
| $U_2 = 8[-18Q_1^2 + 5Q_2 + 12T_2 + T_3]$ | $U_{16} = 18[5Q_2 + T_3 + 15T_2 - 14Q_1^2]$ |
| $U_3 = 6[4T_5 - 5Q_1T_1]$ | $U_{17} = 72T_8$ |
| $U_4 = 4[20Q_2 - 45Q_1^2 + 48T_2]$ | $U_{18} = 24[6T_5 + 3T_6 - 7T_1Q_1]$ |
| $U_5 = 42Q_1$ | $U_{19} = 48Q_1$ |
| $U_6 = 10[18T_2 + 5Q_2 - 24Q_1^2]$ | $U_{20} = 12[5Q_2 + 25T_2 - 31Q_1^2]$ |
| $U_7 = 6[T_9 + 18T_7 + 60Q_1^3 + 7Q_3 - 44Q_1Q_2$ | $U_{21} = 8[7Q_3 + 30T_7 + 10T_{10} + 5T_{11} - 84T_2Q_1$ |
| $- 42Q_1T_2]$ | $- 56Q_2Q_1 - 7T_3Q_1 + 95Q_1^3]$ |
| $U_8 = 108Q_1$ | $U_{22} = 120Q_1$ |
| $U_9 = 72T_1$ | $U_{23} = 60Q_1$ |
| $U_{10} = 54Q_1$ | $U_{24} = 40T_1$ |
| $U_{11} = 36T_1$ | $U_{25} = 40T_4$ |
| $U_{11} = 36T_1$ | $U_{25} = 40T_4$ |
| $U_{12} = 36T_4$ | $U_{26} = 96[10T_2 + 7Q_1^2]$ |
| $U_{13} = 18T_1$ | $U_{27} = 4[10T_3 + 90T_2 + 25Q_2 - 84Q_1^2]$ |
| $U_{14} = 162T_2$ | $U_{28} = 24[5T_5 + 10T_6 - 14T_1Q_1]$ |

comparison with eqn (14) of Sykes (1961). A second partial check arises if we use the planar model (cf. Table II of Stanley, 1968a) or the spherical model (Stanley 1969c).

By using the recursion relation of Table 8.2 to change variables from y_D to J in eqn (9.5a), we can write

$$E(T, H = 0) = - \frac{1}{2\beta} \sum_{l=2}^{\infty} b_l J^l. \quad (9.5b)$$

Note that the recursion relation of Table 8.2 must be "shifted" by one order since the leading term of the series being transformed is not unity, so that here

$$b_2 = B_2 \quad (9.6a)$$

$$b_3 = B_3 \quad (9.6b)$$

$$b_4 = B_4 + Q_1 B_2 \quad (9.6c)$$

$$b_5 = B_5 + 2Q_1 B_3 \quad (9.6d)$$

and so forth. The reader can easily verify the above relations by consulting Table V of Joyce, Volume 1, Chapter 10, which lists the coefficients b_l (which he denotes ε_n) for the spherical model; the Q_j are given in Table 7.1.

The specific heat is obtained by simply differentiating the enthalpy with respect to temperature [cf. (9.1)]. Since this step often has led to errors and much confusion in the literature, we carry it out in some detail. Writing (9.5b) in the form

$$E(T, 0) = - \frac{J}{2} \sum_{l=1}^{\infty} b_{l+1} J^l, \quad (9.7)$$

and using the fact that $\partial/\partial T = (-J/kT^2)\partial/\partial J$, we have

$$C_H(T, 0) = \left(-\frac{J}{2} \right) \left(\frac{-J}{kT^2} \right) \sum_{l=1}^{\infty} l b_{l+1} J^{l-1}. \quad (9.8)$$

Making (9.8) dimensionless,

$$\begin{aligned} k^{-1} C_H(T, 0) &= \frac{1}{2} \sum_{l=1}^{\infty} l b_{l+1} J^{l+1} \\ &= \frac{1}{2} \sum_{l=2}^{\infty} (l-1) b_l J^l \\ &= \sum_{l=2}^{\infty} c_l J^l, \end{aligned} \quad (9.9)$$

TABLE 9.3. The coefficients $c_l(D)$ in the specific heat expansion (9.9) for $D = 1, 2, 3, 4, 5, 8, 10$, and ∞ through order $l = 9$ for a f.c.c. lattice.

| l | $D = 1$ | $D = 2$ | $D = 3$ | $D = 4$ | $D = 5$ | $D = 8$ | $D = 10$ | $D = \infty$ |
|-----|---------------|---------------|---------------|---------------|---------------|---------------|---------------|--------------|
| 2 | 6·0000 | 6·0000 | 6·0000 | 6·0000 | 6·0000 | 6·0000 | 6·0000 | 6 |
| 3 | 48·0000 | 48·0000 | 48·0000 | 48·0000 | 48·0000 | 48·0000 | 48·0000 | 48 |
| 4 | 390·0000 | 387·0000 | 385·2000 | 384·0000 | 383·1429 | 381·6000 | 381·0000 | 378 |
| 5 | 3200·0000 | 3120·0000 | 3072·0000 | 3040·0000 | 3017·1429 | 2976·0000 | 2960·0000 | 2880 |
| 6 | 26584·0000 | 25300·0000 | 24521·8286 | 2400·0000 | 23625·8503 | 22949·6000 | 22685·7143 | 21360 |
| 7 | 226374·4000 | 209496·0000 | 199215·3600 | 192304·0000 | 187431·7143 | 178362·2400 | 174856·0000 | 157248 |
| 8 | 1971091·3333 | 1771749·8750 | 1650281·7120 | 1568660·8000 | 1510101·9159 | 1404293·8240 | 1363055·7708 | 1157058 |
| 9 | 17428723·8095 | 15223406·6667 | 13883970·9571 | 12986589·8667 | 12344427·6360 | 11188545·9261 | 10739911·1156 | 8520960 |

where the specific heat coefficients c_l are given in terms of the enthalpy coefficients by the simple equation

$$c_l = \left(\frac{l-1}{2} \right) b_l \quad [l \geq 2]. \quad (9.10)$$

Note that (9.9) predicts that the leading term in C_H is $1/T^2$, with a constant coefficient $J^2 q/2k$ that is *independent* of D .

B. Numerical values for the f.c.c. lattice

In Table 9.3, we list for the f.c.c. lattice numerical values for the coefficients of eqn (9.9), obtained by using (9.10) and (9.6) (i.e., Table 9.2). The specific heat coefficients of odd order are zero for the loose-packed lattices, so that the only really useful analysis must be carried out on the f.c.c. lattice. Even the f.c.c. series is less reliable than the corresponding susceptibility series treated in Section VIII.B, so that we can only attach mild confidence limits to the mnemonic formula (Stanley and Betts, 1971).

$$\alpha(D, d = 3) \cong \frac{2 - D}{7 + D}, \quad (9.11)$$

in analogy with (8.10). Written in the form of a renormalised spherical model exponent, (9.11) becomes

$$\alpha(D) = \alpha(\infty) R_\alpha(D), \quad (9.12a)$$

where $\alpha(\infty) = -1$, the spherical model value, and

$$R_\alpha(D) \cong \frac{-2 + D}{7 + D}. \quad (9.12b)$$

Using (8.10) and (9.11), and the thermodynamic scaling hypothesis for the Gibbs potential (Hankey and Stanley, 1972 and references contained therein), it is possible to write a similar mnemonic formula for the critical-point exponents for all other thermodynamic functions; in particular, one finds that

$$\delta(D, d = 3) = 5, \quad (9.13)$$

independent of spin dimensionality D ; these arguments will be amplified below in Section X.

X. Dependence of Exponents upon D for $d = 3$: A Bilinear Form Hypothesis

A. Definition of the bilinear form hypothesis

We have argued in the preceding sections that exponents for most physical systems depend principally upon the parameters spin dimensionality D and lattice dimensionality d . In this section we systematically study the estimates that exist for various values of D for the special case $d = 3$. In Sections XI and XII we shall consider successively the cases $d = 2$ and $d = 1$, while in Sections XIII and XIV we consider $d > 3$.

In this section we direct our attention to the dependence of each $d = 3$ critical point exponent λ upon the only parameter left—the spin space dimensionality D . It is convenient to express the variation of λ with D in terms of the spherical model value $\lambda(\infty) = \lambda_{SM}$ as

$$\lambda(D) = \lambda(\infty)R_\lambda(D) \quad (10.1)$$

where $R_\lambda(D)$ is a “renormalisation factor”. It is our object to guess whether there might be a common form of the renormalisation factor for all exponents λ (Stanley and Betts, 1971).

Criteria governing our guess of a plausible form for $R_\lambda(D)$ include the following:

- (1) $R_\lambda(D)$ should vary monotonically with D [Stanley, 1968b].
- (2) $R_\lambda(D)$ might be a rational fraction for all D , since for those cases where exponents are known exactly they are invariably rational fractions. Thus we write $R_\lambda(D) = P_\lambda(D)/Q_\lambda(D)$.
- (3) $P_\lambda(D)$ and $Q_\lambda(D)$ should be of the same functional form, the reason being that it is arbitrary whether one defines an index or its inverse (e.g., $H \sim M^\delta$ or $M \sim H^{1/\delta}$).

The simplest function satisfying these criteria is the *bilinear form*

$$R_\lambda(D) = (b_\lambda + D)/(c_\lambda + D). \quad (10.2)$$

The assumption that for each critical-point exponent λ it is possible to find a pair of numbers b_λ, c_λ such that eqns (10.1) and (10.2) are satisfied we call the *bilinear form hypothesis*. The reader can easily verify by differentiation that (10.2) guarantees that each exponent will be a monotonic function of D , so that criterion (1) is satisfied; criteria (2) and (3) are also clearly satisfied.

B. Numerical evidence favouring the approximate validity of the bilinear hypothesis

Estimates for testing the bilinear form hypothesis are assembled in Table 10.1.

TABLE 10.1. Test of the bilinear form hypothesis. For each critical point exponent λ we show the value calculated from series expansions for various values of spin quantum number s ; for the spherical model ($D = \infty$) we give the exact value. Also shown are the coefficients b_λ , c_λ and the predictions obtained from the bilinear form hypothesis of eqns (10.1) and (10.2). We obtain the same expressions if we use either of two procedures: (i) We choose those values of b_λ and c_λ that lead to an expression that fits most closely with the series expansion data for all D (for $s = \infty$, exponents were calculated for $D = 1, 2, 3, \dots, 49, 50, 100, \dots$, so that the values shown here are only representative), and (ii) if we assume $\delta = 5$, $\gamma(D) = 2(4 + D)/(7 + D)$, and the validity of the static scaling hypothesis. Exponents are defined in Stanley (1971a).

| δ | $b = c$ | b_λ | c_λ | s | $D = 1^r$ | $D = 2$ | $D = 3^s$ | $D = 5$ | $D = 8$ | $D = \infty$ |
|----------|---------|-------------|---------------|-----------------------|---------------------|-------------------|---------------------|-----------------|---------------|----------------|
| γ | 4 | 7 | $\frac{5}{4}$ | 5 | 5.00 ± 0.05^a | — | 5.0 ± 0.1^b | 5 | 5 | 5 |
| | | | | 1 | 5.02 ± 0.13^c | — | — | — | — | — |
| | | | | ∞ | — | — | — | — | — | 5^d |
| Δ | 4 | 7 | $\frac{2}{3}$ | 1.2500 ± 0.0001^e | 1.33 ± 0.02^f | $\frac{7}{3}$ | $\frac{3}{2}$ | $\frac{8}{5}$ | 2 | 2 |
| | | | | 0 | 1.23 ± 0.02^h | 1.32 ± 0.02^i | 1.405 ± 0.02^j | — | — | — |
| | | | | ∞ | — | 1.38 ± 0.02 | 1.50 ± 0.02 | 1.60 ± 0.03 | 2^d | — |
| α | -2 | 7 | $\frac{1}{8}$ | $\frac{2}{6}$ | $\frac{5}{3}$ | $\frac{7}{4}$ | $\frac{25}{8}$ | 2 | $\frac{5}{2}$ | $\frac{5}{2}$ |
| | | | | 0 | 1.563 ± 0.003^k | 1.66 ± 0.05^l | 1.815 ± 0.015^g | — | — | — |
| | | | | ∞ | — | — | 1.73 ± 0.10^m | — | — | $\frac{5d}{2}$ |
| α | -2 | 7 | $\frac{1}{2}$ | 0.125^n | 0 | $-\frac{1}{10}$ | $-\frac{1}{4}$ | $-\frac{6}{15}$ | -1 | -1 |
| | | | | ∞ | — | — | — | — | — | — |

| | | | | | | | |
|---------|---------------|----------|-----------------|-------------------------------|---------------|--------------------------------|-----------------|
| β | 4 | 7 | $\frac{5}{16}$ | $\frac{1}{2} 0.311 \pm 0.008$ | $\frac{1}{3}$ | $\frac{7}{20} 0.35 \pm 0.05^p$ | $\frac{3}{8}$ |
| | | ∞ | — | — | 0 | $-\frac{2}{3}\frac{2}{5}$ | $-\frac{2}{15}$ |
| ϕ | -2 | 4 | $\frac{2}{5}$ | | | $\frac{2}{3}\frac{2}{5}$ | $\frac{2}{5}$ |
| ψ | $\frac{5}{2}$ | 4 | $\frac{14}{26}$ | | $\frac{3}{5}$ | $\frac{3}{5}$ | $\frac{4}{5}$ |
| a_x | 7 | 4 | $\frac{8}{15}$ | | $\frac{1}{2}$ | $\frac{1}{2}\frac{1}{1}$ | $\frac{1}{3}$ |
| a_H | | | $b = c$ | | $\frac{5}{6}$ | $\frac{5}{6}$ | $\frac{5}{6}$ |

- ^a Gaunt, and Sykes (1972)
^b Baker, Eve and Rushbrooke. (1970)
^c Fox and Gaunt (1970)
^d Berlin and Kac (1952); Joyce (1972)
^e Domb and Sykes (1957); Leu, Betts and Elliott (1969);
 Essam and Hunter (1968), Gaunt and Baker (1970)
^f Betts, Elliott and Lee (1970)
^g Baker, Gilbert, Eve and Rushbrooke (1967)
^h Jasnow and Wortis (1968); Ferer, Moore and Wortis
 (1971)
ⁱ Bowers and Joyce (1967)
^j Ferer, Moore and Wortis (1971)
^k Essam and Hunter (1968)
^l Ditzian and Betts (1970)
^m Stephenson and Wood (1968)
ⁿ Sykes, Martin and Hunter (1967)
^p Domb and Bowers (1969); Stanley (1969a)
^q Stephenson and Wood (1970)
^r For Ising critical exponents see also Domb, this
 volume, Chapter 6
^s For Heisenberg critical exponents see also Rushbrooke
 et al, this volume, Chapter 5

The first exponent in Table 10.1 is the index $\delta(M \sim H^{1/\delta}, T = T_c)$. For the spherical model, $\delta = 5$, for the spin $\frac{1}{2}$ Ising model, $\delta = 5.00 \pm 0.05$ (Gaunt and Sykes 1972), and for the Heisenberg model, $\delta = 5.00 \pm 0.20$ (Baker, Eve and Rushbrooke, 1970; Stephenson and Wood, 1970). Recently, theoretical support has been given to the hypothesis that $\delta(D) = 5$ for all D ; this suggestion was first put forward by Gunton and Buckingham (1968) and was taken up by Domb (1969); an attempt to give a theoretical justification has been made by Brout (1971). If this proves correct it follows from (10.1) and (10.2) that $R_\delta(D) = 1$ [or $b_\delta = c_\delta$].

The second through fifth rows of Table 10.1 consider the dependence of the exponents γ , Δ , α , and β upon D . Here these exponents are defined by the relations $\chi_T \sim (\tau)^{-\gamma}$, $G^{(n)}/G^{(n-2)} \sim (\tau)^{-\Delta}$, $C_H \sim (\tau)^{-\alpha}$, and $M \sim (-\tau)^\beta$ where χ_T , G , C_H , and M denote, respectively, the isothermal zero-field susceptibility, the Gibbs potential, the constant field specific heat, and the zero field magnetisation. We have proceeded to calculate γ and α for $s = \infty$ for $D = 4, 5, 6, \dots, 9, 10, 20, \dots, \dots$; for the sake of economy, we display the values only for $D = 5$ and 8 in Table 10.1. The estimates are remarkably well fit by the simple bilinear forms

$$\gamma(D) = \gamma(\infty)(4 + D)/(7 + D) \quad (10.3)$$

where $\gamma(\infty) = 2$,

$$\Delta(D) = \Delta(\infty)(4 + D)/(7 + D) \quad (10.4)$$

where $\Delta(\infty) = \frac{1}{2}$,

$$\alpha(D) = \alpha(\infty)(-2 + D)/(7 + D) \quad (10.5)$$

where $\alpha(\infty) = -1$, and

$$\beta(D) = \beta(\infty)(4 + D)/(7 + D) \quad (10.6)$$

where $\beta(\infty) = \frac{1}{2}$.

Of course we could have "determined" eqns (10.3)–(10.6) by *assuming* the validity of the bilinear form hypothesis (10.2) and then specifying the exponent in question for any two values of D ; thus, e.g., eqn (10.3) could have been obtained from the reliable estimates $\gamma(1) = \frac{5}{6}$ and $\gamma(2) = \frac{4}{3}$, eqn (10.4) from the estimates $\Delta(1) = \frac{2}{16}$ and $\Delta(2) = \frac{1}{3}$, and eqn (10.5) from the estimates $\alpha(1) = \frac{1}{6}$ and $\alpha(2) = 0$ (generally the estimates for critical exponents are more reliable for smaller D). In fact, eqn (10.6) was obtained from the estimates $\beta(1) = \frac{5}{16}$ and $\beta(3) = \frac{7}{20}$.

It is important to emphasise that the estimates of eqns (10.3)–(10.6) are by no means the *only* bilinear forms that are consistent with the data. For

example, the susceptibility exponent $\gamma(D)$ is almost as well fit by the expression

$$\gamma(D) = \gamma(\infty)(21 + 4D)/(36 + 4D). \quad (10.7)$$

Both expressions (10.3) and (10.7) predict that $\gamma(D = 1) = \frac{5}{4}$, while (10.7) predicts the slightly *smaller* values $\gamma(2) = \frac{29}{22} = 1.318$, $\gamma(3) = \frac{11}{8} = 1.375$, $\gamma(5) = \frac{41}{28} = 1.465$, and $\gamma(8) = \frac{53}{34} = 1.557$. These latter numbers are consistently a few percent smaller than our estimates for $\gamma(D)$ with $D = 4, 5, 6, \dots, 50$, but they are more consistent with the values $\gamma(2) \cong 1.32$ and $\gamma(3) \cong 1.38$ that some authors have previously proposed.

C. Connection with the scaling hypothesis for thermodynamic functions

The reader will observe that the “best fit” choices of the numbers b_λ, c_λ (where $\lambda = \delta, \gamma, \Delta, \alpha$, and β) lead to predictions for all the critical point exponents that are consistent with the static scaling hypothesis for thermodynamic functions. Moreover, the answer to the question of why some (but not all) exponents are renormalised by the *same* renormalisation function (e.g., from Table 10.1 or else from eqns (10.3), (10.4) and (10.6) we see that $R_\lambda(D) = (4 + D)/7 + D$ for $\lambda = \gamma, \Delta$, and β) is made clear also through the static scaling hypothesis [cf. (5.1) above]. Equation (5.1) holds for the spherical model ($D = \infty$), with $a_\tau = \frac{1}{3}$ and $a_H = \frac{5}{6}$; in this section we shall *assume* it holds for finite D as well.

All critical point exponents can be expressed directly in terms of the “unknown” scaling parameters a_τ and a_H and the numbers a_τ, a_H may be written in the form

$$a_\tau(D) = a_\tau(\infty)R_\tau(D) \quad [a_\tau(\infty) = \frac{1}{3}] \quad (10.8a)$$

and

$$a_H(D) = a_H(\infty)R_H(D) \quad [a_H(\infty) = \frac{5}{6}], \quad (10.8b)$$

where

$$R_\tau(D) = (7 + D)/(4 + D) \quad (10.9a)$$

and

$$R_H(D) = 1. \quad (10.9b)$$

Since all critical point exponents $\lambda(D)$ are expressible in terms of $a_\tau(D)$ and $a_H(D)$, and since $R_H(D) = 1$, the renormalisation function $R_\lambda(D)$ for each exponent λ can be expressed in terms of $R_\tau(D)$ alone. Thus directly from the definitions $M \sim (\partial G / \partial H)_T$ and $\chi_T \sim (\partial^2 G / \partial H^2)_T$ it follows that

$$R_\beta(D) = R_\gamma(D) = R_\Delta(D) = [R_\tau(D)]^{-1}. \quad (10.10)$$

For $C_H \sim (\partial^2 G / \partial T^2)_H$, we have

$$R_\alpha(D) = 3/R_\tau(D) - 2 \quad (10.11)$$

and

$$R_\phi(D) = 3 - 2R_\tau(D), \quad (10.12)$$

where the exponent ϕ is defined by the relation $C_H(T = T_c, H) \sim H^{-\phi}$. Similarly, we find

$$R_\psi(D) = \frac{3}{2} - \frac{1}{2}R_\tau(D), \quad (10.13)$$

where ψ is defined by $S(T = T_c, H) \sim H^\psi$.

D. Correlation function critical point exponents

Stanley and Betts (1973) have extended the sort of "numerology" described above to include the case of the exponents v , μ that describe the behaviour of the pair correlation function $C_2(T, H, r)$, where v , μ describe the variation of the correlation length as $T \rightarrow T_c$ with $H = 0$ and as $H \rightarrow 0$ with $T = T_c$, respectively. Here the numerical estimates are rather less precise than for the thermodynamic functions, and accordingly a variety of bilinear forms work with varying degrees of accuracy. Stanley and Betts (1971) favour the forms

$$v(D) = v(\infty)[(24 + 6D)/(41 + 6D)], \quad (10.14a)$$

where $v(\infty) = 1$. We then find for η [the $H = 0, T = T_c$ decay of the correlation function]

$$\eta(D) = 1/(21 + 3D) \quad (10.14b)$$

and

$$\mu(D) = \mu(\infty)[(42 + 6D)/(41 + 6D)], \quad (10.14c)$$

Here $\mu(\infty) = 0$, and we have used the scaling laws

$$\gamma = (2 - \eta)v \quad (10.15a)$$

and

$$(\delta - 1)/\delta = (2 - \eta)\mu, \quad (10.15b)$$

which follow from the hypothesis that $C_2(\tau, H, \mathbf{r})$ is a generalised homogeneous function, i.e. that we can find three numbers b_τ , b_H and b_r such that for all positive values of L ,

$$C_2(L^{b_\tau}\tau, L^{b_H}H, L^{b_r}\mathbf{r}) = LC_2(\tau, H, \mathbf{r}). \quad (10.16)$$

XI. Possible Dependencies of Critical Properties Upon D for $d = 2$

A. Calculations for $R \equiv J_z/J_{xy} = 0$

The series extrapolation methods that produce such regular and plausible results for $d = 3$ lattices produce some curious questions when applied to $d = 2$ lattices.

To begin with, the earliest spin-wave arguments showed that for the Heisenberg model (including the classical Heisenberg model) there could exist no zero field magnetisation at non-zero temperature. In 1966, Stanley and Kaplan (1966b) showed that the spin-wave arguments were far from rigorous and, as others had pointed out, the limited number of terms available in the high-temperature series expansion for the case $D = 3$ suggest that the zero field susceptibility diverges at a non-zero temperature—in fact, a temperature that was on the order of *half* the critical temperature predicted on the basis of the unrealistic mean-field theory (cf. Fig. 2.4 for $D = 1$). Since there existed other heuristic arguments—in addition to the spin-wave argument—precluding a spontaneous magnetisation for $T > 0$ in the Heisenberg model, Stanley and Kaplan suggested that perhaps there was a non-zero temperature at which the susceptibility diverged *but below which the spontaneous magnetisation remained zero*.

A few months after their suggestion, Mermin and Wagner (1966) proved rigorously that $M = 0$ for all $T > 0$. Thus either the unusual susceptibility divergence was an “artifact” of the series extrapolation procedures (due, presumably, to the series being too short) or else there was indeed a transition to a new type of “quasi-ordered phase”—one with sufficient *long-range order* that the susceptibility, given by

$$\bar{\chi} \propto \sum_r C_2(r), \quad (11.1)$$

diverged, but one without *infinite range order* so that the magnetisation, defined by

$$M^2 \propto \lim_{|r| \rightarrow \infty} C_2(r), \quad (11.2)$$

remained zero.

For example, if $C_2(r)$ varied as

$$C_2(r) \sim \frac{1}{|r|^{\lambda T}}, \quad (11.3)$$

then for small λT ($\lambda T < 2$), (11.1) would be infinite for a two-dimensional lattice, while (11.2) would be zero for all non-zero T . Dyson (unpublished

TABLE 11.1 The susceptibility coefficients $a_i(D)$ in the expansion (8.3) for the plane triangular lattice. The coefficient $a_0(D) = 1$ for all D .

| i | $D = 1$ | $D = 2$ | $D = 3$ | $D = 4$ | $D = 5$ | $D = 6$ | $D = 7$ | $D = 8$ | $D = 9$ | $D = \infty$ |
|-----|-------------|-------------|------------|------------|------------|------------|------------|------------|------------|--------------|
| 1 | 6·0000 | 6·0000 | 6·0000 | 6·0000 | 6·0000 | 6·0000 | 6·0000 | 6·0000 | 6·0000 | 6 |
| 2 | 30·0000 | 30·000 | 30·0000 | 30·0000 | 30·0000 | 30·0000 | 30·0000 | 30·0000 | 30·0000 | 30 |
| 3 | 135·0000 | 136·0000 | 134·4000 | 134·0000 | 133·7143 | 133·2000 | 133·0000 | 133·0000 | 133·0000 | 132 |
| 4 | 570·0000 | 586·0000 | 560·4000 | 554·0000 | 549·4286 | 541·2000 | 538·0000 | 538·0000 | 538·0000 | 522 |
| 5 | 2306·0000 | 2448·8000 | 2219·7257 | 2162·0000 | 2120·6803 | 2046·1600 | 2017·1429 | 2017·1429 | 2017·1429 | 1872 |
| 6 | 9041·5000 | 10021·3333 | 8450·1943 | 8055·3333 | 7773·2789 | 7266·3200 | 7069·6905 | 7069·6905 | 7069·6905 | 6096 |
| 7 | 34582·1250 | 40364·8762 | 31131·4560 | 28848·4000 | 27230·0599 | 24352·6834 | 23249·3958 | 23249·3958 | 23249·3958 | 17928 |
| 8 | 129634·1667 | 160627·2952 | 11528·7357 | 99750·2667 | 91515·7884 | 77156·3651 | 71762·8913 | 71762·8913 | 71762·8913 | 46962 |

TABLE 11.2. The specific heat coefficients $c_l(D)$ in the expansion (9.9) for the plane triangular lattice. Note that the specific heat displays no sign of divergent behaviour except for $D = 1$ (the Ising model).

| <i>l</i> | $D = 1$ | $D = 2$ | $D = 3$ | $D = 4$ | $D = 5$ | $D = 6$ | $D = 8$ | $D = 10$ | $D = \infty$ |
|----------|-----------|------------|------------|------------|------------|------------|------------|------------|--------------|
| 2 | 3·0000 | 3·0000 | 3·0000 | 3·0000 | 3·0000 | 3·0000 | 3·0000 | 3·0000 | 3 |
| 3 | 12·0000 | 12·0000 | 12·0000 | 12·0000 | 12·0000 | 12·0000 | 12·0000 | 12·0000 | 12 |
| 4 | 33·0000 | 31·5000 | 30·6000 | 30·0000 | 29·5714 | 28·8000 | 28·5000 | 28·5000 | 27 |
| 5 | 80·0000 | 60·0000 | 48·0000 | 40·0000 | 34·2857 | 24·0000 | 20·0000 | 20·0000 | 0 |
| 6 | 212·0000 | 87·5000 | 11·3143 | -40·0000 | -76·8707 | -143·6000 | -169·6429 | -169·6429 | -300 |
| 7 | 649·6000 | 84·0000 | -253·4400 | -476·0000 | -633·1429 | -910·5600 | -1016·0000 | -1016·0000 | -1512 |
| 8 | 2076·4667 | -106·3125 | -1291·9920 | -2012·2667 | -2484·8108 | -3228·8640 | -3474·8646 | -3474·8646 | -4221 |
| 9 | 6652·9524 | -1256·3333 | -4821·0024 | -6568·5333 | -7453·6274 | -8151·7105 | -8067·3639 | -8067·3639 | -3840 |

work at the 1966 Brandeis Summer Institute) produced a non-rigorous "spin-wave type" argument that predicted just such a dependence as (11.3) at low temperature.

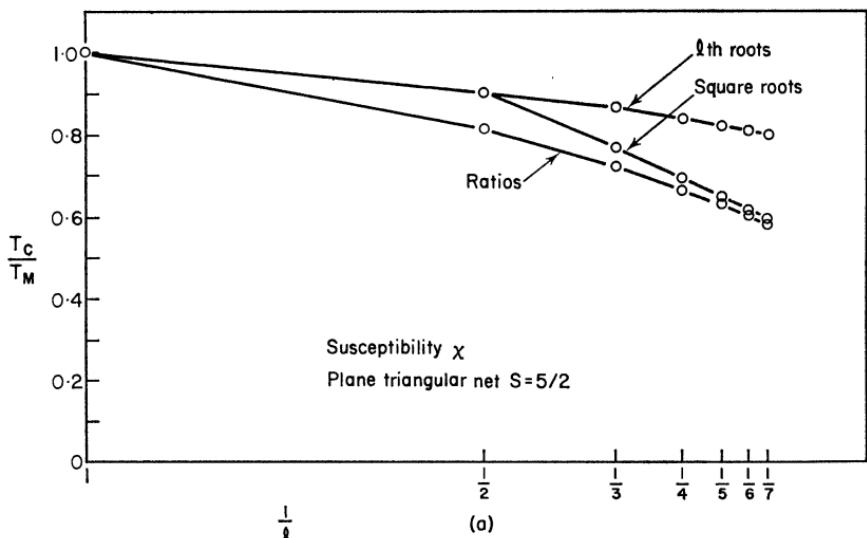
Subsequent work using longer series (Stanley and Kaplan, 1967a, Stanley, 1967a; Moore, 1969; Lambeth and Stanley, 1974) seemed to confirm the proposed susceptibility divergence, thus leaving people with the dilemma that either the very methods that they were comparing with experiment for $d = 3$ lattices were failing for $d = 2$ lattices—or that there was indeed such a peculiar phase transition!

To settle the matter unequivocally by experiment was not possible, for although there existed quasi two-dimensional magnetic materials [e.g., the antiferromagnet K_2NiF referred to in Section VI] for which the series (Stanley, 1969b) also predict a transition, these systems were neither strictly isotropic nor strictly two-dimensional. Thus despite the fact that the careful neutron experiments on K_2NiF_4 of Birgeneau, Guggenheim and Shirane (1969) displayed two-dimensional correlations above a critical temperature that was in rough accord with the series prediction (cf. Fig. 11.1), these results prove nothing about the *isotropic* Hamiltonian (2.1).

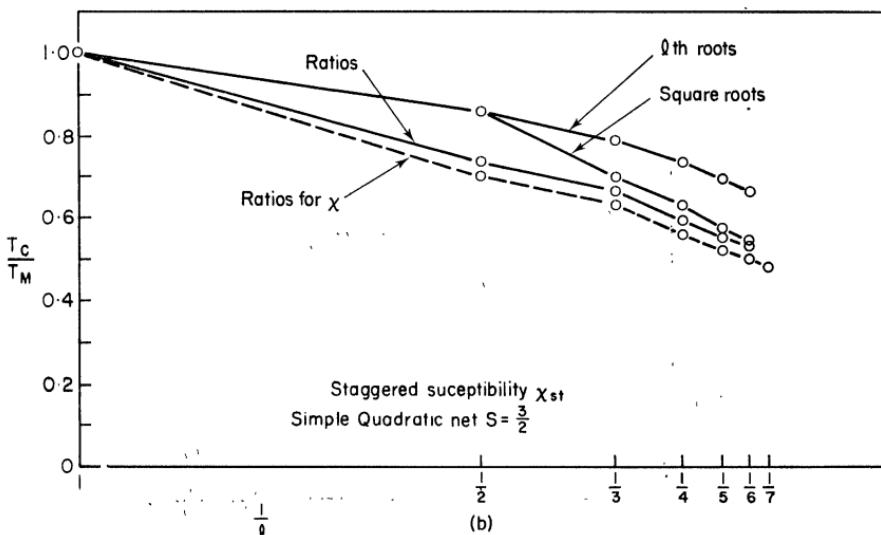
The unusual behaviour was not confined to the Heisenberg model ($D = 3$) (cf. Fig. 11.2). In fact, the evidence in $D = 2$ systems (Stanley, 1968a; Moore, 1969; Betts, Elliott and Ditzian 1971; Lambeth and Stanley, 1974), appeared to some to be more convincing than that for $D = 3$ systems. For several small values of D the series suggest a susceptibility divergence at a non-zero T_c , while for the rigorously-solvable spherical model ($D = \infty$) they *correctly* do not predict a transition; for the $D = 1$ limit they predict *quite accurately* the rigorous Kramers-Wannier transition temperature, and were able to predict the value of the susceptibility exponent $\gamma = \frac{7}{4}$ before this had been established analytically. In fact, these results for $D = 1$ have long been used as evidence of the reliability of extrapolations based upon a limited number of terms in a series expansion.

B. Calculations for arbitrary R

Very recently Lambeth and co-workers (Lambeth and Stanley, 1974; Harbus, Krasnow, Lambeth, Liu and Stanley, 1973) have studied the series for the Hamiltonian (3.2) for $D = 2, 3$. They have obtained a full ten terms for the f.c.c. lattice for general values of the anisotropy parameter $R \equiv J_z/J_{xy}$. Their evidence also appears to favour the existence of a transition in the $R = 0$ limit, though the series are somewhat less regular than the corresponding series for $D = 1$ (Harbus, Krasnow, Liu, and Stanley, 1972; Harbus and Stanley, 1973a; Krasnow, Harbus, Liu and Stanley, 1973). In particular, they find that successive derivatives with respect to R of the susceptibility χ and second moment μ_2 appear to diverge at about the same



(a)



(b)

FIG. 11.1. Comparison between series for (a) the ordinary susceptibility χ (p.t. spin $5/2$) and (b) the staggered susceptibility χ_{st} (sq. spin $3/2$) for two-dimensional lattices. All plots are normalised by dividing by a_1 in order that the intercept at $1/l = 0$ will be the ratio of the critical temperature to the mean-field critical temperature. Here s denotes the spin quantum number. The general spin series for χ and χ_{st} were obtained from Stephenson and Wood (1970) and from Rushbrooke and Wood (1963), respectively.

transition temperature, $T_c/T_M \cong 0.5$. If the Gibbs potential scales in R about $R = 0$ then it follows directly from differentiation of (6.1) that

$$\chi^{(n)}(\lambda^{a_\tau}\tau, \lambda^{a_H}H, \lambda^{a_R}R) = \lambda^{1-2a_H-na_R}\chi^{(n)}(\tau, H, R), \quad (11.4)$$

where here

$$\chi^{(n)}(\tau, H, R) \equiv \left(\frac{\partial^n \chi}{\partial R^n} \right) \equiv \left(\frac{\partial^{n+2} G}{\partial R^n \partial H^2} \right). \quad (11.5)$$

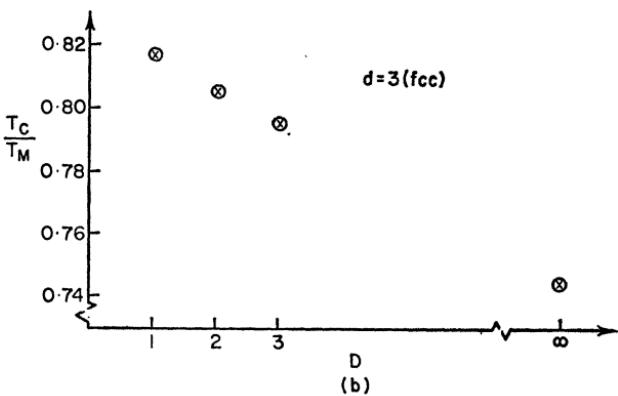
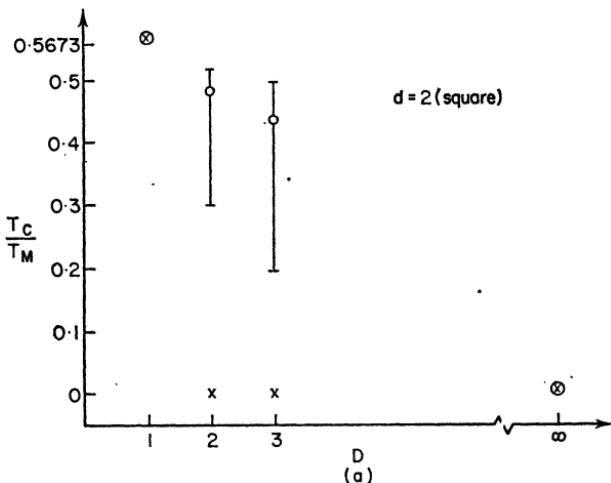


FIG. 11.2. Schematic illustration of the dependence upon D of the temperature " T_c " at which the susceptibility appears to diverge for (a) $d = 2$ (s.q.) and (b) $d = 3$ (f.c.c.) lattices. Shown by crosses are the temperatures below which a non-zero magnetisation exists. The error bars for $d = 2$ are only approximate, and indeed cannot truly exclude the possibility " $T_c = 0$ ".

Setting $H = R = 0$ in eqn (11.4) and choosing λ such that $\lambda^{a_r} = 1$, we have that

$$\chi^{(n)}(\tau, 0, 0) \sim |\tau|^{-\gamma_n} \quad (11.6)$$

with

$$\gamma_n = \gamma_0 + n\phi, \quad (11.7)$$

where

$$\phi \equiv a_R/a_r. \quad (11.8)$$

Liu and Stanley (1972a, b, 1973) have shown rigorously that for all D ,

$$\chi^{(1)} \propto [\chi^{(0)}]^2, \quad (11.9)$$

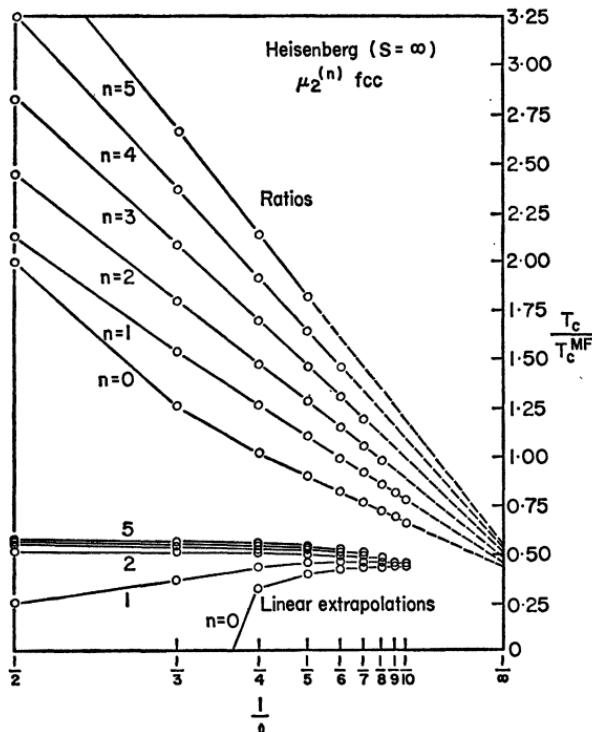


FIG. 11.3. The upper solid lines are the ratio plots $\rho_l^{(n)} = [a_l^{(n)}/a_{l-1}^{(n)}]/a_1^{(0)}$ for the coefficients in the high-temperature series of the function $\mu_2^{(n)}(\tau, H = 0, R)$ defined in analogy to (11.5), where μ_2 is the second moment of the correlation function. Here $kT_c^{MF}/J_{xy} = 4$, the mean field value of the critical temperature for a square lattice. The dashed lines are formed by taking the $l = \infty$ intercept to be the linear extrapolation of the last two ratios. The lower curves are the family of linear extrapolations $l\rho_l^{(n)} - (l-1)\rho_{l-1}^{(n)}$. The curves for $n = 6, 7$ behave similarly. Note that a total of 10 terms were calculated in the general- R series for $D = 1-3$ for the f.c.c. lattice (Lambeth and Stanley, 1974).

so that $\gamma_1 = 2\gamma_0$. Hence from (11.7) for $n = 1$ it follows that $\gamma_1 = \gamma_0 + \phi$ or

$$\phi = \gamma_0, \quad (11.10)$$

and the scaling prediction of (6.1) becomes

$$\gamma_n = (n + 1)\gamma_0. \quad (11.11)$$

[The result (11.11) had been previously obtained only by making the unwarranted assumption that $d\nu = 2 - \alpha$, which is probably not valid for $d = 3$ systems. See Abe (1970) and Suzuki (1971).]

Thus plots of the ratios of successive terms in the series for $\chi^{(n)}(\tau, 0, 0)$ should tend to a constant intercept, $T_c(R = 0)$, with a limiting slope proportional to $\gamma_n = \gamma_0 + n\gamma_0$ (cf. Fig. 11.3)

$$\rho_l^{(n)} \equiv a_l^{(n)}/a_{l-1}^{(n)} = \frac{\gamma_n - 1}{l\mathcal{J}_c} - \frac{1}{\mathcal{J}_c}. \quad (11.12)$$

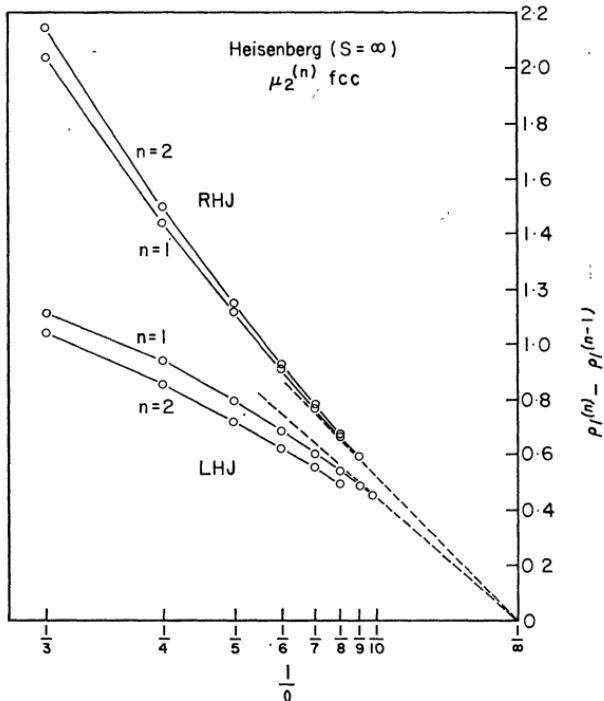


FIG. 11.4. The sequences of (11.13) for the second moment series $\mu_2^{(n)}$. These sequences should approach the origin with limiting slopes γ_0/\mathcal{J}_c , where $\mathcal{J}_c \equiv J_{xy}/kT_c = T_c^{MF}/4T_c$ (Lambeth and Stanley, 1974).

Using (11.11), we note that the sequence

$$\rho_l^{(n)} - \rho_l^{(n-1)} \sim \frac{\gamma_0}{l\mathcal{J}_c} + \mathcal{O}\left(\frac{1}{l^2}\right), \quad (11.13)$$

so that plots of this sequence *vs* $1/l$ should approach the *origin* with a limiting slope of γ_0/\mathcal{J}_c . This prediction is borne out for $D = 1 - 3$ and affords a reliable estimate of the ratio of γ_0 , the two-dimensional susceptibility exponent, to \mathcal{J}_c , *without requiring knowledge of the intercept* (cf. Fig. 11.4 for $D = 3$).

C. Recent rigorous results

The principal recent rigorous results are those Jasnow and Fisher (Jasnow and Fisher, 1969, 1971; Fisher and Jasnow 1971) on finite systems (see Vol. 4) and some arguments of Berezinskii (1971, 1972) which claim to afford a rigorous proof that there is indeed a non-zero transition temperature for $D = 2, 3$. Many authors have questioned the validity of their claim for $D = 3$, but their work for $D = 2$ has withstood the critics rather better and many now believe that $T_c \neq 0$ at least for $D = 2$.

XII. Exact Solution of Zero-Field Thermodynamic Properties and Correlation Functions for all D when $d = 1$ [†]

A. Functions calculated

It is possible to solve exactly for the zero field Gibbs potential and the zero field two spin correlation function $\langle \mathbf{s}_0 \cdot \mathbf{s}_r \rangle$ for the model Hamiltonian (2.1) in the case of a linear chain ($d = 1$) lattice.

The specific thermodynamic functions that have been obtained [and plotted, for $D = 1, 2, 3, 4, 6$, and ∞ , as functions of J/kT and kT/J] are the zero field Gibbs potential (free energy),

$$G(T, H = 0) \equiv -kT \ln Z, \quad (12.1)$$

entropy,

$$S(T, H = 0) \equiv -\left(\frac{\partial G}{\partial T}\right)_H, \quad (12.2)$$

specific heat,

$$C_H(T, H = 0) \equiv T\left(\frac{\partial S}{\partial T}\right)_H, \quad (12.3)$$

magnetic enthalpy,

$$E(T, H = 0) \equiv G + TS = -\frac{\partial}{\partial \beta} (\ln Z), \quad (12.4)$$

[†]See also Thompson, Volume 1, Chapter 5

and susceptibility,

$$\chi(T, H = 0) \propto \sum_r \langle \mathbf{s}_0 \cdot \mathbf{s}_r \rangle. \quad (12.5)$$

The solution has been carried out both for an open chain of N spins (Stanley, 1969b) and for a closed ring [i.e., a linear chain with periodic boundary conditions imposed: $\mathbf{s}_{N+1} = \mathbf{s}_1$] (Stanley, Blume, Matsuno, and Milošević, 1970). The results of the chain and ring problems are, of course, identical in the limit $N \rightarrow \infty$.

The solution itself is rather straightforward [indeed, Ising (1925) had treated the case $D = 1$, Joyce (1967) the case of $D = 2$ for a ring, and Nakamura (1952) and Fisher (1964) the case of $D = 3$], so we shall not repeat the derivation here, but shall instead simply comment upon two interesting features of the solution.

B. Properties of the $d = 1$ solution with implications for $d > 1$

(i) Although the linear chain of D -dimensional classical spins does not display infinite range (or even long-range) order at any temperature except $T = 0$, the detailed plots of the functions obtained reveal graphically that most quantities vary monotonically and smoothly with spin dimensionality D for fixed T . Milošević, Matsuno, and Stanley (1970) in fact proved rigorously that the two-spin correlation function $\langle \mathbf{s}_0 \cdot \mathbf{s}_r \rangle$ was a monotonic function of D ; i.e., for fixed T and r ,

$$\langle \mathbf{s}_0^{(D)} \cdot \mathbf{s}_r^{(D)} \rangle \geq \langle \mathbf{s}_0^{(D+1)} \cdot \mathbf{s}_r^{(D+1)} \rangle. \quad (12.6)$$

In particular the enthalpy, proportional to the nearest-neighbour correlation function, is a monotonic function of D (cf. Fig. 8.1). So also is the entropy—even though the limit $T = 0$ is quite different for $D = 1$ than for the systems with continuous symmetry (cf. Fig. 12.1). This monotonicity does not hold for all functions—e.g. the specific heat and the antiferromagnetic susceptibility (cf. Figs. 12.2 and 12.3, respectively) are monotonic with D only for $D > 1$. For an *antiferromagnet* the correlation function oscillates with site separation vector r , (cf. Fig. 8.7 of Stanley, 1971a) but the monotonicity with D is still true (Milošević *et al.*, 1970) provided one considers the *absolute* values of the correlation function.

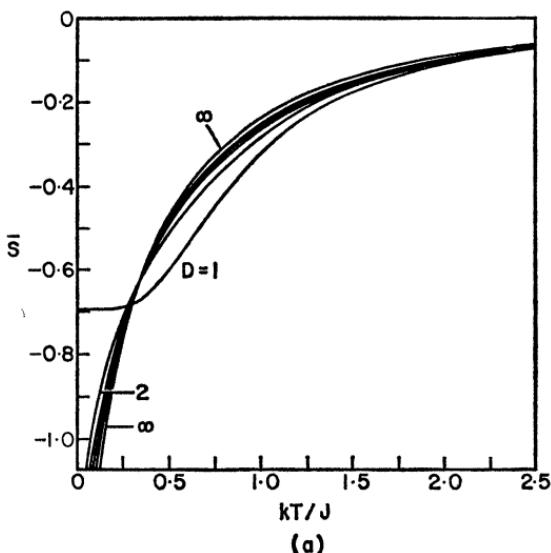
(ii) As D increases without limit, the Gibbs potential and susceptibility approach those obtained for the Berlin-Kac spherical model (Berlin and Kac, 1952),

$$\mathcal{H}_{SM} = -J \sum_{i=1}^{N-1} \mu_i \mu_{i+1}, \quad (12.7a)$$

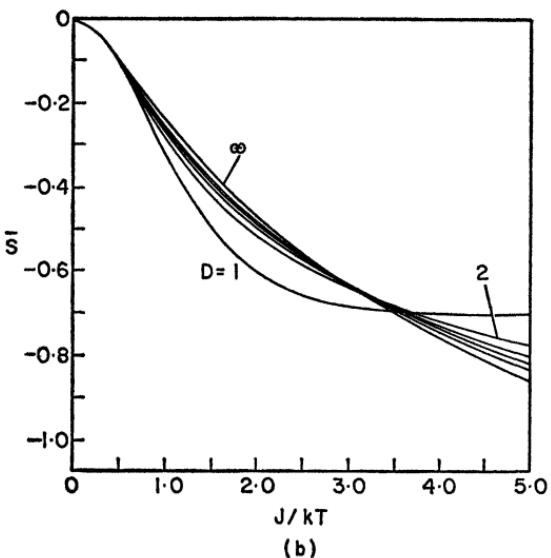
where here the "spins" μ_i are not discrete but rather are continuous variables subject only to the single constraint

$$\sum_{i=1}^N \mu_i^2 = N, \quad (12.7b)$$

and N is the total number of particles in the system (cf. Fig. 2.2 for $N = 2$).



(a)



(b)

FIG. 12.1. Temperature dependence of the reduced entropy for the linear chain lattice.

Properties (i) and (ii) of the one-dimensional lattice are of interest principally because they appear to be reflected in features of the system for higher lattice dimensionality.

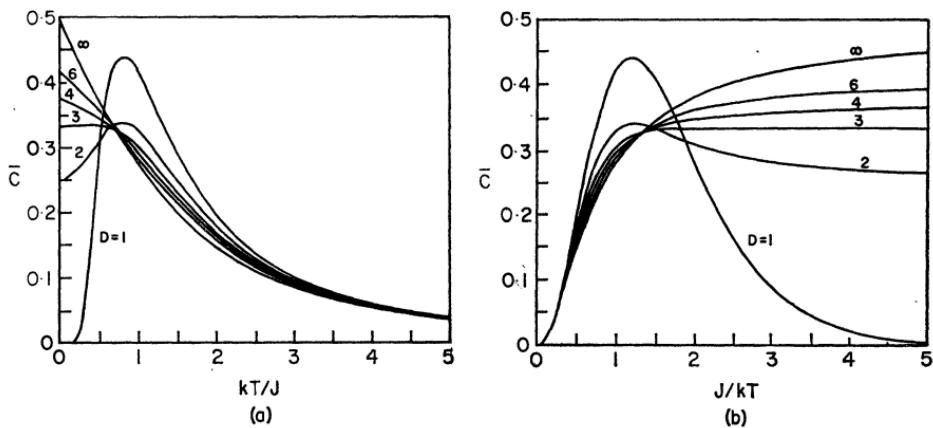


FIG. 12.2. Temperature dependence of the reduced specific heat for the linear chain lattice.

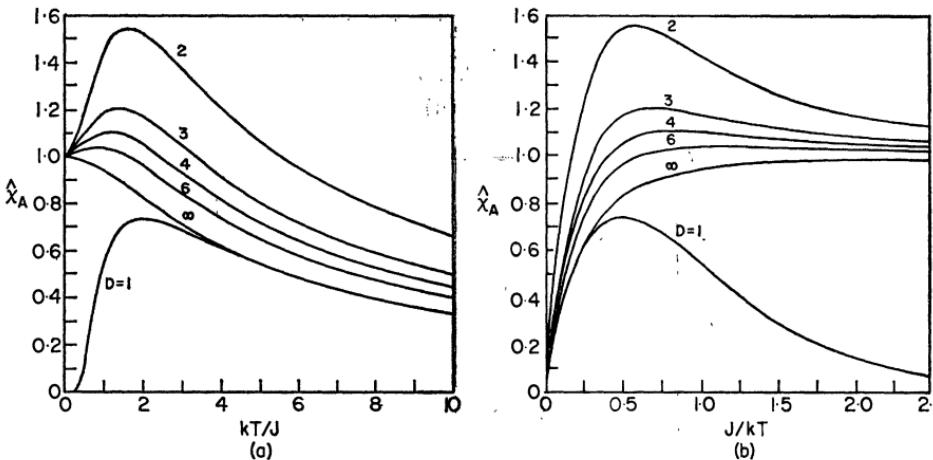


FIG. 12.3. Temperature dependence of the reduced antiferromagnetic susceptibility for the linear chain lattice.

Property (i) [i.e. (12.6)] is intuitively plausible since if we increase the spin dimensionality, then the spins have more phase space in which to "flop about" and hence they are less well correlated. This intuitive reasoning is independent of considerations involving lattice dimensionality, and hence (12.6) is a reasonable conjecture for all D . We have not succeeded in proving

(12.6) except for $d = 1$ [and for a model in which each spin vector lies on the surface of a D -dimensional "hypercone" (Milošević *et al.*, 1970)], but if (12.6) were true, one might expect that the critical temperature would decrease monotonically with lattice dimensionality d . Indeed, the results of series expansions for $d = 2, 3, 4, 5, \dots$ indicate that $T_c(D, d)$ decreases monotonically with D (cf. Fig. 11.2b for a $d = 3$, f.c.c., lattice).

Property (ii) appears to be valid for higher lattice dimensionality (Stanley, 1968c), and has proved extremely useful as an "anchor point" in connection with series expansion methods and also in connection with recent developments utilising expansions, exact in D , in powers of $\epsilon \equiv 4 - d$ (Wilson and Kogut, 1974) and, most recently, expansions in $1/D$ itself (Abe, 1973). Accordingly, we devote the next section to this general- d result.

XIII. Exact Solution of Thermodynamic Properties and Correlation Functions for all d when $D = \infty$ [†]

In 1949 Kac was introduced by Uhlenbeck to the problems involved in trying to generalise to the case $d = 3, D = 1$ Onsager's exact solution for the zero field partition function of the case $d = 2, D = 1$. In a lucid personal account [cf. Section 8.4 of Stanley (1971a) and references contained therein] Kac describes the fashion in which he discovered the spherical model:

"in the best mathematical traditional, not being able to solve the original problem, I looked around for a similar problem which I could solve..."

The basic idea of the spherical model, defined formally in (12.7), is to replace the Ising model with its N constraints that each of N spins be of unit magnitude [cf. (2.3)] by a single constraint that the sum of the magnitude of all N spin vectors equal N . This approximation is indicated schematically in Fig. 2.2. It came to be called the spherical model because the continuous set of allowed states are representable as the surface of a N -dimensional *hypersphere* (just as the discrete set of allowed states for the Ising model are representable as the corners of a N -dimensional *hypercube*). The important point is that the spherical model was very much an "approximation to the Ising model" and, in fact, did not even possess a *bona fide* interaction Hamiltonian. The exact solution of (2.1) in the limit $D \rightarrow \infty$ and its correspondence with the spherical model serves to establish this model at a limiting location in a hierarchy of model Hamiltonians.

[†] See also Joyce Vol. 2, Chapter 10

For those interested principally in closed-form approximate solutions to model Hamiltonians, we might also remark that in light of the monotonicity discussed in Section XII, the apparent result (cf. discussion in Section XII) that the critical properties of (2.1) are monotonic functions of D would suggest that the critical properties of the fairly realistic but hopelessly insoluble Heisenberg model ($D = 3$) are bounded on one side by those of the

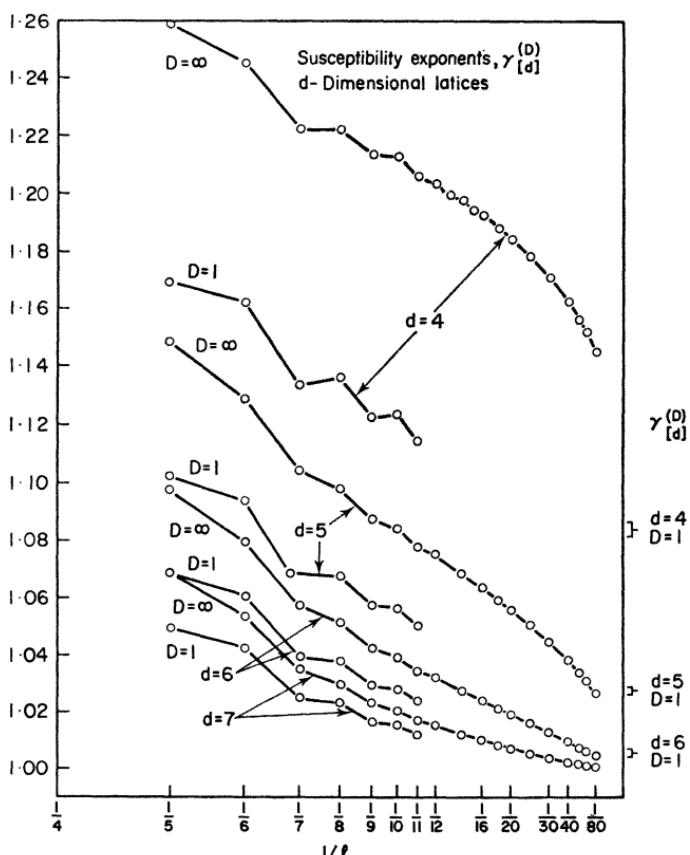


FIG. 13.1. Evidence from series expansion for the value of the susceptibility exponent $\gamma_{t,d}^{(D)}$. Only the Ising model ($D = 1$) and the spherical model ($D = \infty$) are shown. Analogous plots for other values of D lie in between the $D = 1$ and $D = \infty$ curves, and extrapolations support the hypothesis that the critical index γ is a monotonic function of D . The function shown is given by $\gamma_{t,l-1} \equiv 1 - l + l\rho_l/t_{l,l-1}$, where $t_{l,l-1} \equiv l\rho_l - (l-1)\rho_{l-1}$, $\rho_l \equiv a_l/a_1 a_{l-1}$. The point of this figure is that the ratios are not indicating the exactly known spherical model exponents ($\gamma = 1$ for $d > 3$), or at least this is not apparent for the first dozen or so terms. Hence, one might have reason to question the estimates of Fisher and Gaunt (1964) shown by the small brackets. In light of the monotonicity arguments given in the text, Milošević and Stanley (1971) conjecture that $\gamma(D, d) = 1$ for all D if $d \geq 4$.

Ising model ($D = 1$) and on the other by those of the spherical model ($D = \infty$). Moreover, rather than interpret the spherical model as a soluble approximation to the Ising model, it should perhaps have the "finer" honour of being an even better approximation to the Heisenberg model.

The proof of the equivalence is rather lengthy (Stanley, 1968c) and will not be given here. Suffice it to say that it has been generalised to include a uniaxial anisotropic interaction by Okamoto (1970), and that very recently it has provided the basis of Wilson method expansions of critical point exponents in powers of $1/D$ (Abe, 1973).

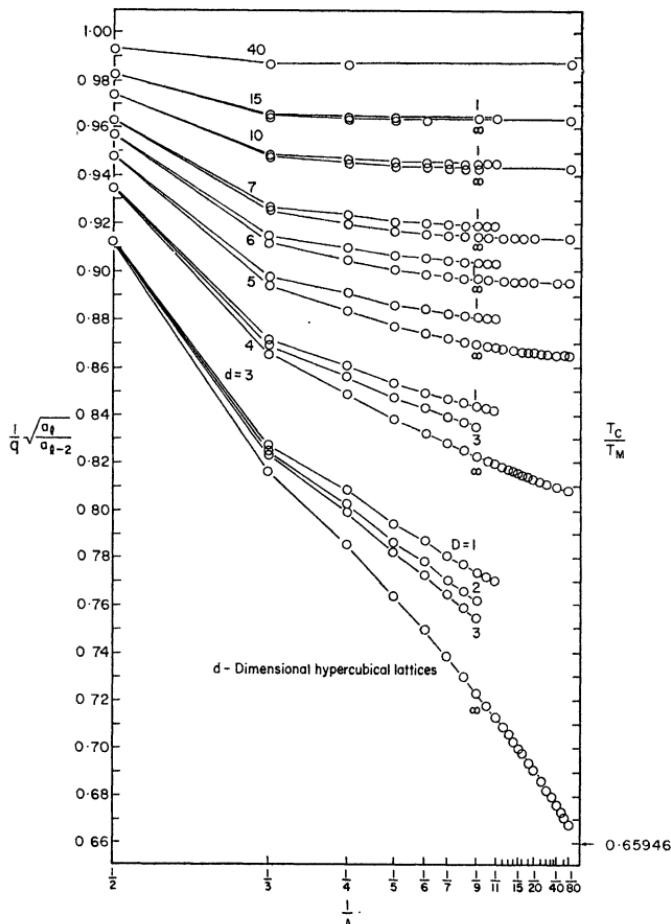


FIG. 14.1. Ratio plot for the susceptibility series indicating the variation of $T_c(D, d)$ with D and d . The additional terms for the spherical model ($D = \infty$) come from a direct expansion of the analytic expressions themselves (H. E. Stanley, unpublished work), and the additional terms for $D = 1$ come from Fisher and Gaunt (1964).

It has also been a "touchstone" with which to compare extrapolations based upon limit numbers of terms in high-temperature series expansions—for example, it was once believed (Fisher and Gaunt, 1964) that the susceptibility exponent $\gamma(D = 1, d)$ decreased to unity with increasing lattice dimensionality d sufficiently slowly that for $d = 4$ and 5, $\gamma(D = 1, d)$ was larger than the mean field ($d = \infty$) limit, $\gamma(D, \infty) = 1$. However, comparison with the spherical model series—which can be carried out to arbitrarily high order—strongly suggested that in fact $\gamma(D, d) = 1$ for all $d > 4$ (cf. Fig. 13.1). In particular, we see from Fig. 13.1 that the approach to the rigorous value $\gamma(D = \infty, d = 4) = 1$ is "tediously slow", even given the 80 terms that are plotted. This behaviour is likely connected with the presence of logarithmic factors in the spherical model solution as first pointed out by Stell (private communication). A second example is provided by Fig. 3.4.

XIV. Dependence of the Critical Point Exponents upon D for $d > 3$: Hypercubical Lattices

We conclude this chapter by pointing out that the information obtained thus far permits one to obtain the series through ninth order for loose-packed and through eighth order for close-packed lattices for any value of D or d —including values of $d > 3$ —all that is needed are the lattice constants. The lattice constants for the hypercubical lattices are listed in Table 8.1,

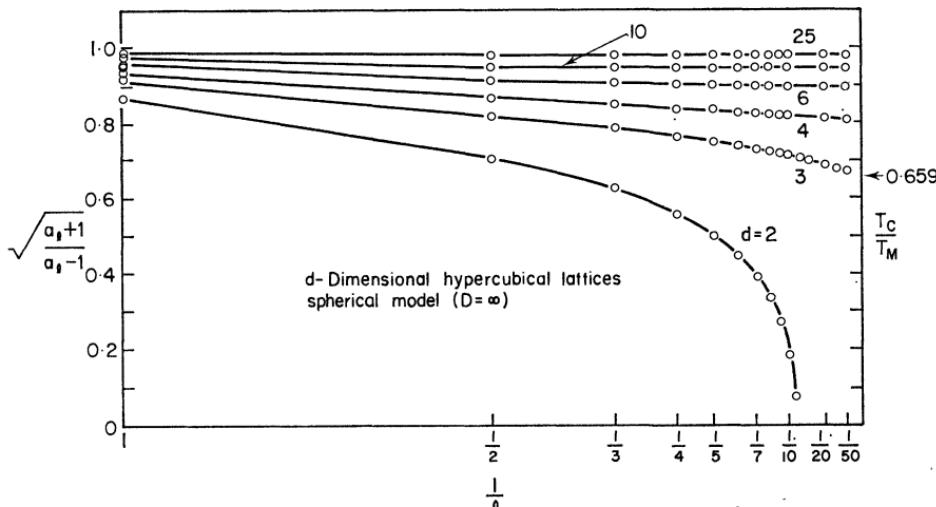


FIG. 14.2. Ratio plot for the susceptibility series for the spherical model ($D = \infty$) for various lattice dimensionalities d . Note that for $d = 2$, the series do not indicate a non-zero transition temperature, in accordance with the rigorous result (Berlin and Kac, 1952).

so that we can obtain the \tilde{A}_l of Table 8.3 and the B_l of Table 9.1 for arbitrary d and study, for example, the fashion in which T_c/T_M approaches unity as $d \rightarrow \infty$.

Simple ratio plots for the susceptibility are shown in Figs. 14.1 and 14.2.

XV. Conclusion and Outlook

In this chapter we have aimed at a presentation that is clear and understandable to the novice; where there have been oversimplifications, we apologise to the experts, and where the references have been inadequate, we refer the interested reader to a recent 2,500-entry bibliography which provides more comprehensiveness (Stanley, 1973). In our survey of the properties of the model system (2.1), we have treated a wide range of cases for which there may be few known experimental systems at the present time. However, Kittel once said that given a model, the half-time for discovery of an appropriate physical system is about 5 years; and indeed the plethora of applications of $d = 1$ and $d = 2$ models to, say, biological systems and of $d = 4$ models to, say, the singlet ground state problem gives evidence supporting the wisdom of Kittel's adage (for references to some of these novel applications, see Stanley, 1972a, b, 1973, 1974; Herzfeld and Stanley, 1974).

Even if there never exist real systems to which some cases correspond, study of a model can help elucidate general principles (e.g., the universality hypothesis of Section III.E), which in turn prove extremely useful in understanding real systems.

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8. X-Y Model

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I. Introduction

The subject of this chapter is basically the spin $\frac{1}{2}$ $X-Y$ model. This model is defined by an interaction Hamiltonian,

$$\mathcal{H}_0 = -\frac{J^\perp}{2} \sum_{\mathbf{r}, \mathbf{r}'} (\sigma_{\mathbf{r}}^x \sigma_{\mathbf{r}'}^x + \sigma_{\mathbf{r}}^y \sigma_{\mathbf{r}'}^y), \quad (1.1)$$

where the σ 's are the well known Pauli matrices, \mathbf{r} and \mathbf{r}' denote the sites or vertices of a lattice and J^\perp is a constant with the dimensions of energy.

The $X-Y$ model, as a special case of quantum lattice fluid model, was introduced by Matsubara and Matsuda in 1956. It has been studied in mean field approximation by them and by Whitlock and Zilsel (1963) and Zilsel (1965). Fisher (1967) has discussed the physics of the model to some extent. Lieb, Schultz, and Mattis (1961) have solved the one-dimensional zero field spin $\frac{1}{2}$ $X-Y$ model. Katsura (1962) and Niemeijer (1967) have calculated exactly a number of further properties of the one-dimensional spin $\frac{1}{2}$ $X-Y$ model. We shall confine ourselves however to discussion of the two- and three-dimensional $X-Y$ models for which no exact solutions are known as the one-dimensional model has been discussed by Thompson (Vol. I Chapter 5).

The discussion throughout this chapter will be based on exact high temperature series expansions including the series analysis and consequences of the results. We shall not discuss mean field and similar closed form approximations. We consider in detail only the isotropic $X-Y$ model as defined by (1.1). Results for spin infinity will be brought in although

only the detailed analysis of the spin $\frac{1}{2}$ case will be considered. Low temperature expansions present particular difficulties and there is no progress to report in this area.

The X-Y model, like the Ising, Heisenberg, and spherical models, which are the subjects of companion chapters, is believed to have a phase transition in three dimensions to an ordered phase at sufficiently low temperature. Because of the form of the Hamiltonian the natural order parameter operator is the perpendicular magnetization in the X-Y plane,

$$M^x = m \sum_{\mathbf{r}} \sigma_{\mathbf{r}}^x. \quad (1.2)$$

The critical phase transition temperature, T_c , is that temperature at and above which the thermal expectation value of the perpendicular magnetization vanishes, $\langle M^x \rangle = 0$. Near T_c large fluctuations in M^x and other quantities are expected. It is these and other anomalous critical properties which we discuss.

The X-Y model differs from the other three models mentioned in an interesting way; for the X-Y model the order parameter, (1.2), does not commute with the interaction Hamiltonian, (1.1). Statically this means for example that since M^x and \mathcal{H}_0 are not simultaneous observables, the equilibrium ground state does not consist of the state with all spins aligned in the X-Y plane. Indeed the ground state is not known, so no low temperature spin wave expansion has yet been made. Dynamically the non-commutation of M^x and \mathcal{H}_0 means that the decay of the order parameter to equilibrium can be studied. In this way the X-Y model resembles the *antiferromagnetic* Heisenberg model.

There are a number of important questions on which in principle a study by series expansion methods of the critical properties of the spin $\frac{1}{2}$ X-Y model should shed some light:

1. To what extent do the calculated critical properties of the spin $\frac{1}{2}$ X-Y model agree with the measured properties of real physical systems such as planar magnets and quantum fluids?
2. To what extent do the calculated critical exponents and critical amplitudes satisfy relations derived from homogeneity or scaling hypotheses?
3. To what extent do the critical properties of the X-Y model depend on spin, hence testing the universality hypothesis?
4. Do the dynamic properties such as the frequency dependent susceptibility have critical singularities in agreement with dynamic scaling?
5. What are the collective modes of the model?
6. Does the two-dimensional X-Y model have a phase transition, and if so what is the nature of the low temperature phase?

Section II is concerned with the detailed introduction of the spin $\frac{1}{2}$ *X-Y* model as an abstract model, a model of a quantum fluid, and a model of a certain class of insulating ferromagnets. A smoothness postulate is also introduced here. Section III discusses other planar systems and the unifying principle of universality.

Section IV deals with the simplest of the high temperature series expansions, the expansion of the zero field partition function, which serves as a prototype for the later expansions. In this Section, various needed graphical concepts and theorems are obtained.

Parallel and perpendicular susceptibilities and fluctuations in the parallel and perpendicular magnetizations are discussed in Section V. In Section VI, the expansion of the order parameter (perpendicular magnetization) fluctuation, perpendicular and parallel susceptibility and fourth order fluctuation high temperature expansions are presented.

Results obtained directly by analysis of the series expansions are given in Section VII; in Section VIII further results are obtained through the use of scaling theory.

Section IX contains the high temperature, high frequency expansion of the frequency-dependent perpendicular susceptibility. Analysis of the series reveals collective modes of the three-dimensional *X-Y* model.

Section X is devoted to the issue of the existence of a phase transition in the two dimensional planar models based on analysis of high temperature expansions of the spin $\frac{1}{2}$ *X-Y* model and the classical plane rotator model.

Section XI makes what comparison is possible with the as yet scanty experimental data, with a particular emphasis on the lambda transition in liquid helium. Finally, discussion, conclusions and outlook are contained in Section XII.

II. *X-Y* Model

In this section we arrive at the *X-Y* model by several different paths, and thus we see that for a variety of reasons, the model is of scientific interest.

A. An abstract model for theoretical studies

Without reference to any particular physical system, it is possible simply to write down, without derivation, the Hamiltonian for the general spin anisotropic Heisenberg model as

$$\begin{aligned} \mathcal{H} = & - (4s^2)^{-1} \sum_{\mathbf{r}, \mathbf{r}'} \{ J_{\mathbf{r}-\mathbf{r}'}^\perp (S_{\mathbf{r}}^x S_{\mathbf{r}'}^x + S_{\mathbf{r}}^y S_{\mathbf{r}'}^y) + J_{\mathbf{r}-\mathbf{r}'}^{\parallel} S_{\mathbf{r}}^z S_{\mathbf{r}'}^z \} \\ & - s^{-1} \sum_{\mathbf{r}} \{ m_\perp H^x S_{\mathbf{r}}^x + m_\parallel H^z S_{\mathbf{r}}^z \} \end{aligned} \quad (2.1)$$

where S_r^z is the α Cartesian component matrix of spin S for lattice site r , H^x and H^z are external fields, the J^\perp and $J\parallel$'s are spin-spin coupling constants and m_\perp and $m\parallel$ are spin-field coupling constants.

In detailed studies, the first summation is usually restricted for simplicity to nearest neighbour pairs of sites (indicated by $\langle r, r' \rangle$) without, it is believed, significantly altering the physics of the model. Even then the model specified by (2.1) admits of two types of anisotropy. If the J 's depend on the direction of the vector $r - r'$ we say the model has *lattice anisotropy*; if $J^\perp \neq J\parallel$ the model has *spin space anisotropy*.

Three special cases of particular interest because of their relative simplicity are obtained by setting, respectively, $J^\perp = 0$ (the Ising model) $J^\perp = J\parallel$, (the isotropic Heisenberg model) and $J\parallel = 0$ (the X - Y model). The Ising and isotropic Heisenberg models have been much studied and are the subject of separate companion chapters in this volume (Rushbrooke, *et al.* Chapter 5; Domb Chapter 6). The X - Y model, the subject of this chapter, has been much less thoroughly studied so far. Indeed for the X - Y model only the two extreme special cases of infinite spin and spin $\frac{1}{2}$ have been investigated.

The spin $\frac{1}{2}$ X - Y model is particularly interesting as perhaps the simplest possible fully quantum mechanical many body system. Admittedly, the Ising model is a simpler model, but it lacks full quantum properties because the Ising Hamiltonian is known in fully diagonal form as are most of the other thermodynamic operators.

In the Ising model the order parameter operator,

$$M^z = m\parallel s^{-1} \sum_r S_r^z,$$

commutes with the interaction Hamiltonian and so has no time dependence. If the Ising magnet is in a non-equilibrium state of magnetization it will remain in that state forever. The same is true of the isotropic Heisenberg model. For the X - Y model on the other hand it is of some theoretical interest that the order parameter,

$$M^x = m_\perp s^{-1} \sum_r S_r^x \quad (2.2)$$

does not commute with the interaction Hamiltonian,

$$\mathcal{H}_0 = -(J^\perp/2s^2) \sum_{\langle r, r' \rangle} (S_r^x S_{r'}^x + S_r^y S_{r'}^y), \quad (2.3)$$

and so has a time dependent behaviour, which is the subject of discussion in Section IX.

B. Quantum lattice fluids

The correspondence between the spin $\frac{1}{2}$ Ising model and a classical lattice fluid has been well known since the work of Yang and Lee (1952) and Fisher (1964) and indeed is closely related to the pioneering work of Lennard-Jones and Devonshire (1937, 1938). Matsubara and Matsuda (1956) extended the correspondence to relate the spin space anisotropic spin $\frac{1}{2}$ Heisenberg model to a quantum lattice fluid. This connection has also been reviewed by Fisher (1967) and Stephenson (1971). In the extreme quantum limit the quantum lattice fluid corresponds to the spin $\frac{1}{2}$ $X-Y$ model.

To develop the connection between the anisotropic Heisenberg model and the quantum fluid we follow rather closely the derivation of Stephenson (1971). We wish to construct a Hamiltonian for a quantum many body system in which the continuous coordinates are replaced by coordinates having a set of discrete values at the sites of a regular lattice. Further we want to specify that the Wigner-Seitz cell surrounding each site as either vacant or occupied by only one molecule.

We choose first a basis of 2^N -dimensions in which for each site (cell) there are two states. Specifically, in the subspace associated with the site \mathbf{r} ,

$$u_{\mathbf{r}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

can represent an occupied site at \mathbf{r} and

$$v_{\mathbf{r}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

a vacant site at \mathbf{r} . Then the molecule creation operator, $a_{\mathbf{r}}^\dagger$ defined by $a_{\mathbf{r}}^\dagger v_{\mathbf{r}} = u_{\mathbf{r}}$, $a_{\mathbf{r}}^\dagger u_{\mathbf{r}} = 0$ and the molecule destruction operator defined by $a_{\mathbf{r}} u_{\mathbf{r}} = v_{\mathbf{r}}$, $a_{\mathbf{r}} v_{\mathbf{r}} = 0$ are represented by

$$a_{\mathbf{r}}^\dagger = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad a_{\mathbf{r}} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \quad (2.4)$$

The number of molecules in the cell defined by $n_{\mathbf{r}} u_{\mathbf{r}} = 1 u_{\mathbf{r}}$ and $n v_{\mathbf{r}} = 0 v_{\mathbf{r}}$ is represented by

$$n_{\mathbf{r}} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = a_{\mathbf{r}}^\dagger a_{\mathbf{r}}. \quad (2.5)$$

The operator for the total number of molecules in the 2^N -dimensional direct product space is thus

$$\mathcal{N} = \sum_{\mathbf{r}} a_{\mathbf{r}}^\dagger a_{\mathbf{r}}. \quad (2.6)$$

Actually for purposes of statistical physics an explicit representation of the annihilation and creation operators is not needed; it is sufficient to know that operators for different sites commute, that for the same site the anticommutation relations

$$[a_r, a_r] = [a_r^\dagger, a_r^\dagger] = 0$$

and

$$[a_r, a_r^\dagger] = 1 \quad (2.7)$$

are satisfied and that

$$\text{tr } a_r = \text{tr } a_r^\dagger = 0$$

and

$$\text{tr } a_r a_r^\dagger = 2^{N-1} \quad (2.8)$$

The connection between these lattice operators and continuum quantum field creation and annihilation operators $\psi^\dagger(\mathbf{r})$ and $\psi(\mathbf{r})$ and density operator $\bar{\rho}(\mathbf{r}) = \psi^\dagger(\mathbf{r})\psi(\mathbf{r})$ must clearly be

$$a_r^\dagger = \psi^\dagger(\mathbf{r})v_0^{\frac{1}{2}}, \quad a_r = \psi(\mathbf{r})v_0^{\frac{1}{2}} \quad (2.9)$$

and

$$n_r = v_0 \bar{\rho}(\mathbf{r})$$

where v_0 is the cell volume.

Next we must discover the lattice fluid operators for the potential and kinetic energies. In order to represent qualitatively, yet simply, the real intermolecular potential between spherically symmetric molecules we assume that (a) there is an infinite repulsion between two molecules in the same cell, (b) there is a finite attraction between two molecules in adjacent cells and (c) there is no interaction between molecules in any other pair of cells. (We also neglect many body forces.) The infinite repulsion has been taken care of by excluding double occupancy of the cells. Then we have the potential energy operator for the lattice fluid,

$$U_{\text{latt}} = -u_0 \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} n_r n_{r'} = -u_0 \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} a_r^\dagger a_r a_{r'}^\dagger a_{r'}. \quad (2.10)$$

The lattice fluid kinetic energy operator is derived from the quantum field theory operator

$$T = -\frac{\hbar^2}{2m} \int \psi^\dagger(\mathbf{r}) \nabla^2 \psi(\mathbf{r}) d\mathbf{r}, \quad (2.11)$$

where m is the molecular mass. For the lattice case the integral must be replaced by a sum, the Laplacian by a finite difference operator and the

ψ 's by a 's. Thus (2.11) is replaced by

$$T_{\text{latt}} = -\frac{\hbar^2}{2m} \sum_{\mathbf{r}} a_{\mathbf{r}}^\dagger \frac{2d}{q\delta^2} \sum_{\mathbf{s}} (a_{\mathbf{r+s}} - a_{\mathbf{r}}) \quad (2.12)$$

where d is the dimensionality of the lattice, q the coordination number and δ a nearest neighbour vector. The second sum is over all nearest neighbour sites to the site at \mathbf{r} .

To see that we have introduced the correct finite difference expression for the Laplacian consider the operator, \mathcal{T} , for finite translation by a vector δ , such that $\mathcal{T}\psi(\mathbf{r}) = \psi(\mathbf{r} + \delta)$,

$$\mathcal{T} = \exp(\delta \cdot \nabla). \quad (2.13)$$

If the scale of variation of the wave function (coherence length) is large compared with δ , a condition which should be valid in the critical region, we may replace (2.13) by the first three terms in its expansion

$$\mathcal{T} = 1 + \delta \cdot \nabla + \frac{1}{2}(\delta \cdot \nabla)^2, \quad (2.14)$$

then

$$\psi(\mathbf{r} + \delta) - \psi(\mathbf{r}) = \delta \cdot \nabla \psi(\mathbf{r}) + \frac{1}{2}(\delta \cdot \nabla)^2 \psi(\mathbf{r}). \quad (2.15)$$

If we next sum (2.13) over all nearest neighbour sites to a given site, then on all the common lattices the first term on the right vanishes by symmetry and we obtain

$$\sum_{\delta} [\psi(\mathbf{r} + \delta) - \psi(\mathbf{r})] = \sum_{\delta} \frac{1}{2}(\delta \cdot \nabla)^2 \psi(\mathbf{r}) = \frac{q\delta^2}{2d} \nabla^2 \psi(\mathbf{r}). \quad (2.16)$$

By slight rearrangement (2.12) can be put in a form facilitating comparison with the anisotropic Heisenberg model

$$T_{\text{latt}} = -\frac{\hbar^2 d}{qm\delta^2} \left\{ \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} (a_{\mathbf{r}}^\dagger a_{\mathbf{r}'} + a_{\mathbf{r}} a_{\mathbf{r}'}^\dagger) - q \sum_{\mathbf{r}} n_{\mathbf{r}} \right\}. \quad (2.17)$$

We can now write the grand partition function for a quantum lattice fluid,

$$\Xi(T, \mu) = \text{tr} \exp \beta \left\{ \left(\mu - \frac{\hbar^2 d}{m\delta^2} \right) \mathcal{N} + \frac{\hbar^2 d}{qm\delta^2} \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} (a_{\mathbf{r}}^\dagger a_{\mathbf{r}'} + a_{\mathbf{r}} a_{\mathbf{r}'}^\dagger) \right. \\ \left. + u_0 \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} n_{\mathbf{r}} n_{\mathbf{r}'} \right\} \quad (2.18)$$

where μ is the chemical potential. To compare (2.18) with (2.1), make the substitutions

$$a_r = S_r^x - iS_r^y, \quad a_r^\dagger = S_r^x + iS_r^y, \quad n_r = S_r^z + \frac{1}{2} \quad (2.19)$$

(2.18) then becomes

$$\Xi = \text{tr} \exp \beta \left\{ \left(\mu - \frac{\hbar^2 d}{m\delta^2} + \frac{qu_0}{4} \right) \frac{N}{2} + \left(\mu + \frac{qu_0}{2} - \frac{\hbar^2 d}{m\delta^2} \right) \sum_r S_r^z + \frac{2\hbar^2 d}{qm\delta^2} \sum_{\langle r, r' \rangle} (S_r^x S_{r'}^x + S_r^y S_{r'}^y) + u_0 \sum_{\langle r, r' \rangle} S_r^z S_{r'}^z \right\}. \quad (2.20)$$

By comparison with (2.1), for the lattice isotropic, nearest neighbour spin $\frac{1}{2}$ case with (2.20)

$$2m_{||}H^z = \mu + \frac{qu_0}{2} - \frac{\hbar^2 d}{m\delta^2}, \quad m_{\perp} = 0, \quad J^{\perp} = \hbar^2 d/qm\delta^2, \\ J^{||} = u_0/2. \quad (2.21)$$

The spin space anisotropy, measuring the relative importance of quantum to classical interactions is

$$\eta \equiv J_{\perp}/J_{||} = 2\hbar^2 d/qm\delta^2 u_0. \quad (2.22)$$

In particular, we see that the pure spin $\frac{1}{2}$ X-Y model corresponds to the extreme quantum limit in which the attractive tail of the potential energy can be neglected.

C. Planar magnetic insulators

It is less generally realized that the spin $\frac{1}{2}$ X-Y model is a reasonable model for a class of ferromagnetic or antiferromagnetic insulators. There are a large number of insulating compounds which are ferromagnetic or, more commonly, antiferromagnetic due to the presence of rare earth ions of high total angular momentum quantum number (in the context of magnetic studies usually called loosely "spin"). Examples of such ions and corresponding spins include Gd³⁺(7/2), Dy³⁺(15/2), Er³⁺(15/2).

Following Betts *et al.* (1970), let us consider then a crystal of magnetic ions of high half odd integral spin embedded in a matrix of non-magnetic ions. We shall assume that the ions interact via an isotropic Heisenberg (exchange) interaction. In addition, the non-magnetic crystalline environment will have the effect of introducing single ion terms in the spin Hamiltonian. For most symmetries the leading single ion anisotropy

term is proportional to $(S^z)^2$. Thus, we take the spin Hamiltonian (in the absence of external field) to be

$$\mathcal{H} = D \sum_{\mathbf{r}} (S_{\mathbf{r}}^z)^2 - \mathcal{J} \sum_{\mathbf{r}, \mathbf{r}'} S_{\mathbf{r}} \cdot S_{\mathbf{r}'} . \quad (2.23)$$

Further, let us take the case $D \gg |\mathcal{J}|$. In the critical region $k_B T_C \sim \mathcal{J}$ therefore, only the lowest Kramers doublet with $S^z = \pm \frac{1}{2}$ is expected to be appreciably populated in this region and effectively we have a spin $\frac{1}{2}$ system.

Next we examine the relative importance of the Ising and $X-Y$ terms in the Heisenberg interaction within the populated subspace. Consider a system of two spins governed by the Hamiltonian (2.23). In the subspace of $S_1^z = \pm \frac{1}{2}$ and $S_2^z = \pm \frac{1}{2}$ (the populated subspace), the first order perturbation matrix for the $X-Y$ interaction, $-\mathcal{J}(S_1^x S_2^x + S_1^y S_2^y)$, is, in the representation in which S_i^z is diagonal,

$$\mathcal{H}'_{XY} = -\frac{\mathcal{J}(s + \frac{1}{2})^2}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} . \quad (2.24)$$

For the Ising interaction, $-\mathcal{J}S_1^z S_2^z$, the perturbation matrix is

$$\mathcal{H}'_I = -\frac{\mathcal{J}}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} . \quad (2.25)$$

The ratio of the magnitudes of the non-zero matrix elements is $2(s + \frac{1}{2})^2$, which for example for Gd^{3+} is 32 and for Dy^{3+} is 128. For such crystals, the approximation of the spin Hamiltonian by the pure spin $\frac{1}{2}$ $X-Y$ model seems not unreasonable for most applications.

Here we might point out that the spin $\frac{1}{2}$ Ising model of a magnetic system can arise in just the same way from (2.23) except that we must take D to be negative. Then the populated subspace in the critical region corresponds to $S^z = \pm s$, and it is matrix elements of the Ising term which are large in this subspace. Incidentally, there appears to be no simple way in which the higher spin $X-Y$ model (or the higher spin Ising model) can arise as a model of a real magnetic system.

D. Perturbed $X-Y$ model

In Section II.B we have seen how the pure $X-Y$ model corresponds to the extreme quantum limit of the quantum lattice fluid model; in

In Section II.C we have seen how the pure *X-Y* model corresponds to the high spin, high single-ion anisotropy limit of a magnetic insulator.

Real systems will contain terms other than the *X-Y* term in the interaction Hamiltonian. Thus, apart from its theoretical interest as discussed in Section II.A, the question arises of the physical relevance of the pure *X-Y* model.

The physically realistic class of models we have already discussed can be encompassed by the perturbed *X-Y* model Hamiltonian

$$\mathcal{H}'_{XY} = \mathcal{H}_{XY} + \eta \mathcal{H}' \quad (2.26)$$

where \mathcal{H}_{X-Y} is the pure spin $\frac{1}{2}$ lattice-isotropic nearest-neighbour *X-Y* model Hamiltonian

$$\mathcal{H}_{X-Y} = -(J^\perp/2) \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} (\sigma_r^x \sigma_{r'}^x + \sigma_r^y \sigma_{r'}^y) = -J^\perp \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} (a_r a_{r'}^\dagger + a_r^\dagger a_{r'}). \quad (2.27)$$

The second term of (2.26) is supposed to be small in some sense and could include any, or all, of second neighbour, Ising, single-ion anisotropy, lattice anisotropy, Dzialoshinsky-Moriya or other interactions.

According to the ideas of smoothness (Dalton and Wood, 1965; Jasnow and Wortis, 1968; Griffiths, 1970), the critical exponents of the perturbed model with Hamiltonian \mathcal{H}'_{XY} (2.26) will be the same as those of the unperturbed model for all η less than some crossover value η_c . For $\eta > \eta_c$, the critical exponents will jump suddenly to those values characteristic of the dominant term in \mathcal{H}' , which then can no longer be regarded as small.

An exception to this behaviour is the eight vertex model (Baxter, 1971) in which the critical exponents depend continuously on η , which measures (in the eight vertex model) the strength of the four spin Ising interaction relative to the two spin Ising interaction. As Kadanoff and Wegner (1971) have pointed out, the eight-vertex model is special in that the interaction contains a term scaling as r^d . In such a case they show that scaling theory allows the observed η dependence of the critical exponents.

III. Planar Models, Planar Systems and the Universality Hypothesis

In this Section are considered a variety of models and systems which are either directly equivalent to the *X-Y* model or at least resemble the *X-Y* model in that they are planar. By a planar system we mean one in which the order parameter, like a vector in a plane, is specified by two real numbers.

A. $X-Y$ antiferromagnets

As observed by Halperin and Hohenberg (1969) and others, the Hamiltonian of the antiferromagnetic $X-Y$ model is identical in form to that of the ferromagnetic $X-Y$ model, at least for loose packed lattices. Following Halperin and Hohenberg, we divide the lattice into two equivalent sublattices A and B and define new dynamical variables

$$Q_r^\alpha = \eta_r S_r^\alpha \quad (3.1)$$

with

$$\eta_r = \begin{cases} +1 & r \text{ on sublattice } A \\ -1 & r \text{ on sublattice } B \end{cases}$$

The three variables Q_r^x , Q_r^y and S_r^z obey exactly the same commutation relations as the original variables S_r^x , S_r^y and S_r^z . Let us also define the "staggered" magnetic field components

$$G_r^\alpha = \eta_r H_r^\alpha. \quad (3.2)$$

The Hamiltonian (2.1), rewritten in terms of the new variables, retains the same form, namely

$$\begin{aligned} \mathcal{H} = & -(4s^2)^{-1} \sum_{r,r'} \{ \eta_r \eta_{r'} J_{r-r'}^\perp (Q_r^x Q_{r'}^x + Q_r^y Q_{r'}^y) + J_{r-r'}^\parallel S_r^z S_{r'}^z \} \\ & - s^{-1} \sum_r \{ m_\perp G_r^x Q_r^x + m_\parallel H^z S_r^z \}. \end{aligned} \quad (3.3)$$

If the original coupling constant $J_{r-r'}^\perp < 0$ (antiferromagnetic), then the new coupling constant, $\bar{J}_{r-r'}^\perp \equiv \eta_r \eta_{r'} J_{r-r'}^\perp > 0$ (ferromagnetic). Thus, it is clear that the $X-Y$ antiferromagnet is isomorphic to the $X-Y$ ferromagnet and, in particular, should have the same critical properties.

The order parameter conjugate to the ordering staggered perpendicular field G_r^x is thus the "staggered" perpendicular magnetization,

$$N_\perp = s^{-1} \sum_r m_\perp Q_r^x = m_\perp s^{-1} \sum_r \eta_r S_r^x. \quad (3.4)$$

Some magnetic insulators which have been mentioned in the literature as being planar antiferromagnets (though not necessarily representatives of the $X-Y$ model) include:

- | | |
|---|--|
| $\text{Gd}_2(\text{SO}_4)_3 \cdot 8\text{H}_2\text{O}$ | (Bogle and Tutenhoofd, 1962; Wielinga <i>et al.</i> , 1967). |
| CsMnF_3 | (Lee <i>et al.</i> , 1963). |
| $\text{La}_2\text{Ni}_3(\text{NO}_3)_{12} \cdot 24\text{H}_2\text{O}$ | (Mess <i>et al.</i> , 1967). |

| | | |
|--|---|---------------------------------------|
| $\text{Er}_{\frac{1}{2}}\text{Na}_{\frac{1}{2}}\text{MoO}_4$ | } | (Holmes and Schieber, 1968). |
| $\text{Yb}_{\frac{1}{2}}\text{Na}_{\frac{1}{2}}\text{MoO}_4$ | | |
| $\text{Yb}_2\text{O}_2\text{S}$ | | (Rossat-Mignod <i>et al.</i> , 1971). |
| ErVO_4 | | (Metcalfe and Rosenberg, 1972). |

Some two-dimensional X-Y-like magnetic systems include CoCl_2 , $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ and $\text{CoBr}_2 \cdot 6\text{H}_2\text{O}$ (de Jongh and Miedema, 1973).

B. Weak ferromagnets

By "weak ferromagnets" we mean magnets in which the principal interaction is the Dzialoshinsky-Moriya interaction (Dzialoshinsky, 1958; Moriya, 1960)

$$\mathcal{H}_{\text{DM}} = \sum_{\mathbf{r}, \mathbf{r}'} \mathbf{d}_{\mathbf{r}, \mathbf{r}'} \cdot (\mathbf{S}_{\mathbf{r}} \times \mathbf{S}_{\mathbf{r}'}) . \quad (3.5)$$

For an extensive discussion of weak ferromagnets, see Moriya (1963). Although the interaction (3.5) is thought to be usually weak in comparison with other competing interactions, this may not be so in all cases (Wolf, 1971).

Symmetry considerations place constraints on the $\mathbf{d}_{\mathbf{r}, \mathbf{r}'}$ (Moriya, 1963). For instance, if the point $(\mathbf{r} + \mathbf{r}')/2$ is an inversion centre, then $\mathbf{d}_{\mathbf{r}, \mathbf{r}'} = 0$. Thus, the Dzialoshinsky-Moriya interaction cannot occur on the s.c., b.c.c., f.c.c. or diamond lattices; it can occur on the B-site spinel (or cristobalite) lattice, the hydrogen peroxide lattice and other lattices of low symmetry. On the hydrogen peroxide lattice (Leu *et al.* 1969), each lattice site is surrounded symmetrically by three nearest neighbour sites with all four sites in the same plane. All sites on this coordination number $q = 3$ lattice are equivalent under a combination of translation and improper rotation. However the symmetry is sufficiently low that no restrictions are placed on the $\mathbf{d}_{\mathbf{r}, \mathbf{r}'}$ for the nearest neighbour sites \mathbf{r}, \mathbf{r}' .

Let us then consider a model in which all the $\mathbf{d}_{\mathbf{r}, \mathbf{r}'}$ are equal in magnitude and point in the z direction on some loose packed lattice where this is allowed, such as the hydrogen peroxide lattice, and only nearest neighbour interactions occur. The interaction Hamiltonian (3.4) then becomes

$$\mathcal{H}_{\text{DM}} = 2d^z \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} (S_{\mathbf{r}}^x S_{\mathbf{r}'}^y - S_{\mathbf{r}}^y S_{\mathbf{r}'}^x) . \quad (3.6)$$

Now, for atoms on the B (primed) sublattice only let us perform a 90° rotation of the coordinate system about z axis so that

$$\begin{aligned} S_{\mathbf{r}'}^y &\rightarrow -S_{\mathbf{r}'}^x \\ S_{\mathbf{r}'}^x &\rightarrow +S_{\mathbf{r}'}^y . \end{aligned} \quad (3.7)$$

Then (3.6) is transformed to the $X-Y$ interaction with $2d^z = J^\perp$. On most lattices the Dzialoshinsky-Moriya interaction Hamiltonian cannot be transformed into the $X-Y$ Hamiltonian, but nevertheless the critical behaviour should be the same as the $X-Y$ critical behaviour because of the expected lattice independence of critical exponents.

The $D-M$ interaction, even when not dominant, may however be solely responsible for the (weak) magnetization. We then expect this magnetization and corresponding susceptibility to have the same critical exponents as the $X-Y$ model.

Some weak ferromagnets which have been identified include:

| | |
|--|-------------------------------------|
| $\alpha\text{-Fe}_2\text{O}_3$ | (Néel, 1953). |
| NiF_2 | (Matarrese and Stout, 1954). |
| MnCO_3 | |
| CoCO_3 | |
| $\text{Fe}_3(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ | (Borovik-Romanov and Orlova, 1956). |
| NiCO_3 | (Prozorova, 1967). |

C. Universality hypothesis*

In this subsection we wish to introduce the *universality hypothesis* of Kadanoff (1970) which we distinguish from the *smoothness hypothesis* discussed in Section II.

There is strong and abundant evidence that the critical exponents for a given interaction Hamiltonian depend on d , the dimensionality of the lattice or the dimensionality of the space occupied by a continuum system. An additional parameter upon which critical exponents seem to depend is D , the dimensionality of the order parameter. By D we mean simply the number of real numbers needed to completely specify the order parameter. For example, in the Ising model with order parameter M_z , $D = 1$, in the $X-Y$ model with order parameter M_\perp , $D = 2$, while in the Heisenberg isotropic ferromagnet with order parameter \mathbf{M} , $D = 3$. The dimensionality of the order parameter may be less than, equal to or greater than the lattice dimensionality. For Hamiltonians representing short range interactions, it is not at all clear that the critical exponents depend on any further parameters, although there has in the past been considerable speculation on the form of critical exponent dependence on spin for example.

This lack of clear evidence for dependence of critical exponents on parameters other than D and d has led to the *universality hypothesis* (Kadanoff, 1970) that all systems of the same "lattice" dimensionality, d , order parameter dimensionality, D , and range of interaction, σ , can be

* See also Stanley, this volume Chapter 7

described in the critical region by an equation of state of the same form. That is, the critical region equations of state of system of the same *universality class* will differ only in the values of coefficients and not in the values of exponents. Most lattice models and most real physical systems have essentially the interaction range $\sigma = 0$ and so their critical exponents $\varepsilon(d, D, s, \dots) = \varepsilon(d, D)$. An exception to universality has already been discussed in Section II, the eight vertex model for which $\varepsilon = \varepsilon(d, D, \eta)$. It is also understood however that the η dependence is due to a special form of the interaction (Kadanoff and Wegner, 1971), so that the universality hypothesis is not vitiated.

The universality hypothesis is at present subject to test in several ways, by experiment, by generation and analysis of exact series expansions, by exact solutions and by general theoretical developments. The study by exact series expansion methods of the spin $\frac{1}{2}$ X-Y model described in the following sections, will *inter alia* contribute to the confirmation or otherwise of this hypothesis.

The universality hypothesis means for example that the critical exponents of the X-Y model should be spin-independent. We discuss the evidence for this in Sections VII and X. The universality hypothesis means further that all planar systems have the same critical exponents as the X-Y model. There is experimental evidence on this point which we discuss in Section XI.

D. Structural phase transitions

In this last subsection of Section III, we mention perovskite-type crystals which undergo displacive type phase transitions, which have been the subject of considerable interest lately (Pytte and Feder, 1969; Müller and Berlinger, 1971; Höchli and Scott, 1971 and references therein). In ABO_3 crystal such as SrTiO_3 and LaAlO_3 , the crystal makes a transition from a more symmetrical high temperature phase to a lower symmetry low temperature phase in which nearly rigid BO_6 octahedra undergo an average net rotation. Regarding the oxygen atoms (each of which is shared between two octahedra) as the elements in the cooperative system, we see that these elements each have freedom of displacement in a plane, albeit in only certain preferred directions in general. In contrast therefore to Müller and Berlinger (1971), who regard the rotation angle of the tetrahedra as the (one-dimensional) order parameter, it may be more appropriate to regard the order parameter as the sum of the two-dimensional displacements of the oxygen atoms. Of course we must include a weighting factor analogous to the η , of the X-Y antiferromagnet and appropriate to the particular crystal because of the "staggered" nature of the order. We shall not here attempt to go into the detail of the nature of these displacive type phase

transitions further. We simply point out that the observation of critical exponents equal to those of the $X-Y$ model should not be unexpected.

IV. Zero Field Partition Function

In this section we consider the exact high temperature series expansion of the partition function of the nearest neighbour spin $\frac{1}{2}$ $X-Y$ model in zero external field. The Hamiltonian can be written

$$\mathcal{H}_0 = -J^\perp \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} (a_{\mathbf{r}}^\dagger a_{\mathbf{r}'} + a_{\mathbf{r}} a_{\mathbf{r}'}^\dagger). \quad (4.1)$$

We seek the expansion of the partition function

$$Z_0 \equiv \text{tr exp}(-\beta \mathcal{H}_0) = \text{tr} \{1 - \beta \mathcal{H}_0 + \beta^2 \mathcal{H}_0^2 / 2! - \dots\} \quad (4.2)$$

where $\beta = 1/k_B T$. From the series for the zero field partition function one can immediately obtain high temperature series expansions for the entropy, internal energy and specific heat.

A. Partition function graphs*

As is usual in perturbation expansions, we introduce a correspondence between graphs and terms in the expansion, following the method of Betts, Elliott and Lee (1970). In \mathcal{H}_0 each term corresponds to a selection of n ordered nearest neighbour pairs of annihilation and creation operators. Each pair factor, $a_{\mathbf{r}}^\dagger a_{\mathbf{r}'}$, is represented by an arrow from site \mathbf{r}' to the nearest neighbour site \mathbf{r} . An entire term corresponds to n arrows connecting s vertices of the lattice ($2 \leq s \leq 2n$). As the creation and annihilation operators for a given site do not commute, the order of the arrows must be taken into account, which we do through the introduction of an extra non-spatial dimension ("time"). The set of arrows corresponding to a given term in \mathcal{H}_0 then forms an *ordered directed linear graph*.

In general, several ordered directed graphs will correspond to one *directed* or *shadow graph* in which the order is neglected. In other words the shadow graph is the spatial projection of the ordered directed graph. Finally, in general several shadow or directed graphs will correspond to one *bare* or *undirected graph*, in which every subset of arrows connecting a nearest neighbour pair of sites is replaced by a single line.

These types of graph are illustrated in Fig. 4.1 for the term in \mathcal{H}_0^5 ,

$$a_1^\dagger a_3 a_2^\dagger a_1 a_3^\dagger a_2 a_3^\dagger a_4 a_4^\dagger a_3$$

(which incidentally has zero trace).

* For a general introduction to graph theory and notation see Domb, this volume, Chapter 1.

Because of the commutation relations (2.7) and trace properties (2.8), non-zero contributions to the partition function correspond to only those graphs for which: (a) an equal number of heads and tails meet at each site or vertex of the shadow graph and (b) arrow heads and tails alternate in the ordered graph above each site of the shadow graph. Graphs which satisfy these criteria are *allowed* graphs. For each allowed ordered directed graph the contribution to the coefficient of $K^l/l!$ in the partition function is 2^{N-s} where s is the number of sites of the corresponding bare graph.

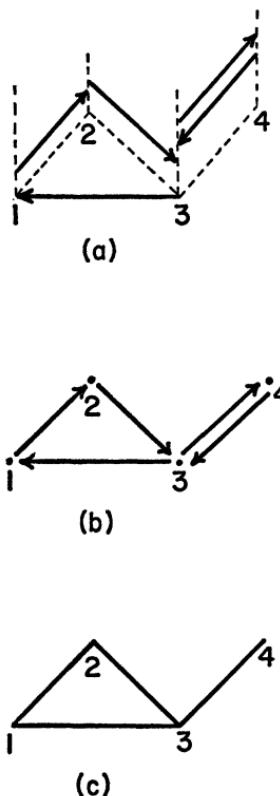


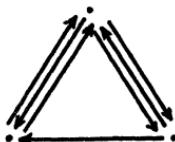
FIG. 4.1. (a) Ordered directed graph, g'' , corresponding to the term

$$a_1^\dagger a_3 a_2^\dagger a_1 a_3^\dagger a_2 a_3^\dagger a_4 a_4^\dagger a_3$$

in the high temperature expansion of the partition function. (b) Corresponding shadow graph, g' . (c) Corresponding bare graph, g .

Among the terms in \mathcal{H}_0^l will be subsets whose members satisfy rule (b) above and differ from one another only in the order of their pair factors. In graph language there are $v(g')$ ordered directed graphs, g'' , in each of which arrow heads and tails alternate in "vertical" order at each vertex and

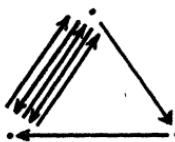
which differ from one another in the overall vertical order of their arrows but all of which correspond to the same shadow graph g' . Hence we call $v(g')$ the *vertical weight* of the graph g' . By direct methods the reader can satisfy himself that the vertical weight of the shadow graph in Fig. 4.1(b) is 40.



(a)



(b)



(c)

FIG. 4.2. Three shadow graphs of order 7 corresponding to the same bare graph. The horizontal weights $h(g_a') = h(g_b') \neq h(g_c')$.

Next we note that, in general, many different shadow graphs correspond to the same bare graph. Figure 4.2 illustrates three different shadow graphs of order $n = 7$ all of which correspond to the same bare graph, the triangle. Graphs (a) and (b) differ from one another only via labelling of the vertices; graph (c) differs from the other two in a more fundamental way. Graphs (a) and (b) have of course the same vertical weight, $v(a) = v(b) = 28$, while graph (c) has vertical weight $v(c) = 12$, as can be verified directly. Shadow graphs such as (a) and (b) in Fig. 4.2 which differ only in the labelling of their vertices we call *equivalent* shadow graphs. The number $h(g')$ of shadow graphs equivalent to a given shadow graph is called the *horizontal weight* of the graph g' . If we denote the symmetry

number of the underlying bare graph g by $s(g)$ and the symmetry number of the shadow graph $s(g')$, then

$$h(g') = \varepsilon(g') s(g)/s(g') \quad (4.3)$$

where $\varepsilon = 1$ if g' is invariant under reversal of all arrows and $\varepsilon = 2$ otherwise.

Finally, for the set of inequivalent shadow graphs, g' , we need to know the weak lattice constants of the corresponding bare graphs, g . The weak lattice constant $(g; \mathcal{L})$ of a graph g embedded in a lattice \mathcal{L} of N sites is the coefficient of N in the polynomial $\mathcal{N}(g; \mathcal{L})$ where $\mathcal{N}(g; \mathcal{L})$ is the number of weak embeddings of g in \mathcal{L} (Sykes *et al.*, 1966; Domb, this volume Chapter 1). The lattice constant concept is of course well known, and lattice constants have many applications in lattice statistics including the Ising and Heisenberg models.

The expression for the zero field partition function can be written

$$Z_N^{\mathcal{L}}(T) = \sum_{l=0}^{aN/2} \frac{K^l}{l!} \sum_{s=2}^l 2^{N-s} \sum_i \mathcal{N}(g_{si}; \mathcal{L}) \sum_j h(g_{si}^{(j)}) v(g_{si}^{(j)}) \quad (4.4)$$

or using the lattice version of the first Mayer theorem (Domb, 1960; this volume, Chapter 1).

$$\begin{aligned} \ln \Lambda^{\mathcal{L}}(T) &= \lim_{N \rightarrow \infty} \left(\frac{1}{N} \ln Z_N^{\mathcal{L}} \right) = \ln 2 + \sum_{l=0}^{\infty} \frac{K^l}{l!} \sum_{s=2}^l 2^{-s} \sum_i (g_{si}; \mathcal{L}) \\ &\quad \times \sum_j h(g_{si}^{(j)}) v(g_{si}^{(j)}). \end{aligned} \quad (4.5)$$

In (4.4) and (4.5) g_{si} is the i th bare graph with s vertices, and $g_{si}^{(j)}$ is the j th inequivalent shadow graph corresponding to g_{si} . The other symbols have already been defined.

Table IV.I illustrates these concepts with the specific examples of all graphs contributing to coefficients of K^l for all $l \leq 5$. For these simple graphs the horizontal and vertical weights can readily be found by inspection. Using Table IV.I in eqn (4.5), we obtain for an arbitrary lattice

$$\begin{aligned} \ln(\Lambda/2) &= \frac{1}{4}(\diagup) K^2 + \frac{1}{4}(\Delta) K^3 \\ &\quad + \left\{ \frac{1}{8}(\square) + \frac{1}{16}(\diagup, \diagdown) + \frac{1}{24}(\diagup\diagdown) + \frac{1}{48}(\diagup\diagdown) \right\} K^4 \\ &\quad + \left\{ \frac{1}{16}(\square) + \frac{1}{24}(\Delta\diagup) + \frac{1}{16}(\Delta) + \frac{1}{16}(\Delta, \diagup) \right\} K^5 \\ &\quad + \dots \end{aligned} \quad (4.6)$$

TABLE IV.1. Spin $\frac{1}{2}$ $X-Y$ model partition function shadow graphs and their weights

| Order l | Shadow graph g' | Vertical graph $v(g')$ | Horiz- ontal weight $h(g')$ | Bare graph g | Weak f.c.c. lattice constant (g ; f.c.c.) |
|--------------|----------------------|------------------------------|--------------------------------------|-------------------|---|
| 2 | | 2 | 1 | — | 6 |
| 3 | | 6 | 2 | | 8 |
| 4 | | 24 | 2 | | 33 |
| | | 8 | 1 | | 66 |
| | | 2 | 1 | — | 6 |
| | | 24 | 1 | | -69 |
| 5 | | 120 | 2 | | 168 |
| | | 40 | 2 | | 240 |
| | | 10 | 6 | | 8 |
| | | 120 | 2 | | -264 |

For the special case of the f.c.c. lattice (4.6) becomes

$$\ln(\Lambda/2) = 1\frac{1}{2}K^2 + 2K^3 + 2\frac{1}{16}K^4 + 4\frac{1}{2}K^5 + \dots \quad (4.7)$$

To obtain reasonably long series for $\ln \Lambda$ however it is necessary to computerize the operations.

B. Representation and generation of shadow graphs

For computer applications it is convenient to represent a shadow graph by an adjacency matrix A such that the matrix element A_{ij} equals the number

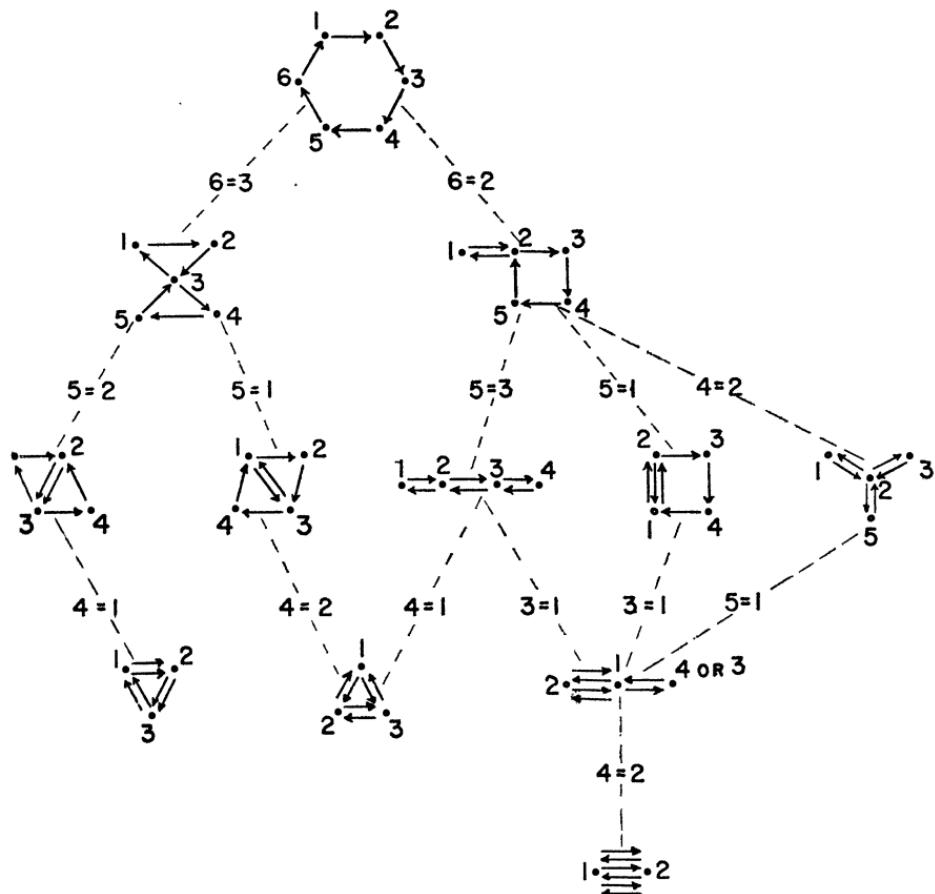
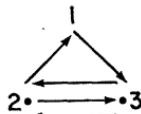


FIG. 4.3. Generation of all sixth order connected shadow graphs from the directed hexagon by successive identification of pairs of vertices.

of arrows from vertex i to vertex j . For example the shadow graph



is represented by

$$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & 2 & 0 \end{pmatrix}.$$

The corresponding bare graph is represented by an adjacency matrix B such that the matrix element B_{ij} is unity if i and j are connected and zero otherwise.

All directed or shadow graphs of l arrows can be generated from the polygon of l arrows by the *method of identification of vertices*, a method with a simple geometrical basis. Consider first as an example the directed hexagon of Fig. 4.3 and the eleven other shadow graphs which can be obtained from it, step by step by identifying pairs of vertices. In general, this process can be carried out readily by computer operations on the adjacency matrix for the directed polygon of l sides.

A new shadow graph \bar{g} of $\bar{s} = s - 1$ vertices is formed by identifying vertices i and k of the original graph g' of s vertices. The corresponding adjacency matrix \bar{A} is formed from the original adjacency matrix A by omitting the k th row and k th column and letting $\bar{A}_{ij} = A_{ij} + A_{kj}$ and $\bar{A}_{mi} = A_{mi} + A_{mk}$. The resulting matrix represents an acceptable shadow graph \bar{g} if all of the diagonal elements $\bar{A}_{ii} = 0$.

C. Vertical weight theorems

In extending the series (4.5) to useful length the calculation of the vertical weights is the most difficult part of the problem. The calculation of vertical weights is facilitated by the use of the following three theorems.

THEOREM I. Let g be a disconnected shadow graph of l arrows consisting of two subgraphs g_1 and g_2 having no vertices in common. If g_1 and g_2 , consisting of l_1 and l_2 arrows respectively, have vertical weights v_1 and v_2 , then the vertical weight, v , of g is given by

$$v = (l! / l_1! l_2!) v_1 v_2. \quad (4.8)$$

Proof: As there is no interference between the arrangements in the two subgraphs the vertical weight of the graph g is given by the product of two factors. The first is the number of ways of assigning l vertical levels such that l_1 are occupied by the arrows of g_1 and the remaining $l_2 = l - l_1$ are

occupied by the arrows of g_2 . The other factor is then the product of the vertical weights of the component subgraphs and the theorem is established.

THEOREM II. Let a connected shadow graph g of l arrows be composed of two subgraphs g_1 and g_2 of l_1 and l_2 arrows, respectively, such that g_1 and g_2 have m common vertices of order 2 in g (hence of order 1 in each of g_1 and g_2) and no other common vertices. Then the vertical weight, v , of g is given by the same expression (4.8) as in Theorem I.

Proof: As there is no restriction on head and tail vertical sequence at vertices of order 2 the vertical weight of g must be the same as that of a separated graph g' consisting of subgraphs g_1 and g_2 . But the vertical weight of g' is given by (4.8) and so the theorem is established.

We now present an example of the application of Theorem II to a shadow graph which contributes to the partition function in sixth order:

$$v\left(\begin{array}{c} \text{square with two arrows} \\ \downarrow \quad \downarrow \end{array} \middle| \begin{array}{c} \nearrow \searrow \\ \nearrow \searrow \end{array}\right) = v\left(\begin{array}{c} \text{square with two arrows} \\ \downarrow \quad \downarrow \end{array}\right) \cdot v\left(\begin{array}{c} \text{square with two arrows} \\ \downarrow \quad \downarrow \end{array} \middle| \begin{array}{c} \nearrow \searrow \\ \nearrow \searrow \end{array}\right) \cdot 6!/2!4!$$

Note that the subgraphs in this case are not allowed graphs in the partition function expansion. However, they have well defined vertical weights, which are readily determined by inspection, so that

$$v\left(\begin{array}{c} \text{square with two arrows} \\ \downarrow \quad \downarrow \end{array} \middle| \begin{array}{c} \nearrow \searrow \\ \nearrow \searrow \end{array}\right) = 2 \cdot 8 \cdot 15 = 240.$$

COROLLARY. For a connected shadow graph g of l arrows of which $l_1 = l - l_2$ are connected at vertices of order 2 only, the vertical weight

$$v(g) = (l!/l_2!) v_2 \quad (4.9)$$

where v_2 is the vertical weight of the shadow graph of l_2 bonds formed by deleting the above mentioned l_1 arrows.

Proof: This corollary follows readily by successive application of Theorem 2 and can be proved by induction.

Consider the last example:

$$v\left(\begin{array}{c} \text{square with two arrows} \\ \downarrow \quad \downarrow \end{array} \middle| \begin{array}{c} \nearrow \searrow \\ \nearrow \searrow \end{array}\right) = (6!/4!) v\left(\begin{array}{c} \nearrow \searrow \\ \nearrow \searrow \end{array}\right) = 30 \times 8 = 240.$$

THEOREM III. Consider a shadow graph g of order l composed of two subgraphs g_1 and g_2 of $l_1 - 1$ and $l_2 - 1$ arrows respectively and a third subgraph g_3 consisting of a single arrow. The subgraphs g_1 and g_2 have in common m vertices of order 2 in g and no other common vertices. The subgraph g_3 (the single

arrow) connects vertices of arbitrary (even) orders r_1 and r_2 in g_1 and g_2 , respectively. Then the vertical weight of g is given by (4.8) again. However now v_1 and v_2 are the vertical weights of the graphs g_1' and g_2' where g_1' is a subgraph of g consisting of g_1 and g_3 and g_2' is a subgraph of g consisting of g_2 and g_3 . It is important to note that $l_1 + l_2 = l + 1$.

Proof: Observe first that the vertical weight of g is the same as that of the graph g' obtained from g by separating all the second order vertices. Next observe that in counting the number of allowed arrow configurations for any shadow graph of order l we may assume that one arrow is at a fixed level and compute the number, n , of allowed configurations of the remaining arrows. Then the vertical weight, $v = ln$.

In g' let the arrow forming g_3 be fixed. The remaining $l - 1$ arrows belong to g_1 or g_2 . The $l_1 - 1$ arrows may be arranged among the $l_1 - 1$ levels assigned to g_1 in n_1 ways independently of the arrangement, in n_2 ways, of the $l_2 - 1$ arrows of g_2 among the $l_2 - 1$ levels assigned to g_2 . The $l - 1$ levels may be assigned in $(l - 1)!/(l_1 - 1)!(l_2 - 1)!$ ways giving

$$n = n_1 n_2 (l - 1)!/(l_1 - 1)!(l_2 - 1)!$$

Noting that $n_1 = v_1/l_1$ and $n_2 = v_2/l_2$, the result (4.8) follows.

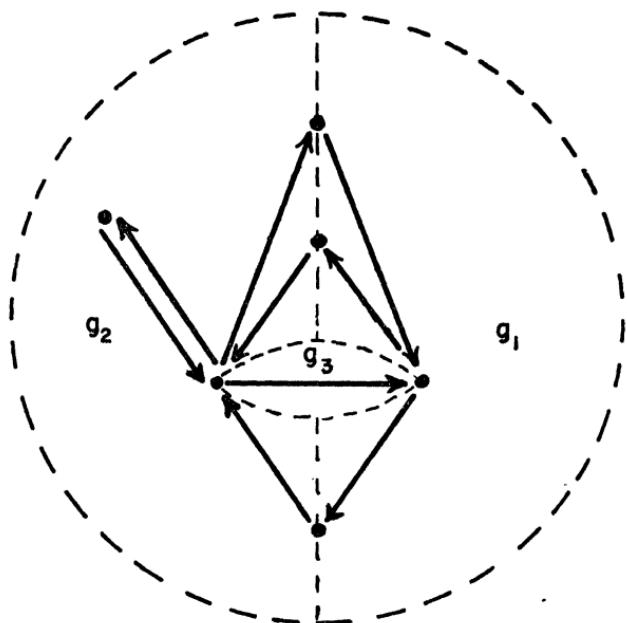
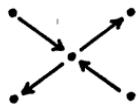
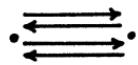
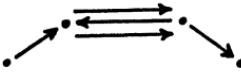
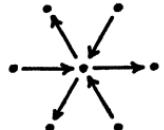
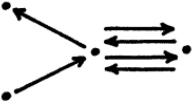
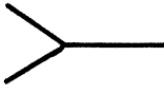
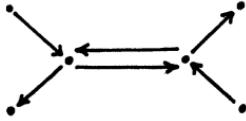
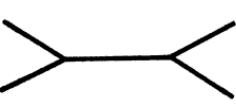


FIG. 4.4. A shadow graph of order 9 considered as two subgraphs g_1 and g_2 connected at vertices of order 2 and a single arrow g_3 .

TABLE IV.2. Elementary shadow graphs and their vertical weights

| Order l | Elementary shadow graph g' | Corresponding bare graph g | Vertical weight $v(g')$ |
|--------------|---|---|-------------------------------|
| 4 |  |  | 8 |
| |  |  | 2 |
| 5 |  |  | 8 |
| 6 |  |  | 72 |
| |  |  | 18 |
| |  |  | 2 |
| |  |  | 72 |
| |  |  | 36 |
| |  |  | 12 |

As an example of the application of Theorem III, let us compute the vertical weight of the shadow graph, g , of Fig. 4.4, a rather difficult task to compute directly by hand. The dashed curves indicate how the whole graph is to be divided into the single arrow, g_3 , and subgraphs g_1 and g_2 . The graph $g'_1 = g_1 \cup g_3$ has vertical weight $v(g'_1) = 8$ and $g'_2 = g_2 \cup g_3$ has vertical weight $v(g'_2) = 72$. Then by (4.7) $v(g) = 8 \cdot 72 \cdot 9! / 4! 6! = 12096$.

In computer applications, Theorems I and II and the Corollary are always used first to reduce considerably in most cases the effort required to compute the vertical weight. (Theorem III has proved useful in spot checking by hand vertical weights of some of the more complicated graphs.) The shadow graphs then whose vertical weights are calculated directly have all vertices of even degree 4 or higher and of degree 1. The first few of these *elementary shadow graphs* and their vertical weights are listed in Table IV.2.

D. Series expansion results

All coefficients of K^l for $l \leq 11$ in the exact series expansion of the logarithm of the zero field partition function have been obtained for the f.c.c. and b.c.c. lattices (Betts *et al.*, 1969, 1970) in the form of series for $\ln(\Lambda/2)$ where

$$\ln \Lambda = \lim_{N \rightarrow \infty} \frac{1}{N} \ln Z. \quad (4.10)$$

From the series for $\ln \Lambda$ we can readily derive series for the dimensionless energy per site

$$-\frac{E}{NJ} = \frac{\partial}{\partial K} (\ln \Lambda) \quad (4.11)$$

the dimensionless specific heat per site

$$\frac{C}{Nk_B} = K^2 \frac{\partial^2}{\partial K^2} (\ln \Lambda) \quad (4.12)$$

and the dimensionless entropy per site

$$\frac{S}{Nk_B} = -K^2 \frac{\partial}{\partial K} \left(\frac{\ln \Lambda}{K} \right). \quad (4.13)$$

For the f.c.c. lattice the partition function series is

$$\begin{aligned} \ln(\Lambda^F/2) = & 1\frac{1}{2}K^2 + 2K^3 + 2\frac{1}{16}K^4 + 4\frac{1}{2}K^5 + 10\frac{1}{240}K^6 + 31\frac{2}{20}K^7 \\ & + 97\frac{3}{5}\frac{2}{3}\frac{5}{7}\frac{3}{6}K^8 + 313\frac{1}{8}\frac{7}{64}K^9 + 1,025\frac{2}{5}\frac{6}{4}\frac{5}{6}K^{10} + 3,444\frac{3}{5}\frac{3}{3}\frac{7}{2}\frac{1}{2}\frac{1}{4}K^{11} \\ & + \dots \end{aligned} \quad (4.14)$$

From (4.14) and (4.11) the f.c.c. energy is

$$\begin{aligned} -E^F/k_B T = & 3K + 6K^2 + 10\frac{3}{4}K^3 + 22\frac{1}{2}K^4 + 64\frac{7}{40}K^5 + 218\frac{83}{120}K^6 \\ & + 780\frac{5659}{6720}K^7 + 2817\frac{17}{96}K^8 + 10,255\frac{1319}{5040}K^9 + 37,890\frac{46807}{48384}K^{10} \\ & + \dots \end{aligned} \quad (4.15)$$

From (4.14) and (4.12) the f.c.c. specific heat is

$$\begin{aligned} C^F/Nk_B = & 3K^2 + 12K^3 + 32\frac{1}{4}K^4 + 90K^5 + 320\frac{7}{8}K^6 + 1312\frac{3}{20}K^7 \\ & + 5465\frac{859}{960}K^8 + 22,537\frac{5}{12}K^9 + 92,297\frac{199}{560}K^{10} + 378,909\frac{16307}{24192}K^{11} \\ & + \dots \end{aligned} \quad (4.16)$$

From (4.14) and (4.13) the f.c.c. entropy is

$$\begin{aligned} S^F/Nk_B = & \ln 2 - 1\frac{1}{2}K^2 - 4K^3 - 8\frac{1}{6}K^4 - 18K^5 - 53\frac{23}{48}K^6 \\ & - 187\frac{9}{20}K^7 - 683\frac{1819}{7600}K^8 - 2504\frac{17}{108}K^9 - 9229\frac{1373}{5600}K^{10} \\ & - 34,446\frac{8883}{266112}K^{11} - \dots \end{aligned} \quad (4.17)$$

For the b.c.c. lattice the partition function series is

$$\ln(\Lambda^B/2) = K^2 + \frac{7}{8}K^4 + 1\frac{181}{360}K^6 + 5\frac{50213}{80640}K^8 + 21\frac{23893}{28800}K^{10} + \dots \quad (4.18)$$

From (4.18) the b.c.c. energy is

$$-E^B/k_B T = 2K + 3\frac{1}{2}K^3 + 9\frac{1}{60}K^5 + 44\frac{9893}{10080}K^7 + 218\frac{853}{2880}K^9 + \dots \quad (4.19)$$

The b.c.c. specific heat is

$$\begin{aligned} C^B/Nk_B = & 2K^2 + 10\frac{1}{2}K^4 + 45\frac{1}{12}K^6 + 314\frac{1253}{1440}K^8 + 1964\frac{917}{2880}K^{10} \\ & + \dots \end{aligned} \quad (4.20)$$

The b.c.c. entropy is

$$\begin{aligned} S^B/Nk_B = & \ln 2 - K^2 - 2\frac{5}{8}K^4 - 7\frac{37}{72}K^6 - 39\frac{4133}{11520}K^8 - 196\frac{13437}{2880}K^{10} \\ & - \dots \end{aligned} \quad (4.21)$$

The analysis of the series (4.14)–(4.21) is discussed in Section VII in conjunction with series for other properties discussed in Sections V and VI.

V. Susceptibilities and Magnetization Fluctuations

A. Quantities of interest

For the anisotropic Heisenberg model governed by the Hamiltonian (2.1), there are two independent magnetization operators

$$M_{\perp} = m_{\perp} s^{-1} \sum_{\mathbf{r}} S_{\mathbf{r}}^x \quad \text{and} \quad M_{\parallel} = m_{\parallel} s^{-1} \sum_{\mathbf{r}} S_{\mathbf{r}}^z.$$

For the case of $J^{\parallel} > J^{\perp}$ (including the Ising model with $J^{\perp} = 0$) the order parameter is M_{\parallel} , while for $J^{\parallel} < J^{\perp}$ (including the X - Y model with $J^{\parallel} = 0$) the order parameter is M_{\perp} . The critical point is determined as the temperature in zero field above which the order parameter vanishes. Thus, the more interesting of the two magnetizations is that which, for the given anisotropy, corresponds to the order parameter.

Also of interest are the *parallel* and *perpendicular* susceptibilities, $\chi_{\parallel} = \partial M_{\parallel} / \partial H_{\parallel}$, and $\chi_{\perp} = \partial M_{\perp} / \partial H_{\perp}$. Closely related quantities are the magnetization fluctuations,

$$Y_{\parallel} = (\Delta M_{\parallel})^2 = \langle M_{\parallel}^2 \rangle - \langle M_{\parallel} \rangle^2 \quad \text{and} \quad Y_{\perp} = (\Delta M_{\perp})^2 = \langle M_{\perp}^2 \rangle - \langle M_{\perp} \rangle^2.$$

In the limiting case of zero magnetic field, the only case we are considering in detail, the magnetization fluctuations become simply $(\Delta M)^2 = \langle M^2 \rangle$.

It is possible to generate in zero field high temperature series expansions for any of the two susceptibilities and the two fluctuations. For $J^{\parallel} > J^{\perp}$ the parallel susceptibility and fluctuation are expected to diverge at T_c while the perpendicular susceptibility and fluctuation remain finite but have an infinite temperature derivative at T_c (Fisher and Sykes, 1962). For $J^{\parallel} < J^{\perp}$, including the pure X - Y model, perpendicular and parallel quantities interchange roles.

B. Relation between susceptibilities and fluctuations

For the anisotropic Heisenberg model, the Hamiltonian (2.1) is of the form

$$\mathcal{H} = \mathcal{H}_0 - H_{\parallel} M_{\parallel} - H_{\perp} M_{\perp} \quad (5.1)$$

where

$$[M_{\parallel}, \mathcal{H}_0] = 0 \quad (5.2a)$$

but

$$[M_{\perp}, \mathcal{H}_0] \neq 0. \quad (5.2b)$$

Thus in zero perpendicular field, $H_{\perp} = 0$, we have

$$\exp(-\beta \mathcal{H}) = \exp(-\beta \mathcal{H}_0) \exp(\beta H_{\parallel} M_{\parallel}) \quad (5.3a)$$

whereas in zero parallel field

$$\exp(-\beta\mathcal{H}) \neq \exp(-\beta\mathcal{H}_0) \exp(\beta H_{\perp} M_{\perp}). \quad (5.3b)$$

For any operator, A , the thermal expectation value,

$$\langle A \rangle = \text{tr}(A \exp(-\beta\mathcal{H})) / \text{tr} \exp(-\beta\mathcal{H}) \quad (5.4)$$

For $H_{\perp} = 0$, the parallel magnetization

$$\begin{aligned} \langle M_{\parallel} \rangle &\equiv \text{tr}(M_{\parallel} \exp(-\beta\mathcal{H}_0) \exp(\beta H_{\parallel} M_{\parallel})) / \text{tr} \exp(-\beta\mathcal{H}) \\ &= \beta^{-1} (\partial/\partial H_{\parallel}) \ln \text{tr} \exp(-\beta\mathcal{H}). \end{aligned} \quad (5.5)$$

The parallel susceptibility, χ_{\parallel} , is given by

$$\beta^{-1} \chi_{\parallel} = \beta^{-1} \partial \langle M_{\parallel} \rangle / \partial H_{\parallel} = \langle M_{\parallel}^2 \rangle - \langle M_{\parallel} \rangle^2 = Y_{\parallel}, \quad (5.6)$$

the parallel fluctuation, where we again make use of (5.3a).

For $H_{\parallel} = 0$, the perpendicular magnetization

$$\begin{aligned} \langle M_{\perp} \rangle &\equiv \text{tr}(M_{\perp} \exp(-\beta\mathcal{H})) / \text{tr} \exp(-\beta\mathcal{H}) \\ &= \beta^{-1} (\partial/\partial H_{\perp}) \ln \text{tr} \exp(-\beta\mathcal{H}), \end{aligned} \quad (5.7)$$

in spite of (5.3b), when use is made of the property of invariance of the trace of a product of operators under cyclic permutation of the operators. However the analogue of (5.6) does not hold for χ_{\perp} . By directly differentiating the expansion of $\exp(-\beta\mathcal{H})$,

$$\begin{aligned} \beta^{-1} \chi_{\perp} &= \text{tr} M^2 \left[1 - \beta\mathcal{H} + \frac{(\beta\mathcal{H})^2}{2!} - \frac{\beta^2}{6} (\mathcal{H}_0^2 - \mathcal{H}_0 M \mathcal{H}_0 M^{-1}) + \dots \right] / Z \\ &\quad - \langle M \rangle^2 \end{aligned} \quad (5.8)$$

where we have carried the expansion as far as the first correction term.

Alternatively, we may express χ_{\perp} in terms of Kubo's *canonical correlation* (Kubo, 1957) defined by

$$(A, B) = \int_0^{\beta} d\lambda \langle \exp(\lambda\mathcal{H}) A \exp(-\lambda\mathcal{H}) B \rangle - \beta \langle A \rangle \langle B \rangle. \quad (5.9)$$

Consider the Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 - \sum_i \mu_i A_i \quad (5.10)$$

where the A_i are operators which in general do not commute with \mathcal{H}_0 .

Following Okubo and Isihara (1972) we first establish the operator identity.

$$\frac{\partial}{\partial \mu_i} \exp(-\beta \mathcal{H}) = \int_0^\beta \exp(\lambda - \beta) \mathcal{H} A_i \exp(-\lambda \mathcal{H}) d\lambda. \quad (5.11)$$

Let

$$f(\beta, \mu_i) = \exp(\beta \mathcal{H}) \frac{\partial}{\partial \mu_i} \exp(-\beta \mathcal{H}) \quad (5.12)$$

then

$$\frac{\partial}{\partial \beta} f = -\exp(+\beta \mathcal{H}) \frac{\partial \mathcal{H}}{\partial \mu_i} \exp(-\beta \mathcal{H}) = \exp(\beta \mathcal{H}) A_i \exp(-\beta \mathcal{H}). \quad (5.13)$$

Integrating (5.13) we obtain (5.11). Taking the trace of (5.11) and using the cyclic invariance property we obtain

$$\frac{\partial}{\partial \mu_i} Z = \beta \operatorname{tr}[A_i \exp(-\beta \mathcal{H})] \quad (5.14a)$$

or

$$\frac{\partial}{\partial \mu_i} \ln Z = \beta \langle A_i \rangle \quad (5.14b)$$

of which (5.7) is a special case.

Differentiating both sides of (5.14a) with respect to μ_j and using (5.11) again plus the cyclic invariance property of the trace we get

$$\begin{aligned} \frac{\partial^2}{\partial \mu_i \partial \mu_j} Z &= \frac{\partial}{\partial \mu_j} \beta \operatorname{tr}[A_i \exp(-\beta \mathcal{H})] \\ &= \beta \int_0^\beta d\lambda \langle \exp(\lambda \mathcal{H}) A_j \exp(-\lambda \mathcal{H}) A_i \rangle. \end{aligned} \quad (5.15)$$

But differentiating (5.14b)

$$\beta \partial \langle A_i \rangle / \partial \mu_j = (\partial^2 / \partial \mu_i \partial \mu_j) \ln Z = \frac{1}{Z} \frac{\partial^2 Z}{\partial \mu_i \partial \mu_j} - \frac{1}{Z^2} \frac{\partial Z}{\partial \mu_i} \frac{\partial Z}{\partial \mu_j}$$

using (5.15) and (5.14a)

$$\partial \langle A_i \rangle / \partial \mu_j = \int_0^\beta d\lambda \langle \exp(\lambda \mathcal{H}) A_j \exp(-\lambda \mathcal{H}) A_i \rangle - \beta \langle A_i \rangle \langle A_j \rangle = (A_i, A_j) \quad (5.16)$$

or, in the special case of the perpendicular susceptibility,

$$\beta^{-1} \chi_\perp = \beta^{-1} \int_0^\beta \langle \exp(\lambda \mathcal{H}) M_\perp \exp(-\lambda \mathcal{H}) M_\perp \rangle d\lambda - \langle M_\perp \rangle^2. \quad (5.17)$$

C. Equivalence of the perpendicular susceptibility and fluctuation in the critical region

Here we follow the developments of Falk and Bruch (1969) in establishing that χ_{\perp} and Y_{\perp} have the same behaviour in the critical region.

In (15.17) the integrand, $K(\lambda)$, has its maximum for $\lambda = 0$, which establishes an upper bound on χ .

$$\chi_{\perp} \leq \beta K(0) - \beta \langle M_{\perp} \rangle^2$$

or

$$\beta^{-1} \chi_{\perp} \leq \langle M_{\perp}^2 \rangle - \langle M_{\perp} \rangle^2. \quad (5.18)$$

By a somewhat more involved argument Falk and Bruch establish, for $H_{\perp} = 0$, a lower bound on χ_{\perp} also,

$$\frac{\chi_{\perp}}{\beta \langle M_{\perp}^2 \rangle} \geq \frac{1 - \exp(-\beta \bar{\omega})}{\beta \bar{\omega}} \quad (5.19)$$

where

$$\bar{\omega} = d \ln K(\lambda) / d\lambda|_{\lambda=0} = \langle [M_{\perp}, [\mathcal{H}_0, M_{\perp}]] \rangle / \langle M_{\perp}^2 \rangle \quad (5.20)$$

which becomes in the case of the pure X-Y model

$$\bar{\omega} = 2m^2 \langle \mathcal{H}_0 \rangle / \langle M_{\perp}^2 \rangle s^2. \quad (5.21)$$

Now in the critical region $\langle \mathcal{H}_0 \rangle$ remains of order N whereas $\langle M_{\perp}^2 \rangle$ becomes of order N^2 , thus the lower bound in (5.19) tends to unity. The equality of the upper and lower bounds on $\chi_{\perp}/\beta \langle M_{\perp}^2 \rangle$ yields the desired identity of $\beta^{-1} \chi_{\perp}$ and Y_{\perp} in the critical region.

D. Higher order fluctuations

For the same reason that it is simpler to investigate by high temperature series expansions the perpendicular fluctuation than the perpendicular susceptibility it is also simpler to investigate the higher order perpendicular fluctuations than the higher field derivatives of the free energy.

In the critical region we expect the higher order field derivatives of the free energy to behave as follows:

$$\partial^{2n} F / \partial H^{2n}|_{H=0} \sim (T - T_c)^{-\gamma_n}, \quad T > T_c. \quad (5.22)$$

As shown by Domb and Hunter (1965), the homogeneity postulate of scaling theory can be established if

$$\gamma_n = \gamma + 2(n - 1)\Delta \quad (5.23)$$

i.e. if there exists a constant gap exponent, Δ . Thus the higher field derivatives or equivalently the higher order fluctuations are of great theoretical interest.

It is a straightforward combinatorial problem to compute the infinite temperature zero field expectation values of the even powers of the magnetization. Thus we find for either $M = M_{\perp}$ or $M = M_{\parallel}$

$$\langle M^2 \rangle_{\infty} = m^2 N \quad (5.24)$$

$$\langle M^4 \rangle_{\infty} = m^4(3N^2 - 2N) \quad (5.25)$$

$$\langle M^6 \rangle_{\infty} = m^6(15N^3 - 30N^2 + 16N) \quad (5.26)$$

$$\langle M^8 \rangle_{\infty} = m^8(105N^4 - 420N^3 + 588N^2 - 272N). \quad (5.27)$$

....

In order to form, as intensive quantities, higher order fluctuations, Y_n , we must construct combinations of M_x^{2n} of the same degree in m and form linear combinations for which the coefficients of powers of N at $T \rightarrow \infty$ vanish. Thus, we define the following:

$$Y_1 = \langle M_x^2 \rangle / m^2 N \quad (5.28)$$

$$Y_2 = (3\langle M_x^2 \rangle^2 - \langle M_x^4 \rangle) / 2m^4 N \quad (5.29)$$

$$Y_3 = (30\langle M_x^2 \rangle^3 - 15\langle M_x^4 \rangle \langle M_x^2 \rangle + \langle M_x^6 \rangle) / 16m^6 N \quad (5.30)$$

$$Y_4 = (2310\langle M_x^2 \rangle^4 - 1365\langle M_x^4 \rangle \langle M_x^2 \rangle^2 + 147\langle M_x^6 \rangle \langle M_x^2 \rangle - 4\langle M_x^8 \rangle) / 1088m^8 N \quad (5.31)$$

The above Y_n are all normalized so that $Y_n(T \rightarrow \infty) = 1$.

By arguments of the sort described in Subsection C we expect that in the critical region

$$Y_n \sim (T - T_c)^{-\gamma_n}. \quad (5.32)$$

Thus scaling theory for the spin $\frac{1}{2}$ X-Y model could be tested by examining the critical behaviour of the higher order fluctuations.

VI. Expansions for Fluctuations and Susceptibilities

This Section is devoted to techniques for obtaining zero field high temperature expansions for thermodynamic properties of the spin $\frac{1}{2}$ X-Y model. The quantities considered are the order parameter fluctuation, the perpendicular susceptibility, the fourth order fluctuation and the parallel susceptibility. For each quantity we have first a general expansion expression in terms of lattice constants and appropriate vertical and horizontal weights.

Next, a table giving the values of the low order weights is given. By use of the table, an expression in terms of lattice constants only for the first few terms is given. Finally, for each function the explicit high temperature series expansion is quoted for each lattice as far as it is known. For purposes of later comparison the series expansion data for the spin infinity X-Y model are also included.

A. Order parameter fluctuation

The fluctuation of the perpendicular magnetization in zero field has been investigated by Betts and Lee (1968) and Betts, Elliott and Lee (1970) and explicit series worked out for the s.c., b.c.c. and f.c.c. lattices. The general expression for the dimensionless second order fluctuation per site (5.28) can be written

$$Y = \langle M_x^2 \rangle / m^2 N = N^{-1} \sum_{\mathbf{r}, \mathbf{r}'} \langle a_{\mathbf{r}}^\dagger a_{\mathbf{r}'} + a_{\mathbf{r}} a_{\mathbf{r}'}^\dagger \rangle \\ = - \lim_{\lambda \rightarrow 0} \frac{\partial}{\partial \lambda} \ln \text{tr} \exp \left\{ -\beta \left[\mathcal{H}_0 + \lambda \sum_{\mathbf{r}, \mathbf{r}'} (a_{\mathbf{r}}^\dagger a_{\mathbf{r}'} + a_{\mathbf{r}} a_{\mathbf{r}'}^\dagger) \right] \right\} / \beta. \quad (6.1)$$

In geometrical language, the terms in the expansion of Y give rise to ordered directed shadow graphs which differ from the partition function graphs discussed in Section IV by the addition of a single extra (dashed) arrow of arbitrary length which however always appears at the bottom in the vertical order. Otherwise, the same rules as for the partition function apply and, in particular, the definitions of horizontal and vertical weights are the same. The vertical weight theorems need only slight modification due to the fact that the extra arrow is (a) distinguishable (dashed) even when of nearest neighbour length and (b) is always at the bottom in vertical order.

The general expression then for the reduced parallel zero field fluctuation is

$$Y = 1 + 2 \sum_{l=1}^{\infty} \frac{K^l}{l!} \sum_{s=2}^{l+1} 2^{-s} \sum_i (g_{si}; \mathcal{L}) \sum_j h_Y(g_{si}^{(j)}) v_Y(g_{si}^{(j)}). \quad (6.2)$$

Now $g_{si}^{(j)}$ stands for the j th shadow graph, including a dashed arrow, corresponding to the nearest neighbour bare graph g_{si} . The horizontal weight $h_Y(g_{si}^{(j)})$ is the number of ways of constructing a shadow graph of l nearest neighbour arrows and one dashed arrow of arbitrary length corresponding to the bare graph g_{si} . The vertical weight $v_Y(g_{si}^{(j)})$ is the number of allowed vertical arrangements of the l nearest neighbours of the fluctuation shadow graph $g_{si}^{(j)}$. Other symbols have the same meanings as before.

TABLE VI.1. Spin $\frac{1}{2}$ $X-Y$ model perpendicular magnetization fluctuation shadow graphs and their weights

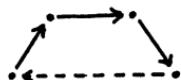
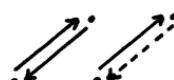
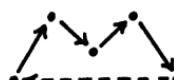
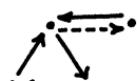
| Order l | Shadow graph g' | Vertical weight $v_Y(g')$ | Horizontal weight $h_Y(g')$ | Bare graph g | Weak f.c.c. lattice constant (g ; f.c.c.) |
|--------------|---|------------------------------|--------------------------------|---|---|
| 1 |  | 1 | 2 |  | 6 |
| 2 |  | 2 | 2 |  | 66 |
| 3 |  | 6 | 2 |  | 702 |
| |  | 2 | 4 |  | 66 |
| |  | 1 | 2 |  | 6 |
| |  | 6 | 4 |  | -69 |
| 4 |  | 24 | 2 |  | 7350 |
| |  | 8 | 6 |  | 220 |
| |  | 8 | 4 |  | 240 |
| |  | 8 | 4 |  | 702 |

TABLE VI.1. (continued)

| Order <i>l</i> | Shadow graph <i>g'</i> | Vertical weight <i>v_Y(g')</i> | Horiz- ontal weight <i>h_Y(g')</i> | Bare graph <i>g</i> | Weak f.c.c. lattice constant (<i>g</i> ; f.c.c.) |
|-------------------|---------------------------|--|---|------------------------|--|
| | | 2 | 4 | | 66 |
| | | 2 | 6 | | 8 |
| | | 4 | 6 | | 8 |
| | | 24 | 4 | | -264 |
| | | 24 | 2 | | -2220 |

In Table VI.1 are contained the vertical and horizontal weights of the decorated shadow graphs which enter the high temperature expansion of the reduced zero field perpendicular fluctuation. This Table is to be compared with Table IV.1 for the partition function.

By use of Table VI.1 in (6.2) for arbitrary lattice we obtain

$$\begin{aligned}
 Y = & 1 + (\swarrow) K + \frac{1}{2}(\nwarrow) K^2 \\
 & + [\frac{1}{4}(\nearrow\nearrow\nearrow) + \frac{1}{3}(\nearrow\nearrow) + \frac{1}{6}(\nearrow) + \frac{1}{2}(\swarrow, \nearrow)] K^3 \\
 & + [\frac{1}{8}(\nearrow\nearrow\nearrow\nearrow) + \frac{1}{4}(\lambda) + \frac{1}{6}(\triangle) + \frac{1}{6}(\nwarrow\nwarrow) \\
 & + \frac{1}{12}(\nwarrow) + \frac{3}{8}(\Delta) + \frac{1}{4}(\Delta, \nearrow) + \frac{1}{6}(\nwarrow, \nearrow)] K^4 + \dots \quad (6.3)
 \end{aligned}$$

To obtain series of useful length, the whole process has been computerized. The same principles have been used as to obtain the partition function series of Section IV. To distinguish the dashed arrow in the adjacency matrix, a negative sign has been used in those cases where the dashed arrow is of

greater than unit length. It is roughly of equal difficulty to obtain the coefficient of K^l in Y as to get the coefficient of K^{l+1} in $\ln \Lambda$. Thus, from this point of view Betts, Elliott and Lee (1970) have gone one step further in obtaining the coefficient of K^{11} in $\ln \Lambda$ than in getting the coefficient of K^9 in Y . Again, the computer calculations have been extensively spot checked as well as checked by hand to K^7 . Thus, we have considerable confidence in their correctness.

The results are for the f.c.c. lattice

$$\begin{aligned} Y^F = 1 + 6K + 33K^2 + 164K^3 + 795\frac{3}{4}K^4 + 3829\frac{5}{8}K^5 + 18,282\frac{1}{2}\frac{3}{4}K^6 \\ + 86,645\frac{1}{6}\frac{3}{7}\frac{1}{2}K^7 + 408,302\frac{4}{5}\frac{2}{6}\frac{3}{0}K^8 + 1,915,573\frac{7}{18}\frac{2}{1}\frac{7}{4}\frac{6}{4}\frac{9}{0}K^9 + \dots \end{aligned} \quad (6.4)$$

For the b.c.c. lattice

$$\begin{aligned} Y^B = 1 + 4K + 14K^2 + 44K^3 + 137\frac{1}{2}K^4 + 425\frac{7}{6}K^5 + 1,302\frac{4}{6}\frac{9}{0}K^6 \\ + 3965\frac{1}{2}\frac{6}{0}\frac{3}{0}\frac{7}{7}K^7 + 11,998\frac{2}{2}\frac{1}{4}\frac{0}{0}K^8 + 36,154\frac{1}{8}\frac{5}{6}\frac{4}{4}\frac{7}{0}K^9 + \dots \end{aligned} \quad (6.5)$$

For the s.c. lattice

$$\begin{aligned} Y^S = 1 + 3K + 7\frac{1}{2}K^2 + 16K^3 + 34\frac{1}{8}K^4 + 74\frac{7}{8}K^5 + 158\frac{7}{16}K^6 \\ + 334\frac{2}{6}\frac{6}{7}\frac{0}{2}K^7 + 701\frac{6}{4}\frac{1}{4}K^8 + 1468\frac{2}{4}\frac{0}{8}\frac{6}{3}\frac{5}{8}K^9 + \dots \end{aligned} \quad (6.6)$$

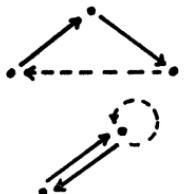
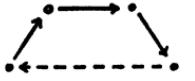
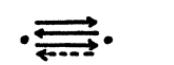
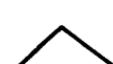
The above series are analysed in Section VII to obtain their critical properties.

B. Perpendicular susceptibility

The perpendicular susceptibility has been investigated by Ditzian (1970). As discussed in Section V, the perpendicular susceptibility does not equal the fluctuation of the perpendicular magnetization. Rather than writing the analogue of (6.1), which would require the establishment of further notation, let us proceed directly to the analogue of (6.2), the graphical expansion.

In geometrical language, the ordered directed shadow graphs corresponding to terms in the high temperature expansion of χ_{\perp} differ from those for the fluctuation in that the dashed arrow of arbitrary length is now slanted vertically. This has the consequence that the vertical weights are different from those for Y . Also, those susceptibility shadow graphs for which head and tail of the dashed arrow occupy the same lattice vertex, "bubble graphs," because solid arrow heads and tails may interleave the dashed arrow head and tail, must be explicitly included.

TABLE VI.2. Spin $\frac{1}{2}$ X-Y model perpendicular susceptibility shadow graphs and their weights

| Order l | Shadow graph g' | Vertical weight $v_{\perp}(g')$ | Horizontal weight $h_{\perp}(g')$ | Bare graph g | Weak f.c.c. lattice constant (g ; f.c.c.) |
|--------------|---|------------------------------------|--------------------------------------|---|---|
| 1 |  | 2 | 2 |  | 6 |
| 2 |  | 6 | 2 |  | 66 |
| |  | 2 | 2 |  | 6 |
| |  | 6 | 1 |  | -12 |
| 3 |  | 24 | 2 |  | 702 |
| |  | 8 | 4 |  | 66 |
| |  | 2 | 2 |  | 6 |
| |  | 24 | 4 |  | -69 |
| |  | 8 | 6 |  | 8 |
| |  | 24 | 2 |  | -24 |

The general graphical expression for the reduced perpendicular susceptibility, $\chi \equiv kT\chi_{\perp}/m^2$, is then

$$\chi = 1 + 2 \sum_{l=1}^{\infty} \frac{K^l}{(l+1)!} \sum_{s=2}^{l+1} 2^{-s} \sum_t (g_{si}; \mathcal{L}) \sum_j h_{\perp}(g_{si}^{(j)}) v_{\perp}(g_{si}^{(j)}). \quad (6.7)$$

The meaning of the symbols in (6.7) is the same as in (6.2) except that the level dashed arrow of the fluctuation has been replaced by the slanted dashed arrow. If $g_{si}^{(j)}$ is not a bubble graph $h_{\perp}(g_{si}^{(j)}) = h_Y(g_{si}^{(j)})$, but the vertical weights are not equal.

In Table VI.2 the perpendicular susceptibility graphs of orders 1, 2 and 3 are illustrated together with their vertical and horizontal weights, the corresponding bare graphs and their f.c.c. lattice constants. This Table is to be compared with Table VI.1. Approximately the same amount of effort is required to obtain the l th term in the expansion of χ as the $l+1$ th term in the expansion of Y . This fact plus the knowledge that the critical behaviour of χ and Y are identical, means that the expansion of χ has not been pursued very far. From Table VI.2 we find for an arbitrary lattice,

$$\begin{aligned} \chi = 1 &+ (\nearrow)K + [\tfrac{1}{2}(\nearrow) + \tfrac{1}{2}(\nwarrow) + \tfrac{1}{4}(\nearrow, \cdot)] K^2 \\ &+ [\tfrac{1}{4}(\nwarrow\nearrow) + \tfrac{1}{3}(\nwarrow) + \tfrac{1}{12}(\nearrow) + \tfrac{1}{2}(\nearrow, \nwarrow) \\ &+ \tfrac{1}{2}(\Delta) + \tfrac{1}{4}(\Delta, \cdot)] K^3 + \dots \end{aligned} \quad (6.8)$$

which may be compared with (6.3).

For the f.c.c. lattice, with the aid of a computer, Ditzian (1970) has found

$$\begin{aligned} \chi^F = 1 &+ 6K + 32K^2 + 161\frac{1}{2}K^3 + 792\frac{3}{10}K^4 + 3823\frac{2}{5}\frac{3}{10}K^5 \\ &+ 18,262\frac{3}{2}\frac{1}{5}K^6 + 86,567\frac{2}{5}\frac{3}{10}K^7 + \dots \end{aligned} \quad (6.9)$$

TABLE VI.3. Ratio of the coefficient of K^l in Y^F to the coefficient of K^l in χ^F

| l | 2 | 3 | 4 | 5 | 6 | 7 |
|-------|---------|---------|---------|---------|---------|---------|
| ratio | 1.03125 | 1.01548 | 1.00435 | 1.00149 | 1.00112 | 1.00090 |

Table VI.3 shows how the ratios of coefficients of Y^F and χ^F rapidly approach unity illustrating for a specific example the general result of Falk and Bruch (1969).

For spin ∞ the perpendicular susceptibility (or equivalently the perpendicular fluctuation since for spin ∞ $[M_{\perp}, \mathcal{H}_0] = 0$) of the $X-Y$ model

has been calculated by Jasnow and Wortis (1968) by the linked cluster method (Wortis, this volume, Chapter 3). For comparison with the spin $\frac{1}{2}$ case, we quote here only the results for the spin infinity *X-Y* model perpendicular susceptibility series for the f.c.c. lattice (Jasnow and Wortis, (1968)) and b.c.c. and s.c. lattices (Ferer, 1972). Note that we have multiplied their K variable by a factor of $\frac{2}{3}$ to convert it into our K variable. For the f.c.c. lattice,

$$\begin{aligned}\chi_{\perp}^F = & 1 + 6K + 33\frac{3}{5}K^2 + 182\frac{2}{25}K^3 + 978\frac{9}{175}K^4 + 5176.87396 \dots K^5 \\ & + 27170.9180 \dots K^6 + 141768.151 \dots K^7 + 736335.734 \dots K^8 \\ & + 3810664.08 \dots K^9 + 19662770.9 \dots K^{10} + \dots\end{aligned}\quad (6.10)$$

For the b.c.c. lattice,

$$\begin{aligned}\chi_{\perp}^B = & 1 + 4K + 14\frac{2}{5}K^2 + 51\frac{1}{25}K^3 + 178.731428 \dots K^4 \\ & + 618.019592 \dots K^5 + 2107.96261 \dots K^6 + 7175.30193 \dots K^7 \\ & + 24240.1060 \dots K^8 + 81772.5738 \dots K^9 \\ & + 274547.165 \dots K^{10} + 920793.62 \dots K^{11} + \dots\end{aligned}\quad (6.11)$$

For the s.c. lattice

$$\begin{aligned}\chi_{\perp}^S = & 1 + 3K + 7\frac{4}{5}K^2 + 20\frac{1}{25}K^3 + 49\frac{4}{5}K^4 + 123.468980 \dots K^5 \\ & + 301.370204 \dots K^6 + 733.486641 \dots K^7 + 1771.30947 \dots K^8 \\ & + 4269.25179 \dots K^9 + 10240.3781 \dots K^{10} \\ & + 24528.4140 \dots K^{11} + \dots\end{aligned}\quad (6.12)$$

The analysis of series (6.10–6.12) is reported in Section VII.

C. Fourth order fluctuation

As we have seen in Section VI.A, it is easier to compute the second order fluctuation of the perpendicular magnetization than the second perpendicular field derivative of the free energy, the perpendicular susceptibility. The computational advantage of computing the fourth order fluctuation of the perpendicular magnetization, rather than the fourth perpendicular field derivative of the free energy, is even greater. It requires roughly the same effort to compute the coefficient of K^{l+2} in the expansion of the former quantity as to compute the coefficient of K^l in the expansion of the latter. Again, by arguments of the Falk–Bruch type, we expect the two fourth order quantities to have the same behaviour in the critical region.

TABLE VI.4. Spin $\frac{1}{2}$ $X-Y$ model fourth order fluctuation graphs with their weights

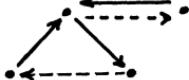
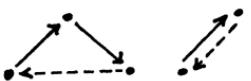
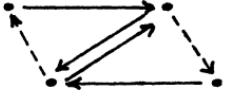
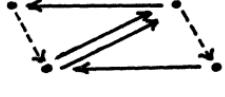
| Order l | Shadow graph g' | Vertical weight $v(g')$ | Horiz- ontal weight $h(g')$ | Bare graph g | Weak f.c.c. lattice constant (g ; f.c.c.) |
|--------------|---|-------------------------------|--------------------------------------|---|---|
| 2 |  | 2 | 4 | / / | -69 |
| |  | 2 | 4 | / / | -69 |
| 3 |  | 2 | 12 |  | 220 |
| |  | 6 | 4 |  | -2220 |
| |  | 6 | 4 |  | -2220 |
| 4 |  | 2 | 2 |  | 702 |
| |  | 4 | 2 |  | 702 |
| |  | 2 | 2 |  | 702 |
| |  | 2 | 2 |  | 702 |
| |  | 4 | 2 |  | 702 |

TABLE VI.4. (continued)

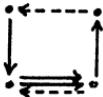
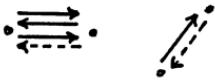
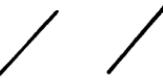
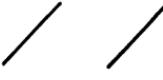
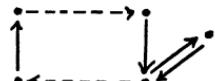
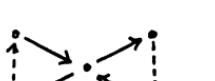
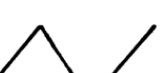
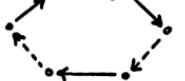
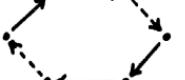
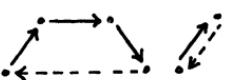
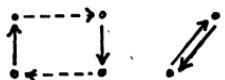
| Order l | Shadow graph g' | Vertical weight $v(g')$ | Horizontal weight $h(g')$ | Bare graph g | Weak f.c.c. lattice constant (g ; f.c.c.) |
|--------------|---|----------------------------|------------------------------|---|---|
| |  | 2 | 2 |  | 702 |
| |  | 4 | 8 |  | -69 |
| |  | 4 | 8 |  | -69 |
| |  | 8 | 8 |  | 6780 |
| |  | 8 | 8 |  | -2220 |
| |  | 8 | 4 |  | 6780 |
| |  | 8 | 12 |  | 495 |
| |  | | |  | -2220 |
| |  | 24 | 4 |  | -30978 |
| |  | 24 | 4 |  | -17580 |

TABLE VI.4. (continued)

| Order <i>l</i> | Shadow graph <i>g'</i> | Vertical weight <i>v</i> (<i>g'</i>) | Horizontal weight <i>h</i> (<i>g'</i>) | Bare graph <i>g</i> | Weak f.c.c. lattice constant (<i>g</i> ; f.c.c.) |
|-------------------|---|---|---|---|---|
| |  | 24 | 4 |  | -30978 |
| |  | 24 | 12 |  | 1292 |
| |  | 24 | 4 |  | -17580 |
| |  | 24 | 12 |  | 1292 |

The general expression for the fourth order fluctuation Y_2 , is given by eqn (5.29). Now, because of the presence of fourth powers of the magnetization, there will be contributions from bare graphs with four odd vertices as well as contributions from bare graphs with two odd vertices. The latter have been dealt with in the expansion of the second order fluctuation. Thus, we concentrate on the new graphs. The new fourth order shadow graphs consist of *l* solid nearest neighbour arrows and two dashed arrows of arbitrary length. In the vertical order, the dashed arrows are fixed at the bottom while the nearest neighbour, solid arrows are permuted among themselves. Let us then define a quantity, *Q*, consisting of the contributions to Y_2 from fourth order bare graphs

$$Q = 6 \sum_{l=2}^{\infty} \frac{K^{l+2}}{l!} \sum_{s=2}^{\infty} 2^{-s} \sum_i (g_{si}; \mathcal{L}) \sum_j h_4(g_{si}^{(j)}) v_4(g_{si}^{(j)}). \quad (6.13)$$

The meaning of the symbols in (6.13) is the same as before but new vertical and horizontal weights must be calculated appropriately.

Table VI.4 contains a list of those fourth order fluctuation shadow graphs of orders 2, 3 and 4 corresponding to bare graphs with four odd

vertices, together with their horizontal and vertical weights. From Table VI.4 we find for arbitrary lattice

$$\begin{aligned} Q = & 3(\swarrow, \nearrow)K^2 + [\tfrac{3}{2}(\lambda) + \tfrac{3}{2}(\nwarrow, \nearrow)]K^3 + [\tfrac{1}{2}(\nwarrow \nearrow \nearrow) + (\swarrow, \nearrow) \\ & + \tfrac{3}{4}(\nwarrow \swarrow) + \tfrac{3}{4}(X) + (\nwarrow, \nearrow) + \tfrac{3}{4}(\nwarrow \nearrow \nearrow, \nearrow) \\ & + \tfrac{3}{4}(\nwarrow, \nwarrow) + \tfrac{9}{4}(\swarrow, \nearrow, \nearrow)]K^4 + \dots \end{aligned} \quad (6.14)$$

The complete fourth order fluctuation series is obtained as

$$Y_2 = 4Y - 3 - Q. \quad (6.15)$$

Again to obtain reliable series of usable length the calculations must be computerized. Ditzian and Betts (1970) have obtained on the f.c.c. lattice all coefficients of Y_2 up to K^6 and Mattingly and Elliott (1973) have added the coefficient of K^7 . The result is

$$\begin{aligned} Y_2^F = & 1 + 24K + 339K^2 + 3656K^3 + 33,176\frac{1}{4}K^4 + 268,835\frac{3}{5}K^5 \\ & + 2010,187\frac{12}{240}K^6 + 14,147,667\frac{19}{20}K^7 + \dots \end{aligned} \quad (6.16)$$

D. Parallel susceptibility

For the $X-Y$ model, the parallel susceptibility is expected to have a weak singularity while the perpendicular (order parameter) susceptibility diverges strongly. In the Ising model, the roles of the two susceptibilities are reversed, and it is known (Sykes and Fisher, 1962; Fisher and Sykes, 1962) that at least in two dimensions and probably in three dimensions the perpendicular susceptibility behaves like the energy. Thus, it is reasonable also to expect that the parallel susceptibility of the $X-Y$ model has an equally weak singularity and hence is difficult to detect from series expansions. Nevertheless, the parallel susceptibility has been investigated by Obokata *et al.*, (1967), Pirnie (1968) and Wood and Dalton (1972) as a special case of the anisotropic Heisenberg model and by Lee (1971) for the pure $X-Y$ model. The results of all other workers are contained in the work of Wood and Dalton, which is valid for arbitrary spin and arbitrary anisotropy. However, if one restricts oneself to the special case of spin $\frac{1}{2}$ and pure $X-Y$ model, certain simplifications arise.

The parallel susceptibility in the limit of zero external field is

$$\chi_{||}^0 = \beta m^2 \sum_{\mathbf{r}, \mathbf{r}'} \text{tr}[\sigma_{\mathbf{r}}^z \sigma_{\mathbf{r}'}^z \exp(-\beta \mathcal{H}_0)] / \text{tr} \exp(-\beta \mathcal{H}_0) \quad (6.17)$$

which leads to the reduced initial parallel susceptibility per site

$$\bar{\chi}_{||}^0 = k_B T \chi_{||}^0 / Nm^2 = - \lim_{\lambda \rightarrow 0} \frac{\partial}{\partial \lambda} \ln \text{tr} \exp \left\{ -\beta \left[\mathcal{H}_0 + \lambda \sum'_{\mathbf{r}, \mathbf{r}'} \sigma_{\mathbf{r}}^z \sigma_{\mathbf{r}'}^z \right] \right\} / \beta \quad (6.18)$$

where the prime on the summation excludes terms with $\mathbf{r} = \mathbf{r}'$.

As the Pauli matrices σ_r^z are traceless, the only terms contributing to $\bar{\chi}_{\parallel}^0$ will be those which also contribute to the free energy per site, but with different weights. Note that

$$\text{tr}(\sigma^z aa^\dagger aa^\dagger \dots) = 1$$

while

(6.19)

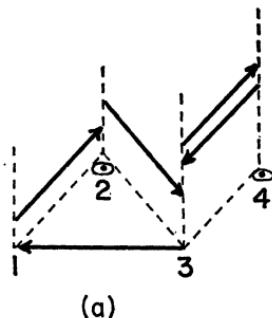
$$\text{tr}(\sigma^z a^\dagger aa^\dagger a \dots) = -1$$

for an alternating sequence of an equal number of annihilation and creation operators. The trace of σ^z times any other sequence of a 's and a^\dagger 's is zero.

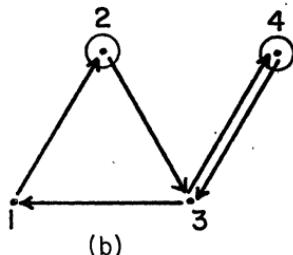
In geometrical terms we must decorate the partition function shadow graphs with two circles corresponding to the two σ^z 's. For example the term in $\Sigma' \sigma_r^z \sigma_r^z \mathcal{H}_0^5$ corresponding to

$$\sigma_2^z \sigma_4^z a_1^\dagger a_3 a_2^\dagger a_1 a_3^\dagger a_2 a_3^\dagger a_4 a_4^\dagger a_3 \quad (6.20)$$

is represented by the decorated shadow graph of Fig. 6.1(b). There will be a number of terms corresponding to this same decorated shadow graph but



(a)



(b)

FIG. 6.1. (a) Ordered directed graph, g'' , corresponding to the term

$$\sigma_2^z \sigma_4^z a_1^\dagger a_3 a_2^\dagger a_1 a_3^\dagger a_2 a_3^\dagger a_4 a_4^\dagger a_3$$

in the high temperature expansion of the parallel susceptibility. (b) Corresponding shadow graph, g' .

TABLE VI.5. Spin $\frac{1}{2}$ X-Y model parallel susceptibility graphs with their weights

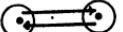
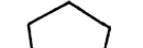
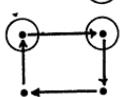
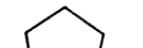
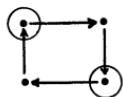
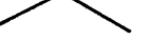
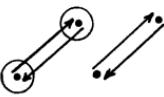
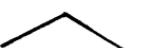
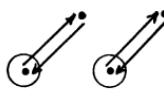
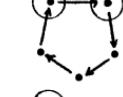
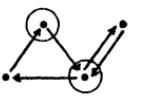
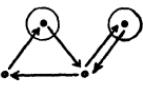
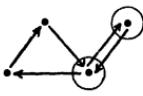
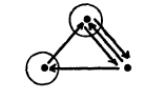
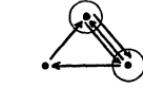
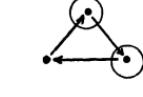
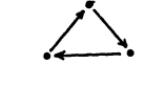
| Order l | Shadow graph g' | Vertical weight $v_{\parallel}(g')$ | Horizontal weight $h_{\parallel}(g')$ | Bare graph g | Weak f.c.c. lattice constant (g ; f.c.c.) |
|--------------|---|--|--|---|---|
| 2 |  | -2 | 1 |  | 6 |
| 3 |  | -2 | 6 |  | 8 |
| 4 |  | -8 | 8 |  | 33 |
| |  | 0 | 4 |  | 33 |
| |  | 0 | 1 |  | 66 |
| |  | -4 | 2 |  | 66 |
| |  | -2 | 1 |  | 6 |
| |  | -24 | 2 |  | -69 |
| |  | 0 | 4 |  | -69 |
| 5 |  | -40 | 10 |  | 168 |
| |  | 0 | 10 |  | 168 |
| |  | -16 | 2 |  | 240 |

TABLE VI.5. (continued)

| Order l | Shadow graph g' | Vertical weight $v_{\parallel}(g')$ | Horiz- ontal weight $h_{\parallel}(g')$ | Bare graph g | Weak f.c.c. lattice constant (g ; f.c.c.) |
|--------------|---|---|--|---|---|
| |  | -8 | 4 |  | 240 |
| |  | -4 | 4 |  | 240 |
| |  | -20 | 2 |  | 240 |
| |  | -2 | 12 |  | 8 |
| |  | -6 | 6 |  | 8 |
| |  | -40 | 6 |  | -264 |
| |  | 0 | 12 |  | -264 |
| |  | -120 | 2 |  | -264 |

differing in the order of the factors. In geometrical terms we again have a number of *ordered decorated shadow graphs*, and the graph corresponding to (6.20) is illustrated in Fig. 6.1(a). However, in computing $\bar{\chi}_{\parallel}^0$ we do not merely count the number of such graphs to find the vertical weight of the underlying decorated shadow graph; we must also take account of whether, immediately above the two decorated vertices, there are on the one hand two arrow heads or two tails (which contribute +1 to the vertical weight) or on the other hand one head and one tail (which contribute -1 to the vertical weight).

The general expression then for the reduced initial parallel susceptibility per site is

$$\bar{\chi}_{\parallel}^0 = 1 + 2 \sum_{l=2}^{\infty} \frac{K^l}{l!} \sum_{s=2}^l 2^{-s} \sum_i (g_{si}; \mathcal{L}) \sum_j h_{\parallel}(g_{si}^{(j)}) v_{\parallel}(g_{si}^{(j)}) \quad (6.21)$$

where now $g_{si}^{(j)}$ stands for the j th decorated shadow graph corresponding to the bare graph g_{si} , the parallel susceptibility horizontal and vertical weights h_{\parallel} and v_{\parallel} have been defined above and other symbols have the same meaning as before.

Table VI.5 contains the vertical and horizontal weights of the decorated shadow graphs which enter the initial parallel susceptibility high temperature expansion. This table is the analogue of Table IV.1 for the partition function and Table VI.2 below for the perpendicular fluctuation.

Using Table VI.5 in (6.21) we obtain for an arbitrary lattice

$$\begin{aligned} \bar{\chi}_{\parallel}^0 = & 1 - \frac{1}{2}(\diagup)K^2 - \frac{1}{2}(\Delta)K^3 - \{ \frac{1}{3}(\square) + \frac{1}{4}(\diagup, \diagdown) + \frac{1}{12}(\diagup\diagdown) \\ & + \frac{1}{24}(\diagup)\}K^4 - \{ \frac{5}{24}(\square\square) + \frac{1}{4}(\Delta, \diagup) + \frac{1}{8}(\diagup\diagdown\diagup) \\ & + \frac{1}{8}(\Delta)\}K^5 + \dots \end{aligned} \quad (6.22)$$

For the special case of the f.c.c. lattice (6.22) becomes

$$\bar{\chi}_{\parallel}^0 = 1 - 3K^2 - 4K^3 + \frac{1}{2}K^4 + 0K^5 + \dots \quad (6.23)$$

To make further progress it is again more efficient to use vertical weight theorems and to computerize the operations as much as possible. Theorem I of Section IV holds for decorated shadow graphs which are unaltered except that the appropriate parallel susceptibility vertical weights must be used. Theorems II and III also apply except that the common vertices must not be decorated vertices.

Without using a computer, Lee (1971) has extended (6.22) by two terms. With the aid of a computer and using techniques very similar to those found useful in obtaining the partition function expansion, it should be feasible to add about four more terms to Lee's series. This has not yet been done, largely because for the $X-Y$ model the parallel susceptibility is the less interesting susceptibility as it is expected to remain finite everywhere.

VII. Critical Properties from Analysis of Series*

In this Section we consider analyses which yield direct estimates of critical temperatures, critical exponents and critical amplitudes for the

* For a general survey see Gaunt and Guttman, this volume, Chapter 4.

various series listed in previous sections. Indirect estimates made with the use of scaling theory are reserved for Section VIII.

A. Critical points and the critical exponent γ from fluctuations

Experience has shown that the zero field (initial) high temperature expansion of the susceptibility yields, for a constant amount of effort, more accurate and more precise estimates of the critical temperature than any of the other commonly calculated series expansions. As noted in Section VI, it is easier to compute the fluctuation series, and so the fluctuation series (6.4)–(6.6) are those we examine first.

The oldest method of analysis of exact series expansions, to determine the nature of a dominant singularity on the real axis, is the ratio method (Domb and Sykes, 1957).

Assume that for the function of interest, $F(K)$, we know the values of the first L coefficients in the expansion

$$F(K) = \sum_{n=0}^{\infty} a_n K^n. \quad (7.1)$$

For many of the functions of interest, their behaviour in the critical region, $K_c - K \equiv \Delta K \ll K_c$, is known or believed to be

$$F(K) \sim A(1 - K/K_c)^{-\varepsilon} + \phi(K) \quad (7.2)$$

where K_c is the critical point, ε the critical exponent and A the critical amplitude. $\phi(K)$ is less singular in the neighbourhood of K_c . If K_c is the singularity nearest to the origin in the complex K plane then the asymptotic behaviour of the ratios is

$$\frac{a_n}{a_{n-1}} \sim \frac{1}{K_c} \left(1 + \frac{\varepsilon - 1}{n} \right). \quad (7.3)$$

The ratio method consists of plotting a_n/a_{n-1} versus $1/n$ and using the “best” line through the points to estimate K_c from the intercept and then ε from the slope.

Applying the ratio method to (6.4) Betts, *et. al.* (1970) have estimated that for the f.c.c. lattice

$$\gamma = 1.335 \pm 0.020. \quad (7.4)$$

This plot is reproduced in Fig. 7.1. Estimates for the other lattices are consistent with this γ value but somewhat less precise. Corresponding ratio estimates of K_c^{-1} are given in Table VII.1 (first line).

TABLE VII.1. Ratio estimates of the dimensionless critical temperatures $kT_c/J \equiv K_c^{-1}$, for the spin $\frac{1}{2}$ X-Y model

| Lattice | f.c.c. | b.c.c. | s.c. |
|---------------------------|-------------------|-------------------|-------------------|
| K_c^{-1} | 4.523 ± 0.010 | 2.908 ± 0.020 | 2.020 ± 0.020 |
| $K_c^{-1} (\gamma = 4/3)$ | 4.524 ± 0.010 | 2.906 ± 0.020 | 2.016 ± 0.020 |

If we now assume γ known the modified ratios $na_n/(n + \gamma - 1)a_{n-1}$ should tend to K_c^{-1} with zero slope as $1/n \rightarrow 0$. The second line of Table VII.1 lists the values of K_c^{-1} by this latter ratio method assuming $\gamma = \frac{4}{3}$.

An alternative to the ratio method is the method of Padé approximants introduced to the world of critical phenomena by Baker (1961). In this method the function to be studied is approximated by a Padé approximant, which is the ratio of two polynomials of degree N and D , respectively. The coefficients in the Padé approximant, $[N, D]$, are chosen so as to agree in series expansion with the first $L + 1 = N + D$ coefficients in the expansion of the approximated function. As the Padé approximant has only simple

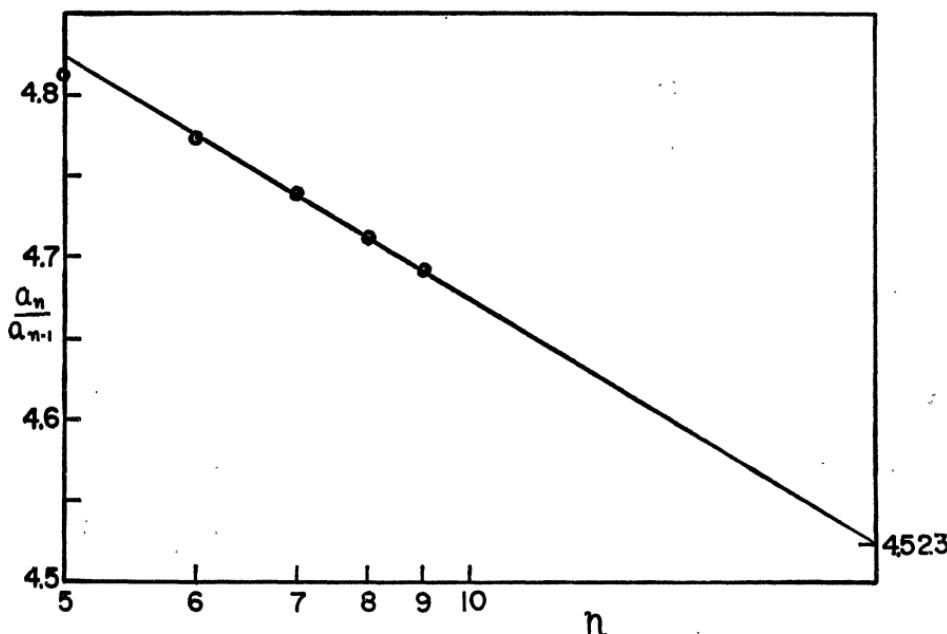


FIG. 7.1. Ratios of coefficients, a_n/a_{n-1} , for the series for the fluctuation in the long range order versus $1/n$. $K_c^{-1} \approx 4.523$ is indicated. (After Betts *et al.*, 1970).

poles and zeros it is usually applied not to the original function of interest but to a related function expected to have a simple pole at the critical point.

We therefore first examine Padé approximants to

$$(d/dK) \log Y(K) \quad (7.5)$$

for each of the three lattices. The poles of (7.5) give estimates of K_c and the residues estimates of γ . Table VII.2 gives estimates of the critical point and critical exponent (in brackets) for the f.c.c. lattice from poles and residues of Padé approximants to (7.5). We see that the results are consistent with the ratio method but more scattered.

TABLE VII.2. Estimates of K_c and in brackets γ for the spin $\frac{1}{2}$ $X-Y$ model on the f.c.c. lattice from the poles and residues respectively of Padé approximants to $(d/dK) \log Y(K)$

| D | $N = 2$ | $N = 3$ | $N = 4$ | $N = 5$ | $N = 6$ |
|-----|--------------------|--------------------|--------------------|--------------------|--------------------|
| 2 | | | 0.22513 (1.523) | 0.22203 (1.381) | 0.22047 (1.306) |
| 3 | | 0.21937 (1.272) | 0.22064 (1.318) | 0.22105 (1.337) | |
| 4 | 0.22136 (1.359) | 0.22302 (1.464) | 0.22135 (1.353) | | |
| 5 | 0.22199 (1.393) | 0.22193 (1.390) | | | |
| 6 | 0.22193 (1.390) | | | | |

If however the value of γ is known, Padé approximant estimates to K_c can be obtained by examining $[Y(K)]^{1/\gamma}$, which also should have a simple pole at K_c . Again $[(d/dK)Y(K)]^{1/\gamma+1}$ should have a simple pole at K_c . If the wrong value of γ is assumed, then the estimates of K_c from the above two functions will not agree. Betts *et al.*, (1970) have exploited this feature to estimate γ as that value for which the two above functions give consistent values of K_c . In this way they found $\gamma = 1.34 \pm 0.02$.

Thus, it is very suggestive from both ratio and Padé approximant methods that γ has the simple fractional value, $\gamma = \frac{4}{3}$. If so, then the most precise Padé approximant values of K_c can be found by examining $[Y(K)]^{1/\gamma}$. Such estimates for the f.c.c., b.c.c and s.c. lattices are tabulated in Tables VII.3, VII.4 and VII.5, respectively. From these Tables we adopt for further analysis as "best" values for K_c those listed in Table VII.6.

TABLE VII.3. Estimates of K_C for the spin $\frac{1}{2}$ X-Y model on the f.c.c. lattice from Padé approximants to $[Y(K)]^{3/4}$

| D | $N = 2$ | $N = 3$ | $N = 4$ | $N = 5$ | $N = 6$ | $N = 7$ |
|-----|----------|----------|----------|----------|----------|----------|
| 2 | | | | 0.220815 | 0.221013 | 0.220989 |
| 3 | | 0.220978 | | 0.220959 | | 0.220986 |
| 4 | | 0.220968 | 0.220954 | 0.220969 | | |
| 5 | 0.221059 | 0.220955 | 0.220965 | | | |
| 6 | 0.220991 | 0.220982 | | | | |
| 7 | 0.220983 | | | | | |

TABLE VII.4. Estimates of K_C for the spin $\frac{1}{2}$ X-Y model on the b.c.c. lattice from Padé approximants to $[Y(K)]^{3/4}$

| D | $N = 2$ | $N = 3$ | $N = 4$ | $N = 5$ | $N = 6$ | $N = 7$ |
|-----|---------|---------|---------|---------|---------|---------|
| 2 | | | | 0.34390 | 0.34389 | 0.34406 |
| 3 | | 0.34385 | | 0.34389 | | 0.34390 |
| 4 | | 0.34370 | 0.34389 | 0.34378 | | |
| 5 | 0.34410 | 0.34370 | 0.34406 | | | |
| 6 | 0.34410 | 0.34391 | | | | |
| 7 | 0.34405 | | | | | |

TABLE VII.5. Estimates of K_C for the spin $\frac{1}{2}$ X-Y model on the s.c. lattice from Padé approximants to $[Y(K)]^{3/4}$

| D | $N = 2$ | $N = 3$ | $N = 4$ | $N = 5$ | $N = 6$ | $N = 7$ |
|-----|---------|---------|---------|---------|---------|---------|
| 2 | | | | 0.4955 | 0.4977 | 0.4837 |
| 3 | | 0.4959 | | 0.4956 | | 0.4954 |
| 4 | | 0.4959 | 0.4960 | 0.4952 | | |
| 5 | 0.4960 | 0.4953 | 0.4951 | | | |
| 6 | 0.4957 | 0.4951 | | | | |
| 7 | 0.4955 | | | | | |

TABLE VII.6. Best estimates of critical point and amplitude of the critical fluctuation for the spin $\frac{1}{2}$ X-Y model

| Lattice | f.c.c. | b.c.c. | s.c. |
|------------|---------------------|---------------------|-------------------|
| K_C | 0.2210 ± 0.0005 | 0.3440 ± 0.0010 | 0.495 ± 0.002 |
| K_C^{-1} | 4.525 | 2.907 | 2.02 |
| C | 1.012 | 1.016 | 1.095 |

Finally, we are interested in estimates of the critical amplitudes, C , in

$$Y \sim C(1 - K/K_c)^{-\gamma}$$

which are obtained from the residues of the singularities of $[Y(K)]^{1/\gamma}$. The best estimates of C are also listed in Table VII.6.

B. Specific heat singularity, critical entropy and critical energy

Specific heat series are notoriously difficult to analyse; the $X-Y$ model series are no exception. As $X-Y$ model specific heat series on loose packed lattices contain only even powers of K we concentrate our analysis on series (4.16) for the f.c.c. lattice.

A ratio plot displays a long period large amplitude oscillation which prevents any precise estimate of the specific heat critical exponent α in

$$C/Nk_B \sim A(1 - K/K_c)^{-\alpha} + \phi(K). \quad (7.6)$$

Certain conformal transformations succeed in reducing but not in eliminating the oscillation (Lothian, 1972), and at best such studies indicate that $\alpha = 0.05 \pm 0.15$.

Padé approximant analysis of the logarithmic derivative of the specific heat and/or its derivatives also give very ragged results. However, there is good reason to believe (see below) that the specific heat may have a logarithmic singularity.

Following Betts and Lothian (1973), we assume

$$C/Nk_B \sim -A \log(1 - K/K_c) + \phi(K) \quad (7.7)$$

where the non-singular term is

$$\phi(K) = \sum_l B_l (1 - K/K_c)^l. \quad (7.8)$$

If $\phi(K)$ is nearly constant near K_c , the $B_l \ll 1$ for $l \neq 0$, and temperature derivatives of C will be more suitable objects for Padé analysis than C itself. Such turns out to be the case for the spin $\frac{1}{2}$ $X-Y$ model (but not for the spin $\frac{1}{2}$ Ising model!).

Anyway, if $B_1 \approx 0$, then dC/dK has a simple pole and Padé approximants to $d(C/Nk_B)/dK$ should give estimates of K_c in agreement with the values obtained from the analysis of the fluctuation series. The result of such analysis are given in Table VII.7. Also included are the residues, which provide estimates of A .

The agreement between the Table VII.7 estimates of K_c and the best value from the fluctuation series analysis, $K_c = 0.2210$, is quite gratifying.

By replacing the logarithmic singularity in (7.7) by a power with exponent α and examining $[d(C/Nk_B)/dK]^{1/1+\alpha}$ Betts and Lothian (1973) conclude that $\alpha = 0.02 \pm 0.05$. Accepting therefore the logarithmic singularity Table VII.7 gives $A = 0.255 \pm 0.015$ for the amplitude in (7.7).

TABLE VII.7. Estimates of K_C from Padé approximants to $(d/dK) C/Nk$

| Degree | Approximant [N, D] | Pole K_C | Residue AK_C |
|--------|-----------------------|---------------|-------------------|
| 10 | [4, 6] | 0.2199 | 0.2510 |
| | [5, 5] | 0.2199 | 0.2365 |
| | [6, 4] | 0.2208 | 0.2548 |
| | [7, 3] | 0.2205 | 0.2547 |
| 9 | [3, 6] | 0.2201 | 0.2583 |
| | [4, 5] | 0.2200 | 0.2586 |
| | [5, 4] | 0.2111 | 0.2533 |
| | [6, 3] | 0.2219 | 0.2546 |
| 8 | [3, 5] | 0.2198 | 0.2542 |
| | [4, 4] | 0.2176 | 0.2516 |
| | [5, 3] | 0.2181 | 0.2596 |
| | [6, 2] | 0.2096 | 0.2554 |

It is then possible to evaluate the B_l by evaluating at K_C Padé approximants to the difference series,

$$B_l(K) = (d/dK)^l [C/Nk + A \ln(1 - K/K_C)]. \quad (7.9)$$

Betts and Lothian (1973) have estimated the first four B_l . In particular they find $B_0 = -0.1901 \pm 0.002$, a value which can be compared with experiment. They also find $B_1 = -0.051$, in support of the original conjecture that $|B_1| \ll 1$. In contrast, the analogous quantity for the spin $\frac{1}{2}$ Ising model on the f.c.c. lattice has the value $B_1 = -1.67$, indicating why analysis of the above type fails for the Ising model.

For all ordering spin $\frac{1}{2}$ models, the dimensionless entropy per site, S/Nk_B , increases from its value of zero at zero temperature to $\ln 2$ at infinite temperature. It is of some theoretical as well as experimental interest to find the value of the entropy at the critical temperature. We obtain estimates of the critical entropy by evaluating at T_C Padé approximants to S/Nk_B obtained using the series (4.17) and (4.21). The estimates from analysis of the series for the b.c.c. lattice are rather scattered; the estimates for the f.c.c. lattice are well converged however. The results are listed in Table VII.8 with for comparison the results for the spin $\frac{1}{2}$ Ising and Heisenberg models. As expected the $X-Y$ ($D = 2$) result is near the mean of the Ising ($D = 1$) and Heisenberg ($D = 3$) results.

Although of lesser theoretical interest we also include estimates of the critical energy, $-E/Nk_B T_C$ in Table VII.8. These values were obtained in the same way as the critical entropy estimates using the energy series (4.15) and (4.19).

TABLE VII.8. Critical entropy, S_C/Nk_B , and in brackets, critical energy, $-E_C/Nk_B T_C$ for the spin $\frac{1}{2}$ Ising, $X-Y$ and Heisenberg models

| Lattice | Ising ¹ | $X-Y$ | Heisenberg ² |
|---------|----------------------|------------------|-------------------------|
| f.c.c. | 0.59023 (0.15155) | 0.518 (0.283) | 0.45 (0.87) |
| b.c.c. | 0.58203 (0.17201) | 0.52 (0.25) | 0.45 (0.92) |
| s.c. | 0.55793 (0.21996) | | 0.43 (1.20) |

¹ Sykes *et al.* (1972). Domb this volume, Chapter 6.

² Rushbrooke, *et al.* this volume, Chapter 5.

It is also of interest to see the actual shape of the specific heat curves. To plot the curves for the spin $\frac{1}{2}$ Ising and $X-Y$ models we have first formed the difference series for the non-singular part, $\phi(K)$, given by

$$\phi(K) = \begin{cases} C/Nk_B - A_I(1 - K/K_C)^{-1/8} & (\text{Ising}) \\ C/Nk_B + A_{XY} \ln(1 - K/K_C) & (X-Y) \end{cases} \quad (7.10)$$

Next we have formed Padé approximants to $\phi(K)$ and evaluated them

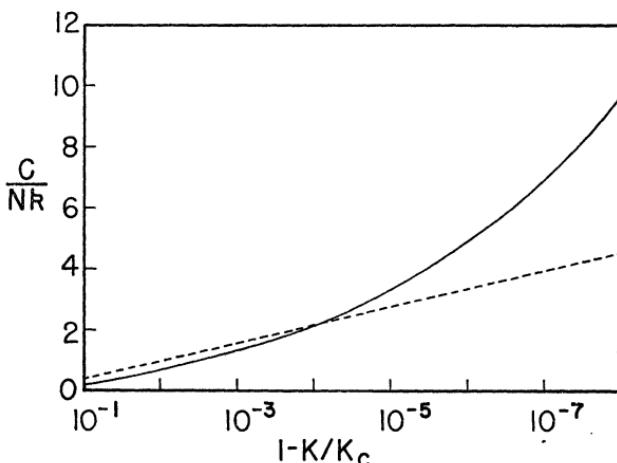


FIG. 7.2. Specific heat of the spin $\frac{1}{2}$ $X-Y$ model (dashed curve) compared with the specific heat of spin $\frac{1}{2}$ Ising model (solid curve) on the f.c.c. lattice.

for the range $0 < K < K_c$ for each model. Then the singular part is evaluated and added to $\phi(K)$ to form values for plotting the specific heat. The resulting specific heat curves are displayed in Fig. 7.2. Observe the sharper peaking in the Ising model versus the larger area enclosed under the $X-Y$ curve.

C. Analysis of fourth order fluctuations

Although a proof has not yet been supplied it seems clear that just as the perpendicular susceptibility, $\partial^2 F / \partial H^2 \equiv \chi_{\perp}$, and the second order fluctuation, Y_{\perp} , become asymptotically identical (apart from a constant) in the critical regions, so will the fourth derivative of the free energy, $\partial^4 F / \partial H^4$, and the fourth order fluctuation, Y_2 . Here we report estimates of the critical exponent, γ_2 , and the critical amplitude, C_2 , for the f.c.c. lattice in

$$Y_2 \sim C_2(1 - K/K_c)^{-\gamma_2} \quad (7.11)$$

where we take K_c as given from the analysis of Y above.

First, a standard ratio plot gives points which are not yet completely linear and leads to an estimate of $K_c^{-1} = 4.40$ versus the best estimate of $K_c^{-1} = 4.525$. Accordingly the companion estimate of γ_2 must be regarded as too high. Padé approximants to the logarithmic derivative of Y_2 yield rather scattered results for K_c and γ_2 which, however, are nearly linearly related. Taking the accepted value of K_c yields the corresponding value of $\gamma_2 = 4.54 \pm 0.15$.

Given the value of K_c , an alternative ratio method is to extrapolate the estimates

$$\gamma_2(n) = [(a_n/a_{n-1})K_c - 1]n + 1 \quad (7.12)$$

on a $1/n$ plot to $1/n = 0$. Such a plot is illustrated in Fig. 7.3 from which $\gamma_2 = 4.71 \pm 0.05$.

We may estimate K_c from Padé approximants to $[Y_2(K)]^{1/\gamma}$ for a set of γ_2 and pick the correct γ_2 as that which best reproduces the known K_c . In this way we estimate $\gamma_2 = 4.61 \pm 0.20$.

It would be highly desirable, but very laborious, to have more terms in the series (6.16) for Y_2 . At present, we adopt $\gamma_2 = 4.65 \pm 0.10$ as our best estimate of γ_2 . If γ_2 is a simple fraction, then $\gamma_2 = 14/3$ is a likely value.

Finally, assuming $\gamma_2 = 14/3$, we estimate the amplitude C_2 from the residues of the Padé approximants to $[Y_2(K)]^{+3/14}$. The poles of this function give estimates to K_c and the residues give estimates to $C_2^{3/14}K_c$.

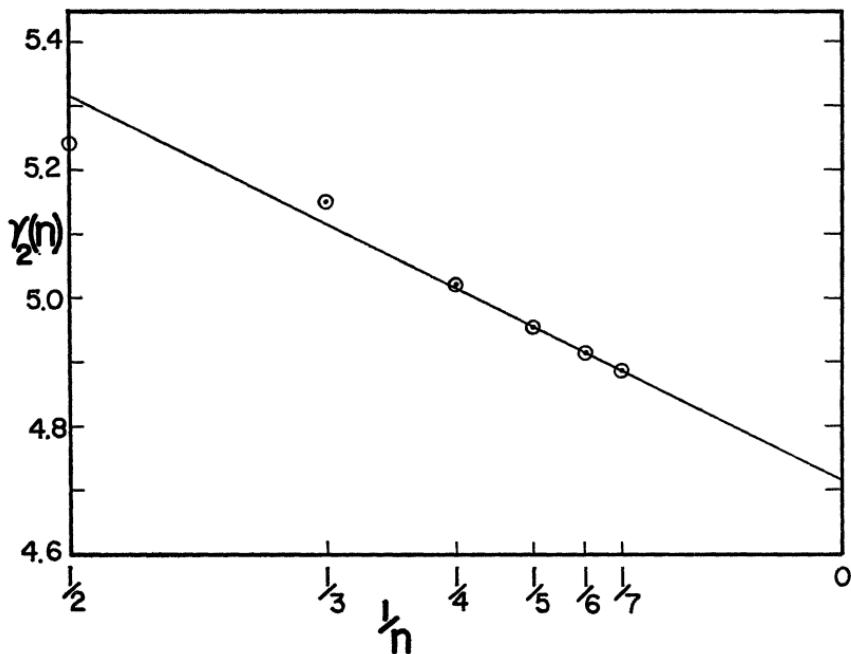


FIG. 7.3. For the fluctuation, $Y_2(K)$, on the f.c.c. lattice are plotted the critical exponent estimates $\gamma_2(n) = [(a_{2,n}/a_{2,n-1})K_c - 1]n + 1$ versus $1/n$.

Again, there is considerable scatter among the approximants but again they form a rather smooth curve. Taking the point on the curve corresponding to the accepted value of K_c gives $C_2 = 1.78 \pm 0.10$ for the f.c.c. lattice.

D. Spin infinity model

Unlike either the spin ∞ Heisenberg model on the one hand or the spin $\frac{1}{2} X-Y$ model on the other hand the spin $\infty X-Y$ model does not seem to be of direct experimental interest. The model is however of theoretical interest for tests of scaling theory and universality.

Jasnow and Wortis (1968) have reported an analysis of the perpendicular susceptibility series using ratio methods, Padé approximants and Neville tables to estimate $\gamma = 1.32 \pm 0.01$. Within the confidence limits, this estimate agrees with the spin $\frac{1}{2} X-Y$ model for γ . Thus, universality or at least spin independence of γ seems to be indicated. However, more recently

Grover (1972) using renormalization methods has found for the spin ∞ X-Y model the lower value $\gamma = 1.29$. This estimate is not consistent with the spin $\frac{1}{2}$ X-Y value and calls universality into question.

TABLE VII.9. Estimates of the critical point, K_C , and critical amplitude, C , of the perpendicular susceptibility for the spin ∞ X-Y model assuming $\gamma = \frac{4}{3}$

| | f.c.c. | b.c.c. | s.c. |
|-------|-------------------|-------------------|-------------------|
| K_C | 0.200 ± 0.001 | 0.307 ± 0.001 | 0.429 ± 0.003 |
| C | 0.805 ± 0.005 | 0.808 ± 0.005 | 0.860 ± 0.020 |

Nevertheless, assuming the universal value of $\gamma = \frac{4}{3}$ for the X-Y model for all s , Table VII.9 lists the values of critical temperatures and amplitudes for the spin ∞ X-Y model on the s.c., b.c.c. and f.c.c. lattices as estimated from poles and residues of $[\chi_{\perp}(K)]^{3/4}$. These estimates may be compared with the corresponding estimates for the spin $\frac{1}{2}$ X-Y model as given in Table VII.6, which shows that the critical temperatures for the spin ∞ model are slightly higher than for the spin $\frac{1}{2}$ X-Y model on the same lattice.

VIII. Critical Properties from Scaling Relations*

In this Section the results obtained directly from the series analysis of Section VII are used to obtain supplementary results using scaling theory. Ordinary scaling theory is used to obtain values for further critical exponents while lattice-lattice scaling theory yields additional critical amplitude estimates.

A. Scaling theory for critical exponents

Ordinary scaling theory for bulk properties in the critical region (Widom, 1965; Domb and Hunter, 1965; Kadanoff, 1966; Kadanoff *et al.*, 1967; Patashinskii and Pokrovskii, 1966; Griffiths, 1967) may be stated in terms of the magnetization, M , magnetic field H , and reduced temperature $\varepsilon = (T - T_C)/T_C$. To oversimplify somewhat, instead of regarding $M = M(H, \varepsilon)$ (or $H = H(M, \varepsilon)$) as a function of the two independent variables, two new variables, x and y say, are constructed from M , H and ε such that $y = y(x)$ or $x = x(y)$. x and y may be taken to be any two of M/ε^{β} , H/M^{δ} and H/ε^{Δ} where $\Delta = \beta\delta$. Actually, care must be taken with regard to signs of M , H and ε and it must be noted that the relations apply

* See also Domb, this volume, Chapter 6, Section IIIc.

only to the most singular parts of the functions. A thorough review of scaling may be found in a companion chapter (Vicentini-Missoni Vol. 2, Chapter 2).

For example, to obtain relations at zero field for $T > T_c$, assume

$$M \sim \varepsilon^\beta f(H/\varepsilon^\Delta). \quad (8.1)$$

Then differentiating with respect to field once

$$\chi \sim \begin{cases} \varepsilon^{-\gamma} & \text{by definition} \\ \varepsilon^{\beta-\Delta} & \text{by scaling} \end{cases}, \quad H = 0 \quad (8.2)$$

and twice more

$$\frac{\partial^2 \chi}{\partial H^2} \sim \begin{cases} \varepsilon^{-\gamma_2} & \text{by definition} \\ \varepsilon^{\beta-3\Delta} & \text{by scaling} \end{cases}, \quad H = 0. \quad (8.3)$$

In other words the scaling identities

$$\Delta = \gamma + \beta \quad (8.4)$$

and .

$$\gamma_2 = \gamma + 2\Delta \quad (8.5)$$

have been established.

Integrating (8.1) with respect to field and then differentiating twice with respect to temperature establishes the specific heat behaviour.

$$C \sim \begin{cases} \varepsilon^{-\alpha} & \text{by definition} \\ \varepsilon^{\beta+\Delta-2} & \text{by scaling} \end{cases}, \quad H = 0 \quad (8.6)$$

i.e.

$$\alpha = 2 - \Delta - \beta. \quad (8.7)$$

Combining (8.4), (8.5) and (8.7) yields the scaling relation,

$$\gamma_2 + \alpha - 2\gamma = 2. \quad (8.8)$$

For the spin $\frac{1}{2}$ X-Y model we now have a direct test of relation (8.8). Using the estimates $\gamma_2 = 4.65 \pm 0.10$, $\gamma = 1.33 \pm 0.02$, $\alpha = 0.02 \pm 0.05$ the left side of (8.8) becomes 2.01 ± 0.12 . Thus we have one piece of evidence in support of scaling for the spin $\frac{1}{2}$ X-Y model.

When we turn from bulk properties to correlations we have the scaling relation (Kadanoff *et al.*, 1967; Fisher, 1967)

$$\Gamma(r, \varepsilon, h) \sim r^{-d+2-\eta} G(\varepsilon r^{1/\nu}, h/\varepsilon^\Delta). \quad (8.9)$$

According to scaling theory

$$\nu = (2 - \alpha)/d. \quad (8.10)$$

which for the logarithmic divergence of the $d = 3$ X-Y model gives $\nu = \frac{2}{3}$ in good agreement with the direct estimates of Jasnow and Wortis (1968) from analysis of the second moment of the correlations for the spin ∞ X-Y model, in agreement with universality.

We have seen that the set of four critical exponents α , γ , γ_2 and ν directly calculated for the X-Y model seem to satisfy scaling theory, in which there are only 2 independent exponents. Thus we adopt the simple fractional values $\alpha = 0$, $\gamma = \frac{4}{3}$, consistent with our direct estimates, and using scaling theory present a complete set of critical exponents in Table VIII.1.

TABLE VIII.1. Scaling theory values of X-Y model critical exponents consistent with numerical estimates

| Exponent | $\alpha = \alpha'$ | $\gamma = \gamma'$ | $\nu = \nu'$ | Δ | β | η |
|----------|--------------------|--------------------|--------------|----------|---------|--------|
| Value | 0 | 4/3 | 2/3 | 5/3 | 1/3 | 0 |

B. Scaling theory for critical amplitude ratios

Not only critical exponents but also ratios of critical amplitudes on two different lattices are objects which can be related for one thermodynamic function to their values for two other functions by scaling theory (Watson, 1969a, 1969b; Betts *et al.*, 1971). The basic postulate of the lattice-lattice scaling theory expressed in terms of the reduced temperature, ε , dimensionless magnetic field, $h = mH/kT_C$, magnetization, $m(T, H)/M(0, 0 +)$ is

$$m_X(\varepsilon_X, h_X) = m_Y(\varepsilon_Y, h_Y) \quad (8.11)$$

for lattices X and Y where the temperature and field variables are scaled by,

$$n_X h_X = n_Y h_Y \quad (8.12)$$

$$g_X \varepsilon_X = g_Y \varepsilon_Y. \quad (8.13)$$

By use of (8.11)–(8.13), it is straightforward to express any amplitude ratio in terms of powers of the ratios of the parameters n_X and g_X . If we also assume the exponent scaling relations such expressions become particularly simple.

For example, the ratio of susceptibility amplitudes.

$$C_X/C_Y = (n_X/n_Y)(g_Y/g_X)^\gamma \quad (8.14)$$

while the specific heat amplitudes satisfy

$$A_X/A_Y = (n_Y/n_X)(g_X/g_Y)^{2-\alpha}. \quad (8.15)$$

Unfortunately, for the $X-Y$ model we only know the critical amplitudes of the susceptibility (order parameter fluctuation) on lattices other than the f.c.c. so we cannot yet test lattice-lattice scaling on the $X-Y$ model. However, lattice-lattice scaling has been fully verified for other models so this could be utilised to predict additional amplitudes; but we cannot yet do even this for the $X-Y$ model without an additional assumption.

Betts *et al.* (1971) introduced a further independent hypothesis, which is by no means established, but which is in agreement with the present scanty evidence. The additional hypothesis is that one of the two critical parameters, the spin density parameter n_X , is independent of the model. (In contrast, g_X depends at least on the universality class of the model.) If this hypothesis is true, we may use in (8.14) the values of n_X obtained from another model such as the Ising model or still better the spherical model and the susceptibility amplitude ratios of the $X-Y$ model to compute the ratios g_X/g_Y . The results are given in Table VIII.2, where as usual we have taken the f.c.c. lattice as standard.

TABLE VIII.2. Temperature scaling parameter, $g_X(s)$, for the $X-Y$ model determined from the spherical model values of n_X and the $X-Y$ susceptibility amplitudes

| | f.c.c. | b.c.c. | s.c. |
|-------------------------------------|--------|-----------|-----------|
| n_X | 1 | 1.0655670 | 1.3945666 |
| $C_X(\frac{1}{2})/C_Y(\frac{1}{2})$ | 1 | 1.004 | 1.082 |
| $g_X(\frac{1}{2})$ | 1 | 1.045 | 1.209 |
| $C_X(\infty)/C_Y(\infty)$ | 1 | 1.003 | 1.068 |
| $g_X(\infty)$ | 1 | 1.046 | 1.222 |

Given g_X, n_X and A , the specific heat amplitude on the f.c.c. lattice, we can calculate the specific heat amplitude on lattice X from the lattice-lattice scaling result (Betts *et al.*, 1971).

$$A_X = A_F g_X^{2-\alpha} n_X^{-1}. \quad (8.16)$$

Similarly, we can calculate the critical amplitude

$$C_2 \text{ of } \partial^4 F / \partial H^4|_{H=0} \text{ from } C_{2,X} = C_{2,F} g_X^{-\gamma} n_X. \quad (8.17)$$

We do not now have estimates of A_X for the loose packed lattices and, because only coefficients of even powers of K occur on such lattices, direct determination of the specific heat amplitude from the series cannot be expected for some time. Thus, alternative indirect estimates are of some interest. The results of calculations using (8.16) and (8.17) are given in Table VIII.3.

TABLE VIII.3. Lattice-lattice scaling estimates of critical amplitudes of the specific heat and fourth order fluctuation for the X-Y model on loose packed lattices

| | f.c.c. | b.c.c. | s.c |
|-----------------------------|--------|--------|-------|
| $A_X (s = \frac{1}{2})$ | 0.255 | 0.261 | 0.267 |
| $A_X (s = \infty)$ | 2.40 | 2.46 | 2.57 |
| $C_{2,X} (s = \frac{1}{2})$ | 1.78 | 1.75 | 1.99 |

Stauffer *et al.*, (1972) have recently extended the lattice-lattice scaling idea to correlations by introducing a third (length) critical scale parameter, l_X , for which (8.12) and (8.13) are supplemented by

$$\mathbf{q}_X l_X = \mathbf{q}_Y l_Y \quad (8.18)$$

in the Fourier transform of the correlation function (8.9),

$$n_X \chi_X(\mathbf{q}_X, \varepsilon_X, h_X) / (g_X \varepsilon_X)^\gamma = n_Y \chi_Y(\mathbf{q}_Y, \varepsilon_Y, h_Y) / (g_Y \varepsilon_Y)^\gamma. \quad (8.19)$$

Actually, l_X is not an independent critical parameter but is related to n_X by

$$\rho_X l_X^d / n_X = \rho_Y l_Y^d / n_Y \quad (8.20)$$

where d is the dimensionality of the lattice and ρ_X is the site density of lattice X . This extension of lattice-lattice scaling has been shown to be satisfied exactly in the two-dimensional Ising model and to within 1% in the three-dimensional Ising model. An assumption of its general validity would allow us to compute the critical amplitude of the Fourier transform of the correlation function of the X-Y model on all lattices for which g_X and n_X are known given the value of the same amplitude on one lattice.

IX. Dynamical Properties of the X-Y Model

The dynamical properties of the X-Y model have as yet not received a great deal of attention. For the anisotropic Heisenberg model, described by the interaction Hamiltonian (2.1), as pointed out in Section II, there is a very important difference, dynamically, between the parallel magnetization, M_{\parallel} , and the perpendicular magnetization, M_{\perp} . M_{\parallel} commutes with \mathcal{H}_0 and is thus a constant of the motion while M_{\perp} does not commute with \mathcal{H}_0 and so may decay to zero. Consequently the perpendicular susceptibility is frequency dependent, $\partial M_{\perp} / \partial H_{\perp} = \chi_{\perp}(T, \omega)$. Allan and Betts (1968) and Essam and Garelick (1969) have found exact solutions to the problem of the frequency dependent perpendicular susceptibility of the pure Ising model in two dimensions. The frequency dependent perpendicular susceptibility of the three-dimensional Ising model has not been studied. Indeed, for arbitrary anisotropy of the Heisenberg model, even the zero frequency or static perpendicular susceptibility has not been studied.

The frequency dependent perpendicular susceptibility for the Heisenberg model for anisotropy $\eta \equiv J^{\parallel}/J^{\perp} < 1$ is of particular interest because for this range of anisotropy M_{\perp} is the order parameter. Ditzian and Betts (1972) and Mattingly and Betts (1972) have studied the frequency dependent perpendicular susceptibility of the pure X-Y model on the f.c.c. lattice, using Kubo's (1957) linear response theory.

A. Linear response of the X-Y model to a perpendicular field

In the Kubo theory we seek the response $\Delta B(t)$ of an observable B due to an external force $F(t) = F_0 \exp(i\omega t + \delta t)$ ($\delta \rightarrow 0$) conjugate to the observable A (which may be identical to B). The appropriate density matrix of the perturbed system is found by solving in the linear approximation the equation of motion,

$$\frac{d\rho}{dt} = [\mathcal{H}, \rho(t)]/i\hbar, \quad (9.1)$$

where $\mathcal{H} = \mathcal{H}_0 - AF(t)$, subject to the initial condition

$$\rho_0 \equiv \rho(-\infty) = \exp(-\beta\mathcal{H}_0)/\text{tr exp}(-\beta\mathcal{H}_0). \quad (9.2)$$

Then

$$\Delta B = \text{tr } B[\rho(t) - \rho(-\infty)]. \quad (9.3)$$

It follows that

$$\Delta B = (1/i\hbar) \text{tr} \int_{-\infty}^t [\rho_0, A] B(t - t') F(t') dt', \quad (9.4)$$

where

$$B(t) = \exp(it\mathcal{H}_0/\hbar) B \exp(-it\mathcal{H}_0/\hbar). \quad (9.5)$$

The linear response function ϕ_{BA} , the response of the observable B to the disturbance by the field conjugate to A , is defined by

$$\Delta B = \int_{-\infty}^t \phi_{BA}(t-t') F(t') dt'. \quad (9.6)$$

Thus,

$$\phi_{BA}(t) = (1/i\hbar) \operatorname{tr} \rho_0 [A, B(t)]. \quad (9.7)$$

The frequency-dependent susceptibility, $\chi_{BA}(\omega)$, is defined by

$$\Delta B(t) = \operatorname{Re} \chi_{BA}(\omega) F_0 \exp(i\omega t). \quad (9.8)$$

Combining (9.6) and (9.8) gives

$$\chi_{BA}(\omega) = \lim_{\delta \rightarrow 0+} \int_0^\infty \phi_{BA} \exp(-i\omega t - \delta t) dt. \quad (9.9)$$

For short times the response function can be expanded in a power series,

$$\phi_{BA} = (1/i\hbar) \operatorname{tr} \rho_0 \left[A, \left\{ B + it/\hbar [\mathcal{H}_0, B] + (it/\hbar)^2 [\mathcal{H}_0, [\mathcal{H}_0, B]] + \dots \right\} \right]. \quad (9.10)$$

The series (9.10) is either even or odd in t . Substitution of (9.10) in (9.9) results in a moment expansion of $\chi_{BA}(\omega)$ in either odd or even moments (powers of $1/\omega$).

As the order parameter for the X - Y model is M^x (or M^y) the small time expansion of ϕ^{xx} is required where

$$\langle M^x \rangle = \int_0^t \phi^{xx}(t-t') H^x(t') dt'. \quad (9.11)$$

Since ϕ^{xx} must be proportional to N , ρ_0 can be replaced in (9.7) or (9.10) by the part of its numerator linear in N times 2^{-N} . Letting

$$P = - \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} (a_{\mathbf{r}}^\dagger a_{\mathbf{r}'} + a_{\mathbf{r}} a_{\mathbf{r}'}^\dagger) \quad (9.12)$$

and $s = J^\perp t/\hbar$ and using the cyclic property of the trace, after some manipulation we get the short time, high temperature expansion of the response function for the spin $\frac{1}{2}$ X - Y model.

$$\begin{aligned} \phi^{xx}(t, T) &= \frac{im^2}{2^{N+1}\hbar} \sum_{n=0}^{\infty} \frac{K^n}{n!} \sum_{k=0}^{\infty} \frac{(is)^{2k+1}}{(2k+1)!} \sum_{j=0}^{2k+1} \binom{2k+1}{j} (-1)^j \\ &\times \operatorname{tr} \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} (P^{n+j} a_{\mathbf{r}}^\dagger P^{2k+1-j} a_{\mathbf{r}'} + P^{n+j} a_{\mathbf{r}} P^{2k+1-j} a_{\mathbf{r}'}^\dagger). \end{aligned} \quad (9.13)$$

The high temperature, high frequency expansion of $\chi_{\perp}(\omega, T)$ is obtained from (9.13) by Fourier transformation.

As in the case of static properties discussed in Section VI, it is convenient to use a graphical representation of the terms in the expansion of (9.3). Indeed, the diagrams are just those needed for the static perpendicular susceptibility. The concepts of vertical weight and horizontal weight previously introduced retain their validity and the vertical weight theorems for the static susceptibility still hold. Thus, we rewrite the expansion (9.13) as a diagram expansion for the reduced response function

$$\bar{\phi}_\perp = 2\hbar\phi^{xx}/m^2 = \sum_{l,n} \frac{K^n(-1)^l}{n!} \frac{s^{2l+1}}{(2l+1)!} \sum_{g'} \frac{\varepsilon(g')h_\omega(g')(g; \mathcal{L})V_l(g')}{2^{M(g')}} \quad (9.14)$$

where $h_\omega(g')$ is the dynamic horizontal weight of the shadow graph g' , $\varepsilon(g') = 1$ if in g' the two special vertices coincide (bubble graphs) and $\varepsilon(g') = 0$ if the two special vertices are distinct, M is the number of vertices of g' and $V_l(g')$ is a composite vertical weight given by

$$V_l(g') = \sum_{m=0}^{2l+1} \binom{2l+1}{m} (-1)^m v(2l+1-m). \quad (9.15)$$

One simplification occurs with the response function expansion when the vertical weight is independent of the level difference between the arrow head and tail, i.e. $v(2l+1-m) = v$. Then, $V_l = 0$.

This result means that all directed graphs in which the slanted, dashed arrow has a vertex of order 2 do not contribute to $\bar{\phi}$ in (9.14). From this result and the appropriately modified Theorems I, II and III (Ditzian, 1970), we find that for arbitrary lattice

$$\begin{aligned} \bar{\phi}_\perp &= \frac{1}{2}(\nearrow)Ks + [\frac{3}{2}(\Delta) + (\nearrow)] \frac{K^2 s}{2} + [\frac{1}{2}(\nearrow) + (\nearrow\nearrow) + 3(\Delta) + 3(\square) \\ &\quad + \frac{3}{2}(\nearrow, \nearrow)] \frac{K^3 s}{6} + [-\frac{1}{2}(\nearrow) - \frac{5}{2}(\nearrow\nearrow) + 6(\Delta)] \frac{K s^3}{6} + \dots \end{aligned} \quad (9.16)$$

For the f.c.c. lattice Ditzian and Betts (1972) with the aid of a computer have given all coefficients of total degree 9 or less in the expansion of $\chi_\perp(\omega, T)$ in $1/\omega$ and $1/T$. Mattingly and Betts (1972) have repeated their calculations and obtained further the set of all four coefficients of degree 10 in $1/\omega$ and $1/T$. The result in terms of K and $L = J^\perp/\hbar\omega$ is

$$\begin{aligned} \bar{\chi} &\equiv 2J\chi/m^2 = (3K + 9K^2 + 14\frac{3}{4}K^3 + 22K^4 + 61\frac{3}{8}K^5 + 237\frac{19}{240}K^6 \\ &\quad + 880\frac{941}{960}K^7 + 3161\frac{29}{420}K^8 + \dots)L^2 + (120K + 36K^2 - 897K^3 \\ &\quad - 3451\frac{3}{4}K^4 - 8601\frac{3}{10}K^5 - 22,794\frac{19}{24}K^6 + \dots)L^4 + (10,980K \\ &\quad + 10,059K^2 - 35,534\frac{1}{2}K^3 - 170,293\frac{1}{2}K^4 + \dots)L^6 + (1,973,244K \\ &\quad + 6,305,892K^2 + \dots)L^8 + \dots \end{aligned} \quad (9.17)$$

B. Analysis of the frequency dependent perpendicular susceptibility

Equation (9.17) must contain a substantial amount of information about the dynamical properties of the X-Y model. In particular, collective oscillatory modes of the system at finite frequencies $\omega_i(T)$ should be revealed by infinities in χ_{\perp} at $\omega = \omega_i(T)$ [or $L = L_i(K)$]. Secondly it is expected from hydrodynamic theory (Halperin and Hohenberg, 1969) that for $T \leq T_c$ a zero frequency spin wave mode should exist, also resulting in an infinity in χ_{\perp} . According to dynamic scaling theory (Halperin and Hohenberg, 1967; Ferrell *et al.*, 1967)

$$\chi_{\perp}(\omega, T_c) \sim \omega^{-\gamma}. \quad (9.18)$$

It should be possible to discover such singular behaviour in $\chi_{\perp}(K, L)$ through Padé approximant analysis of the series expansion (9.17). For the Ising model in the low temperature expansion of the thermodynamic functions, $M_{\parallel}(z, y)$ or $\chi_{\parallel}(z, y)$ in powers of z and y (Sykes *et al.*, 1965; Domb, this volume, Chapter 6 Section II.C) it is possible to set $z = z_c$ and obtain a series expansion in y valid on the critical isotherm because the coefficients of each power of y are finite polynomials in z (and vice versa). In contrast, for the X-Y model perpendicular susceptibility, the coefficients of each power of K are infinite series in L and vice versa, so one can not, for example, test the validity of (9.18) by studying the series expansion (9.17) for the $K = K_c$.

Mattingly and Betts (1972) have analyzed (9.17) by setting $K = \rho L$ instead and used Padé approximants to study the series expansion $\chi_{\rho}(L) \equiv \chi_{\perp}(\rho L, L)$ for a set of values of the parameter ρ . Two techniques were used. Assuming

$$\chi_{\rho} \sim (L_i(\rho) - L)^{-\gamma_i(\rho)},$$

poles and residues of Padé approximants to $d(\log \chi_{\rho})/dL$ yielded estimates of L_i and γ_i , respectively. Secondly, each Padé approximant to χ_{ρ}^{1/γ_i} gave a curve of L_i versus γ_i and the region where the curves for the central high degree approximants most nearly coincided gave estimates of the true L_i and γ_i . In this way, a weak high frequency singularity was found at a frequency $\omega_1 = (14 \pm 2) J/\hbar$ with an exponent $\gamma_1 = 0.20 \pm 0.05$, both nearly independent of temperature.

In order to examine lower temperature behaviour Euler transformations such as

$$K = K^*/(1 - K^*) \quad (9.19)$$

were introduced by Mattingly and Betts (1972), and to study lower frequency behaviour, transformations were used such as

$$L = L^*/(1 - L^*)\sqrt{12}. \quad (9.20)$$

The above two transformations used together, map the entire physical quadrant of the (ω, T) plane on to the unit square in the (K^*, L^*) plane. With the aid of (9.20), (9.21) and other transformations, Mattingly and Betts discovered another stronger lower frequency singularity. The information about singularities and their exponents is summarized in Fig. 9.1. The values of ω_1 and ω_2 and, *a fortiori*, γ_1 and γ_2 are rather uncertain, but of the existence of the two collective finite frequency modes there seems little doubt.

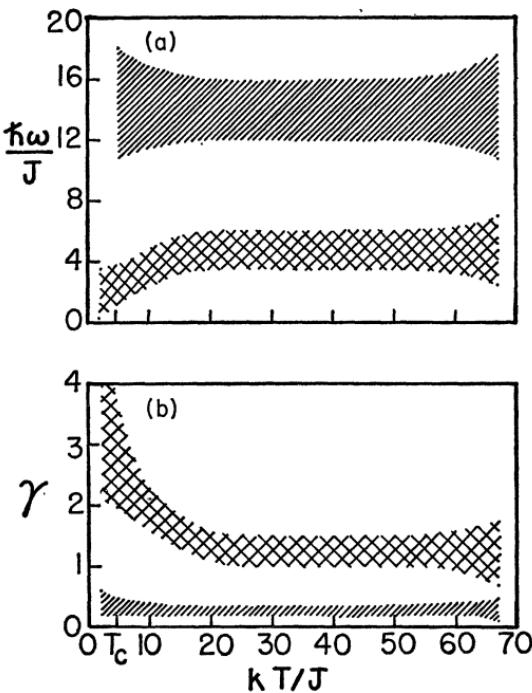


FIG. 9.1. Frequency, ω , and exponent, γ , of singularities in the frequency dependent susceptibility, $\chi_{\perp}(\omega, T)$ of the spin $\frac{1}{2}$ $X-Y$ model on the f.c.c. lattice for the high frequency collective mode (shaded) and low frequency collective mode (crosshatched).

Because of the two finite frequency singularities encountered at values of $L^* < 1$, it has not proved possible to estimate the zero frequency exponent or even indeed to ascertain the existence of the expected singularity in χ_{\perp} at $L^* = 1$, $K \geq K_c$ from the finite series presently available.

The next task is to find a physical explanation for the two finite frequency modes. Mattingly and Betts (1972) have offered a "quasi-atomic" explanation of the higher frequency singularity. Except for $T \gg T_c$, there

will be many clusters of spins in which a central spin and its twelve neighbours will be aligned parallel to one another. The central spin will have energy $-12J^{\perp}$. The introduction of a small frequency-dependent perpendicular field will excite many such central spins into rotation in phase with the field thus giving the rotating spin zero energy. Other than for complete alignment, there is no special energy state for the first neighbour shell of spins; hence only one resonance, that at $\omega_1 \sim 12J_{\perp}/\hbar$, is observed. No convincing simple physical explanation for the lower frequency mode has yet been put forward. It would be desirable to study other dynamical functions in order to elucidate the exact nature of the collective modes of the spin $\frac{1}{2}$ *X-Y* model.

X. Two-Dimensional Planar Models*

During the past half dozen years there has been great interest in the question of the existence and nature of phase transitions in two-dimensional systems. For the two-dimensional Ising model Peierls (1936) proved the existence of an ordered phase at low temperatures and in a classic work Onsager (1944) found the zero field partition function exactly. However, arguments of Bloch (1930) and others had convinced most physicists that the two-dimensional Heisenberg model does not undergo a phase transition. Then Rushbrooke and Wood (1958), and later and more emphatically Stanley and Kaplan (1966), presented numerical evidence based on analysis of the high temperature series for the susceptibility derived by Rushbrooke and Wood (1958), that for $s > \frac{1}{2}$ the two-dimensional isotropic Heisenberg model has a finite transition temperature. Very soon thereafter Mermin and Wagner (1966) proved for a variety of one and two dimensional models that no state of long range order can exist at non-zero temperatures. Their proof includes the isotropic Heisenberg model and the *X-Y* model. However, as Stanley and Kaplan (1966) had pointed out, it is possible that a low temperature phase can exist without long range order but with sufficiently slowly attenuated spin-spin correlations that the susceptibility could become infinite.

A. The models

It is by no means certain that the isotropic Heisenberg model with $D = 3$ undergoes any type of phase transition. Indeed for the fully quantum mechanical spin $\frac{1}{2}$ case there is little evidence for a phase transition. Thus, it is of interest to consider the evidence for phase transitions in planar ($D = 2$) systems in two dimensions ($d = 2$).

* See also Stanley, this volume, Chapter 7, Section XI.

Consider the planar Hamiltonian

$$\mathcal{H}_2 = -(J^\perp/2s^2) \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} (S_{\mathbf{r}}^x S_{\mathbf{r}'}^x + S_{\mathbf{r}}^y S_{\mathbf{r}'}^y) + (D'/s^2) \sum_{\mathbf{r}} (S_{\mathbf{r}}^z)^2 - (m_1 H^x/s) \sum_{\mathbf{r}} S_{\mathbf{r}}^x. \quad (10.1)$$

When $s = \frac{1}{2}$, the second term reduces to an additive constant and the pure $X-Y$ model is recovered. When $s = \infty$, there are two cases of interest. For $D' = 0$, the classical $X-Y$ model is obtained. For $D'/|J^\perp| \gg 0$, the states in which the spins lie near in direction to the $X-Y$ plane are highly favoured energetically and the Hamiltonian describes the so called classical planar or plane rotator model.

If universality holds, all three models should have the same critical exponents. Further, in two dimensions all or none of the three models should have a phase transition. The classical planar model has been introduced at this point because, although in three dimensions the classical $X-Y$ model has been studied by the method of exact series expansions, the classical planar model has been studied in two dimensions only.

B. Series expansions

For the spin $\frac{1}{2}$ $X-Y$ model on lattices of two dimensions, the techniques used to obtain high temperature series expansions do not differ from those for three dimensions and have been described in earlier sections. Betts *et al.*, (1971) have found the order parameter fluctuation for the p.t. lattice;

$$\begin{aligned} Y^T = & 1 + 3K + 7\frac{1}{2}K^2 + 14\frac{1}{2}K^3 + 24\frac{3}{8}K^4 + 39\frac{6}{8}K^5 + 66\frac{11}{16}K^6 \\ & + 110.75907738 \dots K^7 + 175.09226190 \dots K^8 \\ & + 262.6967552 \dots K^9 + \dots, \end{aligned} \quad (10.2)$$

and for the s.q. lattice;

$$\begin{aligned} Y^Q = & 1 + 2K + 3K^2 + 3\frac{1}{3}K^3 + 3\frac{1}{4}K^4 + 3\frac{11}{40}K^5 + 3\frac{31}{72}K^6 \\ & + 3.391964286 \dots K^7 + 3.099007936 \dots K^8 \\ & + 2.728331680 \dots K^9 + \dots. \end{aligned} \quad (10.3)$$

The fourth order fluctuation has been expanded for the p.t. lattice only. The result is

$$\begin{aligned} Y_2^T = & 1 + 12K + 79\frac{1}{2}K^2 + 379K^3 + 1432\frac{7}{8}K^4 + 4621\frac{1}{2}K^5 \\ & + 13,336\frac{1}{4}K^6 + 35,115\frac{481}{30}K^7 + \dots \end{aligned} \quad (10.4)$$

For general spin the results of Wood and Dalton (1972) may be used to obtain expansions of the zero field partition function to order K^7 and parallel susceptibility to order K^6 . Ishikawa and Oguchi (1971) have also obtained expansions for the parallel susceptibility to order K^5 . The results of Dalton and Wood are not quoted here because the general expression is rather lengthy and because the series are nevertheless too short for analysis to yield meaningful estimates of critical properties.

For the classical planar model Stanley (1968) has given for arbitrary lattice the coefficients to order 8 for the perpendicular susceptibility (and order 9 for loose packed lattices) and of the energy (hence specific heat) to order 9 (and order 10 for loose packed lattices). Moore (1969) has found the high temperature series expansion of the perpendicular spin-spin correlation function to order 10 on the p.t. lattice. From the correlations the perpendicular susceptibility expansion for the plane rotator model on the p.t. lattice is

$$\begin{aligned}\chi_{\perp}^T = & 1 + 3K + 7\frac{1}{2}K^2 + 16\frac{7}{8}K^3 + 35\frac{5}{8}K^4 + 72\frac{5}{8}K^5 + 141\frac{3}{12}\frac{5}{8}K^6 \\ & + 270\frac{177}{2024}K^7 + 506.383465 \dots K^8 + 933.57038 \dots K^9 \\ & + 1,697.512102 \dots K^{10} + \dots\end{aligned}\quad (10.5)$$

C. Analysis of series

For the spin $\frac{1}{2}$ model in two dimensions, unlike the three-dimensional model, the fluctuation series ratios do not become linear in $1/n$. Padé approximant analysis of the logarithmic derivative of the fluctuation series on the s.q. and p.t. lattices reveals the cause.

TABLE X.1. Estimates of location of dominant singularities in the long range order fluctuation for the spin $\frac{1}{2}$ X-Y model on the p.t. lattice from Padé approximants to $(d/dK) \log Y(K)$

| D | $N = 1$ | $N = 2$ | $N = 3$ | $N = 4$ | $N = 5$ |
|-----|--------------------|--------------------|--------------------|--------------------|---------|
| 3 | | 0.664 | 0.738 | 0.872 | |
| | | $0.027 \pm 0.588i$ | $0.071 \pm 0.593i$ | $0.083 \pm 0.644i$ | |
| 4 | | 0.643 | 0.597 $\pm 0.184i$ | | |
| | | $0.039 \pm 0.596i$ | $0.027 \pm 0.601i$ | $0.046 \pm 0.617i$ | |
| 5 | $0.772 \pm 0.086i$ | $0.587 \pm 0.139i$ | $0.545 \pm 0.094i$ | | |
| | $0.038 \pm 0.596i$ | $0.048 \pm 0.605i$ | $0.044 \pm 0.608i$ | | |
| 6 | 0.700 | 0.540 $\pm 0.079i$ | | | |
| | $0.037 \pm 0.600i$ | $0.044 \pm 0.607i$ | | | |
| 7 | 0.561 $\pm 0.130i$ | | | | |
| | $0.044 \pm 0.611i$ | | | | |

Table X.1 gives the resulting estimates of the singularities of $Y^T(K)$ nearest to the origin in the complex K plane. The singularities nearest to the origin seem to be a complex conjugate pair near to the imaginary axis at a distance of about 0.6 from the origin and either a second complex conjugate pair about the same distance from the origin but near to the positive real axis or a single positive real singularity at a slightly greater distance from the origin of about 0.7. The first possibility would indicate no phase transition, whereas the second possibility would indicate a phase transition. The results for the s.q. lattice are qualitatively very similar.

In order to discriminate between these two possibilities Betts *et al.*, (1971) introduced conformal transformations of K which moved points near the real axis nearer to the origin while moving points near the imaginary axis farther from the origin. Typical of the more satisfactory choices, many of which were tried, is the transformation

$$K = \bar{K}/(1 - \bar{K}^2). \quad (10.6)$$

This particular transformation has the effect of transforming the points $K \approx \pm 0.7$ into the pairs of points $\bar{K} \approx \pm 0.5$ and $\bar{K} \approx \pm 2$, while transforming the pair of points $K \approx \pm 0.6i$ into the four points $\bar{K} \approx \pm 0.6 \pm 0.8i$. Thus, the distance of the physical singularity (if it exists) from the origin has been reduced to 0.5 while the now four non-physical singularities are at unit distance from the origin.

TABLE X.2. Estimates of K_C and, in parentheses, γ for the spin $\frac{1}{2}$ $X-Y$ model on the p.t. lattice from Padé approximants to $(d/dK) \log Y(K)$ where $K = \bar{K}/(1 - \bar{K}^2)$

| D | $N = 2$ | $N = 3$ | $N = 4$ | $N = 5$ |
|-----|------------------|------------------|------------------|------------------|
| 3 | | 0.5025 (1.52) | 0.5001 (1.49) | 0.5025 (1.53) |
| 4 | 0.5026 (1.52) | 0.5017 (1.51) | 0.5013 (1.51) | |
| 5 | 0.5001 (1.49) | 0.5012 (1.51) | | |
| 6 | 0.5025 (1.53) | | | |

Padé approximant analysis of the logarithmic derivative of $Y^T(K)$ now yields consistently a single positive real singularity and no longer gives consistent evidence for any non physical singularities. Table X.2 contains

estimates from the central, higher degree approximants of the location of the singularity and, in brackets, the residue as an estimate of γ . From Table X.2 we are encouraged to believe not only that there is a phase transition but that its location is $\bar{K}_c^T \approx 0.501 \pm 0.002$ and the critical exponent $\gamma \approx 1.51$. Analogous results are found for the s.q. lattice.

TABLE X.3. Estimates of K_c for the spin $\frac{1}{2}$ $X-Y$ model on the p.t. lattice from Padé approximants to $[Y(K)]^{2/3}$ with $K = \bar{K}/(1 - K^2)$

| D | $N = 2$ | $N = 3$ | $N = 4$ | $N = 5$ | $N = 6$ |
|-----|---------|---------|---------|---------|---------|
| 3 | | | 0.50097 | 0.50084 | 0.50111 |
| 4 | | 0.50000 | 0.50087 | 0.50093 | |
| 5 | 0.50098 | 0.50088 | 0.50105 | | |
| 6 | 0.50084 | 0.50093 | | | |
| 7 | 0.50011 | | | | |

If γ is a simple fraction then it is likely that $\gamma = \frac{3}{2}$. If $\gamma = \frac{3}{2}$ then Padé approximant analysis of $[Y^T(K)]^{2/3}$ should give better estimates of \bar{K}_c (hence K_c). Table X.3 gives estimates for central, high degree Padé approximants of \bar{K}_c from singularities of $[Y^T(K)]^{2/3}$. If $\gamma = \frac{3}{2}$ then

$$(d/d\bar{K})Y(\bar{K}) \sim (\bar{K}_c - \bar{K})^{-5/2} \quad (10.7)$$

and singularities in Padé approximants to $[(d/d\bar{K})Y(\bar{K})]^{2/5}$ should give estimates of \bar{K}_c consistent with other methods. Central, high degree Padé approximants to this last function for the p.t. lattice are given in Table X.4. From Tables X.2, X.3 and X.4 the best estimate of \bar{K}_c^T is $\bar{K}_c^T = 0.501 \pm 0.001$. For the s.q. lattice Betts *et al.* (1971) have followed the same procedure to find $X^Q = 0.647 \pm 0.002$.

TABLE X.4. Estimates of K_c for the spin $\frac{1}{2}$ $X-Y$ model on the p.t. lattice from Padé approximants to $[(d/d\bar{K})Y(\bar{K})]^{2/5}$

| D | $N = 3$ | $N = 4$ | $N = 5$ | $N = 6$ |
|-----|---------|---------|---------|---------|
| 3 | | 0.5012 | 0.5006 | 0.5014 |
| 4 | 0.5012 | 0.5009 | 0.5010 | |
| 5 | 0.5006 | 0.5010 | | |
| 6 | 0.5014 | | | |

The residues of Padé approximants to $Y^{1/\gamma}(\bar{K})$ yield estimates of the critical amplitude, \bar{A} , of $Y(\bar{K})$. The amplitude of $Y(K)$ is then obtained from the relation

$$A = \bar{A} \left(\frac{1 - K_c^2 + 2\bar{K}_c}{1 - \bar{K}_c^2} \right)^\gamma. \quad (10.8)$$

From such analysis our best estimates of the fluctuation (perpendicular susceptibility) amplitudes for the two-dimensional $X-Y$ model are contained Table X.5.

TABLE X.5. Critical properties of the spin $\frac{1}{2}$ $X-Y$ model in two dimensions

| Lattice | γ | K_c | A | $K_{B\pm}$ | γ_2 |
|---------|-----------------|-------------------|-----------------|--|-----------------|
| p.t. | 1.50 ± 0.02 | 0.667 ± 0.003 | 2.34 ± 0.04 | $+0.04 \pm 0.03$ $\pm i(0.95 \pm 0.03)$ | 5.35 ± 0.30 |
| s.q. | 1.50 ± 0.03 | 1.111 ± 0.005 | 1.53 ± 0.10 | -0.02 ± 0.03 $\pm i(0.95 \pm 0.03)$ | |

The series (10.4) for the fourth order fluctuation on the p.t. lattice is rather short, so results from the analysis of this series must be treated very cautiously. Betts *et al.* (1971) using the same transformation (10.5) have estimated that the critical exponent $\gamma_2 = 5.35 \pm 0.30$.

Finally returning to the fluctuation series Betts *et al.* (1971) have introduced a transformation

$$K = K^*/(1 + K^{*2}) \quad (10.9)$$

which stretches the real axis and shrinks the imaginary axis in order to estimate better the location of the dominant non-physical singularities. Singularities in Padé approximants to $(d/dK^*)Y(K^*)$ yield estimates of the non-physical singularities at $K_{B\pm}^*$ which are consistent with earlier estimates of $K_{B\pm}$ but better converged. From these results for $K_{B\pm}^*$ the estimates of $K_{B\pm}$ in Table X.5 are obtained. Figure 10.1 shows the position in the complex K/K_c plane of the non-physical singularities for the two two-dimensional lattices and the three three-dimensional lattices studied as determined from analysis of the corresponding fluctuation series. On all five lattices there is one complex conjugate pair of non-physical singularities

near to the imaginary axis. However, for the two-dimensional lattices, they lie inside the unit circle while for the three-dimensional lattices they lie well outside the unit circle.

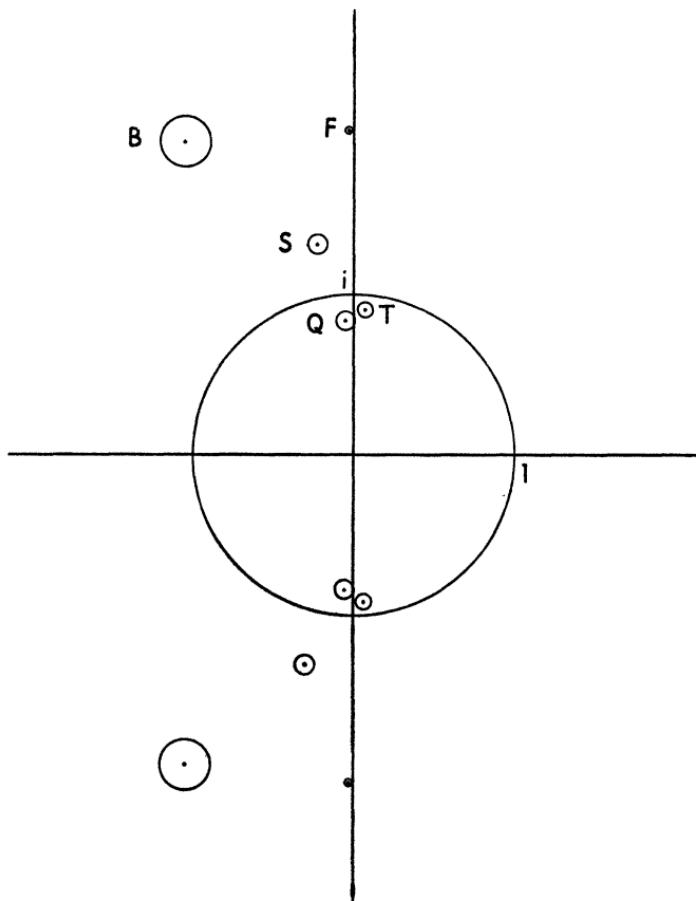


FIG. 10.1. Location of non-physical singularities in the complex K/K_c plane from the fluctuation series for the spin $\frac{1}{2}$ X-Y model on the s.q. (Q), p.t. (T), s.c. (S), b.c.c. (B) and f.c.c. (F) lattices. Size of circles represents relative confidence in the location of the singularities.

Moore (1969) has analysed (10.5) by the Neville table method and concluded that $K_c = 0.635 \pm 0.020$ and $\gamma = 3.0 \pm 0.5$. His estimate of γ is for the plane rotator *twice* that of Betts *et al.* (1971) for the two dimensional X-Y model.

We report here a re-analysis of (10.5) using Padé approximants. Analysis of $(d/dK) \log \chi_{\perp}^T$ reveals consistently a real singularity, $K_c \approx 0.64$ with

residue, $\gamma \approx 3.0$, in agreement with Moore's analysis, and a complex conjugate pair of singularities near the imaginary axis but somewhat *further* from the origin than K_C . Use of the transformation (10.6) gave results consistent with but, as we expected, not appreciably better than, analysis of the original series when applied to the logarithmic derivative. Finally we examined Padé approximants to $[\chi_{\perp}^T(\bar{K})]^{1/\gamma}$ and to $[(d/d\bar{K})\chi_{\perp}^T(\bar{K})]^{1/\gamma+1}$ for a set of values of γ near $\gamma = 3$. Best consistency for K_C was obtained when $\gamma = 3$. Finally we conclude that $K_C^{-T} = 0.643 \pm 0.010$ and $\gamma = 3.0 \pm 0.3$ for the plane rotator model.

D. Universality and scaling

Although the analysis of the series expansions for the three dimensional spin $\frac{1}{2}$ and spin ∞ models yields results in agreement with universality, such does not seem to be the case in two dimensions. It seems most doubtful that either or both of the estimates $\gamma = 1.5$ for spin $\frac{1}{2}$ and $\gamma = 3.0$ for spin ∞ could be sufficiently in error for the true γ values to be in agreement. In other words for $d = 2$ the universality class may depend on s as well as D .

The application of scaling theory to the two dimensional $X-Y$ and classical planar models is beset by the handicap that in both models, of the two critical exponents needed as input, only one, γ , is known moderately well. In both models also there is no spontaneous magnetization. However the homogeneity postulate can be cast in the form

$$\chi \sim \varepsilon^{-\gamma} f(h/\varepsilon^{\Delta}). \quad (10.10)$$

The exponent δ can then be defined for example by

$$\chi \sim h^{-(1-1/\delta)} \quad \varepsilon = 0. \quad (10.11)$$

TABLE X.6. Some possible choices for scaling exponents for two-dimensional planar models

| γ | δ | Δ | α | ν | η |
|----------|----------|----------|----------|-------|--------|
| 3/2 | 5 | 15/8 | -1/4 | 9/8 | 3/2 |
| 3/2 | 7 | 7/4 | 0 | 1 | 1/2 |
| 3 | 5 | 15/4 | -5/2 | 9/4 | 2/3 |
| 3 | 7 | 7/2 | -2 | 2 | 1/2 |

The choice of scaling exponents can be reduced by demanding that δ be an odd integer. Then $\delta = 5$ is the most likely choice for the spin $X-Y$ model whereas $\delta = 7$ is the best choice for the plane rotator, but either value is a

good choice for either model within the error of the estimates for Δ and v respectively. Table X.6 gives, for what little it is worth, the scaling values of the other exponents for $\gamma = 3$ or $\frac{3}{2}$ and $\delta = 5$ or 7. Incidentally, the spin $\frac{1}{2}$ Ising value of $\delta = 15$ seems firmly excluded. Note that a cusp not an infinity in the specific heat is indicated for all plausible choices of critical exponents.

XI. Comparison with Experiment

In Section II and especially Section III, a number of magnetic systems have been mentioned as possibly behaving in the critical region like the X-Y model. For most of these systems there has been little, if any, study of their critical properties. Such comparison as is possible between X-Y model results and magnetic system is made in Section XI.B below. The comparison of X-Y model results with experimental results for helium near the λ transition is made in Section XI.A. In Section XI.C, experimental results for other planar systems are presented.

A. The λ transition in liquid helium

From the discussion in Section II.B it is clear that the spin $\frac{1}{2}$ X-Y model is a model for liquid helium near the λ transition. The main approximations made were to replace the real potential by a hard core potential and to confine the molecules to sites of a regular lattice. It is not obvious how serious the approximations are. However, at least neither should affect the universality class of the transition, and hence the right critical exponents in agreement with experiment for helium, may be expected. Beyond that, the lattice approximation should not be too inaccurate when the correlation length is sufficiently great (when the λ line is approached sufficiently closely). It is not clear *a priori* how serious the hard core approximation is.

Ditzian and Betts (1970) have compared theoretical and experimental critical exponents near T_λ . Their results are reproduced in Table XI.1.

TABLE XI.1. Comparison of values of critical exponents of the X-Y model and liquid helium

| Exponent | X-Y Model | Liquid helium | Reference |
|-----------|-----------|----------------------------|--|
| α | 0 | $0\cdot000 \pm 0\cdot003$ | Ahlers (1969) |
| α' | $1/3$ | $-0\cdot020 \pm 0\cdot003$ | Ahlers (1969) |
| β | 0 | $0\cdot333 \pm 0\cdot010$ | Clow and Reppy (1966) Tyson and Douglass (1966) |
| v' | $2/3$ | $0\cdot67 \pm 0\cdot04$ | Henkel, <i>et al.</i> (1969) |

Apart from the discrepancy that for helium, α' is not quite equal to α , the agreement between experiment and theory is very gratifying. Note that the theoretical exponents, except for α , are obtained with the aid of scaling theory, and that simple rational fractions have been assumed.

For the specific heat above T_λ more direct and detailed comparison is possible between liquid helium and the $X-Y$ model, because in this case both the series expansion and the experimental measurements are available. In the spin $\frac{1}{2}$ $X-Y$ model the specific heat series expansion, in fluid terms, is for $C_\mu(T, \mu_Q)$ where the value μ_Q of the chemical potential has been chosen for calculational convenience to be that value for which $H_{\parallel} = 0$,

$$\mu_Q = 3\hbar^2/m\delta^2. \quad (11.1)$$

The nearest neighbour distance, δ , is at this point still arbitrary.

Betts and Lothian (1973) choose the point, Q , on the λ line for which experiment is to be compared with theory by requiring that the experimental critical ratio equal the theoretical critical ratio for lattice X , i.e.

$$m\rho_Q/\rho_Q k_B T_Q = 2 \ln \Lambda_C^X. \quad (11.2)$$

The factor 2 occurs as above in converting from partition function per site to partition function per molecule. For the f.c.c. and b.c.c. lattices $\ln \Lambda_C$ is obtained by evaluating at K_C Padé approximants to (4.14) and (4.18) respectively. From the density, ρ_Q^X , then δ^X is immediately obtained for both lattices. The results are contained in Table XI.2.

TABLE XI.2. Values of thermodynamic variables at that point, Q , on the lambda for which the critical ratios of the spin $\frac{1}{2}$ $X-Y$ model and liquid helium are equal.

| lattice | $T_Q [K]$ | $P_Q [\text{bar}]$ | $\rho_Q [\text{g./cm.}^3]$ | $\delta [\text{cm.} \times 10^{-8}]$ |
|---------|-----------|--------------------|----------------------------|--------------------------------------|
| b.c.c. | 2.046 | 11.36 | 0.1632 | 3.00 |
| f.c.c. | 2.051 | 10.96 | 0.1628 | 3.07 |

Examination of Table XI.2 shows that the point Q lies near the middle of the lambda line and is insensitive to the choice of lattice. The resulting values of nearest neighbour spacings, δ^X , are close to the experimental value, $\delta_{Q}^{He} = 3.1 \times 10^{-8} \text{ cm.}$

Because of the up-down symmetry of the zero field $X-Y$ model the shape of the λ line of the $X-Y$ model near Q is given by

$$T_\lambda - T_Q \propto (P_\lambda - P_Q)^2, \quad (11.3)$$

so that the lambda line is vertical at Q . The lambda line in He has a finite but large slope at Q

$$\left(\frac{\partial \log P_\lambda}{\partial \log T_\lambda} \right)_Q = -15 \quad (11.4)$$

Again because of the symmetry of the X - Y model $C_\mu(T, \mu_Q) = C_p(T, \mu_Q) = C_V(T, \mu_Q)$ for all $T > T_c$ but $C_\mu(T, \mu_Q) = C_p(T, \mu_Q)$ only as $T \rightarrow T_c$. Thus for helium it is C_V and not C_p which is to be compared with the model results. Buckingham and Fairbank (1961) have used the experimental facts of the finiteness of $(\partial p / \partial T)_\lambda$ and the infinity of C_p and $(\partial V / \partial T)_p$ on the lambda line to prove thermodynamically that C_V must remain finite at the lambda line. However since on the one hand the slope of the lambda line is very large and on the other hand a specific heat with a logarithmic singularity rises to infinity very slowly (Fig. 7.2) it is not surprising that Ahlers (1973) has found that C_V for helium can be well represented by

$$C_V/R = -A(p) \log [1 - T_\lambda(p)/T] + B_0(p) \quad T > T_\lambda(p) \quad (11.5)$$

Betts and Lothian (1973) have therefore interpolated Ahlers' (1973) results to obtain $A(p_Q)$ and $B_0(p_Q)$ for helium to compare with the spin $\frac{1}{2}$ X - Y model results. The results are contained in Table XI.3. The X - Y model values for A and B_0 from Section VII have been multiplied by a factor 2 to convert from specific heat per site to specific heat per molecule.

TABLE XI.3. Comparison of critical amplitude, A , and critical constant, B_0 , for the specific heat of the X - Y model and of helium.

| System | A | B_0 |
|--|-------|--------|
| spin $\frac{1}{2}$ X - Y model on f.c.c. lattice | 0.510 | -0.380 |
| helium for $T_\lambda = 2.051 K$ | 0.511 | -0.39 |
| spin $\frac{1}{2}$ X - Y model on b.c.c. lattice | 0.522 | — |
| helium for $T_\lambda = 2.046 K$ | 0.507 | -0.39 |
| spin ∞ X - Y model on f.c.c. lattice | 2.4 | -4.0 |
| helium near saturated vapour pressure | 0.61 | -0.34 |
| helium near solidification pressure | 0.38 | -0.38 |

The amplitude, A_B , for the b.c.c. lattice has not been directly determined because of the shortness of the series. However, according to lattice-lattice

scaling theory (Betts *et al.*, 1971) A_B can be found from A_F using

$$A_B = A_F g_B^{2-\alpha}/n_B \quad (11.6)$$

where g_B and n_B are critical scaling parameters. B_0 cannot be found from lattice-lattice scaling, but at least for the Ising model (Sykes *et al.*, 1972) seems to be almost independent of lattice.

Also included in Table XI.3 are estimates of A and B_0 for the spin ∞ X-Y model and experimental values for pressures near either extreme of the lambda line.

Table XI.3 shows that agreement between experiment on helium near $p_Q \approx 11$ bar and the spin $\frac{1}{2}$ X-Y model is remarkably good for A and B_0 for either the b.c.c. or f.c.c. lattice. On the other hand the spin ∞ X-Y model results for A and B_0 are nearly an order of magnitude larger than the experimental results. It seems that the *spin one half* X-Y model is the "right" model for the lambda transition in helium in more ways than simply having the right order parameter dimensionality ($D = 2$), which the spin ∞ model also has.

B. Three-dimensional magnetic systems

For most of the planar magnetic systems discussed in Section III no precise measurements of their critical properties have been made. An exception is the rare earth metal terbium. Although, being a metal, terbium is far from being an ideal X-Y magnetic system, it does at least have a planar order parameter. The spin correlations in terbium have been carefully studied by Dietrich and Als Nielsen (1968). They find $\nu = 0.66 \pm 0.02$ in good agreement with the value $\nu = \frac{2}{3}$ expected for the X-Y model if scaling is valid and ν is a simple rational fraction. Admittedly this result is not substantially in disagreement with the value for the spin $\frac{1}{2}$ Ising model, $\nu = 0.643 \pm 0.003$ (Fisher and Burford, 1967) or the value for the spin $\frac{1}{2}$ Heisenberg model, $\nu = 0.71 \pm 0.01$ (Ritchie and Fisher, 1972). However it fits best the expected X-Y model result. It will be of interest to see how the directly calculated critical exponent and critical amplitude of the correlation length for the spin $\frac{1}{2}$ X-Y model agree with the measured quantities for terbium.

C. Displacive transitions

A number of measurements have been made recently of critical properties of ferroelectrics which undergo displacive transitions. Von Waldkirch *et al.*, (1972) have determined ν and η by measuring the broadening of the EPR line width as $T \rightarrow T_c^+$. They find $\nu = 0.63 \pm 0.07$ and $\eta = 0$ within

experimental error. These values with their quoted errors encompass the theoretical values for all three of the theoretical models, the Ising, X-Y and Heisenberg models, and thus cannot at present discriminate among models.

The critical exponent, β , for the order parameter has been measured for at least three displacive ferroelectrics. For both SrTiO_3 and LaAlO_3 , Müller and Berlanger (1971) find $\beta = 0.33 \pm 0.02$ in good agreement with the X-Y model result but not quite excluding the Ising model value $\beta \approx \frac{5}{16}$ (Essam and Fisher, 1963) nor the Heisenberg model estimate of $\beta = 0.35$ (Baker *et al.*, 1970). For quartz, Höchli and Scott (1971) find $\beta = 0.34 \pm 0.02$, spanning the X-Y and Heisenberg model estimates for β . Clearly, it would be highly desirable to have measurements of other critical exponents, measurements on additional dielectric substances and more precise measurements to determine definitely the critical behaviour of displacive ferroelectrics.

XII. Discussion, Conclusions and Outlook

In Section II we have seen that the spin $\frac{1}{2}$ X-Y model is a plausible model for liquid helium near the λ transition and for a class of magnetic insulators near the Curie point. If the principle of smoothness holds, then the perturbations to the model introduced to make it resemble more closely the real physical system should not affect the critical exponents. A broader class of physical systems and theoretical models are encompassed by invoking the universality principle, discussed in Section III, according to which the critical exponents, for short range forces, depend only on the dimensionality of the lattice, d , and the dimensionality of the order parameter, D . If the universality principle is valid the spin infinity X-Y model, liquid helium near the λ transition, planar ferro- and antiferromagnetic insulators and metals and some types of ferroelectrics should all have the same critical exponents as the spin $\frac{1}{2}$ X-Y model.

The thermodynamic properties for which series expansions are to be obtained, the techniques for obtaining the series and the series themselves have been presented in Sections IV to VI. Series to $1/T^{11}$ have been obtained for the free energy, to $1/T^9$ for the (second order) fluctuation in the order parameter and to $1/T^7$ for the fourth order fluctuation.

Analysis of these series (Section VII) by standard techniques has yielded estimates of the critical temperatures on the s.c., b.c.c. and f.c.c. lattices and estimates of critical amplitudes for each function. Of probably greatest interest are the estimates of the critical exponents, $\gamma = 1.33 \pm 0.02$, $\alpha = 0.02 \pm 0.05$ and $\Delta = 1.67 \pm 0.10$. Within the confidence limits, these estimates agree with the scaling relation connecting them. Tentatively, we have assumed the simple fractional values $\gamma = \frac{4}{3}$, $\alpha = 0$ and $\Delta = \frac{5}{3}$, although

clearly it would be highly desirable to have longer series in order to make more precise estimates of these critical exponents. Using the assigned simple fractions the other critical exponents from standard scaling theory have the values $\alpha = \alpha'$, $\gamma = \gamma'$, $\delta = 5$, $\beta = \frac{1}{3}$, $v = v' = \frac{2}{3}$ and $\eta = 0$. Lattice-lattice scaling theory has also been used to determine for example amplitudes for the specific heat on the s.c. and b.c.c. lattices.

One test of universality is provided by comparison of the estimates of the critical exponents of the spin $\frac{1}{2}$ and spin ∞ X - Y models. As far as the evidence from series expansion goes the corresponding exponents are equal within the confidence limits, thus supporting universality. However, the recent results of Grover (1972) for spin ∞ are in conflict with the series results for both spin values.

Besides extending the existing series, it would be highly desirable to have high temperature series expansion for the perpendicular spin-spin correlations, for the spin $\frac{1}{2}$ X - Y model. The spin-spin correlations are measured directly in both magnetic substances and liquid helium. A direct estimate of v would provide a further test of scaling, and finally, by comparison with v already estimated for the spin ∞ X - Y model, a further test of universality. It would also be useful to have series expansions for the higher order fluctuations to test the constancy of the gap index (hence scaling).

Section IX has been devoted to dynamic properties of the X - Y model, particularly the high frequency, high temperature expansion of the perpendicular (order parameter) susceptibility. The hope of testing dynamic scaling has not been realized because of the apparent presence of two finite frequency collective modes. The conclusions of this Section must be regarded as quite tentative. It would be of interest to discover more concerning the nature of the collective modes, perhaps through series expansion of appropriate combinations of time dependent correlations.

The two-dimensional spin $\frac{1}{2}$ X - Y model fluctuation series (Section X) seem to give clear evidence of a phase transition with exponent $\gamma \approx \frac{3}{2}$. On the other hand, while the plane rotator ($s = \infty$) model also gives clear evidence of a phase transition in two dimensions, the exponent $\gamma \approx 3$. Although there are fairly wide confidence limits on both exponents, it is difficult to believe that they are really equal. Thus, universality with respect to spin value may not hold in two dimensions even though it holds in three dimensions. Such a failure could be connected with the peculiar nature of the low temperature phase in two dimensional spin systems. This is a question clearly demanding further investigation.

The only planar system several of whose critical properties have been carefully measured is liquid helium near the λ transition. In that case there is gratifying agreement between the experimentally measured critical

exponents, α , α' , ν' and β and the theoretical exponents for the $X-Y$ model as obtained from series expansions augmented by scaling. Even more gratifying is the surprisingly good agreement between the liquid helium and $X-Y$ model values, for spin $\frac{1}{2}$ only, for the critical amplitude and critical constant for the specific heat. These results show that the spin $\frac{1}{2}$ $X-Y$ model should be taken quite seriously as a model for liquid helium near T_λ .

There are a fair number of magnetic insulators that are $X-Y$ -like or at least planar. Unfortunately almost no precise measurements have been made of the critical properties of any of them. Some attention has been given to the critical properties of rare earth metals, particularly terbium, with planar order parameters, but measurements of further properties are called for. It would also be desirable to have a thorough experimental study of the critical properties of at least one displacive type ferroelectric such as SrTiO_3 .

Theoretically, we are awaiting a breakthrough on the low temperature properties of the spin $\frac{1}{2}$ $X-Y$ model, starting presumably with the elucidation of the nature of the ground state.

On the high temperature side, besides investigating series expansions for thermodynamic properties, if we are to take the spin $\frac{1}{2}$ $X-Y$ model seriously as a model of a quantum fluid, transport properties should be investigated. Presumably high temperature series expansions can be derived for such properties as thermal conductivity, bulk and shear viscosity, thermal diffusivity, etc. and analysed to estimate the corresponding critical exponents.

The next few years should encompass some exciting developments in this field.

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9. Ferroelectric Models*

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I. Weak Graph Generating Function

Suppose we have a crystallographic lattice L with periodic boundary conditions. Let there be N vertices, each of which has coordination number q , so that there are $(qN/2)$ edges in the lattice L . A central mathematical object in this volume is the weak graph generating function $F_L(Z_0, Z_1, Z_2, \dots, Z_q)$ where the set of variables $(Z_0, Z_1, Z_2, \dots, Z_q)$ will be designated by Z . The weak graph generating function is defined (Nagle and Temperley, 1968) to be a weighted summation over the weak subgraphs G contained in the lattice L . (Weak subgraphs or embeddings were defined by Domb, this volume, Chapter 1 Section IV. For our purposes a weak subgraph may be thought of as a subset of the $(qN/2)$ edges of the lattice plus all the vertices. The vertices of the lattice not incident to any edge of

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the subset simply have degree zero.) The weight w_G of a weak subgraph G is a product over all vertices in L of vertex weights. Each vertex of the lattice L has a vertex weight Z_s where s is the number of edges of the subgraph G incident to that vertex. Thus, $w_G = \prod_{s=0}^q Z_s^{p_s}$ where p_s is defined to be the number of vertices of degree s in the weak subgraph G . The set of integers $(p_0, p_1, p_2, \dots, p_q)$ may be abbreviated by p . In general there may be more than one weak subgraph with vertex description p ; the number of such graphs will be designated $g(p)$ and the weight of each of these graphs will be $w(p, Z) = \prod_{s=0}^q Z_s^{p_s}$. Finally, the weak graph generating function is defined as

$$F_L(Z) = \sum_p g(p) w(p, Z)$$

where the p summation is essentially a summation over subgraphs.

A number of problems, i.e. partition functions, of physical interest can be rigorously transformed into weak graph generating functions. This method of transformation will be called the weak graph series expansion method. The prototypical problem is the spin $\frac{1}{2}$ Ising problem in a field. The particular weak graph transformation for this problem is known as the hyperbolic tangent expansion (Domb, 1960, and this volume Chapter 6.) The identification of variables is $Z_s = w^{s/2}$ when s is even and $Z_s = \tau w^{s/2}$ when s is odd, where $w = \tanh \beta J$ and $\tau = \tanh \beta mH$. A low temperature expansion may also be obtained via a different transformation (Nagle, 1968); the identification is $Z_0 = 1 + yz^q$ and $Z_s = (z^2 - 1)^{s/2} yz^q$, for $s > 0$, where $z = \exp(-2\beta J)$ and $y = \exp(-2\beta mH)$. The monomer-dimer grand partition function is naturally defined as a weak graph generating function, without the need for any transformation. The identification is simply $Z_0 = x_1$, $Z_1 = x_2^{1/2}$, and $Z_s = 0$, $s \geq 2$, where x_1 is the activity of a monomer and x_2 is the activity of a dimer. Some other problems which can be formulated in terms of weak graph generating functions are described by Nagle (1968). The largest class of such problems is the hydrogen-bonded crystal class which will be discussed in some detail in Sections II and III.

Thus, the weak graph generating function approach unifies and generalizes a class of lattice statistical problems. An exact calculation of the weak graph generating function, even in two dimensions, would obviously be very desirable, although this looks to be a very formidable task. However, it should at least be mentioned that *not all* difficult problems can be transformed into weak graph generating functions with *known* weights. An example of such a problem is to compute the number of ways to color the vertices of the lattice such that no edge is incident to two vertices of the

same color. Although one can transform this problem into a weak graph generating function, the weights are known only through a recursion relation (Nagle, 1971). Temperley and Lieb (1971) have also taken a different approach to the coloring problem in which the central mathematical object is the Whitney polynomial; contact is also made with the percolation problem.

One use of the weak graph series expansion is to provide transformed formal expressions for partition functions for various problems. These transformed expressions, i.e. the weak graph generating functions, have sometimes been useful in exact analyses as is reviewed in Section III.A.

Another use of the weak graph expansion is to provide approximations for the thermodynamic behavior of various systems. If one is fortunate, the weak graph generating function appropriate to a specific problem may be arranged into a series in terms of one variable. One then counts weak subgraphs to obtain the $g(p)$ necessary to evaluate as many coefficients in the series as feasible. Then, series extrapolation techniques such as the Padé approximant and the ratio method (Gaunt and Guttmann, this volume, Chapter 4) may be used to estimate the asymptotic behavior of the series. Some results of this procedure are reviewed in Section III.B.

The numerical labor involved in obtaining the relevant $g(p)$ is greatly reduced if many graphs have zero weight. For this reason, the spin $\frac{1}{2}$ Ising specific heat series in zero field are far easier to obtain than series in which the field is non-zero, because vertices of odd degree have zero weight in the former series but not in the latter (Domb, 1960). However, it was observed by Sykes (1961) that the susceptibility series in the limit of zero field could be rearranged in such a way that no graphs with vertices of degree one were required. This is a special case of a general combinational theorem proved subsequently by Nagle and Temperley (1968) which shows that the weak graph generating function can be transformed into itself, but with different vertex weights. In particular, the vertex weight for vertices of degree one can be made equal to zero, thereby obviating the necessity to count most of the weak graphs. Using the $g(p)$ for the remaining and much smaller subset of graphs, one can invert the transformation to obtain the $g(p)$ for all types of p . The algebraic transformation is far easier to perform (and has been programmed for a computer) and more certain to be accurate than the corresponding graph counting.

For an illustrative example one may consider the monomer-dimer grand partition function on the square lattice expanded in the dimer activity x . To obtain the coefficient to x^4 by the straightforward method of counting the number of ways to place four non-overlapping dimers on the lattice is a non-trivial exercise. To obtain the same coefficient using the transformed series requires only the simple counting of the number of squares on the lattice and the expansion of an algebraic expression. The coefficient

of x^{11} was obtained in this way without the use of a computer (Nagle, 1966a). However, it should be mentioned that the most extensive results (to x^{15}) in this particular problem are due to Gaunt (1969) who used a different transformation starting from the low temperature Ising spin $\frac{1}{2}$ series. For the Ising problem itself, other series expansion methods are certainly competitive and are currently being pursued more vigorously than the weak graph method so it is appropriate that we should turn to the hydrogen bonded problems, for which no competitive method exists.

II. Weak Graph Expansion Method Applied to Hydrogen-Bonded Models

Let us consider the Slater (1941) KDP model, which has been discussed earlier in this volume by Lieb and Wu (Volume 1, Chapter 8). For ease of discussion we shall consider the two-dimensional case where the underlying lattice is the s.q. lattice. However, we emphasize that, unlike the exact methods, the series methods are easily generalized to any dimensionality. The allowed configurations of arrows adjacent to each vertex in the Slater KDP model and energies are shown in Fig. 1(a). Physically, the vertices correspond to PO_4^{\pm} groups, the edges correspond to the hydrogen-bonds, and the arrows designate which of the two off-centre positions on each hydrogen bond is occupied by a proton. The vertex configurations in Fig. 1(a) all correspond to H_2PO_4^- groups, that is, each phosphate group has precisely two protons. This condition is analogous to the Pauling model for ice in which each oxygen has precisely two protons and is therefore often called the "ice rule". However, whereas the ice rule is a very good approximation for the equilibrium properties of ice, it is somewhat poorer for KH_2PO_4 and the Slater model is therefore only a first order approximation to KDP. A more realistic model, known as the Takagi model (Takagi, 1948) allows H_3PO_4 and HPO_4^{\pm} groups which constitute regions of net charge ± 1 (remembering the K^+ ion) and are therefore called ionic faults. Thus, in addition to the vertex configurations in Fig. 1(a), the Takagi model involves four vertex configurations with three arrows pointed towards the vertex and four vertex configurations with one arrow pointed toward the vertex. The Takagi model has been intractable using known methods of exact solutions, even in two dimensions, but it involves no additional difficulties to series methods as compared to the Slater model except that the notation becomes more complicated; for this reason we illustrate the series methods using the Slater model.

In Fig. 1(b) a simple transformation is shown which yields a weak graph description involving only vertices of degree zero, two and four. The transformation involves drawing a solid line when an arrow points down or

to the left and a dotted line (i.e. an empty edge) otherwise. This transformation is useful in showing the existence of the phase transition for the KDP model (Nagle, 1969a). However, it is not so useful as the basis for a series or perturbation expansion for the KDP problem

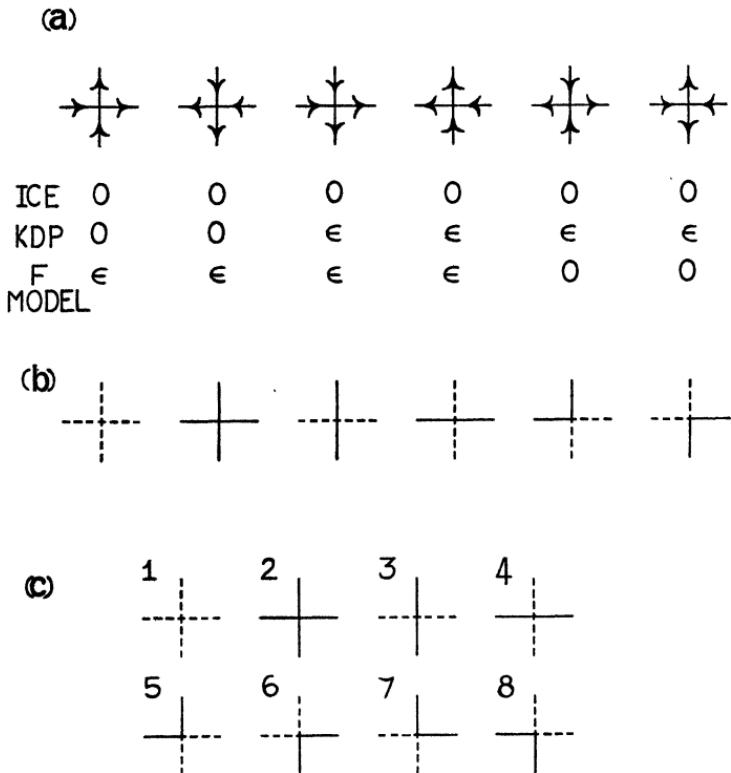


FIG. 1. In (a) the six allowed vertex configurations are shown for the ice, KDP and F model problems along with their energies. The vertex configurations in (a) may be transformed to those in (b) under the rule that an arrow to the left or down is replaced by a solid edge and otherwise is replaced by a vacant or dotted edge. Finally, (c) shows the vertex configurations which occur in the weak graph series expansion of the ice, KDP and F model problems.

because the smallest perturbation or configuration must involve at least one chain of vertices of degree two running from the southwest edge of the crystal to the northeast edge, and this involves an infinite perturbation energy for an infinite crystal.

The initial step in obtaining a useful series expansion for hydrogen bonded problems was taken by DiMarzio and Stillinger (1964). A number of simplifications and generalizations have been made which have made the procedure rather simple and routine (Nagle, 1968). Let us define a variable $\xi_i = 1, 2, \dots, 6$ which identifies the particular vertex configuration in Fig. 1(a) at the i th vertex of the lattice. The vertex energy at the i th vertex is then $E_i(\xi_i) = 0$ if $\xi_i = 1, 2$ and $E_i(\xi_i) = \varepsilon$ if $\xi_i = 3, 4, 5$ or 6 . Let us define a vertex function $B_i(\xi_i) = \exp[-E_i(\xi_i)/kT]$. Finally, let us define a function for each edge ij and each vertex i incident to that edge by

$$C_{ij}(\xi_i) = 1 \text{ if the arrow of the } \xi_i \text{ vertex configuration which is on the } ij \text{ edge points up or to the right,} \quad (1)$$

$$= -1 \text{ if the arrow of the } \xi_i \text{ vertex configuration which is on the } ij \text{ edge points down or to the left.}$$

We now assert that the partition function for the problem in zero electric field is correctly given by

$$Z = \sum_C \prod_{\substack{\text{edges} \\ ij}} \frac{1}{2}[1 + C_{ij}(\xi_i) C_{ji}(\xi_j)] \prod_i B_i(\xi_i). \quad (2)$$

The edge factor in square brackets simply gives zero whenever the two vertex configurations on the two vertices incident at the edge have arrows pointing in opposite directions on that edge. Such vertex configurations are incompatible and vanish from the summation in eqn (2) which is over all 6^N possible combinations of vertex configurations on the lattice. The remaining configurations are compatible in that each edge has two arrows, one from each vertex configuration, which run in the same direction. To complete the formal equivalence with the Slater KDP problem one replaces two parallel arrows on an edge by one arrow and verifies that the $B_i(\xi_i)$ factors give the appropriate Boltzmann factors.

To obtain a series expansion from eqn (2) the multiple product is expanded into its 2^{2N} terms. Each term may be represented by a subgraph G of the square lattice L_{sq} according to the rule that the edge ij of L_{sq} is contained in G if and only if the $C_{ij}(\xi_i) C_{ji}(\xi_j)$ part (rather than the "1" part) of the edge factor (in square brackets) was used in forming the term. Obviously, this kind of expansion dictates that the subgraphs G be weak subgraphs of the lattice. Next, the summation over the vertex configurations is performed to obtain the contribution of each term, i.e. the weight of each

graph. Formally,

$$Z = \sum_{G \leq L_{sq}} w(G) = \sum_{G \leq L_{sq}} \prod_{i=1}^N \frac{1}{\xi_i} \sum_{\xi_i=1}^6 B_i(\xi_i) \prod_{i,j \text{ in } G} C_{ij}(\xi_i). \quad (3)$$

It is at this stage that the utility of the particular form of the edge factor becomes apparent. The initial developments (DiMarzio and Stillinger, 1964, and Nagle, 1966b) simply wrote $a_{ij}(\xi_i, \xi_j)$ instead of $C_{ij}(\xi_i) C_{ji}(\xi_j)$. However, the factorability of the $a_{ij}(\xi_i, \xi_j)$ means that the 6^N fold summation decouples into single vertex summations as in eqn (3). These summations are easily performed to give the vertex weights in Table I. The types of vertices are shown in Fig. 1(c). These will also be called "vertex configurations" but it must be remembered that they are defined in connection with the transformed partition function and are not the same as the vertex configurations of the original problem. All types of vertex such as vertices of degree one not shown in Fig. 1(c) have zero weight in Table I.

TABLE I

| Vertex Type (From Fig. 1(c)) | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|------------------------|------------------------|---------------|---------------|---------------|---------------|------------------------|------------------------|
| Vertex Weight where $K = \varepsilon/kT$ | $\frac{1}{2} + e^{-K}$ | $\frac{1}{2} + e^{-K}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2} - e^{-K}$ | $\frac{1}{2} - e^{-K}$ |

Notice that there are now eight types of vertex configurations, not just six. Also notice that the vertex weights are not the same for all types of vertices of degree two. This can not be otherwise, since the original Slater KDP model has inherent anisotropy along the southwest-northeast axis. This requires a slight generalization of the weak graph generating function introduced in Section I, but does not fundamentally change the discussion. Fan and Wu (1969) have also considered the most general kind of generating function in the sense that all eight vertex configurations in Fig. 1(c) may have different weights. However, they specialize in the sense that no vertices of odd degree are allowed. This forces a number of symmetry relations; for example, there must be an equal number of vertices of type 7 and of type 8 in each subgraph with non-zero weight. Such symmetry relations seem to be related to the solvability of these models in two dimensions.

Thus far, we have ignored any electric field term in the problem. Superficially, the easiest way to include a field is to simply modify the $B_i(\xi_i)$ Boltzmann factors such that $B_i(1) = y = \exp(2\mu E/kT)$ and $B_i(2) = y^{-1}$. The derivation proceeds as before to yield vertex weights but now vertices of degrees one and three do *not* have zero weight, which makes the graph counting considerably more tedious. As was discussed in the introduction

one can transform the generating function so as to eliminate vertices of degree one. Equivalently, one can simply make use of some of the freedom in choosing values for the $B_i(\xi_i)$ and $C_{ij}(\xi_i)$ functions as follows:

In eqn (1) let

$$C_{ij}(\xi_i) = x \quad \text{or} \quad -\left(\frac{1}{x}\right) \text{ instead of } \pm 1, \text{ respectively.} \quad (4)$$

Let x be temporarily undetermined.

$$\begin{aligned} \text{Let } B_i(\xi_i) &= \frac{y}{(1+x^2)^2}, & \xi_i &= 1 \\ &= \frac{y^{-1}}{(1+x^{-2})^2}, & \xi_i &= 2 \\ &= \frac{e^{-K}}{(1+x^2)(1+x^{-2})}, & \xi_i &= 3, 4, 5, 6. \end{aligned} \quad (5)$$

Equation (2) is valid with these new functions in an electric field. The expansion is performed as before to yield the vertex weights. In particular, vertices of degree one have weight

$$z_1 = \frac{xy}{(1+x^2)^2} - \frac{x^{-1}y^{-1}}{(1+x^{-2})^2} + \frac{2(x-x^{-1})e^{-K}}{(1+x^{-2})(1+x^{-2})}. \quad (6)$$

Eliminating vertices of degree one by setting this equal to zero determines x to be

$$x = \left(\frac{2e^{-K}-y}{2e^{-K}-y^{-1}} \right)^{\frac{1}{2}}.$$

However, the electric field does introduce *some* complication into the series expansion since the weight of vertices of degree three can not be made to vanish simultaneously with the weights of vertices of degree one.

With these examples in mind we can discuss the flexibility and the limitation of the weak graph expansion method. If q is the degree of each vertex then clearly there can be at most 2^q different vertex configurations. The edge factor $[1 + C_{ij}(\xi_i)C_{ji}(\xi_j)]$ can generally be any two-valued function; if an edge factor with more than two values is required, there is no guarantee that this form will suffice, although it may suffice for special cases such as the special ternary model (Nagle, 1968). Thus, the method in this simple "binary-edge" form is rather limited. The more complicated forms which must be introduced to discuss more complex problems severely reduce the

utility and simplicity of the method. However, as we have seen, there is just enough flexibility in the binary edge form to guarantee that graphs with vertices of degree one can be eliminated from computations.

III. Applications of the Weak Graph Expansion to Hydrogen-bonded Models

A. Exact analysis

Often series expansion work is thought to be inherently of an approximate nature. However, one need only recall that the duality relation for Ising models in two dimensions can be derived using the hyperbolic tangent expansion (Domb, 1960) to realize that weak graph series expansions may be useful in exact analysis. Here we describe two additional such instances where the weak graph series expansion has been instrumental in exact analysis and one instance where a near miss can be registered.

As has been mentioned before Fa Yueh Wu has considered variations of the basic hydrogen bonded models. One of the variations consists of the two-dimensional F model with doubly ionized vertices. (Wu, 1969.) The F model is analogous to the two-dimensional Slater KDP model except that the vertex energies as shown in Fig. 1(a) are of antiferroelectric rather than ferroelectric type as can be seen by constructing the ground state. Wu's inclusion of doubly ionized vertices requires an additional vertex configuration which has all four arrows pointed towards the vertex and a vertex configuration which has all four arrows pointed away from the vertex. Using the transformation which takes Fig. 1(a) to Fig. 1(b), the F model with doubly ionized vertices can be described in terms of the vertex configurations in Fig. 1(c). The vertex weights $w(\xi)$ are $w(1) = w(2) = w(3) = w(4) = e^{-\beta e}$; $w(5) = w(6) = 1$ and $w(7) = w(8) = e^{-2\beta e}$. With these vertex weights the two-dimensional problem is not readily solved by the Pfaffian or dimer technique of solution. However, Wu found that this problem can be re-expanded using the weak graph method as follows:

Let $C_{ij}(\xi_i) = 1$ if ξ_i has a bond on the edge ij

$$= -1 \text{ otherwise}$$

Then,

$$Z = \sum_C \prod_{\substack{ij \\ \text{edges}}} \frac{1}{2}[1 + C_{ij}(\xi_i)C_{ji}(\xi_j)] \prod_{i=1}^N w(\xi_i).$$

Carrying out the expansion of Z yields a new weak graph expansion in which

the vertex weights, designated by primes, are:

$$\begin{aligned} w'(1) &= w'(2) = \frac{1}{2}(w(1) + w(3) + w(5) + w(7)) \\ w'(3) &= w'(4) = \frac{1}{2}(w(1) + w(3) - w(5) - w(7)) \\ w'(5) &= w'(6) = \frac{1}{2}(w(1) - w(3) + w(5) - w(7)) \\ w'(7) &= w'(8) = \frac{1}{2}(w(1) - w(3) - w(5) + w(7)). \end{aligned}$$

Using the symmetry that there must be the same number of vertices of type 5 and type 6 in any subgraph with non-zero weight allows $w(5)$ and $w(6)$ to be replaced by $-w(5)$ and $-w(6)$. Then the new weights are in a form such that the Pfaffian method can be immediately applied to solve the model.

The second instance where the weak graph expression has been essential to an exact analysis is the proof that Slater KDP models in any dimension have a first order phase transition at the temperature T_c given by the relation $e^{-\varepsilon/kT_c} = \frac{1}{2}$ (Nagle, 1969a). An argument based on the transformation shown in Fig. 1(b) can be used to prove that the Slater model is perfectly ordered for $T \leq T_c$ and leaves little doubt that there is a transition at $T = T_c$, but it appears very difficult to extend the argument to a rigorous proof. In contrast the series expansion developed in Section II permits an easy proof. First, we note that there are only two subgraphs in the series expansion which each contribute identically $(\frac{1}{2} + e^{-K})^N$ to the expansion, namely, the subgraph with no edges present and the subgraph with all edges of the lattice present. Next, we note that all other subgraphs must have at least one vertex of type 7 in Fig. 1(c) and one vertex of type 8. The contributions from all such subgraphs vanish when $e^{-K} = e^{-\varepsilon/kT} = \frac{1}{2}$, i.e. at T_c , because the vertex weights given in Table I vanish for types 7 and 8. Independently of the argument based on the transformation in Fig. 1(b), this suffices to show that the model is perfectly ordered for $T \leq T_c$ since the partition function must be non-decreasing with T and cannot be less than 2, which is its value at $T = 0$, and must therefore be identically equal to 2 for $0 \leq T \leq T_c$. For $T > T_c$ the fact that the number of vertices of type 7 is the same as the number of vertices of type 8 suffices to show that the contribution from all graphs is positive so that the partition function is bounded below by $2(\frac{1}{2} + e^{-K})^N$. Since the free energy per site is reasonably supposed to be continuous by convexity arguments this yields an energy per lattice site greater than or equal to $\frac{1}{2}\varepsilon$ as $T \rightarrow T_c$ from above as compared to zero energy for $T < T_c$, and thus establishes the discontinuous nature of the phase transition. However, for completeness one may note that even if the free energy per site were discontinuous at T_c one would still have a discontinuous phase transition.

The two-dimensional F model provides an instance where a duality type of argument, reminiscent of the Ising model duality argument, almost

enables one to locate the transition temperature rigorously (Nagle, 1969b). Just as in the Ising model case one develops a low temperature expansion which is represented by graphs which look very much like the graphs in the high temperature expansion, except that for the F model there are extra graphs in the high temperature expansion which spoil the complete duality. However, if one ignores the extra graphs and computes a T_c using only the dual graphs, it then turns out that the contributions of the extra graphs vanish at the trial T_c . Unfortunately, there are ways in which this could happen such that the trial T_c is not the exact T_c , so the argument has not been made rigorous, nor is it likely to be made rigorous since the exact solution gives us the exact T_c . Nevertheless, it is interesting that the trial T_c suggested by the duality argument is the exact T_c (Lieb and Wu, Volume 1, Chapter 8).

B. Numerical approximations

The weak graph series method was first developed in the form presented in this paper for the specific problem of estimating the residual entropy of ice. (DiMarzio and Stillinger, 1964; Nagle, 1966c.) The ice problem can be thought of as the infinite temperature Slater KDP problem, i.e. $e^{-K} = 1$. From the weights in Table I the partition function can then be written as:

$$Z = \left(\frac{3}{2}\right)^N \sum_{G \leq L} \left(\frac{1}{3}\right)^{p_2}$$

where use has been made of symmetry which requires vertices of type 7 and type 8 to come in pairs so that the (-1) factors can be ignored.

The natural way to order the expansion is to let the n th term be the sum of the weights of all graphs with n vertices of degree two. This yields the following series for the partition function per site for the two-dimensional square lattice:

$$Z_{sq}^{1/N}(x) = \frac{3}{2}[1 + x^4 + 4x^6 + 18x^8 + 92x^{10} + 518x^{12} + \dots]$$

which must be evaluated at $x = \frac{1}{3}$ for the ice problem. The term in x^4 comes from the square subgraph, i.e. the polygon with four edges. The x^6 term comes from two orientations of polygons with six edges and two orientations of the "figure-eight" subgraph composed of two squares joined at a common vertex, which is of degree four. This latter graph contributes only to the eighth term in the Ising hyperbolic tangent series, and shows the extra complication involved in obtaining the ice series.

Since the ice series is not expected to be singular at $x = \frac{1}{3}$, rather unsophisticated series extrapolations may be performed to yield $Z_{sq}(\frac{1}{3}) = 1.540 \pm .001$ where the quoted uncertainty is a confidence estimate,

not a rigorous bound. This agrees with the subsequently derived exact value $Z_{sq}(\frac{1}{2}) = 1.5396 \dots$ (Lieb, 1967). For the physically interesting three-dimensional case the series is:

$$Z_3^{1/N}(x) = (\frac{3}{2}) [1 + 2x^6 + 3x^8 + 36x^{10} + 114x^{12} + 1080x^{14} \dots].$$

Notice that there is no x^4 term since the smallest polygonal subgraph which can be formed in the ice lattice has six vertices. This means that the three-dimensional estimate for $Z_3^{1/N}(\frac{1}{2})$ is even closer to $(\frac{3}{2})$ than for the two-dimensional case. Also notice that the series for the three-dimensional case exhibits an odd-even effect which makes it less smooth and somewhat harder to extrapolate than the series for the two-dimensional case. However, the terms in the series when evaluated at $x = \frac{1}{2}$ diminish so rapidly that one can estimate that:

$$1.5067 < Z_3^{1/N}(\frac{1}{2}) < 1.5070.$$

This estimate for $Z_3^{1/N}(\frac{1}{2})$ gives excellent agreement with experiment.

Currently, progress is being made on obtaining estimates for the susceptibility or dielectric constant of ice. In the two-dimensional case R Peacock and I have obtained

$$\chi = \frac{\mu^2}{kT} [1 - 4x^4 - 12x^8 + 48x^{10} + \dots]$$

where again the series is to be evaluated at $x = \frac{1}{2}$. Just adding up the available terms in the series gives $\chi = 0.9496 (\mu/kT)$ and one might suppose that the next few terms in the series may be positive. This agrees with the exact result

$$\chi = \frac{3}{\pi} \frac{\mu^2}{kT} = 0.9549 \dots \frac{\mu^2}{kT}$$

which may be deduced from the paper of Sutherland *et al.* (1967). Preliminary numerical work on the three dimensional diamond lattice indicates that χ will be very much closer to $1(\mu^2/kT)$ for this case.

From the excellent results obtained for the ice problem one might expect that the KDP and F model series should also yield useful approximations to the phase transition. Unfortunately, one immediately runs into the difficulty that there does not exist a single variable in which to expand the series. This is most easily seen from Table I. One may divide out $(\frac{1}{2} + e^{-K})^N$ from the partition function, but one is still left with two incommensurate vertex weights, one for vertices of types 3, 4, 5 and 6 and one for vertices of types 7 and 8. No way has yet been found to rearrange

the series such that there is a single expansion variable *and* such that the subgraphs which contribute to the *n*th order term are finite in number.

It is perhaps not too surprising that the series for these hydrogen-bonded problems are somewhat unusual when compared to, say, the Ising model series in view of the fact that the hydrogen-bonded models are themselves somewhat unusual. For example, Baxter (1970) has shown that the staggered susceptibility for the F model actually diverges at least at one temperature above T_c and Sutherland (1970) has argued that models obeying the ice rule are "critical" in the high temperature phase. This precludes a study of the F model critical "point" by the use of high temperature series. Similarly, the low temperature series for the F model (Nagle, 1969b) are rather pathological. However, it is very reassuring for practitioners of the series method that these pathologies may be detected from the series. Thus, even though one may not obtain excellent approximations each time by the series method, at least one has some hope that careful scrutiny will avoid the drawing of erroneous conclusions.

Finally, we turn briefly to the monomer-dimer problem. Unlike the hydrogen bonded problems the series expansions for the monomer-dimer problem provide good approximations throughout the physical region (Gaunt, 1969). In particular, the form of the weak graph expansion seems to be very useful in estimating the entropy in the limit of maximum concentration of dimers, as can be seen by comparison with the exact results in two dimensions (Nagle, 1966a). Thus, it is to be hoped that problems with pathological series are the exception and not the rule.

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