THE TWO-DIMENSIONAL ISING MODEL

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TO CHEN NING YANG AND SAU-LAN YU

without whom it would have been impossible

PREFACE

Of all the systems in statistical mechanics on which exact calculations have been performed, the two-dimensional Ising model is not only the most thoroughly investigated; it is also the richest and most profound. In 1925, Ising introduced the statistical system which now bears his name and studied some of its properties in one dimension. Although the generalization of Ising's system to higher dimensions was immediately obvious, it was not until 1941 that a quantitative statement about the phase transition in the two-dimensional case was made when Kramers and Wannier and also Montroll computed the Curie (or critical) temperature. However, the most remarkable development was made in 1944 when Onsager was able to compute the thermodynamic properties of the two-dimensional lattice in the absence of a magnetic field. Onsager's approach was greatly simplified by Kaufman in 1949, and in a companion paper Kaufman and Onsager studied spin correlation functions. The spontaneous magnetization was first published, without derivation, by Onsager in 1949, and the first derivation was given by Yang in 1952. For the next decade no new result of fundamental significance was derived, but a great deal was accomplished in simplifying the mathematics of these pioneering papers. The work of Kac, Kasteleyn, Montroll, Potts, Szegö, and Ward, among others, has been especially significant.

The methods of Onsager, Kaufman, and Yang, although very beautiful and powerful, are also extremely complicated. Thus, the two-dimensional Ising model has acquired a notorious reputation for difficulty whereas, in fact, the simplified methods developed by 1963 have reduced the analysis to the point where it may be readily understood. Since then we have actively used these methods as the basis for computing many more quantities of physical interest. Our original concern was with the spin correlation functions of the two-dimensional Ising model. However, it soon became apparent that much more could be studied. In particular, we found that the Ising model has properties which exhibit a hysteresis behavior. Moreover, we discovered that exact results can be obtained even in a much more complicated situation where the interaction between the spins is allowed to be a random variable. On the basis of these results, a quantitative study of the influence of impurities on phase transitions has been carried out. This influence is large and has experimental consequences that have yet to be fully explored.

Since the two-dimensional Ising model forms the basis of much of our theoretical understanding of phase transitions, it is unfortunate that these recent developments have not been easily accessible to the general community of physicists. Perhaps as a result of its notoriety, most physicists tend to think of the two-dimensional Ising model as a closed problem that was completely solved by Onsager, Kaufman, and Yang. Moreover, once a physicist does become aware of the wide variety of open questions there is no convenient place where he can find the known facts collected together and explained in an organized fashion. Furthermore, even if one has the patience to trace the references back to Kasteleyn's paper of 1961, the usual result is a feeling of confusion. This confusion arises not out of any errors in the published work, but out of the fact that in journal articles many things must be omitted owing to lack of space. Therefore, points that can be straightened out and rigorously shown to cause no problems are often treated very briefly. The careful reader therefore has questions that he must resolve for himself and the resolutions are frequently quite time consuming.

The study of the two-dimensional Ising model requires the use of mathematics from such apparently widely separated areas as the theory of determinants and integral equations. Few physicists are knowledgeable in all these branches of mathematics. Therefore, a formula that may have been well known to a mathematician of 100 years ago may be totally unknown to a physicist of today. It is quite impossible to discuss such a formula in a journal article. One must call it "well known," give a reference, and go on. But the reference is often useless because, while correct, it usually is so arranged that the reader must spend an inordinate amount of time in mastering a lot of notation which is mostly superfluous if he wants to derive only one particular formula. For example, in our study of Ising-model spin correlation functions we make extensive use of the theory of Wiener-Hopf sum equations. Except as an afterthought to the theory of Wiener-Hopf integral equations, these sum equations are rarely discussed in the literature. This circumstance often leads one to believe that the sum equations are harder than the integral equations. In fact they are simpler.

W

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For these reasons we feel that it is at this time most desirable to write a book on the two-dimensional Ising model that has the following three goals:

(1) It should be completely up to date and be crystal clear in its statement of what is known and, more important, what is as yet unknown.

(2) It should discuss all topics in complete detail. No significant point should be dismissed with the casual remark "it can be shown."

(3) It should strive to be self-contained. All mathematical statements that are not known by the average graduate student in physics should be proved.

The present book, which sets forth the theory of the two-dimensional Ising model with nearest-neighbor interactions as it has developed through the end of 1969, is our attempt at meeting these three goals. In particular, we have tried to make this book complete in such a manner that the physicist can read it without consulting any additional source. To this end we have assumed that the reader knows no statistical mechanics at all and have included at the beginning a chapter that develops all the statistical mechanics needed for the entire book. Furthermore, though we do not feel justified in including a chapter on special functions, we have not assumed a familiarity with mathematics beyond a basic understanding of complex-variable theory.

For the sake of readability we abandon altogether any attempt at preserving the historical development of the Ising model and, in fact, give no exposition whatsoever of the original work of Onsager, Kaufman, and Yang. The development we follow instead should be obvious from the chapter headings in the table of contents. Only three points deserve special attention. First, the interrelations between the chapters are shown in Fig. 0.1. Secondly, we have chosen to give a thorough treatment of

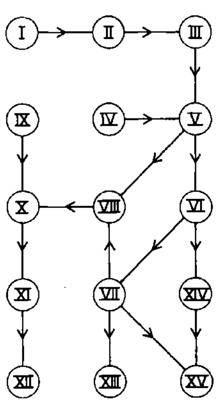

Fig. 0.1. The interrelations of the chapters.

boundary effects before any study is made of bulk spin correlation functions. We have made this choice because the calculations for the boundary are much easier to understand and are more complete than the corresponding calculations for the bulk. Lastly, we wish to call the reader's attention to Chapter IV. This is the most crucial chapter in the book because everything that is done later depends on it. For this reason, in Chapter IV we attempt to give a complete and detailed discussion of all the fine points. However, several of these details have to do only with straightening out certain + and − signs associated with the various boundary conditions that may be imposed on the lattice. Accordingly, if the reader is willing to accept the conclusions of Sections 4 and 5 of Chapter IV, he may omit the derivations without impairing his ability to read the rest of the book. In fact, we will suggest that the book may be profitably read with the omission of Chapter IV altogether, even though this is the most crucial chapter, because the results of this chapter are much more easily stated and used than they are proved. Moreover, the several open questions we will arrive at already incorporate the combinatorics of Chapter IV in their formulation. Therefore, it is perfectly possible to appreciate the current status of the physics of the Ising model without a full understanding of the combinatorial problem involved. Indeed, this was precisely the route that we took ourselves when we first entered the field.

If the authors of any scientific book are to be fair to the reader, it is as important for them to indicate what is omitted as to explain what is covered. Not a book, but an encyclopedia, results if an effort is made to include all related topics, related related topics, and so on. For this book we mention the conspicuous omission of the following five related topics: (1) high- and low-temperature expansions, (2) Padé approximants, (3) the circle theorem of Lee and Yang, (4) decorated lattices, and (5) theorems that prove the existence of limits or of analyticity without actually computing the quantity involved.

One of us (TTW) would like to express special gratitude to Professor Ronold W. P. King and Professor Elliott W. Montroll. Because of the insistence of Professor King that each student must be allowed to decide his own interest and pick his own topic, it has been a most rewarding experience to write a doctorial dissertation under his guidance. Furthermore, without his continual encouragement and help in every respect of this present book, its completion would be impossible. Professor Montroll taught us the Pfaffian approach to the two-dimensional Ising model. The influence of his two papers, "Lattice Statistics" (Chapter IV, *Applied Combinatorial Mathematics*, ed. E. F. Beckenbach, Wiley, New York, 1964) and "Correlations and Spontaneous Magnetization of the Two-Dimensional Ising Model" (with R. B. Potts and J. C. Ward, J. Math. Phys. **4**, 308, 1963), is particularly evident in Chapter IV and Chapter VIII of this book.

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In the course of our study of the Ising model, we have had the benefit of the advices of many friends. In particular, we wish to thank Professor H. Cheng, Professor F. Dyson, Professor K. Huang, Professor T. D. Lee, Professor H. Levine, Professor H. McKean, Professor A. Pais, Professor G. C. Rota, and Professor C. P. Yang for many helpful discussions.

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In Chapters VI, VII, XI, XII, XIII, XIV, and XV, we draw heavily on material we have published separately, jointly, and with Professor H. Cheng in *The Physical Review* and *The Physical Review Letters*. We wish to thank the National Science Foundation and the Alfred P. Sloan Foundation for supporting the research reported in these papers, and the editors of *The Physical Review* and *The Physical Review Letters* for allowing us to use this copyrighted material. We also wish to thank the Pergamon Press Ltd. (Oxford, England) for permitting us to employ the proof of Privalov's theorem as it appears in the book *Trigonometric Series* by N. K. Bary.

Finally, special thanks are due Professor Chen Ning Yang, who has been a constant source of inspiration and who tries to make theoretical physicists out of us.

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State University of New York
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I have developed three criteria to determine
my selection of an issue; I ask myself first
how important it is; second, what kind of
contribution I can make; and third, how many
people are already working in the area.—Ralph Nader

THE TWO-DIMENSIONAL ISING MODEL

CHAPTER I
Introduction

1. INTRODUCTION

Statistical mechanics is an old and venerable branch of physics which has received the attention of many physicists from the time of Gibbs. Since then it has developed in several directions so that at present it is possible to distinguish at least three different theoretical approaches to the subject: (1) the foundational approach, which is concerned with establishing the general properties of, and proving existence theorems for, statistical mechanical systems by rigorous mathematical means, (2) the phenomenological approach, which is concerned with correlating and quantitatively explaining the results of experiments by any available method, and (3) the model-building approach, which attempts to gain insight into practical situations by studying simple models in which at least some physically interesting quantities may be exactly computed. Each of these approaches has made such valuable contributions to our understanding of statistical mechanics that it is neither feasible nor desirable to separate them completely. However, because each approach has developed such a large body of literature, it is likewise not possible to give an adequate treatment of all of them in a single book. Therefore, while we will attempt to make this book self-contained by giving a brief discussion of the foundation of statistical mechanics, and while we will attempt to place the book in a somewhat broader context by making contact with the existing experimental situation, we will concentrate our efforts on the study of certain solvable models.

The number of exactly solvable problems in a field depends on the complexity of the subject. For example, there are innumerable solvable problems in classical mechanics, whereas, at the other extreme, very few problems in relativistic quantum field theory have ever been exactly solved. The scarcity of solvable models in both statistical mechanics and relativistic quantum field theory is due basically to the fact that, in a system with a very large number of particles, each particle may indirectly interact with an enormous number of others even if the fundamental interaction is two-body and of short range. However, it is the purpose of statistical mechanics to study systems with a large number of particles, and the phenomena of greatest interest are precisely those which are not present in the classical or quantum mechanics of a small number of particles. Therefore, a criterion for the usefulness of any model in statistical mechanics is its capability of giving us insight into the new phenomena characteristic of a large number of particles.

The most characteristic feature of statistical mechanical systems is the existence of phase transitions. Surely the most familiar phase transition is either the condensation of steam into water or the freezing of water into ice. Only slightly less familiar is the ferromagnetic phase transition that takes place at the Curie temperature, which, as an example, is roughly 1043°K for iron. Of the several existing models which exhibit a phase transition, the most famous is the Ising model. In three dimensions the model is so complicated that no exact computation has ever been made, while in one dimension the Ising model does not undergo a phase transition. However, it is one of the most beautiful discoveries of twentieth-century physics that in two dimensions the Ising model not only has a ferromagnetic phase transition but also has very many physical properties which may be exactly computed. Indeed, despite the restriction on dimensionality, the two-dimensional Ising model exhibits all of the phenomena peculiar to magnetic systems near the Curie temperature. For that reason, the two-dimensional Ising model forms the basis of almost all our theoretical understanding of the phase transition to the ferromagnetic state.

2. THE ISING MODEL

The model introduced by Ising[1] consists of a lattice of "spin" variables σ_α, which may take on only the values $+1$ and -1. Any two of these "spins" have a mutual interaction energy

$$-E(\alpha, \alpha')\sigma_\alpha\sigma_{\alpha'}. \tag{2.1}$$

The meaning of (2.1) is as follows: the mutual interaction energy is $-E(\alpha, \alpha')$ when σ_α and $\sigma_{\alpha'}$ are both $+1$ or both -1, but is $+E(\alpha, \alpha')$ in the two cases where $\sigma_\alpha = +1$, $\sigma_{\alpha'} = -1$ and $\sigma_\alpha = -1$, $\sigma_{\alpha'} = +1$. In

1. E. Ising, *Z. Physik* **31**, 253 (1925). Some people prefer to refer to this as the Lenz-Ising model because Lenz introduced the model in *Physik. Z.* **21**, 613 (1920). However, Lenz never computed any of the model's properties. Therefore, we will follow the practice of Onsager, Kaufman, and Yang and refer to the model by Ising's name alone.

addition, a spin may interact with an external magnetic field H with an energy

$$-H\sigma_\alpha. \tag{2.2}$$

Like (2.1), (2.2) means that the interaction energy is $-H$ or $+H$ according as the spin σ_α is $+1$ or -1. Throughout this book we will consider only the case where $E(\alpha, \alpha')$ vanishes unless the locations α and α' are nearest neighbors on the lattice. Furthermore, we will restrict ourselves to the square lattice, where all the spins σ_α are situated at the intersections of a square grid. These two restrictions are of quite different natures and deserve comment.

In two dimensions, the restriction to nearest-neighbor interactions has proved essential if we wish to perform exact calculations valid for all temperatures. In one dimension, however, the same remark does not apply, and, in fact, explicit computations on the linear Ising chain have been carried out with interactions which include several neighbors. More important, it has been shown by Dyson[2] that, whereas no phase transition can exist if all interactions are finite and of finite range, a phase transition does exist if the interactions are of infinite range and decrease sufficiently slowly as the separation between the spins becomes large. At present only the existence of this phase transition has been established, but none of its properties have been computed. This one-dimensional work is extremely interesting but does not fall within the scope of this book. It does, however, lead us to believe that in two dimensions a generalization of the interaction to include more than nearest neighbors will change the nature of the phase transition qualitatively only if the range of interaction is infinite. Because dipole-dipole forces are of long range, this is physically an interesting topic, but unfortunately nothing is exactly known at present.

There are numerous two-dimensional lattices other than the square lattice. For example, the triangular, hexagonal, and decorated lattices have all been considered. However, the square lattice is the one which has been most thoroughly studied. Furthermore, the existing work on all of these lattices has been performed by methods quite closely related to those we will develop for the square lattice. Also, with the exception of decorated lattices, most of the physical properties of these lattices reveal no new phenomena not already exhibited by the square lattice. Consequently, for reasons of concreteness and convenience, we will, with one exception in Chapter VIII, not consider these lattices in this book.

With these restrictions, we may now write the total energy of the two-dimensional Ising model as

$$\mathscr{E} = -\sum_j \sum_k \{E_1(j,k)\sigma_{j,k}\sigma_{j,k+1} + E_2(j,k)\sigma_{j,k}\sigma_{j+1,k} + H\sigma_{j,k}\}, \tag{2.3}$$

2. F. Dyson, *Communications in Math. Physics* **12**, 91, 212 (1969).

where the first subscript of σ labels the rows and the second subscript labels the columns of the square lattice. However, further simplifying assumptions on $E_1(j, k)$ and $E_2(j, k)$ are still needed if we wish to obtain explicit results. Throughout the first thirteen chapters of this book we will consider the case first studied by Onsager,[3] namely, the case where $E_1(j, k)$ does not depend on j and k and where $E_2(j, k)$ also does not depend on j and k. We will refer to the square lattice with these conditions on E_1 and E_2 as *Onsager's lattice* and write its total energy explicitly as

$$\mathscr{E} = -E_1 \sum_j \sum_k \sigma_{j,k}\sigma_{j,k+1} - E_2 \sum_j \sum_k \sigma_{j,k}\sigma_{j+1,k} - H \sum_j \sum_k \sigma_{j,k}. \tag{2.4}$$

Onsager's lattice has the property that (ignoring for the moment possible complications at the boundary) each site is equivalent to every other site. In the last two chapters of this book, the restriction to Onsager's lattice is relaxed. Instead, we study lattices where $E_2(j, k)$ is allowed to depend on j but not k although $E_1(j, k)$ is still independent of both j and k.

Our definition of the Ising model is still incomplete, because we have not yet specified the situation at the boundary. In this book, several different choices appear, depending on the physical quantity of interest.

It must be pointed out that the Ising model is a useful model for several physical phenomena other than ferromagnetism. For example, Lee and Yang[4] have used it to study the liquid-gas transition, and it has also proved to be of great value in understanding the order-disorder transition of alloys such as β-brass. However, for the sake of concreteness of interpretation and because the considerations of the last three chapters do not make physical sense with any other interpretation, we will unabashedly think of the Ising model as a ferromagnet.

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We conclude this chapter with a chronological list of the literature on the two-dimensional Ising model that is referred to in the course of this book.

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CHAPTER II
Statistical Mechanics

1. INTRODUCTION

The basic simplification in framing the definition of the Ising model of the preceding chapter is the choosing of the fundamental variables to be the numbers $\sigma_{j,k}$ which can be only $+1$ or -1. Because of this choice there can be no terms in the interaction energy which refer to kinetic energy or to angular momentum. Consequently, the $\sigma_{j,k}$ do not change with time and by necessity we must confine ourselves to a study of those physical properties which depend only on the distribution of energy levels of the system. When the number of energy levels is large, this study requires the use of statistical mechanics. Furthermore the energy levels of the Ising model are discrete and are bounded below. In this chapter we will develop the statistical mechanics needed to study such systems.

2. MICROCANONICAL ENSEMBLE

A thorough and rigorous development of statistical mechanics in a form general enough to apply to all systems of physical interest is a difficult job which is outside the scope of this book. Fortunately, we avoid some of the mathematical difficulties by restricting our attention to systems with discrete energies only. Furthermore we will make the additional technical restriction that the discrete energy levels are commensurable. In particular, we assume: (1) that all differences between energy levels are integral multiples of some ΔE, and (2) that ΔE is the largest of the numbers satisfying (1). For the interaction (2.4) of Chapter I with $H = 0$ this restriction is equivalent to the requirement that E_1/E_2 be rational. It is inconceivable that any quantity of physical interest can depend on the existence of ΔE and, indeed, ΔE will not appear in the final form of statistical mechanics which we shall derive.

Our derivation of statistical mechanics is not going to be logically impeccable. To be truly understandable to the physicist we should take the laws of mechanics, be they classical or quantum, and compute everything from first principles. Unfortunately, this has never been done. Anyone who wants to "derive" the laws of statistical mechanics must at some point wave his hands, intimidate the reader by appealing either to "physical experience" or to "mathematical axioms," and introduce some concept beyond the realm of the laws of mechanics. For the moment we will follow tradition and introduce these extramechanical assumptions. In Sec. 6 we will return to this point and make explicit some of the physical phenomena for which this approach is inadequate.

It is traditional in discussions of statistical mechanics to introduce the concept of thermal equilibrium. Strictly speaking, this is an undefined (or, perhaps better, multiply defined) concept. In introducing it we try by an appeal to our physical intuition to circumnavigate the fact that we are not in general able to study the time development of a system with a large number of particles.

One notion of thermal equilibrium is the intuitive feeling that if a macroscopic system is prepared and then left isolated for a long period of time its macroscopic properties will eventually stop changing and it will be in some sort of equilibrium.

Another notion of equilibrium is embodied in the zeroth law of thermodynamics: If system A and system C are in thermal equilibrium with each other and system B and system C are in thermal equilibrium with each other, then system A and B are also in thermal equilibrium with each other. In this form the zeroth law is a bit abstract. However, in practice it is made concrete by introducing the concept of temperature. Indeed, we will use the zeroth law to characterize temperature by saying that temperature is a quantity which is the same for all bodies which are in thermal equilibrium with each other.

We will use the word temperature to mean "statistical" temperature. On the other hand, once we have used statistical mechanics to give a precise definition of the statistical temperature, we will show that it has all the properties of the temperature of thermodynamics. In particular, we show that the temperatures of two bodies in thermal equilibrium with each other are equal.

By definition it is not possible to speak of the statistical mechanics of one isolated Ising model with a finite, and perhaps small, number of sites. Therefore we must consider that in some way our Ising model is made part of a system which is big enough for statistical concepts to be useful. The actual way in which this contact is established and the nature of the larger system will be irrelevant as long as the forces which make the connection are sufficiently weak. To carry out this construction within the context of discrete energy levels, we will consider a large number N of identical Ising models of $\mathscr{M}$ rows and $\mathscr{N}$ columns connected together by infinitely weak forces which allow the Ising models to exchange energy but that do not contribute to the total energy of the system. One of the Ising models is the system we are interested in; the others will serve to define the temperature. Such a collection of systems is called an ensemble.

We study this ensemble by using the fundamental postulate of the statistical mechanics of discrete energy levels: if we know only the total energy of an ensemble but do not know the energies of each of the Ising models that make it up, then all such distributions of the total energy are equally probable. An ensemble with this probability function is called a microcanonical ensemble.

To state this postulate in mathematical form let $\sigma^{(n)}$ stand for the set of variables which specify the nth Ising model and let $\mathscr{E}^{(n)}(\sigma^{(n)})$ be the energy corresponding to $\sigma^{(n)}$. Then if the only information we have about an ensemble is that its total energy is E^{tot}, the probability that the N Ising models have the configurations specified by $\sigma^{(1)}, \ldots, \sigma^{(N)}$ is

$$P(\sigma^{(1)}, \ldots, \sigma^{(N)}; E^{\text{tot}}) = \frac{\delta_{E^{\text{tot}}, \mathscr{E}^{\text{tot}}}}{\Omega(E^{\text{tot}})}. \tag{2.1}$$

Here

$$\mathscr{E}^{\text{tot}} = \sum_{n=1}^{N} \mathscr{E}^{(n)}(\sigma^{(n)}), \tag{2.2}$$

$\delta_{j,j'}$ is Kronecker's delta which is 1 if $j = j'$ and 0 otherwise, and

$$\Omega(E^{\text{tot}}) = \sum_{\sigma^{(1)}} \cdots \sum_{\sigma^{(N)}} \delta_{E^{\text{tot}}, \mathscr{E}^{\text{tot}}}, \tag{2.3}$$

where $\sum_{\sigma^{(n)}}$ indicates a summation over all configurations $\sigma^{(n)}$ of the nth Ising model.

3. CANONICAL ENSEMBLE

Our interest is not in properties of all N Ising models but rather in the properties of one particular Ising model. We therefore must find the probability $P(\sigma^{(1)}; E^{\text{tot}})$ that one Ising model (say the first one) is in some particular state $\sigma^{(1)}$ while the rest of the Ising models may be in any state subject only to the requirement that E^{tot} be constant. This probability is exactly computed from (2.1) as

$$P(\sigma^{(1)}; E^{\text{tot}}) = \frac{\sum_{\sigma^{(2)}} \cdots \sum_{\sigma^{(N)}} \delta_{E^{\text{tot}}, \mathscr{E}^{\text{tot}}}}{\Omega(E^{\text{tot}})}. \tag{3.1}$$

If N is small this is the final expression and no further simplification is possible. We are, however, interested in the limit where $N \to \infty$, which corresponds to the physical situation of having our one small Ising model connected to an external system or heat bath which has an enormous number of degrees of freedom. A collection of Ising models with a probability determined by (3.1) in the $N \to \infty$ limit is known as a canonical ensemble.

To study (3.1) as $N \to \infty$ we first use the integral representation of Kronecker's delta,

$$\delta_{j,j'} = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta e^{i\theta(j-j')/\Delta E}, \tag{3.2}$$

which is valid since $(j - j')/\Delta E$ is an integer, and we write

$$\begin{aligned}\Omega(E^{\text{tot}}) &= \sum_{\sigma^{(1)}} \cdots \sum_{\sigma^{(N)}} \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta \exp\left\{\frac{i\theta}{\Delta E}\left[E^{\text{tot}} - \sum_{n=1}^{N} \mathscr{E}^{(n)}\right]\right\} \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta \exp\left\{\frac{i\theta}{\Delta E} E^{\text{tot}} + N \ln Z\left(\frac{i\theta}{\Delta E}\right)\right\} \\ &= \frac{\Delta E}{2\pi i}\int_{-i\pi/\Delta E}^{i\pi/\Delta E} d\zeta \exp\{\zeta E^{\text{tot}} + N \ln Z(\zeta)\},\end{aligned} \tag{3.3}$$

where

$$\zeta = \frac{i\theta}{\Delta E} \tag{3.4}$$

and

$$Z(\zeta) = \sum_{\sigma} e^{-\zeta \mathscr{E}(\sigma)}. \tag{3.5}$$

Similarly,

$$\begin{aligned}&\sum_{\sigma^{(2)}} \cdots \sum_{\sigma^{(N)}} \delta_{E^{\text{tot}}, \mathscr{E}^{\text{tot}}} \\ &= \frac{\Delta E}{2\pi i}\int_{-i\pi/\Delta E}^{i\pi/\Delta E} d\zeta \exp\{\zeta[E^{\text{tot}} - \mathscr{E}^{(1)}(\sigma^{(1)})] + (N-1)\ln Z(\zeta)\}.\end{aligned} \tag{3.6}$$

We will approximately evaluate the integrals in (3.3) and (3.6) when $N \to \infty$ by the method of steepest descents.

To carry out this approximation we first show that if

$$\zeta = \beta + iy \tag{3.7}$$

and

$$-\frac{\pi}{\Delta E} < y < \frac{\pi}{\Delta E} \tag{3.8}$$

then the integrand of (3.3) has its absolute maximum for a given value of

β at $y = 0$. We demonstrate this by noting that

$$|[Z(\beta + iy)]^N \exp[E^{\text{tot}}(\beta + iy)]| = |Z(\beta + iy)|^N \exp(E^{\text{tot}}\beta). \tag{3.9}$$

But

$$Z(\beta + iy) = \sum_{\sigma} e^{-(\beta + iy)\mathscr{E}(\sigma)} \tag{3.10}$$

takes on its maximum absolute value when each term in the sum has

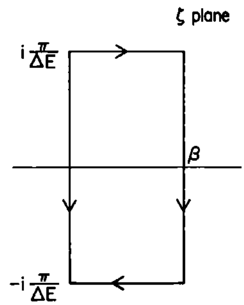


Fig. 2.1. Integration contours used in the steepest-descents evaluation of (3.3) and (3.6).

the same phase (modulo 2π). This occurs either when $y = 0$ or, if $y \neq 0$, when y is such that for all configurations

$$y[\mathscr{E}(\sigma) - \mathscr{E}(\sigma_0)] = 2\pi\,(\text{integer}), \tag{3.11}$$

where σ_0 is some arbitrary fixed configuration. However, we have defined ΔE to be the largest number such that $[\mathscr{E}(\sigma) - \mathscr{E}(\sigma_0)]/\Delta E$ is an integer for all σ and σ_0. Therefore any $y \neq 0$ which satisfies (3.11) must have a magnitude which is at least as big as $2\pi/\Delta E$, which violates (3.8).

The number of energy levels in an Ising model is $2^{\text{number of sites}}$. Therefore, the function $Z(\zeta)$ is a finite sum of analytic functions and therefore is an analytic function itself. This means that the integrands in (3.3) and (3.6) are analytic functions and hence the path of integration may be deformed away from the imaginary ζ axis without altering the value of the integral. Furthermore, these integrals are obviously periodic functions of ζ with period $2\pi i/\Delta E$. Therefore if we deform the path of integration as shown in Fig. 2.1 the contributions from the two parts of the path that are parallel to the real axis cancel because the integrands are equal but the directions of integration are opposite. Thus in (3.3) and (3.6) we can replace ζ by $\beta + iy$ and integrate the variable y from $-\pi/\Delta E$ to $\pi/\Delta E$. The method of steepest descents consists in choosing β so that as $N \to \infty$ the only important contributions to the integrals come from the region very close to $y = 0$.

Consider first $\Omega(E^{\text{tot}})$. Because E^{tot} is proportional to N we define

$$\bar{E} = E^{\text{tot}}/N \tag{3.12}$$

and write the integrand of (3.3) as

$$\exp N\{\zeta\bar{E} + \ln Z(\zeta)\}. \tag{3.13}$$

Consider an expansion of the term in braces into a power series about some point ζ_0 so that

$$\begin{aligned}\exp N\{\zeta\bar{E} + \ln Z(\zeta)\} \sim{}& \exp N\{\zeta_0\bar{E} + \ln Z(\zeta_0)\}\\ &\times \exp N\left\{(\zeta - \zeta_0)\left[\bar{E} + \frac{\partial}{\partial\zeta}\ln Z(\zeta)|_{\zeta_0}\right]\right.\\ &\left.+ \frac{1}{2}(\zeta - \zeta_0)^2\frac{\partial^2}{\partial\zeta^2}\ln Z(\zeta)|_{\zeta_0} + \cdots\right\}.\end{aligned} \tag{3.14}$$

If we try to integrate this approximation along the contour Re $\zeta = \zeta_0$ for large N the term containing $N(\zeta - \zeta_0)^2$ will cause contributions to the integral from that part of the contour where $|\zeta - \zeta_0| \gg N^{-1/2}$ to be negligible. However, when $|\zeta - \zeta_0| \gg N^{-1}$ the term which is proportional to $N(\zeta - \zeta_0)$ oscillates violently. Since $N^{-1} \ll N^{-1/2}$, there will be an enormous number of oscillations from this first term in the region where $e^{N(\zeta-\zeta_0)^2}$ is close to 1. These rapid oscillations tend to cancel each other out and make a direct estimation of the integral extremely difficult. However, we avoid this problem if we choose ζ_0 so that the coefficient of $N(\zeta - \zeta_0)$ vanishes. Therefore we shift the contour of integration to $\zeta = \beta + iy$, where y is real and β satisfies

$$\bar{E} = -\frac{\partial}{\partial\beta}\ln Z(\beta). \tag{3.15}$$

When β is determined from this equation $Z(\beta)$ is called the partition function.

With this contour of integration it is straightforward to obtain an approximate evaluation of $\Omega(E^{\text{tot}})$ by expanding the integrand in (3.3) about $y = 0$. To justify this procedure we must show that there is no more than one value of β that satisfies (3.15).

This will be the case if we prove that $(\partial/\partial\beta)\ln Z(\beta)$ is a monotonic function of β when β is real and, since $(\partial/\partial\beta)\ln Z(\beta)$ is a continuous function of β for real β, this monotonicity will follow if

$$\frac{\partial^2}{\partial\beta^2}\ln Z(\beta) \geq 0. \tag{3.16}$$

But

$$\frac{\partial^2}{\partial\beta^2}\ln Z(\beta) = \frac{\sum_\sigma \mathscr{E}^2 e^{-\beta\mathscr{E}}}{Z(\beta)} - \left(\frac{\sum_\sigma \mathscr{E}e^{-\beta\mathscr{E}}}{Z(\beta)}\right)^2 = \frac{\sum_\sigma \mathscr{E}^2 e^{-\beta\mathscr{E}}}{Z(\beta)} - \bar{E}^2, \tag{3.17}$$

and furthermore for β real

$$0 \leq \frac{\sum_\sigma (\mathscr{E} - \bar{E})^2 e^{-\beta\mathscr{E}}}{Z(\beta)} = \frac{\sum_\sigma \mathscr{E}^2 e^{-\beta\mathscr{E}}}{Z(\beta)} - \frac{2\bar{E}\sum_\sigma \mathscr{E} e^{-\beta\mathscr{E}}}{Z(\beta)} + \bar{E}^2$$

$$= \frac{\sum_\sigma \mathscr{E}^2 e^{-\beta\mathscr{E}}}{Z(\beta)} - \bar{E}^2. \tag{3.18}$$

Therefore (3.16) holds.

We now may proceed to evaluate (3.3) by expanding

$$N\{\zeta\bar{E} + \ln Z(\zeta)\} \sim N\left\{\beta\bar{E} + \ln Z(\beta) - \frac{1}{2}y^2\frac{\partial^2}{\partial\beta^2}\ln Z(\beta) - \frac{i}{6}y^3\frac{\partial^3}{\partial\beta^3}\ln Z(\beta) + \frac{1}{24}y^4\frac{\partial^4}{\partial\beta^4}\ln Z(\beta) + \cdots\right\}. \tag{3.19}$$

The last two terms here do not contribute to the leading term and we retain them only to obtain an estimate of the error involved in our approximation. Let

$$y' = N^{1/2}y \tag{3.20}$$

and so obtain

$$\Omega(E^{\text{tot}}) = \frac{\Delta E}{2\pi}N^{-1/2}e^{N[\beta E + \ln Z(\beta)]}\int_{-\pi N^{1/2}/\Delta E}^{\pi N^{1/2}/\Delta E} dy' e^{-(1/2)y'^2(\partial^2/\partial\beta^2)\ln Z(\beta)}$$
$$\times\left\{1 + N^{-1}\left[\frac{1}{24}y'^4\frac{\partial^4}{\partial\beta^4}\ln Z(\beta) - \frac{1}{2}y'^6\left(\frac{1}{6}\frac{\partial^3}{\partial\beta^3}\ln Z(\beta)\right)^2\right] + o(N^{-1})\right\}. \tag{3.21}$$

We may extend the limits of integration to run from $-\infty$ to $+\infty$ with a negligible error and then evaluate the remaining Gaussian integral to obtain the desired result:

$$\Omega(E^{\text{tot}}) = e^{N[\beta E + \ln Z(\beta)]}\Delta E\left[\frac{1}{2\pi N(\partial^2/\partial\beta^2)\ln Z(\beta)}\right]^{1/2}\{1 + O(N^{-1})\}. \tag{3.22}$$

Essentially the same procedure may be used to evaluate the expression for $\sum_{\sigma^{(2)}}\cdots\sum_{\sigma^{(N)}}\delta_{E^{\text{tot}},\mathscr{E}^{\text{tot}}}$ in (3.6). The only remark which is needed is that for our steepest-descents evaluation to be accurate we do not really need the coefficient of $N(\zeta - \zeta_0)$ in (3.14) to be identically zero but merely need it small enough so that the number of oscillations this linear term contributes in the region where the quadratic term $e^{(1/2)N(\zeta-\zeta_0)^2}$ is of order 1 will not become enormous as $N \to \infty$. This requirement, besides being satisfied if the coefficient of $\zeta - \zeta_0$ is zero, will also be satisfied if that coefficient is $O(N^{-1/2})$ as $N \to \infty$.

We use this remark to evaluate (3.6) by noting that if we followed the previous procedure we would expand the integrand about the point

$\zeta = \beta'$, where β' is determined from

$$\bar{E} - \frac{\mathscr{E}(\sigma^{(1)})}{N} = -(1 - N^{-1})\frac{\partial \ln Z(\beta')}{\partial \beta'}. \tag{3.23}$$

Clearly $\beta - \beta' = O(N^{-1})$, so the foregoing remark indicates that we may just as well expand about β (which is independent of $\sigma^{(1)}$) as about β'. We therefore use (3.15) and expand

$$\begin{aligned}
&\zeta[N\bar{E} - \mathscr{E}(\sigma^{(1)})] + (N-1)\ln Z(\zeta) \\
&\quad \sim \beta[N\bar{E} - \mathscr{E}(\sigma^{(1)})] + (N-1)\ln Z(\beta) \\
&\quad + iy\left[-\mathscr{E}(\sigma^{(1)}) - \frac{\partial \ln Z(\beta)}{\partial \beta}\right] - \frac{1}{2}y^2(N-1)\frac{\partial^2 \ln Z(\beta)}{\partial \beta^2} \\
&\quad - \frac{i}{6}y^3(N-1)\frac{\partial^3 \ln Z(\beta)}{\partial \beta^3} + \frac{1}{24}y^4(N-1)\frac{\partial^4 \ln Z(\beta)}{\partial \beta^4} + \cdots,
\end{aligned} \tag{3.24}$$

where again the last two terms will not contribute to the leading term of our result. If this approximation is used in (3.6) we may again use (3.20), and extend the limits of integration to run from $-\infty$ to $+\infty$, and obtain

$$\begin{aligned}
&\sum_{\sigma^{(2)}} \cdots \sum_{\sigma^{(N)}} \delta_{E^{\text{tot}},\mathscr{E}^{\text{tot}}} \\
&\quad = \frac{\Delta E}{2\pi} N^{-1/2} \exp\{\beta[N\bar{E} - \mathscr{E}(\sigma^{(1)})] + (N-1)\ln Z(\beta)\} \\
&\quad \times \int_{-\infty}^{\infty} dy' \exp\left\{-iy'N^{-1/2}\left[\mathscr{E}(\sigma^{(1)}) + \frac{\partial \ln Z(\beta)}{\partial \beta}\right]\right. \\
&\qquad\qquad \left. - \frac{1}{2}y'^2(1 - N^{-1})\frac{\partial^2 \ln Z(\beta)}{\partial \beta^2}\right\} \\
&\quad \times \left\{1 - \frac{i}{6}N^{-1/2}y'^3\frac{\partial^3 \ln Z(\beta)}{\partial \beta^3} + \frac{1}{24}N^{-1}y'^4\frac{\partial^4 \ln Z(\beta)}{\partial \beta^4}\right. \\
&\qquad\qquad \left. - \frac{1}{2}N^{-1}y'^6\left[\frac{1}{6}\frac{\partial^3 \ln Z(\beta)}{\partial \beta^3}\right]^2 + \cdots\right\}.
\end{aligned} \tag{3.25}$$

These integrals may be evaluated if we first complete the square by writing

$$\begin{aligned}
&-\frac{1}{2}y'^2(1 - N^{-1})\frac{\partial^2 \ln Z(\beta)}{\partial \beta^2} - iy'N^{-1/2}\left[\mathscr{E}(\sigma^{(1)}) + \frac{\partial \ln Z(\beta)}{\partial \beta}\right] \\
&\quad = -\frac{1}{2}(1 - N^{-1})\frac{\partial^2 \ln Z(\beta)}{\partial \beta^2}(y' - y_0)^2 \\
&\qquad - \frac{1}{2}(1 - N^{-1})^{-1}N^{-1}\frac{[\mathscr{E}(\sigma^{(1)}) + (\partial/\partial\beta)\ln Z(\beta)]^2}{(\partial^2/\partial\beta^2)\ln Z(\beta)},
\end{aligned} \tag{3.26}$$

where

$$y_0 = -i(1 - N^{-1})^{-1}N^{-1/2}\frac{\mathscr{E}(\sigma^{(1)}) + (\partial/\partial\beta)\ln Z(\beta)}{(\partial^2/\partial\beta^2)\ln Z(\beta)}, \tag{3.27}$$

and then deform the contour of integration to the line $y'' = y' - y_0$. Thus we obtain the result

$$\sum_{\sigma^{(2)}}\cdots\sum_{\sigma^{(N)}}\delta_{E^{\text{tot}},\mathscr{E}^{\text{tot}}} = \exp\{\beta[\bar{E}N - \mathscr{E}(\sigma^{(1)})] + (N-1)\ln Z(\beta)\}$$
$$\times\ \Delta E\left[\frac{1}{2\pi N(\partial^2/\partial\beta^2)\ln Z(\beta)}\right]^{1/2}\{1 + O(N^{-1})\}. \tag{3.28}$$

It remains to combine (3.22) and (3.28) and obtain the desired result that as $N \to \infty$

$$P(\sigma^{(1)}; E^{\text{tot}}) = \frac{e^{-\beta\mathscr{E}(\sigma^{(1)})}}{Z(\beta)}\{1 + O(N^{-1})\}. \tag{3.29}$$

This is the probability function of systems in a canonical ensemble. The minimum level spacing ΔE no longer appears and the entire effect of the large system to which this Ising model is connected is contained in the parameter β.

From the probability function (3.29) we may study any property f of the Ising model that depends on the variables $\sigma^{(1)}$. In particular we may compute the probability $P_f(\bar{f})$ that the property f has the value $\bar{f}$. However, when the number of sites $\mathscr{M}\mathscr{N}$ of the Ising model becomes large we will see that $P_f(\bar{f})$ is often very sharply peaked about one particular value of $\bar{f}$. In such a case a measurement of f on any one Ising model will almost certainly correspond with the average value which would be obtained if we measured f on many identical Ising models each described by (3.29). Therefore for Ising models with $\mathscr{M}$ rows and $\mathscr{N}$ columns we often will be content to study only such average values, which we denote as $\langle f\rangle_{\mathscr{M},\mathscr{N}}$ and compute from (3.29) as

$$\langle f\rangle_{\mathscr{M},\mathscr{N}} = \lim_{N\to\infty}\sum_{\sigma} f(\sigma)P(\sigma; E^{\text{tot}}) = \frac{\sum_{\sigma} f(\sigma)e^{-\beta\mathscr{E}(\sigma)}}{Z(\beta)}. \tag{3.30}$$

Both the probability function (3.29) and these average values (3.30) are functions of the parameter β. To determine the significance of β, consider two Ising models with different interaction energies $\mathscr{E}_1$ and $\mathscr{E}_2$. From each kind of Ising model construct a microcanonical ensemble, one with N_1 models of energies $\mathscr{E}_1^{(n)}$ and total energy E_1^{tot}; the other with N_2 models of energies $\mathscr{E}_2^{(n)}$ and total energy E_2^{tot}. As we have just seen, if $\sigma_{(j)}$ is a particular state of an Ising model of type j, the probability function $P_j(\sigma_{(j)}; E_j^{\text{tot}})$ that one Ising model of type j is in the state $\sigma_{(j)}$ is, as $N_j \to \infty$,

$$P_j(\sigma_{(j)}; E_j^{\text{tot}}) = \frac{e^{-\beta_j\mathscr{E}_j(\sigma_{(j)})}}{Z_j(\beta_j)}, \qquad j = 1, 2 \tag{3.31}$$

where

$$Z_j(\beta_j) = \sum_{\sigma_{(j)}} e^{-\beta_j \mathscr{E}_j(\sigma_{(j)})} \tag{3.32}$$

and β_j is determined from

$$E_j^{\text{tot}}/N_j = -\frac{\partial}{\partial \beta_j} \ln Z_j(\beta_j). \tag{3.33}$$

Now connect these two microcanonical ensembles together to form one larger microcanonical ensemble of $N_1 + N_2$ Ising models and total energy $E_1^{\text{tot}} + E_2^{\text{tot}}$ and compute the probability function $\tilde{P}_j(\sigma_{(j)}; E_1^{\text{tot}} + E_2^{\text{tot}})$, which describes a single Ising model of type j, when $N_1 + N_2 \to \infty$. By definition

$$\tilde{P}_1(\sigma_{(1)}; E_1^{\text{tot}} + E_2^{\text{tot}}) = \frac{\sum_{\sigma_{(1)}^{(2)}} \cdots \sum_{\sigma_{(1)}^{(N_1)}} \sum_{\sigma_{(2)}^{(1)}} \cdots \sum_{\sigma_{(2)}^{(N_2)}} \delta\left[\left(E_1^{\text{tot}} + E_2^{\text{tot}}\right) - \left(\sum_{n=1}^{N_1} \mathscr{E}_1^{(n)} + \sum_{n=1}^{N_2} \mathscr{E}_2^{(n)}\right)\right]}{\tilde{\Omega}(E_1^{\text{tot}} + E_2^{\text{tot}})} \tag{3.34}$$

where $\delta[x - y]$ is the Kronecker delta $\delta_{x,y}$,

$$\tilde{\Omega}(E_1^{\text{tot}} + E_2^{\text{tot}}) = \sum_{\sigma_{(1)}^{(1)}} \cdots \sum_{\sigma_{(1)}^{(N_1)}} \sum_{\sigma_{(2)}^{(1)}} \cdots \sum_{\sigma_{(2)}^{(N_2)}} \delta\left[(E_1^{\text{tot}} + E_2^{\text{tot}}) - \left(\sum_{n=1}^{N_1} \mathscr{E}_1^{(n)} + \sum_{n=1}^{N_2} \mathscr{E}_2^{(n)}\right)\right], \tag{3.35}$$

and $\tilde{P}_2$ is given by a similar expression with the roles of system 1 and system 2 interchanged. We may evaluate these probabilities as $N_1 + N_2 \to \infty$ exactly as we did in the previous case where we had only one type of Ising model.

In particular we assume that $\mathscr{E}_1$ and $\mathscr{E}_2$, besides each possessing commensurable energy levels, are also mutually commensurable in the sense that there is a ΔE such that all differences in energy levels are integral multiples of ΔE. As before, if there is one such ΔE there is an infinite number, and we define ΔE to be the largest of these possible numbers. With this technical assumption we then find, as $N_1 + N_2 \to \infty$ with E_1^{tot}/N_1 and E_2^{tot}/N_2 fixed,

$$\begin{aligned}
&\tilde{\Omega}(E_1^{\text{tot}} + E_2^{\text{tot}}) \\
&= \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \exp\left\{\frac{i\theta}{\Delta E}(E_1^{\text{tot}} + E_2^{\text{tot}}) + N_1 \ln Z_1\left(\frac{i\theta}{\Delta E}\right) + N_2 \ln Z_2\left(\frac{i\theta}{\Delta E}\right)\right\} \\
&= \exp\{\beta[E_1^{\text{tot}} + E_2^{\text{tot}}] + N_1 \ln Z_1(\beta) + N_2 \ln Z_2(\beta)\} \\
&\quad \times \Delta E(2\pi)^{-1/2}\left[\frac{1}{N_1(\partial^2/\partial\beta^2) \ln Z_1(\beta) + N_2(\partial^2/\partial\beta^2) \ln Z_2(\beta)}\right]^{1/2} \\
&\quad \times \{1 + O[(N_1 + N_2)^{-1}]\},
\end{aligned} \tag{3.36}$$

where β is determined from

$$E_1^{\text{tot}} + E_2^{\text{tot}} = -N_1 \frac{\partial}{\partial\beta} \ln Z_1(\beta) - N_2 \frac{\partial}{\partial\beta} \ln Z_2(\beta) \tag{3.37}$$

and

$$\begin{aligned}
\sum_{\sigma_{(1)}^{(2)}} \cdots \sum_{\sigma_{(1)}^{(N_1)}} \sum_{\sigma_{(2)}^{(1)}} \cdots \sum_{\sigma_{(2)}^{(N_2)}} \delta\left[(E_1^{\text{tot}} + E_2^{\text{tot}}) - \left(\sum_{n=1}^{N_1} \mathscr{E}_1^{(n)} + \sum_{n=1}^{N_2} \mathscr{E}_2^{(n)}\right)\right] \\
= \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta \exp\left\{\frac{i\theta}{\Delta E}[E_1^{\text{tot}} + E_2^{\text{tot}} - \mathscr{E}_1(\sigma_{(1)}^{(1)})]\right. \\
\left. + (N_1 - 1)\ln Z_1\left(\frac{i\theta}{\Delta E}\right) + N_2 \ln Z_2\left(\frac{i\theta}{\Delta E}\right)\right\} \\
= \exp\{\beta[E_1^{\text{tot}} + E_2^{\text{tot}} - \mathscr{E}_1(\sigma_{(1)}^{(1)})] \\
+ (N_1 - 1)\ln Z_1(\beta) + N_2 \ln Z_2(\beta)\} \\
\times \Delta E\,(2\pi)^{-1/2}\left[\frac{1}{N_1(\partial^2/\partial\beta^2)\ln Z_1(\beta) + N_2(\partial^2/\partial\beta^2)\ln Z_2(\beta)}\right]^{1/2} \\
\times \{1 + O[(N_1 + N_2)^{-1}]\}.
\end{aligned} \tag{3.38}$$

Equations (3.36) and (3.38) are valid as they stand if N_1/N_2 is fixed. They are also valid if (say) N_1 is fixed (while $N_2 \to \infty$) and the square root is expanded as a power series in N_1/N_2. Therefore one Ising model of type j obeys the canonical ensemble probability function

$$\tilde{P}_j(\sigma_{(j)}; E_1^{\text{tot}} + E_2^{\text{tot}}) = \frac{e^{-\beta\mathscr{E}_j(\sigma_{(j)})}}{Z_j(\beta)}, \qquad j = 1, 2, \tag{3.39}$$

where β is independent of j. In other words, β is a parameter which is meaningful only when the number of systems is large and which is the same for two (or many) ensembles of systems with discrete mutually commensurable energy levels which are in thermal equilibrium with each other. In fact, as one expects, the restriction to discrete mutually commensurable energy levels is not necessary for the conclusion and β is indeed the same for all systems which are in thermal equilibrium with each other. Therefore β has the property of temperature required by the zeroth law of thermodynamics as discussed in the previous section.

The quantity β itself is not called temperature. When $\beta \to \infty$ it is easily seen from (3.5) that

$$Z \sim e^{-\beta\mathscr{E}_{\min}} \times \text{multiplicity of } \mathscr{E}_{\min}, \tag{3.40}$$

where $\mathscr{E}_{\min}$ is the minimum energy the system may attain. It is customary to associate $T = 0$ with this minimum energy. Therefore, the temperature T, which is measured in Kelvin degrees, is defined as

$$T = \frac{1}{k\beta}, \tag{3.41}$$

where k is called Boltzmann's constant. With this definition the well-known ideal gas can be shown to obey the equation

$$PV = NkT, \tag{3.42}$$

where P is the pressure, V is the volume, and N is the number of molecules. Real gases obey this equation to a good approximation at low enough densities, so in principle we could often measure T by using a gas as a thermometer. If we then use such an ideal-gas thermometer to measure at sea-level pressure the temperatures at which water freezes and boils and arbitrarily define a degree on the Kelvin scale so that the difference between these two temperatures is 100 degrees, we empirically find that

$$k = 1.38 \times 10^{-16} \text{ erg/degree}. \tag{3.43}$$

4. THERMODYNAMICS

The probability distribution of the canonical ensemble allows us to study the properties of an Ising model in thermal equilibrium. Though in principle it is possible to define many properties of an Ising model, in practice only a few properties are of direct physical interest. In addition to $\bar{E}$, the internal energy, the properties of magnetic systems which are of greatest physical interest are the magnetization, heat capacity, entropy, and Helmholtz free energy. These quantities are not all independent but are related by the laws of thermodynamics. For the sake of concreteness it is useful to define these properties and exhibit their general interrelations before embarking upon their detailed calculation.

Heat may be defined as that work which is done on a system by those forces which are ignored in the interaction energy but which couple the system to the external system that defines the temperature. Therefore if we fix H, so that T is the only variable, the change in heat δQ is related to a change $d\bar{E}$ in the internal energy as

$$d\bar{E} = \delta Q. \tag{4.1}$$

In particular, $\bar{E}$ may be changed by changing the temperature so that

$$\left.\frac{\delta Q}{\delta T}\right|_{\delta H=0} = \left.\frac{\partial \bar{E}}{\partial T}\right|_{H}, \tag{4.2}$$

where the notation $|_x$ indicates the variables which are held constant during the partial differentiation. Measurements of $(\delta Q/\delta T)|_{\delta H=0}$ are some of the most common thermal measurements. Thus we define C, the heat capacity at constant magnetic field, as

$$C = \left.\frac{\delta Q}{\delta T}\right|_{\delta H=0} = \left.\frac{\partial \bar{E}}{\partial T}\right|_{H}. \tag{4.3}$$

(This heat capacity is sometimes written as C_H to emphasize that H is held constant. It is to be distinguished from C_M, which refers to a measurement of $\delta Q/\delta T$ in which the magnetization is held constant. In this book C_M will never be discussed.)

The total spin of any Ising model is

$$\sum_{j,k} \sigma_{j,k}. \tag{4.4}$$

Accordingly, the average total magnetization of an Ising model of $\mathcal{M}$ rows and $\mathcal{N}$ columns in the canonical ensemble is (from 3.30)

$$\bar{M} = \left\langle \sum_{j,k} \sigma_{j,k} \right\rangle_{\mathcal{M},\mathcal{N}} = \frac{\sum_{\sigma} \left[\sum_{j,k} \sigma_{j,k}\right] e^{-\beta \mathcal{E}(\sigma)}}{Z(\beta)} = \beta^{-1} \frac{\partial \ln Z(\beta)}{\partial H}\bigg|_{\beta}. \tag{4.5}$$

Therefore if we consider a collection of identical Ising models each of which is in equilibrium at temperature T, and then thermally isolate them and change the external magnetic field from H to $H + dH$, the work done per Ising model will be

$$d\bar{E} = -\bar{M}\, dH. \tag{4.6}$$

For the Ising model the only external forces which are considered are that of the external magnetic field and the forces that connect the Ising model to the external heat bath. Therefore, if the Ising model is connected to the external heat bath (i.e. not thermally isolated) and if the magnetic field is allowed to change we may combine (4.1) and (4.6) to find that the total change in internal energy is

$$d\bar{E} = \delta Q - \bar{M}\, dH. \tag{4.7}$$

This is the first law of thermodynamics.

For our microcanonical ensemble of N identical Ising models and total energy E^{tot} the entropy S^{tot} may be defined as k times the logarithm of the number of ways in which the total energy may be distributed among the N Ising models. In other words,

$$S^{\text{tot}} = k \ln \Omega(E^{\text{tot}}). \tag{4.8}$$

When $N \to \infty$ we see from (3.22) that

$$S^{\text{tot}}/k = N[\beta \bar{E} + \ln Z(\beta)] - \tfrac{1}{2} \ln N + \ln \Delta E + O(1). \tag{4.9}$$

Therefore, we define $\bar{S}$, the entropy per Ising model, as

$$\bar{S} = \lim_{N \to \infty} S^{\text{tot}}/N, \tag{4.10}$$

so that as $N \to \infty$

$$\bar{S} = k[\beta \bar{E} + \ln Z(\beta)]. \tag{4.11}$$

Clearly $\bar{S}$ is a function only of the macroscopic variables T and H, or, equivalently, $\bar{E}$ and H. The significance of entropy may be seen by considering

$$d\bar{S} = \frac{\partial \bar{S}}{\partial \bar{E}}\bigg|_H d\bar{E} + \frac{\partial \bar{S}}{\partial H}\bigg|_E dH. \tag{4.12}$$

We may rewrite this expression by using the relation

$$\bar{E} = -\frac{\partial \ln Z(\beta)}{\partial \beta} \tag{4.13}$$

to express $(\partial/\partial\bar{E})|_{\bar{H}}$ and $(\partial/\partial H)|_E$ in terms of $(\partial/\partial\beta)|_H$ and $(\partial/\partial H)|_\beta$. In particular, the chain rule for partial derivatives gives

$$\frac{\partial}{\partial \bar{E}}\bigg|_H = \frac{\partial \beta}{\partial \bar{E}}\frac{\partial}{\partial \beta}\bigg|_H \tag{4.14a}$$

and

$$\frac{\partial}{\partial H}\bigg|_E = \frac{\partial}{\partial H}\bigg|_\beta - \frac{\partial \bar{E}}{\partial H}\bigg|_\beta \frac{\partial \beta}{\partial \bar{E}}\frac{\partial}{\partial \beta}\bigg|_H. \tag{4.14b}$$

Therefore

$$d\bar{S} = \frac{\partial \beta}{\partial \bar{E}}\frac{\partial \bar{S}}{\partial \beta}\bigg|_H d\bar{E} + \left\{\frac{\partial \bar{S}}{\partial H}\bigg|_\beta - \frac{\partial \bar{E}}{\partial H}\bigg|_\beta \frac{\partial \beta}{\partial \bar{E}}\frac{\partial \bar{S}}{\partial \beta}\bigg|_H\right\} dH. \tag{4.15}$$

Furthermore, from (4.5), (4.11), and (4.13),

$$\frac{\partial \bar{S}}{\partial \beta}\bigg|_H = k\beta\frac{\partial \bar{E}}{\partial \beta}\bigg|_H \tag{4.16}$$

and

$$\frac{\partial \bar{S}}{\partial H}\bigg|_\beta = k\beta\left[\frac{\partial \bar{E}}{\partial H}\bigg|_\beta + \bar{M}\right], \tag{4.17}$$

so we find

$$d\bar{S} = \frac{1}{T}[d\bar{E} + \bar{M}\,dH]. \tag{4.18}$$

If we further use the first law of thermodynamics (4.7), we find

$$d\bar{S} = \frac{\delta Q}{T}, \tag{4.19}$$

which means that

$$\int_{\text{state 1}}^{\text{state 2}} \frac{\delta Q}{T} = \Delta\bar{S} \tag{4.20}$$

depends only on T_1, H_1 and T_2, H_2 and not on the path of integration in the T, H plane. This is the reason why entropy is a useful quantity to consider.

Finally we define the Helmholtz free energy A by

$$Z(\beta) = e^{-\beta A}. \tag{4.21}$$

In terms of A we have

$$\bar{M} = -\frac{\partial A}{\partial H}\bigg|_{\beta}, \tag{4.22}$$

$$\bar{E} = \frac{\partial}{\partial \beta}(\beta A)\bigg|_{H}, \tag{4.23}$$

$$\bar{S} = \frac{1}{T}(\bar{E} - A), \tag{4.24}$$

and, combining the last two expressions,

$$\bar{S} = -\frac{\partial A}{\partial T}\bigg|_{H}. \tag{4.25}$$

5. THE THERMODYNAMIC LIMIT

To define temperature precisely we have considered the limit where N, the number of identical models in the microcanonical ensemble, goes to infinity. In the remainder of this book this $N \to \infty$ limit will always be taken (and, accordingly, the number of identical models in the microcanonical ensemble will never be mentioned again). However, the number $\mathscr{M}$ of rows and $\mathscr{N}$ of columns in each individual Ising model has been kept fixed and finite. For example, consider the case $\mathscr{M} = 1$ and $\mathscr{N} = 1$, where one Ising spin is in thermal equilibrium with an external system at temperature T. In any measurement the energy of this spin can be either $+H$ or $-H$. The partition function is

$$Z(\beta) = e^{-\beta H} + e^{\beta H} = 2 \cosh \beta H \tag{5.1}$$

and the Helmholtz free energy is

$$A = -\beta^{-1} \ln 2 \cosh \beta H. \tag{5.2}$$

Therefore the average total energy is

$$\bar{E} = -H \tanh \beta H, \tag{5.3}$$

which is quite different from $+H$ or $-H$. Similarly, any measurement of the spin can be only $+1$ or -1. However, from (4.22) and (5.2),

$$\bar{M} = \tanh \beta H. \tag{5.4}$$

Again in this very small Ising model the average value computed from the canonical ensemble is quite different from the result of any one measurement.

In actual practice, of course, we are never interested in one isolated spin but rather are interested in macroscopic systems of $\sim 10^{23}$ interacting spins. As mentioned in Chapter I, the most distinctive features of statistical mechanics arise precisely because the system under consideration has such an enormous number of particles. Therefore we are most interested in the Ising model in the case $\mathscr{M} \to \infty$ and $\mathscr{N} \to \infty$. When $\mathscr{M}\mathscr{N}$ is large, the total average magnetization, the total average energy, and the Helmholtz free energy will in general be proportional to $\mathscr{M}\mathscr{N}$. Therefore, one aspect of the investigation of large Ising models is to divide these quantities by $\mathscr{M}\mathscr{N}$ and let $\mathscr{M} \to \infty$ and $\mathscr{N} \to \infty$. This limit is called the thermodynamic limit. We therefore define:

(1) the free energy per spin (or more simply the free energy),

$$F = \lim_{\substack{\mathscr{M}\to\infty \\ \mathscr{N}\to\infty}} A/\mathscr{M}\mathscr{N} = -\lim_{\substack{\mathscr{M}\to\infty \\ \mathscr{N}\to\infty}} (\beta\mathscr{M}\mathscr{N})^{-1} \ln Z(\beta); \tag{5.5}$$

(2) the magnetization per spin (or more simply the magnetization),

$$M = \lim_{\substack{\mathscr{M}\to\infty \\ \mathscr{N}\to\infty}} \overline{M}/\mathscr{M}\mathscr{N}; \tag{5.6}$$

(3) the internal energy per spin (or more simply the internal energy),

$$u = \lim_{\substack{\mathscr{M}\to\infty \\ \mathscr{N}\to\infty}} \overline{E}/\mathscr{M}\mathscr{N}; \tag{5.7}$$

(4) the entropy per spin (or more simply the entropy),

$$S = \lim_{\substack{\mathscr{M}\to\infty \\ \mathscr{N}\to\infty}} \overline{S}/\mathscr{M}\mathscr{N}; \tag{5.8}$$

(5) the specific heat,

$$c = \lim_{\substack{\mathscr{M}\to\infty \\ \mathscr{N}\to\infty}} C/\mathscr{M}\mathscr{N}. \tag{5.9}$$

The last four quantities may be expressed in terms of F by using the relations at the end of the last section. Therefore

$$M = -\frac{\partial F}{\partial H}, \tag{5.10}$$

$$S = -\frac{\partial F}{\partial T}, \tag{5.11}$$

$$u = \frac{\partial}{\partial \beta}(\beta F) = F + TS, \tag{5.12}$$

and

$$c = \frac{\partial E}{\partial T} = \frac{\partial F}{\partial T} + S + T\frac{\partial S}{\partial T} = -T\frac{\partial^2 F}{\partial T^2}. \tag{5.13}$$

Here and in the remainder of this book T (or β) and H are the independent variables. In particular we will never further consider $\bar{E}$ as an independent variable. Hence, without fear of confusion, we have adopted the abbreviated notation

$$\left.\frac{\partial}{\partial H}\right|_{\beta} = \frac{\partial}{\partial H}, \qquad \left.\frac{\partial}{\partial T}\right|_{H} = \frac{\partial}{\partial T}, \quad \text{and} \quad \left.\frac{\partial}{\partial \beta}\right|_{H} = \frac{\partial}{\partial \beta}.$$

The special case $\mathscr{M} = 1$ and $\mathscr{N} = 1$ illustrates a general feature of small systems, namely, that one measurement of a quantity such as the energy or the magnetization may differ substantially from its average computed in the canonical ensemble. To see that this is not the case when $\mathscr{M}\mathscr{N}$ is large, consider the fluctuations in the average energy, one measure of which is $(\mathscr{M}\mathscr{N})^{-1}[\langle \mathscr{E}^2 \rangle_{\mathscr{M},\mathscr{N}} - \bar{E}^2]$. Since

$$\bar{E} = \frac{\sum_{\sigma} \mathscr{E}(\sigma) e^{-\beta \mathscr{E}(\sigma)}}{Z(\beta)}, \tag{5.14}$$

we may differentiate both sides with respect to $-\beta$ and obtain

$$-\frac{\partial \bar{E}}{\partial \beta} = kT^2 C = \langle \mathscr{E}^2 \rangle_{\mathscr{M},\mathscr{N}} - \bar{E}^2.$$

Therefore as long as the specific heat exists we have for large $\mathscr{M}\mathscr{N}$,

$$\langle (\mathscr{E}/\mathscr{M}\mathscr{N})^2 \rangle_{\mathscr{M},\mathscr{N}} - u^2 \sim kT^2 c/\mathscr{M}\mathscr{N}, \tag{5.15}$$

which means that as $\mathscr{M}\mathscr{N} \to \infty$ a measurement of the internal energy per spin will with probability 1 yield the value u. It is important to remark, however, that the specific heat as defined by (5.9) does not have to exist for all temperatures and magnetic fields. At those temperatures where it does not exist the left-hand side of (5.15) will still, in general, vanish as $\mathscr{M}\mathscr{N} \to \infty$ but it will not vanish as rapidly as $(\mathscr{M}\mathscr{N})^{-1}$.

In a similar fashion we may consider fluctuations in the magnetization per spin, which may be measured in terms of

$$(\mathscr{M}\mathscr{N})^{-1}\left[\left\langle \left(\sum_{j,k} \sigma_{j,k}\right)^2 \right\rangle_{\mathscr{M},\mathscr{N}} - \bar{M}^2\right].$$

Since

$$\bar{M} = \frac{\sum_{j,k} \sigma_{j,k} \exp\left\{-\beta\left[\mathscr{E}(\sigma)|_{H=0} - H \sum_{j,k} \sigma_{j,k}\right]\right\}}{Z(\beta)}, \tag{5.16}$$

We find

$$\frac{1}{kT}\frac{\partial \bar{M}}{\partial H} = \left\langle \left(\sum_{j,k} \sigma_{j,k}\right)^2 \right\rangle_{\mathscr{M},\mathscr{N}} - \bar{M}^2. \tag{5.17}$$

The magnetic susceptibility per spin is defined as

$$\chi = \lim_{\substack{\mathcal{M}\to\infty \\ \mathcal{N}\to\infty}} \frac{\partial M}{\partial H}. \tag{5.18}$$

Therefore, if χ exists,

$$\left\langle (\mathcal{M}\mathcal{N})^{-2}\Big(\sum_{j,k}\sigma_{j,k}\Big)^2\right\rangle_{\mathcal{M},\mathcal{N}} - M^2 \sim \frac{1}{kT}\frac{\chi}{\mathcal{M}\mathcal{N}} \tag{5.19}$$

when $\mathcal{M}\mathcal{N}$ is large and so in this case a measurement of the magnetization per spin will almost certainly yield M. However, as was the case with the specific heat, there is no reason that χ must exist for all T and H.

The mathematical significance of the thermodynamic limit may be seen by examining the partition function

$$Z(\beta) = \sum_{\sigma} e^{-\beta\mathscr{E}(\sigma)}. \tag{5.20}$$

When $\mathcal{M}$ and $\mathcal{N}$ are finite, this partition function is a sum of a finite number of analytic functions of β and H, and therefore $Z(\beta)$ must be analytic. Furthermore, when β is positive and H is real, $Z(\beta)$ is a finite sum of positive numbers and hence is positive. Moreover, when $\mathcal{M}$ and $\mathcal{N}$ are finite $Z(\beta)$ must be nonzero for some region where β is sufficiently close to the positive real axis and H is sufficiently close to the real axis. Therefore $\ln Z(\beta)$ must be an analytic function of β and H in this region and so must all properties derivable from $\ln Z(\beta)$ by differentiation. However, when $\mathcal{M}\to\infty$ and $\mathcal{N}\to\infty$, the sum involved in $Z(\beta)$ contains an infinite number of terms. The position of zeros of $Z(\beta)$ may converge to the positive β or real H axis and so in this limit F does *not* have to be an analytic function of β and H for β positive and H real.[1] These new analyticity properties of F correspond to qualitative features that appear in the thermodynamic limit which are not possible in a system with a finite number of particles. These analytic properties are intimately related to the physical notion of phase transition. The major reason for studying the two-dimensional Ising model is to attempt to make this connection more precise.

The interaction energy of the Ising model with $H = 0$ has a symmetry such that if we change all spins into their negatives the interaction energy is unchanged. Therefore neither spin up nor spin down is preferred. In particular,

$$\bar{M}(0) = 0. \tag{5.21}$$

Furthermore, if $H \neq 0$ and if we send $H \to -H$ and all spins into their

1. C. N. Yang and T. D. Lee, *Phys. Rev.* **87**, 404 (1952); T. D. Lee and C. N. Yang, *Phys. Rev.* **87**, 410 (1952).

negatives, $\mathscr{E}$ is unchanged. Therefore

$$\overline{M}(H) = -\overline{M}(-H). \tag{5.22}$$

It is also simple to prove that

$$\overline{M}(H) > 0 \quad \text{if} \quad H > 0. \tag{5.23}$$

Let $\mathscr{E}_0$ denote $\mathscr{E}$ with $H = 0$. Then if we denote by $\sum'_\sigma$ a summation over all states σ satisfying

$$\sum_{j,k} \sigma_{j,k} > 0, \tag{5.24}$$

we have

$$\overline{M}(H) = \frac{\sum'_\sigma e^{-\beta\mathscr{E}_0}\left[\exp\left(\beta H \sum_{j,k} \sigma_{j,k}\right) - \exp\left(-\beta H \sum_{j,k} \sigma_{j,k}\right)\right] \sum_{j,k} \sigma_{j,k}}{\sum_\sigma e^{-\beta\mathscr{E}}}, \tag{5.25}$$

from which (5.23) follows.

If $\mathscr{M}$ and $\mathscr{N}$ are finite, $\overline{M}(H)$, which is derivable from $\ln Z(\beta)$ by differentiation, must be an analytic function of all real H for all positive β. In particular, $\overline{M}(H)$ will be a continuous function of H at $H = 0$ for all T, so that in addition to (5.21) we have

$$\lim_{H \to 0} \overline{M}(H) = 0. \tag{5.26}$$

Now consider the thermodynamic limit. In this limit (5.22) continues to hold, so we have

$$M(H) = -M(-H). \tag{5.27}$$

However, after the thermodynamic limit is taken $M(H)$ does not have to be analytic at $H = 0$ for all T. In particular, $M(H)$ does not have to be continuous at $H = 0$ and we have

$$\lim_{H \to 0^+} \lim_{\substack{\mathscr{M} \to \infty \\ \mathscr{N} \to \infty}} \frac{\overline{M}}{\mathscr{M}\mathscr{N}} \geq \lim_{\substack{\mathscr{M} \to \infty \\ \mathscr{N} \to \infty}} \lim_{H \to 0^+} \frac{\overline{M}}{\mathscr{M}\mathscr{N}}. \tag{5.28}$$

Therefore

$$\lim_{H \to 0^+} M(H) = M(0^+) \geq 0. \tag{5.29}$$

We define $M(0^+)$ as the spontaneous magnetization and call the temperature at which $M(0^+)$ first becomes positive as T is decreased from infinity the critical temperature T_c.[2]

Since analyticity in T at $H = 0$ breaks down for M at T_c, it is most

2. The question can be asked whether the free energy of an Ising model can fail to be analytic in T or H at a value of H other than zero. That this does not happen if all interaction energies are non-negative is proved by T. D. Lee and C. N. Yang, *Phys. Rev.* **87**, 410 (1952).

interesting to investigate the analyticity properties of the specific heat c as a function of temperature at $H = 0$. In the finite case, of course, the heat capacity C must be analytic and hence finite at all temperatures. However, in the thermodynamic limit, c at $H = 0$ does not have to be an analytic function of T at all T, and, indeed, we shall find that in Onsager's lattice c is infinite at T_c.

In order to gain insight into the microscopic behavior of the Ising model, and especially into the peculiar behaviors of M and c that may occur at T_c, it is most useful to study the spin-spin correlation functions

$$\langle \sigma_{M',N'}\sigma_{M,N}\rangle = \lim_{\substack{\mathcal{M}\to\infty \\ \mathcal{N}\to\infty}} \langle \sigma_{M',N'}\sigma_{M,N}\rangle_{\mathcal{M},\mathcal{N}} = \lim_{\substack{\mathcal{M}\to\infty \\ \mathcal{N}\to\infty}} \frac{\sum_{\sigma} \sigma_{M',N'}\sigma_{M,N}e^{-\beta\mathscr{E}(\sigma)}}{Z(\beta)}. \tag{5.30}$$

In Onsager's lattice, at least if we ignore boundary effects (which vanish in the thermodynamic limit), this correlation depends not on four variables but only on $M - M'$ and $N - N'$.

To see some of the connections between spin correlation functions and the macroscopic properties already discussed, we first note that in Onsager's lattice, owing to translational invariance,

$$M(H) = \lim_{\substack{\mathcal{M}\to\infty \\ \mathcal{N}\to\infty}} \left\langle (\mathcal{M}\mathcal{N})^{-1} \sum_{j,k} \sigma_{j,k} \right\rangle_{\mathcal{M},\mathcal{N}} = \lim_{\substack{\mathcal{M}\to\infty \\ \mathcal{N}\to\infty}} \langle \sigma_{0,0}\rangle_{\mathcal{M},\mathcal{N}} \tag{5.31}$$

and

$$\begin{aligned} u = {} & \lim_{\substack{\mathcal{M}\to\infty \\ \mathcal{N}\to\infty}} (\mathcal{M}\mathcal{N})^{-1} \Big\langle \Big[-E_1 \sum_{j,k} \sigma_{j,k}\sigma_{j,k+1} - E_2 \sum_{j,k} \sigma_{j,k}\sigma_{j+1,k} \\ & \qquad\qquad - H \sum_{j,k} \sigma_{j,k} \Big] \Big\rangle_{\mathcal{M},\mathcal{N}} \\ = {} & -E_1\langle \sigma_{0,0}\sigma_{0,1}\rangle - E_2\langle \sigma_{0,0}\sigma_{1,0}\rangle - H\langle \sigma_{0,0}\rangle \\ = {} & -E_1\langle \sigma_{0,0}\sigma_{0,1}\rangle - E_2\langle \sigma_{0,0}\sigma_{1,0}\rangle - HM(H). \end{aligned} \tag{5.32}$$

Furthermore, in a lattice of $\mathcal{M}$ rows and $\mathcal{N}$ columns, we may define the magnetic susceptibility per site $\chi_{\mathcal{M},\mathcal{N}}(H)$ as

$$\chi_{\mathcal{M},\mathcal{N}}(H) = (\mathcal{M}\mathcal{N})^{-1} \frac{\partial \overline{M}(H)}{\partial H}. \tag{5.33}$$

In an arbitrary Ising lattice, $\chi_{\mathcal{M},\mathcal{N}}$ may be expressed in terms of spin-spin correlation functions as

$$\begin{aligned} \chi_{\mathcal{M},\mathcal{N}}(H) = {} & \frac{\partial}{\partial H}\Big\{ Z^{-1} \sum_{\sigma} \Big[(\mathcal{M}\mathcal{N})^{-1} \sum_{j,k} \sigma_{j,k} \Big] \\ & \qquad \times \exp\Big[-\beta\Big(\mathscr{E}_0 - H \sum_{l,m} \sigma_{l,m} \Big) \Big] \Big\} \\ = {} & \beta(\mathcal{M}\mathcal{N})^{-1} \sum_{j,k} \sum_{l,m} [\langle \sigma_{j,k}\sigma_{l,m}\rangle_{\mathcal{M},\mathcal{N}} - \langle \sigma_{j,k}\rangle_{\mathcal{M},\mathcal{N}}\langle \sigma_{l,m}\rangle_{\mathcal{M},\mathcal{N}}]. \end{aligned} \tag{5.34}$$

From (5.34) we may simply prove that

$$\chi_{\mathscr{M},\mathscr{N}}(H) \geq 0. \tag{5.35}$$

To see this we first rewrite (5.34) as

$$\chi_{\mathscr{M},\mathscr{N}}(H) = \beta(\mathscr{M}\mathscr{N})^{-1}Z^{-2}\left\{\sum_{\sigma}\sum_{\sigma'}\sum_{j,k}\sum_{l,m}[\tfrac{1}{2}\sigma_{j,k}\sigma_{l,m} + \tfrac{1}{2}\sigma'_{j,k}\sigma'_{l,m} - \sigma_{j,k}\sigma'_{l,m}]\exp\{-\beta[\mathscr{E}(\sigma) + \mathscr{E}(\sigma')]\}\right\}. \tag{5.36}$$

Consider any configuration of the spins σ and the spins σ' and introduce the following notation:

N_U is the number of $\sigma_{j,k}$ equal to $+1$,
N_D is the number of $\sigma_{j,k}$ equal to -1,
N'_U is the number of $\sigma'_{j,k}$ equal to $+1$,
N'_D is the number of $\sigma'_{j,k}$ equal to -1.

Then it is easily seen that for the configurations of σ and σ'

$$\begin{aligned}\sum_{j,k}\sum_{l,m}(\tfrac{1}{2}\sigma_{j,k}\sigma_{l,m} + \tfrac{1}{2}\sigma'_{j,k}\sigma'_{l,m} - \sigma_{j,k}\sigma'_{l,m})
&= \tfrac{1}{2}(N_U^2 + N_D^2 - 2N_UN_D) + \tfrac{1}{2}(N_U'^2 + N_D'^2 - 2N'_UN'_D) \\
&\quad - (N_U - N_D)(N'_U - N'_D) \\
&= \tfrac{1}{2}(N_U - N_D)^2 + \tfrac{1}{2}(N'_U - N'_D)^2 \\
&\quad - (N_U - N_D)(N'_U - N'_D) \\
&= \tfrac{1}{2}[(N_U - N_D) - (N'_U - N'_D)]^2 \geq 0.\end{aligned} \tag{5.37}$$

Therefore, since $\exp\{-\beta[\mathscr{E}(\sigma) + \mathscr{E}(\sigma')]\}$ is also nonnegative for all σ and σ', each term in the summation over σ and σ' in (5.36) is nonnegative, so (5.35) follows.

In the thermodynamic limit the susceptibility is defined as

$$\chi(H) = \frac{\partial M(H)}{\partial H}. \tag{5.38}$$

In Onsager's lattice we use (5.34) to write

$$\begin{aligned}\chi(H) &= \frac{\partial}{\partial H}\lim_{\substack{\mathscr{M}\to\infty\\ \mathscr{N}\to\infty}}(\mathscr{M}\mathscr{N})^{-1}\overline{M}(H) = \lim_{\substack{\mathscr{M}\to\infty\\ \mathscr{N}\to\infty}}\chi_{\mathscr{M},\mathscr{N}}(H) \\
&= \beta\sum_{j,k}[\langle\sigma_{0,0}\sigma_{j,k}\rangle - \langle\sigma_{0,0}\rangle^2].\end{aligned} \tag{5.39}$$

In particular, the zero-field susceptibility is

$$\chi(0^+) = \lim_{H\to 0^+}\chi(H) = \beta\sum_{j,k}[\langle\sigma_{0,0}\sigma_{j,k}\rangle - M^2]. \tag{5.40}$$

If the limit exists at $H = 0$, the quantity

$$\lim_{j^2+k^2\to\infty}\langle\sigma_{0,0}\sigma_{j,k}\rangle \tag{5.41}$$

is referred to as the long-range order. From (5.40) we see that if $\chi(0^+)$ is finite and if the long-range order exists, then

$$\lim_{j^2+k^2\to\infty} \langle \sigma_{0,0}\sigma_{j,k} \rangle = M^2(0^+). \tag{5.42}$$

More generally, from (5.39) we find that if the limit exists then

$$\lim_{j^2+k^2\to\infty} \langle \sigma_{0,0}\sigma_{j,k} \rangle = M^2(H). \tag{5.43}$$

If M is zero, χ will be infinite if $\langle \sigma_{0,0}\sigma_{j,k} \rangle$ is not a summable function of j and k. These considerations show that the behavior of $\langle \sigma_{0,0}\sigma_{j,k} \rangle$ at $H = 0$ is related to the singularities of F. Indeed, since nobody has managed to compute the free energy exactly when $H \neq 0$, the spin-spin correlation functions will be a major tool in the study of the spontaneous magnetization and the zero-field susceptibility.

6. EXTENSIONS OF STATISTICAL MECHANICS

In Section 2 we gave two distinct definitions of thermal equilibrium; one defined equilibrium as the state to which a system will tend when it has been allowed to sit undisturbed for a long while, and the other defined it in terms of the zeroth law of thermodynamics. The statistical mechanics developed in Sections 2 and 3 was shown to describe an equilibrium system in the sense of the second definition. To be totally convincing, it would be most desirable to prove that this statistical mechanics also describes a system which is in equilibrium in the first sense as well. To be more specific, one would like to prove that, if we begin at time zero with a large number of systems with identical Hamiltonians but different initial conditions, and if we vary at will for some finite amount of time the parameters in this Hamiltonian referring to such things as external electric and magnetic fields, then as time becomes sufficiently large the possible states of this collection of systems should approach the distribution of the canonical (or microcanonical) ensemble. More weakly, we might be satisfied if we could prove such a theorem when the initial distribution of states was in some sense "close" to the equilibrium distribution of states. Unfortunately, without further restrictions on the Hamiltonian such a theorem is not true because there exists an explicit example of a Hamiltonian for which we may begin with a collection of systems with the distribution of the canonical ensemble, vary an external magnetic field, and discover that as time goes to infinity the systems do *not* return to the distribution of a canonical ensemble. It would be most desirable to know what conditions must be imposed on the Hamiltonian of a system so as to avoid this unpleasant phenomenon.

It must be realized that, even if we can overcome this objection to statistical mechanics, there still exist limitations to the statistical mechanics presented here. The removal of this objection would merely say that in the limit as $t \to \infty$ we could describe a system by use of statistical mechanics. However, unless we know how fast this $t \to \infty$ limit is approached, the theorem that removes the objection would be useless from a practical point of view. After all, a thermal equilibrium which requires 10^{23} years to reach is of little use to the average physicist. This question of the time it takes to achieve thermal equilibrium is most important because there do, in fact, exist many cases in which the statistical mechanics we have previously discussed does not apply. For example, the properties of a piece of glass depend not only on the material it is made out of but also on the manner in which these materials are heated and cooled. The very property of being a glass or of being a crystallized solid depends on the thermal history of the system. If the physical properties of a collection of atoms depend upon their past thermal history, this collection obviously cannot be expected to be described by our statistical mechanics. If one waits long enough, presumably the glass will crystallize and the final state can be described by the canonical ensemble. However, it is clearly desirable to extend statistical mechanics to deal with the system which actually confronts us at finite time.

Problems similar to that of glass cannot be ignored in dealing with magnetism because the familiar phenomena of hysteresis cannot be treated on the basis of the (micro) canonical ensemble above. To deal with these phenomena we need some extension of the basic postulate of Section 2. Although no general theory of such extensions exists, these problems are often studied by restricting the sum over all states which occurs in the partition function to an appropriately chosen subset. This assumes that there exists a time scale in which it is extremely improbable that the system can fluctuate out of this subset of states. Such a treatment is vague because, aside from questions related to the time scale, there is usually no unambiguous way of specifying which states are in the subset. Since there is no dynamics in the Ising model, we cannot possibly study problems related to time scales. However, within the context of the Ising model, there does exist a type of hysteresis behavior for which the specification of the subset of states can be made completely precise. This phenomenon will be studied in Chapter XIII.

To conclude this chapter it is important to emphasize that our development of statistical mechanics and thermodynamics has been based on an important and unphysical assumption, namely, that the interaction energy of the system is completely known. Experimentally this assumption is never correct. The exact chemical composition of a substance is never exactly known. Even if it were, one would still not know the spatial arrangement of the atoms unless, for example, the lattice were a pure perfectly periodic lattice which, although sometimes a good approximation, is in fact never the case. If statistical mechanics is to be a truly useful tool for the analysis of real experiments it must be possible to show that in some sense almost all interaction energies consistent with our imperfect knowledge of the experimental situation will lead to the same free energy in the thermodynamic limit. We will return to this important practical question in Chapters XIV and XV and show that it is indeed true that, if the interaction energies $E_2(j)$ of the Ising model are not exactly known but are allowed to be independent random variables described by a known probability distribution $P(E_2)$, then the free energies of all Ising models that are described by $P(E_2)$ will, with probability 1, have the same free energy in the thermodynamic limit. However, this free energy is not the same as the free energy of any Onsager lattice and in the last two chapters we will see in a precise fashion that even a very small amount of randomness will, if we consider temperatures sufficiently close to the critical temperature, cause physically observable properties such as the specific heat to have enormous deviations from the behavior they would have in any Onsager lattice. It is gratifying that this effect has been experimentally observed.

CHAPTER III
The One-Dimensional Ising Model

1. INTRODUCTION

There is an enormous difference between the one-dimensional and two-dimensional Ising models. In one dimension an Ising model with nearest-neighbor forces does not possess a phase transition, whereas in two dimensions it does. The primary goal of this book is to study the phase transition in two dimensions as explicitly as possible. However, that study is long and is complicated by the fact that for many quantities of interest closed-form answers are not available and we must be content with appropriate approximations. Therefore, before commencing the study of the two-dimensional Ising model it is useful to study the one-dimensional model where both the free energy and the spin-spin correlation function may be exactly computed in closed form in the presence of a magnetic field.[1]

In a one-dimensional lattice with $\mathscr{N}$ spins we consider the interaction energy given by (I.2.4) with $j = 1$ and $1 \leq k \leq \mathscr{N}$. However, to complete the specification of the system we need to state precisely what are the interactions of the spins 1 and $\mathscr{N}$ at the two ends. There are two common ways of treating these end spins.

(1) *Cyclic.* We consider the one-dimensional lattice deformed into a circle and join site 1 and site $\mathscr{N}$ by a bond of strength E_1. Then the interaction energy is

$$\mathscr{E}_c = -E_1 \sum_{k=1}^{\mathscr{N}} \sigma_k \sigma_{k+1} - H \sum_{k=1}^{\mathscr{N}} \sigma_k, \tag{1.1}$$

where $\sigma_{\mathscr{N}+1} \equiv \sigma_1$.

1. E. Ising, *Z. Physik*, 31, 253 (1925).

(2) *Free.* We may also consider the more natural arrangement in which spin 1 interacts only with H and with spin 2 and spin $\mathcal{N}$ interacts only with H and with spin $\mathcal{N} - 1$. Then the interaction energy is

$$\mathscr{E}_F = -E_1 \sum_{k=1}^{\mathcal{N}-1} \sigma_k\sigma_{k+1} - H \sum_{k=1}^{\mathcal{N}} \sigma_k. \tag{1.2}$$

We will treat both types of boundary conditions in this chapter not only to show that they both have the same free energy (per site) in the limit $\mathcal{N} \to \infty$ but also to see for systems of finite size how large $\mathcal{N}$ must be before the boundary conditions may safely be ignored.

Though the distinction between these two types of boundary conditions is in general clear, the case $\mathcal{N} = 2$ is slightly peculiar, since if E_1 is the bond between the two spins with the free end conditions we may obtain all properties of the cyclic case merely by replacing E_1 by $2E_1$. In particular, for free boundary conditions there are only four possible states of the system and it is elementary to find

$$\begin{aligned} Z(\beta) &= \sum_{\sigma_1}\sum_{\sigma_2} \exp\{\beta[E_1\sigma_1\sigma_2 + H(\sigma_1 + \sigma_2)]\} \\ &= e^{\beta(E_1+2H)} + 2e^{-\beta E_1} + e^{\beta(E_1-2H)}, \end{aligned} \tag{1.3}$$

$$\begin{aligned} \bar{E} &= -\frac{\partial \ln Z(\beta)}{\partial\beta} \\ &= \frac{-(E_1 + 2H)e^{\beta(E_1+2H)} + 2E_1e^{-\beta E_1} - (E_1 - 2H)e^{\beta(E_1-2H)}}{e^{\beta(E_1+2H)} + 2e^{-\beta E_1} + e^{\beta(E_1-2H)}}, \end{aligned} \tag{1.4}$$

$$\begin{aligned} \bar{M} &= 2\langle\sigma_0\rangle_{1,2} = 2\langle\sigma_1\rangle_{1,2} = \beta^{-1}\frac{\partial \ln Z(\beta)}{\partial H} \\ &= \frac{4e^{\beta E_1}\sinh 2\beta H}{e^{\beta(E_1+2H)} + 2e^{-\beta E_1} + e^{\beta(E_1-2H)}}, \end{aligned} \tag{1.5}$$

$$\begin{aligned} \bar{S} &= \frac{1}{T}\bar{E} + k\ln Z(\beta) \\ &= -\frac{1}{T}\frac{(E_1 + 2H)e^{\beta(E_1+2H)} - 2E_1e^{-\beta E_1} + (E_1 - 2H)e^{\beta(E_1-2H)}}{e^{\beta(E_1+2H)} + 2e^{-\beta E_1} + e^{\beta(E_1-2H)}} \\ &\quad + k\ln[e^{\beta(E_1+2H)} + 2e^{-\beta E_1} + e^{\beta(E_1-2H)}], \end{aligned} \tag{1.6}$$

and

$$\langle\sigma_0\sigma_1\rangle_{1,2} = \frac{e^{\beta(E_1+2H)} - 2e^{-\beta E_1} + e^{\beta(E_1-2H)}}{e^{\beta(E_1+2H)} + 2e^{-\beta E_1} + e^{\beta(E_1-2H)}}. \tag{1.7}$$

In the high-temperature limit, where $\beta \to 0$,

$$Z(\beta) \to 4 = \text{the number of states}, \tag{1.8}$$

$$\bar{E} \sim -\beta(E_1^2 + 2H^2) \to 0, \tag{1.9}$$

$$\bar{M} \sim 2\beta H \to 0, \tag{1.10}$$

$$\bar{S} \to k\ln 4 = k\ln(\text{number of states}), \tag{1.11}$$

and

$$\langle\sigma_0\sigma_1\rangle_{1,2} \sim \beta E_1 \to 0. \tag{1.12}$$

Similarly, in the low-temperature limit, where $\beta \to \infty$,

$$Z(\beta) \sim \left\{\begin{matrix} 2e^{\beta|E_1|} & \text{if } H = 0 \\ e^{\beta[E_1+2|H|]} & \text{if } E_1 > -|H| \neq 0 \\ 3e^{-\beta E_1} & \text{if } E_1 = -|H| \neq 0 \\ 2e^{-\beta E_1} & \text{if } E_1 < -|H| \neq 0 \end{matrix}\right\} = \begin{matrix}\text{degeneracy of } \mathscr{E}_{\min} \\ \times\, e^{-\beta\mathscr{E}_{\min}},\end{matrix} \tag{1.13}$$

$$\bar{E} \to \left\{\begin{matrix} -(E_1 + 2|H|) & \text{if } E_1 \geq -|H| \\ E_1 & \text{if } E_1 \leq -|H| \end{matrix}\right\} = \mathscr{E}_{\min}, \tag{1.14}$$

$$\bar{M} \sim \left\{\begin{matrix} 2\,\mathrm{sgn}\,(H) & \text{if } E_1 > -|H| \\ \frac{2}{3} & \text{if } E_1 = -|H| \neq 0 \\ e^{2\beta(E_1-|H|)} & \text{if } E_1 < -|H| \neq 0 \end{matrix}\right\} = \begin{matrix}\text{average of the} \\ \text{magnetization of all} \\ \text{states with energy } \mathscr{E}_{\min},\end{matrix} \tag{1.15}$$

where sgn (H) is the signature function of H that is $+1$ if $H > 0$, -1 if $H < 0$, and 0 if $H = 0$,

$$\bar{S} \to \left\{\begin{matrix} k \ln 2 & \text{if } H = 0 \\ 0 & \text{if } E_1 > -|H| \neq 0 \\ k \ln 3 & \text{if } E_1 = -|H| \neq 0 \\ k \ln 2 & \text{if } E_1 < -|H| \neq 0 \end{matrix}\right\} = \begin{matrix}\ln\text{ (number of states with} \\ \text{energy } \mathscr{E}_{\min})\end{matrix} \tag{1.16}$$

and

$$\langle\sigma_0\sigma_1\rangle_{1,2} \to \left\{\begin{matrix} \mathrm{sgn}\, E_1 & \text{if } H = 0 \\ 1 & \text{if } E_1 > -|H| \neq 0 \\ -\frac{1}{3} & \text{if } E_1 = -|H| \neq 0 \\ -1 & \text{if } E_1 < -|H| \neq 0 \end{matrix}\right\} = \begin{matrix}\text{average of } \langle\sigma_0\sigma_1\rangle_{1,2} \\ \text{of all states with} \\ \text{energy } \mathscr{E}_{\min}.\end{matrix} \tag{1.17}$$

The statement in (1.16) that $\bar{S} \to 0$ if $E_1 > -|H| \neq 0$ is a general property of entropy for systems which are not degenerate in energy at $T = 0$. Indeed, the final expressions on the right-hand sides of (1.8)–(1.16) are general expressions which will be valid for any Ising model.

2. PARTITION FUNCTION

We now consider the case of an arbitrary value of $\mathscr{N}$. The partition function with cyclic boundary condition is

$$Z^c_{1,\mathscr{N}}(\beta) = \sum_{\sigma_1} \cdots \sum_{\sigma_{\mathscr{N}}} \exp\left\{\beta\left[E_1 \sum_{k=1}^{\mathscr{N}} \sigma_k\sigma_{k+1} + H \sum_{k=1}^{\mathscr{N}} \sigma_k\right]\right\} \tag{2.1}$$

and the partition function for one-dimensional Ising model with free boundary conditions is

$$Z_{1,\mathcal{N}}^F(\beta) = \sum_{\sigma_1} \cdots \sum_{\sigma_{\mathcal{N}}} \exp\left\{\beta\left[E_1 \sum_{k=1}^{\mathcal{N}-1} \sigma_k\sigma_{k+1} + H\sum_{k=1}^{\mathcal{N}} \sigma_k\right]\right\}. \tag{2.2}$$

We will explicitly compute these partition functions for arbitrary $\mathcal{N}$ by use of a matrix formalism introduced by Kramers and Wannier.[2]

Consider the spins σ_k and σ_{k+1} together. If $\sigma_k = \sigma_{k+1}$, these spins give a contribution $-E_1$ to the interaction energy, whereas if $\sigma_k = -\sigma_{k+1}$, they give a contribution of $+E_1$. Furthermore, with this pair of spins we associate the energy $\frac{1}{2}H(\sigma_k + \sigma_{k+1})$. Let the two values which any σ may take on be the basis of a two-dimensional vector space and in this space define the matrix P by

$$\langle\sigma|P|\sigma'\rangle = \exp\{\beta[E_1\sigma\sigma' + \tfrac{1}{2}H(\sigma + \sigma')]\}, \tag{2.3}$$

the vector V by

$$\langle\sigma|V\rangle = e^{\beta H\sigma/2}, \tag{2.4a}$$

and the transposed vector V^T by

$$\langle V^T|\sigma\rangle = e^{\beta H\sigma/2}. \tag{2.4b}$$

More explicitly we have

$$P = \begin{bmatrix} e^{\beta(E_1+H)} & e^{-\beta E_1} \\ e^{-\beta E_1} & e^{\beta(E_1-H)} \end{bmatrix} \tag{2.5}$$

and

$$V = \begin{bmatrix} e^{(1/2)\beta H} \\ e^{-(1/2)\beta H} \end{bmatrix}. \tag{2.6}$$

Then in terms of P we may write $Z_{1,\mathcal{N}}^c$ as

$$\begin{aligned} Z_{1,\mathcal{N}}^c &= \sum_{\sigma_1} \cdots \sum_{\sigma_{\mathcal{N}}} \langle\sigma_1|P|\sigma_2\rangle\langle\sigma_2|P|\sigma_3\rangle \cdots \langle\sigma_{\mathcal{N}-1}|P|\sigma_{\mathcal{N}}\rangle\langle\sigma_{\mathcal{N}}|P|\sigma_1\rangle \\ &= \sum_{\sigma_1} \langle\sigma_1|P^{\mathcal{N}}|\sigma_1\rangle = \operatorname{tr} P^{\mathcal{N}}, \end{aligned} \tag{2.7}$$

where tr stands for the trace of a matrix. Similarly, in terms of P and V we may write $Z_{1,\mathcal{N}}^F$ as

$$\begin{aligned} Z_{1,\mathcal{N}}^F &= \sum_{\sigma_1} \cdots \sum_{\sigma_{\mathcal{N}}} \langle V^T|\sigma_1\rangle\langle\sigma_1|P|\sigma_2\rangle \cdots \langle\sigma_{\mathcal{N}-1}|P|\sigma_{\mathcal{N}}\rangle\langle\sigma_{\mathcal{N}}|V\rangle \\ &= V^T P^{\mathcal{N}-1} V. \end{aligned} \tag{2.8}$$

2. H. A. Kramers and G. H. Wannier, *Phys. Rev.* **60**, 252 (1941).

To evaluate (2.7) and (2.8) we remark that since P is a symmetric matrix it may be diagonalized by a similarity transformation with some matrix U. Therefore define U and $\lambda_\pm$ by

$$U^{-1}PU = \begin{bmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{bmatrix}, \tag{2.9}$$

where the eigenvalues λ_+ and λ_- satisfy the equation

$$(e^{\beta(E_1+H)} - \lambda)(e^{\beta(E_1-H)} - \lambda) - e^{-2\beta E_1} = 0$$

and are found to be

$$\begin{aligned} \lambda_\pm &= e^{\beta E_1}[\cosh \beta H \pm (\cosh^2 \beta H - 2e^{-2\beta E_1} \sinh 2\beta E_1)^{1/2}] \\ &= e^{\beta E_1}[\cosh \beta H \pm (\sinh^2 \beta H + e^{-4\beta E_1})^{1/2}]. \end{aligned} \tag{2.10}$$

Furthermore one possible choice for the matrix U is

$$U = \begin{bmatrix} -e^{\beta E_1}(e^{\beta(E_1-H)} - \lambda_+) & 1 \\ 1 & -e^{\beta E_1}(e^{\beta(E_1+H)} - \lambda_-) \end{bmatrix} \tag{2.11}$$

with

$$U^{-1} = U\begin{bmatrix} -(\det U)^{-1} & 0 \\ 0 & -(\det U)^{-1} \end{bmatrix}. \tag{2.12}$$

We then use the cyclic property of the trace to find

$$\begin{aligned} Z^c_{1,\mathcal{N}} &= \operatorname{tr} P^{\mathcal{N}} = \operatorname{tr}\,[U^{-1}PU]^{\mathcal{N}} = \operatorname{tr} \begin{bmatrix} \lambda_+^{\mathcal{N}} & 0 \\ 0 & \lambda_-^{\mathcal{N}} \end{bmatrix} = \lambda_+^{\mathcal{N}} + \lambda_-^{\mathcal{N}} \\ &= \lambda_+^{\mathcal{N}}[1 + (\lambda_-/\lambda_+)^{\mathcal{N}}]. \end{aligned} \tag{2.13}$$

Similarly we find

$$\begin{aligned} Z^F_{1,\mathcal{N}} &= V^T U \begin{bmatrix} \lambda_+^{\mathcal{N}-1} & 0 \\ 0 & \lambda_-^{\mathcal{N}-1} \end{bmatrix} U^{-1} V \\ &= [1 - e^{2\beta E_1}(e^{\beta(E_1-H)} - \lambda_+)(e^{\beta(E_1+H)} - \lambda_-)]^{-1} \\ &\quad \times \{\lambda_+^{\mathcal{N}-1}[e^{\beta(E_1+(1/2)H)}(e^{\beta(E_1-H)} - \lambda_+) - e^{-(1/2)\beta H}]^2 \\ &\quad + \lambda_-^{\mathcal{N}-1}[e^{\beta(E_1-(1/2)H)}(e^{\beta(E_1+H)} - \lambda_-) - e^{(1/2)\beta H}]^2\} \\ &= \lambda_+^{\mathcal{N}-1}\{\cosh \beta H + (\sinh^2 \beta H + e^{-2\beta E_1})(\sinh^2 \beta H + e^{-4\beta E_1})^{-1/2}\} \\ &\quad + \lambda_-^{\mathcal{N}-1}\{\cosh \beta H - (\sinh^2 \beta H + e^{-2\beta E_1}) \\ &\qquad \times (\sinh^2 \beta H + e^{-4\beta E_1})^{-1/2}\}. \end{aligned} \tag{2.14}$$

When $H = 0$ these reduce to the simpler expressions

$$Z^c_{1,\mathcal{N}} = [2 \cosh \beta E_1]^{\mathcal{N}}[1 + (\tanh \beta E_1)^{\mathcal{N}}] \tag{2.15}$$

and

$$Z_{1,\mathcal{N}}^{F} = 2[2 \cosh \beta E_1]^{\mathcal{N}-1}. \tag{2.16}$$

These expressions have two interesting features which will reappear in our discussion of the two-dimensional model. First of all, we note that $Z_{1,\mathcal{N}}^{F}$ is an even function of E_1, whereas $Z_{1,\mathcal{N}}^{c}$ is an even function of E_1 if $\mathcal{N}$ is even but possesses no such symmetry if $\mathcal{N}$ is odd. These features may be readily understood by considering the interaction energies $\mathscr{E}_F$ and $\mathscr{E}_c$ of (1.1) and (1.2) with $H = 0$. If in (1.2) we make the replacement

$$\sigma_k \to (-1)^k \sigma_k', \tag{2.17}$$

then

$$\mathscr{E}_F(\sigma; E_1) \to \mathscr{E}_F(\sigma'; -E_1). \tag{2.18}$$

Since $Z_{1,\mathcal{N}}^{F}$ is a summation of $e^{-\beta \mathscr{E}_F(\sigma; E_1)}$ over all states, (2.18) guarantees that $Z_{1,\mathcal{N}}^{F}$ will be an even function of E_1. Consider next $\mathscr{E}_c$, given by (1.1). If we make the substitution (2.17) we see that

$$\mathscr{E}_c(\sigma; E_1) = \mathscr{E}_F(\sigma'; -E_1) + [1 - (-1)^{\mathcal{N}}]\sigma_1 \sigma_{\mathcal{N}}. \tag{2.19}$$

If $\mathcal{N}$ is even, $1 - (-1)^{\mathcal{N}}$ vanishes and (2.19) guarantees that $Z_{1,\mathcal{N}}^{c}$ will be an even function of E_1.

The second feature of (2.15) and (2.16) to be noted is their $T \to 0$ limit. As $T \to 0$,

$$Z_{1,\mathcal{N}}^{F} \to 2e^{\beta |E_1|(\mathcal{N}-1)}. \tag{2.20}$$

This limit is in accord with the right-hand side of (1.13) since

$$\mathscr{E}_{F\min} = -|E_1|(\mathcal{N} - 1) \tag{2.21}$$

and the degeneracy of this state is 2. However, the $T \to 0$ limit of $Z_{1,\mathcal{N}}^{c}$ is slightly more complicated. If $E_1 > 0$ or if $E_1 < 0$ and $\mathcal{N}$ is even, then

$$Z_{1,\mathcal{N}}^{c} \to 2e^{\beta \mathcal{N} |E_1|}. \tag{2.22}$$

When $E_1 < 0$ and $\mathcal{N}$ is odd, then

$$Z_{1,\mathcal{N}}^{c} \to 2\mathcal{N} e^{\beta |E_1|(\mathcal{N}-2)}. \tag{2.23}$$

The difference between these two cases is related to the behavior of $\mathscr{E}_c$ under the substitution (2.17) which is shown in (2.19). It can perhaps be best seen in Fig. 3.1. When $E_1 < 0$ and $\mathcal{N}$ is even, $\mathscr{E}_F$ has the two ground states shown there. However, when $E_1 < 0$ and $\mathcal{N}$ is odd, the regular alternation of spins in the ground state which is possible when $\mathcal{N}$ is even must be broken at one bond. At this bond the two neighboring spins must both point either up or down. Since the mismatched bond can be any of the $\mathcal{N}$ bonds in the ring, the degeneracy of this ground state is $2\mathcal{N}$. The bond at which the mismatch occurs is called the "antiferromagnetic

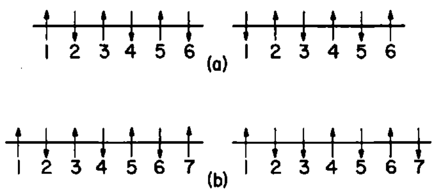


Fig. 3.1. Configurations of minimum energy of the one-dimensional Ising model with $E_1 < 0$ (antiferromagnetic) and $H = 0$. Cyclic boundary conditions are imposed so the two ends of the chain are considered as nearest neighbors. (a) $\mathcal{N}$ is even; both configurations of minimum energy are shown. (b) $\mathcal{N}$ is odd; two of the $2\mathcal{N}$ configurations of minimum energy are shown. The mismatched bond is the antiferromagnetic seam.

seam." It is important in the one-dimensional model only at $T = 0$. We will return to this seam in Chapter V where we will see that in a two-dimensional Ising model a comparable phenomenon exists not only for $T = 0$ but for all T below the critical temperature.

From (2.10) it is clear that when H is real and β is finite and positive

$$\lambda_+ > \lambda_-. \tag{2.24}$$

Therefore if $T > 0$,

$$\lim_{\mathcal{N}\to\infty} \mathcal{N}^{-1} \ln Z^c_{1,\mathcal{N}} = \lim_{\mathcal{N}\to\infty} \mathcal{N}^{-1} \ln Z^F_{1,\mathcal{N}} = \ln \lambda_+ = -\beta F, \tag{2.25}$$

so that, as expected in the thermodynamic limit, the free energy per spin with cyclic boundary conditions and the free energy per spin with free boundary conditions are the same.

The approach of $\mathcal{N}^{-1} \ln Z_{1,\mathcal{N}}$ to this $\mathcal{N} \to \infty$ limit depends strongly on the boundary conditions. From (2.13) we find that for large $\mathcal{N}$

$$\ln Z^c_{1,\mathcal{N}} \sim -\mathcal{N}\beta F + (\lambda_-/\lambda_+)^{\mathcal{N}}, \tag{2.26}$$

whereas from (2.14)

$$\begin{aligned} \ln Z^F_{1,\mathcal{N}} \sim -\mathcal{N}\beta F + \{-\ln \lambda_+ + \ln [\cosh \beta H + (\sinh^2 \beta H + e^{-2\beta E_1}) \\ \times (\sinh^2 \beta H + e^{-4\beta E_1})^{-1/2}]\} + O[(\lambda_-/\lambda_+)^{\mathcal{N}}]. \end{aligned} \tag{2.27}$$

Therefore $\mathcal{N}^{-1} \ln Z^c_{1,\mathcal{N}}$ approaches F exponentially in $\mathcal{N}$ while $\mathcal{N}^{-1} \ln Z^F_{1,\mathcal{N}}$ approaches F at the much slower rate of $\mathcal{N}^{-1}$.

We may interpret this difference as follows. First note that the second term in (2.27) is proportional to the number of free spins at the ends of the lattice. Because this term is lacking in (2.26) we identify $-\frac{1}{2}\beta$ times the second term in (2.27) as an additional free energy of a free end.

We therefore expect that, as long as a sample is large enough that its "surface"-to-"volume" ratio may be neglected, boundary conditions become unimportant for the computation of physical properties derivable from the free energy.

We may now use the formalism of the last chapter to find from the free energy

$$F = -E_1 - \beta^{-1} \ln \{\cosh \beta H + (\sinh^2 \beta H + e^{-4\beta E_1})^{1/2}\}, \tag{2.28}$$

that the internal energy is

$$\begin{aligned} u = \frac{\partial \beta F}{\partial \beta} &= -H \sinh \beta H (\sinh^2 \beta H + e^{-4\beta E_1})^{-1/2} \\ &\quad - E_1 \coth 2\beta E_1 + E_1 e^{-2\beta E_1} \operatorname{csch} 2\beta E_1 \cosh \beta H \\ &\quad \times (\sinh^2 \beta H + e^{-4\beta E_1})^{-1/2}, \end{aligned} \tag{2.29}$$

the specific heat is

$$\begin{aligned} c = \frac{\partial E}{\partial T} &= k\beta^2 \{H e^{-4\beta E_1}[H \cosh \beta H + 2E_1 \sinh \beta H] \\ &\quad \times (\sinh^2 \beta H + e^{-4\beta E_1})^{-3/2} - 2E_1^2 \operatorname{csch}^2 2\beta E_1 \\ &\quad + 2E_1^2 \operatorname{csch}^2 2\beta E_1 \cosh \beta H (\sinh^2 \beta H + e^{-4\beta E_1})^{-1/2} \\ &\quad - [E_1 H \sinh \beta H (e^{-4\beta E_1} - 1) + 2E_1^2 e^{-4\beta E_1} \cosh \beta H] e^{-2\beta E_1} \operatorname{csch} 2\beta E_1 \\ &\quad \times (\sinh^2 \beta H + e^{-4\beta E_1})^{-3/2}\}, \end{aligned} \tag{2.30}$$

and the magnetization is

$$M = -\frac{\partial F}{\partial H} = \sinh \beta H [\sinh^2 \beta H + e^{-4\beta E_1}]^{-1/2}. \tag{2.31}$$

At $H = 0$ these simplify to

$$F = -kT \ln \left[2 \cosh \frac{E_1}{kT}\right], \tag{2.32}$$

$$u = -E_1 \tanh \frac{E_1}{kT}, \tag{2.33}$$

$$c = \frac{E_1^2}{kT^2} \operatorname{sech}^2 \frac{E_1}{kT}. \tag{2.34}$$

For comparison with later work we plot $M(H)$ versus H for $E_1/k = 1$ in Fig. 3.2, $M(H)$ versus H for $E_1/k = -1$ in Fig. 3.3, M versus T at fixed H for $E_1/k = -1$ in Fig. 3.4, and c versus T in Fig. 3.5.

It is clear from the definition that if $\mathcal{N}$ is finite both $Z^c_{1,\mathcal{N}}$ and $Z^F_{1,\mathcal{N}}$ are analytic functions of β and H for all β and H. However, we see explicitly from (2.27) that in the limit $\mathcal{N} \to \infty$ there are values of β and H where

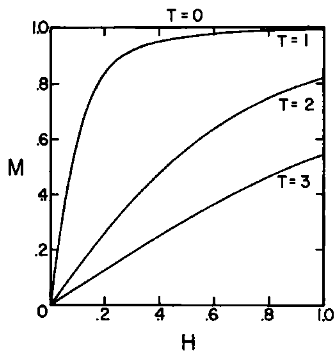


Fig. 3.2. The magnetization $M(H)$ of the one-dimensional Ising model at various temperatures for $E_1/k = 1$.

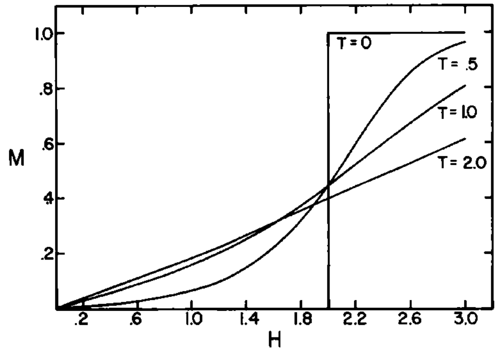


Fig. 3.3. The magnetization $M(H)$ of the one-dimensional Ising model at various temperatures for $E_1/k = -1$.

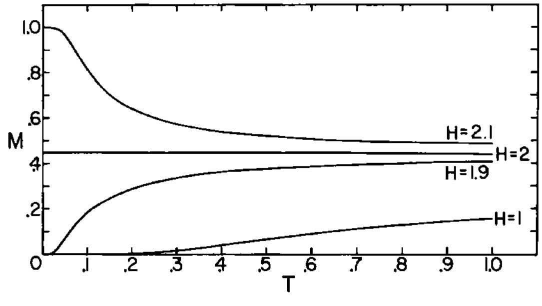


Fig. 3.4. The magnetization of the one-dimensional Ising model as a function of T for various values of H for $E_1/k = -1$.

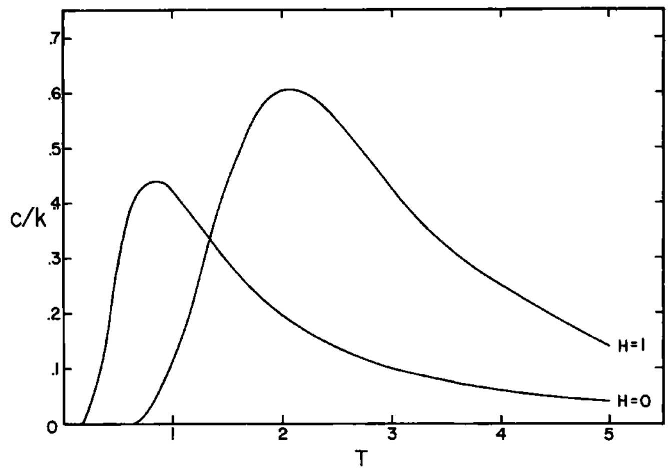


Fig. 3.5. The specific heat of the one-dimensional Ising model as a function of T at various values of H for $E_1/k = 1$.

neither F nor $e^{-\beta F}$ is analytic. This lack of analyticity, however, does not occur for H real and β positive so there is no possibility of a phase transition in this one-dimensional system. In particular, for all $T > 0$ this system cannot be ferromagnetic because $\lim_{H\to 0} M(H)$ is zero.

3. SPIN-SPIN CORRELATION FUNCTIONS

We may compute the spin-spin correlation functions by an extension of this matrix technique. Consider first cyclic boundary conditions and $N' \le N$, so that

$$\langle\sigma_{N'}\sigma_N\rangle^c_{1,\mathcal{N}} = (Z^c_{1,\mathcal{N}})^{-1}\sum_\sigma \sigma_{N'}\sigma_N \exp\left\{\beta\left[E_1\sum_{k=1}^{\mathcal{N}}\sigma_k\sigma_{k+1} + H\sum_{k=1}^{\mathcal{N}}\sigma_k\right]\right\}. \tag{3.1}$$

Using the matrix P we may easily re-express this as

$$\langle\sigma_{N'}\sigma_N\rangle^c_{1,\mathcal{N}} = (Z^c_{1,\mathcal{N}})^{-1}\,\mathrm{tr}\, P^{\mathcal{N}-(N-N')}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}P^{N-N'}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}, \tag{3.2}$$

which, as expected, is a function of $N - N'$ alone. To evaluate the trace we first diagonalize P by use of the matrix U, to find

$$\langle\sigma_{N'}\sigma_N\rangle^c_{1,\mathcal{N}} = (Z^c_{1,\mathcal{N}})^{-1}\,\mathrm{tr}\begin{bmatrix}\lambda_+ & 0\\ 0 & \lambda_-\end{bmatrix}^{\mathcal{N}-(N-N')}U^{-1}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}$$
$$\times\, U\begin{bmatrix}\lambda_+ & 0\\ 0 & \lambda_-\end{bmatrix}^{N-N'}U^{-1}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}U. \tag{3.3}$$

Then, using the explicit form of U given by (2.11), it is straightforward to obtain

$$\begin{aligned}\langle\sigma_{N'}\sigma_N\rangle^c_{1,\mathcal{N}} = {} & (\sinh^2\beta H + e^{-4\beta E_1})^{-1} \\ & \times [\sinh^2\beta H + (\lambda_+^{\mathcal{N}-N+N'}\lambda_-^{N-N'} + \lambda_-^{\mathcal{N}-N+N'}\lambda_+^{N-N'}) \\ & \times (\lambda_+^{\mathcal{N}} + \lambda_-^{\mathcal{N}})^{-1}e^{-4\beta E_1}]. \end{aligned} \tag{3.4}$$

We may then take the thermodynamic limit by keeping $N - N'$ fixed and letting $\mathcal{N} \to \infty$ to find

$$\langle\sigma_{N'}\sigma_N\rangle^c = (\sinh^2\beta H + e^{-4\beta E_1})^{-1}[\sinh^2\beta H + (\lambda_-/\lambda_+)^{N-N'}e^{-4\beta E_1}]. \tag{3.5}$$

By comparison with (2.29) we see, as expected from (II.5.32), that

$$u = -E_1\langle\sigma_0\sigma_1\rangle^c - HM. \tag{3.6}$$

Furthermore, by comparison with (2.31) we see, as expected from (II.5.43), that

$$\lim_{N-N'\to\infty}\langle\sigma_{N'}\sigma_N\rangle^c = M^2. \tag{3.7}$$

The existence of this limiting value is independent of the sign of E_1. However, it is easily seen from (2.10) that the approach to this limit is monotonic if $E_1 > 0$. If $E_1 < 0$ the approach is oscillatory. In general the value of $\langle\sigma_{N'}\sigma_N\rangle^c$ for $E_1 < 0$ is not simply expressible in terms of $\langle\sigma_{N'}\sigma_N\rangle^c$ with E_1 replaced by $-E_1$. However, in the special case $H = 0$ we easily see that

$$\langle\sigma_{N'}\sigma_N\rangle^c = (\tanh\beta E_1)^{N-N'}. \tag{3.8}$$

Therefore

$$\langle\sigma_{N'}\sigma_N\rangle^c|_{E_1} = (-1)^{N-N'}\langle\sigma_{N'}\sigma_N\rangle^c|_{-E_1}. \tag{3.9}$$

This is precisely the relation expected from the behavior (2.18) of $\mathscr{E}_c$ under the substitution (2.17).

In (5.41) of the previous chapter we defined the long-range order as the limit when $N - N' \to \infty$ of $\langle\sigma_{N'}\sigma_N\rangle$ evaluated at $H = 0$. From (3.8) we see that the long-range order so defined is 1 if $T = 0$ and zero otherwise. This absence of long-range order at $T > 0$ has a simple explanation. From (3.9) we may restrict our considerations to $E_1 > 0$. When $T = 0$ the system must be in its lowest energy state and all spins point in the same direction. Therefore $\langle\sigma_0\sigma_N\rangle = 1$. However, if we let $T > 0$ then not only is the lowest energy state important for the computation of $\langle\sigma_0\sigma_N\rangle$ but so are the low-lying excited states. But, because of the one-dimensional nature of this system, if we overturn one spin to put the system in its first excited state we may then overturn one of its nearest neighbors with no additional cost in energy. Indeed, the first excited state is $2\mathcal{N}(\mathcal{N} - 1)$-

fold degenerate. The states contributing to this degenerate level consist of all ways that the one-dimensional chain may be broken up into two blocks of spins with the spins in one block all pointing up and the spins in the other all pointing down. Because of this large degeneracy this first excited state has none of the order possessed by the 2-fold degenerate ground state and hence, for $T > 0$, $\langle\sigma_0\sigma_N\rangle$ must be zero.

The case of free boundary conditions is treated in a similar fashion. By definition, with $N' < N$,

$$\langle\sigma_{N'}\sigma_N\rangle_{1,\mathcal{N}}^F = (Z_{1,\mathcal{N}}^F)^{-1}\sum_\sigma \sigma_{N'}\sigma_N \exp\left\{\beta\left[E_1\sum_{k=1}^{\mathcal{N}-1}\sigma_k\sigma_{k+1} + H\sum_{k=1}^{\mathcal{N}}\sigma_k\right]\right\}, \tag{3.10}$$

which may be rewritten as

$$\begin{aligned}\langle\sigma_{N'}\sigma_N\rangle_{1,\mathcal{N}}^F &= (Z_{1,\mathcal{N}}^F)^{-1}V^T P^{N'-1}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}P^{N'-N}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}P^{\mathcal{N}-N}V\\ &= (Z_{1,\mathcal{N}}^F)^{-1}V^T U\begin{bmatrix}\lambda_+ & 0\\ 0 & \lambda_-\end{bmatrix}^{N'-1}U^{-1}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\\ &\quad\times U\begin{bmatrix}\lambda_+ & 0\\ 0 & \lambda_-\end{bmatrix}^{N-N'}U^{-1}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}U\begin{bmatrix}\lambda_+ & 0\\ 0 & \lambda_-\end{bmatrix}^{\mathcal{N}-N}U^{-1}V.\end{aligned} \tag{3.11}$$

This is now straightforwardly evaluated and we find

$$\begin{aligned}\langle\sigma_{N'}\sigma_N\rangle_{1,\mathcal{N}}^F &= (\sinh^2\beta H + e^{-4\beta E_1})^{-1}\\ &\quad\times\{\sinh^2\beta H + e^{-4\beta E_1}[\![(\lambda_-/\lambda_+)^{N-N'}\lambda_+^{\mathcal{N}-1}\\ &\quad\times[\cosh\beta H(\sinh^2\beta H + e^{-4\beta E_1})^{1/2} + \sinh^2\beta H + e^{-2\beta E_1}]\\ &\quad+(\lambda_+/\lambda_-)^{N-N'}\lambda_-^{\mathcal{N}-1}[\cosh\beta H(\sinh^2\beta H + e^{-4\beta E_1})^{1/2}\\ &\quad-\sinh^2\beta H - e^{-2\beta E_1}]]\!]\\ &\quad\times[\![\lambda_+^{\mathcal{N}-1}[\cosh\beta H(\sinh^2\beta H + e^{-4\beta E_1})^{1/2}\\ &\quad+\sinh^2\beta H + e^{-2\beta E_1}]\\ &\quad+\lambda_-^{\mathcal{N}-1}[\cosh\beta H(\sinh^2\beta H + e^{-4\beta E_1})^{1/2}\\ &\quad-\sinh^2\beta H - e^{-2\beta E_1}]]\!]^{-1} - 4\sinh^2\beta H\, e^{-4\beta E_1}\sinh^2\beta E_1\\ &\quad\times[\![\lambda_+^{\mathcal{N}-1}[(\lambda_-/\lambda_+)^{N'-1} - (\lambda_-/\lambda_+)^{N-1}]\\ &\quad+\lambda_-^{\mathcal{N}-1}[(\lambda_+/\lambda_-)^{N'-1} - (\lambda_+/\lambda_-)^{N-1}]]\!]\\ &\quad\times[\![\lambda_+^{\mathcal{N}-1}[\cosh\beta H(\sinh^2\beta H + e^{-4\beta E_1})^{1/2}\\ &\quad+\sinh^2\beta H + e^{-2\beta E_1}]\\ &\quad+\lambda_-^{\mathcal{N}-1}[\cosh\beta H(\sinh^2\beta H + e^{-4\beta E_1})^{1/2}\\ &\quad-\sinh^2\beta H - e^{-2\beta E_1}]]\!]^{-1}\}.\end{aligned} \tag{3.12}$$

This correlation function is an enormous mess when compared with the much simpler expression (3.4) obtained for the lattice with cyclic boundary conditions. In fact, it is to avoid such complicated expressions that cyclic boundary conditions are often imposed in statistical mechanical problems. However, there are several features of this result which will reappear in our later work on boundary effects in the two-dimensional lattice. In particular, we note that (3.12) does not depend on $N - N'$ alone but on N and N' separately. Therefore there are several ways to take the thermodynamic limit. One possible way is to keep N and N' fixed and let $\mathscr{N} \to \infty$. In this limit we are observing the correlation of two spins each of which is a finite distance from the free boundary. From (3.12) we explicitly obtain

$$\langle \sigma_{N'} \sigma_N \rangle^F = (\sinh^2 \beta H + e^{-4\beta E_1})^{-1} \{\sinh^2 \beta H + e^{-4\beta E_1} (\lambda_-/\lambda_+)^{N-N'} - 4 \sinh^2 \beta H \, e^{-4\beta E_1} \sinh^2 \beta E_1 [(\lambda_-/\lambda_+)^{N'-1} - (\lambda_-/\lambda_+)^{N-1}]\}. \tag{3.13}$$

However, we may also consider the limit where not only does $\mathscr{N} \to \infty$ but also $N \to \infty$, $N' \to \infty$, $\mathscr{N} - N \to \infty$, and $\mathscr{N} - N' \to \infty$. We refer to this limit as the bulk limit, because the two spins to be correlated are infinitely far from the boundary, and find

$$\lim_{\text{bulk}} \langle \sigma_{N'} \sigma_N \rangle^F = (\sinh^2 \beta H + e^{-4\beta E_1})^{-1} \{\sinh^2 \beta H + (\lambda_-/\lambda_+)^{N-N'} e^{-4\beta E_1}\}. \tag{3.14}$$

This limit may be obtained from (3.13) by letting $N \to \infty$ and $N' \to \infty$ while keeping $N - N'$ fixed. It also is identical with the expression (3.5) for $\langle \sigma_{N'} \sigma_N \rangle^c$. We therefore are led to expect that if we are interested only in bulk properties of the Ising model it is immaterial what boundary conditions we apply. In later chapters we will study the two-dimensional Ising model under several different boundary conditions and explicitly verify this conclusion.

If bulk properties of any statistical mechanical model in the thermodynamic limit do depend on the boundary conditions, then the distinction between bulk and surface can no longer be sharply made. While we will not be concerned with such problems in this book, it should be remarked that such difficulties can arise if the forces between particles approach zero sufficiently slowly as the separation between spins becomes infinite. In such cases a discussion of macroscopic properties in terms of a free energy such as that defined by (II.5.5) is inadequate.

CHAPTER IV
Dimer Statistics

1. INTRODUCTION

The matrix method of the previous chapter allowed us to compute the partition function and the spin-spin correlation functions of a one-dimensional Ising model in a very elementary fashion. Accordingly, the most natural way to study the two-dimensional Ising model would be to generalize that procedure to study Ising models of more than one row. One could then hope to study the case of a plane of Ising spins by letting the number of rows tend to infinity. Indeed, this is precisely the procedure followed by Onsager[1] in 1944. However, the mathematics of this procedure is extremely complicated. In order to obtain a simple method of computing the partition function of Onsager's lattice we will use instead the method of Kasteleyn,[2] who many years after Onsager's original computation discovered that the partition function of the two-dimensional Ising model with $H = 0$ is intimately related to a combinatorial problem involving dimers. This problem has an extremely elegant solution in terms of Pfaffians of matrices which may be easily evaluated. We will devote this chapter to the exposition and solution of this dimer problem. In so doing we will introduce all of the mathematical tools needed for the computation of the partition function at $H = 0$ of Onsager's two-dimensional Ising model.

A dimer is a figure that may be drawn on a lattice and that covers two nearest-neighbor sites and the bond that joins them. Consider the bonds

1. L. Onsager, *Phys. Rev.* **65**, 117 (1944).
2. P. W. Kasteleyn, *J. Math. Phys.* **4**, 287 (1963). This paper relates the Ising problem to the dimer problem previously solved in detail by P. W. Kasteleyn, *Physica* **27**, 1209 (1961). The solution of this dimer problem was also communicated by H. N. V. Temperley and M. E. Fisher, *Phil. Mag.* **6**, 1061 (1961).

of the lattice to be divided into several classes—for example, if the lattice is square, the bonds may be horizontal and vertical—and let $g(N_1, N_2, \ldots, N_n)$ be the number of ways we may completely cover all sites of the lattice with dimers such that there are N_1 dimers covering bonds of class 1, N_2 dimers covering bonds of class 2, and so on, with the restriction that only one dimer may occupy any one site. For example, there may be two classes where N_1 = the number of horizontal bonds and N_2 = the number of vertical bonds. One such dimer covering is shown in Fig. 4.1. In this chapter we will be interested in the square lattice of $\mathscr{M}$

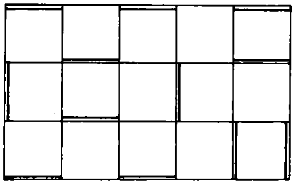


Fig. 4.1. An example of a closest-packed dimer covering of a square lattice. The number of horizontal bonds, N_1, is 8 and the number of vertical bonds, N_2, is 4.

rows and $\mathscr{N}$ columns and, since the total number of sites must be even if the lattice is to be completely filled with dimers, we will require $\mathscr{N}$ to be an even integer. We will study $g(N_1, N_2, \ldots, N_n)$ by computing the generating function for the close-packed dimer configuration

$$Z = \sum_{N_1}\sum_{N_2}\cdots\sum_{N_n} g(N_1, N_2, \ldots, N_n) z_1^{N_1} z_2^{N_2} \cdots z_n^{N_n}. \tag{1.1}$$

To complete the specification of this dimer problem we need to state the boundary conditions of the lattice. In the one-dimensional problems of the previous chapter we considered two different boundary conditions, free and cyclic. For the two-dimensional problems in this book we will consider three boundary conditions: (1) free in both the horizontal and vertical directions, (2) free in one direction but cyclic in the other (that is, the lattice is wrapped on a cylinder) and (3) cyclic in both directions (that is, the lattice is wrapped on a torus). The principal results of this chapter are to show that if the lattice has either free or cylindrical boundary conditions we may find an antisymmetric matrix A such that

$$Z = \operatorname{Pf} A, \tag{1.2}$$

where Pf A indicates the Pfaffian of A (to be explained in detail in the next section) and that if the lattice has toroidal boundary conditions Z is equal to a linear combination of four Pfaffians. In order to do this we will devote the next section to a definition of the Pfaffian and the derivation of some of its most important properties. In the remaining sections we will then use these properties to evaluate the Pfaffian and explicitly evaluate Z in terms of integrals in the limit $\mathscr{M} \to \infty$, $\mathscr{N} \to \infty$.

In this chapter we present a complete discussion of these topics including all of the fine points connected with $\pm$ signs that are related to boundary conditions. To our knowledge such a discussion has never appeared in the literature. Since the result of this discussion is to show that none of these fine points causes any trouble, they may safely be ignored for the purpose of understanding the rest of the book. They are included for the dedicated, as opposed to the interested, reader.[3]

2. THE PFAFFIAN

The Pfaffian of a $2N \times 2N$ antisymmetric matrix A, or more precisely of the set of numbers a_{jk}, where $1 \le j < k \le 2N$, which may be extended to an antisymmetric matrix with the definition

$$a_{kj} = -a_{jk} \quad \text{and} \quad a_{kk} = 0, \tag{2.1}$$

is a number that is defined as

$$\operatorname{Pf} A = \sum_p{}' \delta_p a_{p_1 p_2} a_{p_3 p_4} \cdots a_{p_{2N-1} p_{2N}}. \tag{2.2}$$

Here $p_1, \ldots, p_{2N}$ is some permutation of the numbers $1, 2, \ldots, 2N$, $\sum_p'$ is a summation over all permutations which satisfy the restrictions

$$p_{2m-1} < p_{2m} \qquad 1 < m < N \tag{2.3a}$$

and

$$p_{2m-1} < p_{2m+1} \qquad 1 < m < N-1, \tag{2.3b}$$

and δ_p, the parity of the permutation, is $+1$ if the permutation p is made up of an even number of transpositions and -1 if p is made up of an odd number of transpositions. We note that because of (2.1) $\operatorname{Pf} A$ may be written in the alternative form

$$\operatorname{Pf} A = \frac{1}{N!\,2^N} \sum_p \delta_p a_{p_1 p_2} a_{p_3 p_4} \cdots a_{p_{2N-1} p_{2N}} \tag{2.4}$$

when the sum is over all permutations. For example, if $2N = 4$,

$$\operatorname{Pf} A = a_{12}a_{34} - a_{13}a_{24} + a_{14}a_{23}. \tag{2.5}$$

This contains three terms. For arbitrary N it is laborious to write out all

3. The distinction between the interested and the dedicated reader seems to have been first made by G. F. Chew, M. L. Goldberger, F. E. Low, and Y. Nambu, *Phys. Rev.* **106**, 1337 (1957).

the terms in Pf A but the number of these terms is easily found. In particular, p_1 must always be 1 but p_2 may take on any of the remaining $2N - 1$ values; the value of p_3 is then fixed at 3 if $p_2 = 2$ and 2 if $p_2 > 2$, but p_4 may take on any of the remaining $2N - 3$ values. Continuing in this fashion we find that the number of terms in the Pfaffian of a $2N \times 2N$ antisymmetric matrix is

$$(2N-1)(2N-3)(2N-5)\cdots 5\cdot 3\cdot 1 = (2N-1)!! \tag{2.6}$$

The usefulness of the Pfaffian stems from the formula

$$[\mathrm{Pf}\, A]^2 = \det A. \tag{2.7}$$

This formula is older than statistical mechanics but is not nearly as well known to physicists. Therefore, though it is assumed that the reader is acquainted with the elementary properties of matrices and determinants, we will devote the rest of this section to its proof. We do this by studying $(\det A)^{1/2}$ and demonstrating that it may be written as Pf A.

To obtain (2.7) we first prove a theorem known as Jacobi's theorem. Let A be an arbitrary square matrix of dimension n with the elements a_{jk}. Explicitly,

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}. \tag{2.8}$$

Define the cofactor A_{jk} of the element a_{jk} as $(-1)^{j+k}$ times the determinant of the matrix obtained by deleting the jth row and the kth column from A. It is well known that

$$A\begin{bmatrix} A_{11} & A_{21} & \cdots & A_{n1} \\ A_{12} & A_{22} & \cdots & A_{n2} \\ \vdots & \vdots & & \vdots \\ A_{1n} & A_{2n} & \cdots & A_{nn} \end{bmatrix} = (\det A)\, I, \tag{2.9}$$

where I is the $n \times n$ identity matrix. From this relation we obtain

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & a_{24} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & a_{34} & \cdots & a_{3n} \\ a_{41} & a_{42} & a_{43} & a_{44} & \cdots & a_{4n} \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & a_{n3} & a_{n4} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} A_{11} & A_{21} & 0 & 0 & \cdots & 0 \\ A_{12} & A_{22} & 0 & 0 & \cdots & 0 \\ A_{13} & A_{23} & 1 & 0 & \cdots & 0 \\ A_{14} & A_{24} & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ A_{1n} & A_{2n} & 0 & 0 & \cdots & 1 \end{bmatrix}$$

$$= \begin{bmatrix} \det A & 0 & a_{13} & a_{14} & \cdots & a_{1n} \\ 0 & \det A & a_{23} & a_{24} & \cdots & a_{2n} \\ 0 & 0 & a_{33} & a_{34} & \cdots & a_{3n} \\ 0 & 0 & a_{43} & a_{44} & \cdots & a_{4n} \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & a_{n3} & a_{n4} & \cdots & a_{nn} \end{bmatrix}. \tag{2.10}$$

We further define $A_{jk,lm}$ as $(-1)^{j+k+l+m}$ times the determinant of the matrix obtained by omitting the jth and kth rows and the lth and mth columns from the matrix A. Then we take the determinant of (2.10) and use the elementary relation

$$\det M_1 M_2 = \det M_1 \det M_2 \tag{2.11}$$

to obtain

$$(\det A)(A_{11}A_{22} - A_{12}A_{21}) = A_{12,12}(\det A)^2. \tag{2.12}$$

If $\det A \neq 0$ we may divide by it and obtain

$$A_{11}A_{22} - A_{12}A_{21} = A_{12,12} \det A. \tag{2.13a}$$

However, since both sides of this expression are continuous functions of the elements a_{jk}, the condition $\det A \neq 0$ may be removed. Clearly there is nothing distinguished about 1 and 2 and we more generally have

$$A_{jj}A_{kk} - A_{jk}A_{kj} = A_{jk,jk} \det A. \tag{2.13b}$$

This is Jacobi's theorem.

We now apply this theorem to an $n \times n$ antisymmetric matrix $a_{jk} = -a_{kj}$. Then

$$A = -A^T, \tag{2.14}$$

where T stands for the operation of transposition (that is, of replacing all a_{jk} by a_{kj}). Thus

$$\det A = (-1)^n \det A^T, \tag{2.15}$$

and from the elementary relation

$$\det A^T = \det A \tag{2.16}$$

we conclude from (2.15) that if n is odd $\det A = 0$. We therefore confine our attention to the case $n = 2N$. Then A_{kk} and A_{jj} are determinants of antisymmetric matrices of odd dimensions and hence vanish. Jacobi's theorem thus specializes to

$$-A_{12}A_{21} = A_{12,12} \det A, \tag{2.17}$$

and, since A is antisymmetric,

$$A_{j1} = -A_{1j}, \tag{2.18}$$

we find

$$(A_{1j})^2 = A_{1j,1j} \det A. \tag{2.19}$$

If $n = 2$,

$$\det A = \begin{bmatrix} 0 & a_{12} \\ -a_{12} & 0 \end{bmatrix} = (a_{12})^2, \tag{2.20}$$

which is a perfect square. Therefore by induction on the dimension of A we conclude from (2.19) that $(\det A)^{1/2}$ is a rational function of the elements a_{jk}. Furthermore from (2.9)

$$\det A = \sum_{j=1}^{n} a_{1j} A_{1j} \tag{2.21}$$

so that we may use (2.19) to obtain

$$\pm(\det A)^{1/2} = \sum_{j=1}^{n} \pm a_{1j}(A_{1j,1j})^{1/2}, \tag{2.22}$$

which shows that the square root of the determinant of an $n \times n$ antisymmetric matrix is a combination of square roots of $(n-2) \times (n-2)$ determinants. Therefore, if we recall (2.20), mathematical induction on n proves that $(\det A)^{1/2}$ is not just a rational function of a_{jk} but is a polynomial and, as a consequence of (2.22), must be of the form

$$\pm(\det A)^{1/2} = \sum_{p}{}' \pm a_{p_1p_2} a_{p_3p_4} \cdots a_{p_{2N-1}p_{2N}}, \tag{2.23}$$

where $\sum_p'$ indicates the summation over all permutations p subject to restrictions (2.3).

The $\pm$ signs in (2.23) depend on the permutation p. To determine them it is convenient to use the antisymmetry of a_{jk} to extend the summation to all permutations. Thus if we let $S(p)$ stand for the sign corresponding to the permutation p,

$$\pm (\det A)^{1/2} = \frac{1}{N!\,2^N} \sum_{p} S(p) a_{p_1p_2} a_{p_3p_4} \cdots a_{p_{2N-1}p_{2N}}. \tag{2.24}$$

In this expression there are $N!\,2^N$ terms of the form $a_{p_1p_2} a_{p_3p_4} \cdots a_{p_{n-1}p_n}$, which differs from a term contained in (2.23) only by (1) the transposition of pairs of indices (p_{2k-1}, p_{2k}) and (2) the interchanges of one pair of indices (p_{2k-1}, p_{2k}) with another (p_{2j-1}, p_{2j}). For these terms not contained in (2.23), $S(p)$ is defined to be equal to the $\pm$ sign of that term in (2.23) which may be obtained from the given term by steps (1) and (2) times a factor of -1 for each transposition required in step 1.

We may define in (2.24)

$$S(I) = 1, \tag{2.25}$$

where I is the identity permutation. The remainder of the $S(p)$ may be computed if we make the elementary observation that the value of det A is not changed if two rows are interchanged and two columns are interchanged. Therefore, if p' is any permutation of the numbers 1 through $2N$ and

$$a'_{jk} = a_{p'_j p'_k}, \tag{2.26}$$

then

$$\det A' = \det A, \tag{2.27}$$

which may be combined with (2.24) to give

$$\pm' \sum_p S(p) a'_{p_1 p_2} a'_{p_3 p_4} \cdots a'_{p_{2N-1} p_{2N}} = \sum_p S(p) a_{p_1 p_2} a_{p_3 p_4} \cdots a_{p_{2N-1} p_{2N}}, \tag{2.28}$$

where the notation $\pm'$ is meant to indicate a sign which may be $+$ or $-$ depending on the permutation p'. We may rewrite (2.28) as

$$\pm' \sum_p S(p) a_{(p'p)_1 (p'p)_2} a_{(p'p)_3 (p'p)_4} \cdots a_{(p'p)_{2N-1} (p'p)_{2N}} = \sum_p S(p) a_{p_1 p_2} a_{p_3 p_4} \cdots a_{p_{2N-1} p_{2N}}, \tag{2.29}$$

where $p'p$ stands for the product permutation obtained by first applying p to the numbers 1 through $2N$ and then applying p' to the resulting permutation. Accordingly, since the summations are over all permutations p and the equality holds for arbitrary values of a_{jk}, we find that

$$S(p'p) = \pm' S(p). \tag{2.30}$$

However, if we take into account (2.25) we have

$$\pm' = S(p') \tag{2.31}$$

so that

$$S(p'p) = S(p')S(p).^4 \tag{2.32}$$

Any permutation may be expressed as a product of transpositions $p^{(j,k)}$ which interchange the j and k indices. Clearly,

$$(p^{(j,k)})^2 = I, \tag{2.33}$$

so from (2.25)

$$S[(p^{(j,k)})^2] = 1. \tag{2.34}$$

4. Equation (2.32) means that S is a one-dimensional representation of the permutation group. There are only two such representations, (2.37) and (2.38). We here prove this fact without using group theory.

But it is also elementary to verify that, if j, k, and l are distinct,

$$[p^{(j,k)}p^{(k,l)}]^3 = I. \tag{2.35}$$

Therefore

$$S[(p^{(j,k)})^3] = S[(p^{(k,l)})^3], \tag{2.36}$$

so that either

$$S(p^{(j,k)}) = 1 \qquad \text{for all } j \text{ and } k \tag{2.37}$$

or

$$S(p^{(j,k)}) = -1 \qquad \text{for all } j \text{ and } k. \tag{2.38}$$

But (2.37) is excluded because we know, for example, that $S(p^{(1,2)}) = -1$. Therefore (2.38) is the only possibility and we conclude that,

$$(\det A)^{1/2} = \pm \sum_p{}' \delta_p a_{p_1p_2} a_{p_3p_4} \cdots a_{p_{2N-1}p_{2N}}, \tag{2.39}$$

from which (2.7) follows.

3. DIMER CONFIGURATIONS ON LATTICES WITH FREE BOUNDARY CONDITIONS

The sites of a square lattice may be labeled by the number of the row, j, and the number of the column, k, where $1 \le j \le \mathscr{M}$ and $1 \le k \le \mathscr{N}$ (remember that $\mathscr{N}$ is even). They may also be labeled by a single index p, where

$$(j, k) \leftrightarrow p = k + (j-1)\mathscr{N}. \tag{3.1}$$

We shall refer to the arrangement of dimers which occupies the pairs of sites p_1 and p_2, p_3 and $p_4, \ldots, p_{\mathscr{M}\mathscr{N}-1}$ and $p_{\mathscr{M}\mathscr{N}}$ as the configuration

$$C = |p_1, p_2|p_3, p_4| \cdots |p_{\mathscr{M}\mathscr{N}-1}, p_{\mathscr{M}\mathscr{N}}|. \tag{3.2}$$

For example, one of the possible dimer configurations is (Fig. 4.2)

$$C_0 = |1, 2|3, 4|5, 6| \cdots |\mathscr{M}\mathscr{N} - 1, \mathscr{M}\mathscr{N}|. \tag{3.3}$$

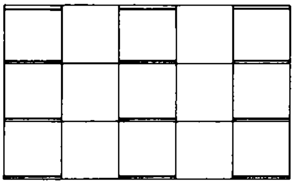


Fig. 4.2. The configuration C_0.

In general the labeling of a dimer configuration by (3.2) is not unique. To make this description unique we impose the additional restriction

$$p_1 < p_2, p_3 < p_4, \ldots, p_{\mathscr{M}\mathscr{N}-1} < p_{\mathscr{M}\mathscr{N}}, \tag{3.4a}$$

and

$$p_1 < p_3 < p_5 \cdots < p_{\mathscr{M}\mathscr{N}-1}. \tag{3.4b}$$

Suppose we let the nonzero elements of $a(p_1, p_2)$ be

$$a(p_1, p_2) = z_i, \tag{3.5}$$

where $p_1 < p_2$ and p_1 and p_2 are connected by a bond of class i. In particular, if the classes of bonds are vertical and horizontal, z_1 refers to horizontal bonds and z_2 refers to vertical bonds. We then may write the generating function for closest-packed dimer configurations as

$$Z^F_{\mathscr{M},\mathscr{N}} = \sum_p{}' a(p_1, p_2)a(p_3, p_4) \cdots a(p_{\mathscr{M}\mathscr{N}-1}, p_{\mathscr{M}\mathscr{N}}), \tag{3.6}$$

where the summation is over all permutations satisfying (3.4). Such an expression is called a Hafnian, but, unfortunately, when $\mathscr{M}$ and $\mathscr{N}$ are large there is no efficient way to evaluate such objects. We note, however, that because the restrictions (3.4) are exactly the same as the restrictions (2.3), (3.6) would be a Pfaffian if in each term we included a factor δ_p. Therefore if we let the nonzero elements of $a(p_1, p_2)$ satisfy

$$a(p_1, p_2) = s(p_1, p_2)z_i \tag{3.7}$$

with $|s(p_1, p_2)| = 1$, where $p_1 < p_2$ and p_1 and p_2 are connected by a bond of class i, and if we can choose $s(p_1, p_2)$ so as to cancel out the factor δ_p that occurs in the definition of the Pfaffian, then $Z^F_{\mathscr{M},\mathscr{N}}$ would equal $\operatorname{Pf} A_F$. This is extremely useful because by (2.7) the Pfaffian is related to the determinant of the associated antisymmetric matrix and this determinant may be efficiently studied when $\mathscr{M}$ and $\mathscr{N}$ are large.

The rest of this section is devoted to showing that such a set of values for $s(p_1, p_2)$ can be found. For concreteness we concentrate on the square lattice with two classes of bonds, vertical and horizontal. In this case our final result is that

$$Z^F_{\mathscr{M},\mathscr{N}} = \operatorname{Pf} A_F, \tag{3.8}$$

where A_F is the $\mathscr{M}\mathscr{N} \times \mathscr{M}\mathscr{N}$ matrix whose nonvanishing elements are

$$a(j, k; j, k+1) = -a(j, k+1; j, k) = z_1,$$
$$1 \le j \le \mathscr{M},\ 1 \le k \le \mathscr{N} - 1, \tag{3.9a}$$

and

$$a(j, k; j+1, k) = -a(j+1, k; j, k) = (-1)^k z_2,$$
$$1 \le j \le \mathscr{M} - 1,\ 1 \le k \le \mathscr{N}. \tag{3.9b}$$

The arguments used, however, will be general enough to apply to any lattice with free boundary conditions and any number of classes provided the lattice may be drawn in a plane with no overlap of bonds. These lattices will be referred to as planar.

Our method of verifying (3.8) and (3.9) consists in giving geometric interpretations to δ_p and $s(p_1, p_2)$ and then proving some geometric theorems.

We first note that to verify (3.8) and (3.9) it is sufficient to show that $s(p_1, p_2)$ can be chosen such that if $p^{(1)}$ and $p^{(2)}$ are any two permutations satisfying (2.3) then

$$\delta_{p^{(1)}} s(p_1^{(1)}, p_2^{(1)}) \cdots s(p_{\mathcal{M}\mathcal{N}-1}^{(1)}, p_{\mathcal{M}\mathcal{N}}^{(1)}) = \delta_{p^{(2)}} s(p_1^{(2)}, p_2^{(2)}) \cdots s(p_{\mathcal{M}\mathcal{N}-1}^{(2)}, p_{\mathcal{M}\mathcal{N}}^{(2)}). \quad (3.10)$$

However, the restriction (2.3) is somewhat awkward. Therefore, it is useful to note that, if we let $\bar{p}$ be any one of the $2^{\mathcal{M}\mathcal{N}/2}(\frac{1}{2}\mathcal{M}\mathcal{N})!$ permutations which, by violating (2.3), may be obtained from a given permutation p that satisfies (2.3), then, as seen in (2.1), (3.10) will hold if we can find one such $\bar{p}^{(1)}$ and $\bar{p}^{(2)}$ such that

$$\delta_{\bar{p}^{(1)}} s(\bar{p}_1^{(1)}, \bar{p}_2^{(1)}) \cdots s(\bar{p}_{\mathcal{M}\mathcal{N}-1}^{(1)}, \bar{p}_{\mathcal{M}\mathcal{N}}^{(1)}) = \delta_{\bar{p}^{(2)}} s(\bar{p}_1^{(2)}, \bar{p}_2^{(2)}) \cdots s(\bar{p}_{\mathcal{M}\mathcal{N}-1}^{(2)}, \bar{p}_{\mathcal{M}\mathcal{N}}^{(2)}). \quad (3.11)$$

With the foregoing definition we proceed to show that for any permutation p there is (at least) one related permutation $\bar{p}$ for which $\delta_{\bar{p}}$ may be computed from geometric considerations.

Consider any two arrangements of dimers specified by the permutations $p^{(1)}$ and $p^{(2)}$. Draw the dimers of $p^{(1)}$ on the lattice as dotted lines and the dimers of $p^{(2)}$ as solid lines. The resulting set of figures is referred to as a transition graph (Fig. 4.3). Then, because any lattice point is the end-

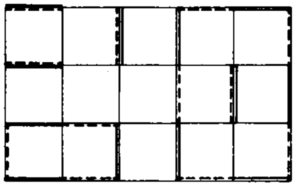


Fig. 4.3. An example of a transition graph.

point of one and only one line of each type of dimer, the figures in the transition graph will consist of: (1) two sites connected by a dotted and by a solid line (these figures are called double bonds), and (2) closed polygons with an even number of bonds in which the dotted and solid lines alternate. We call these closed polygons transition cycles because if the bonds of $p^{(1)}$ are permuted clockwise or counterclockwise one step around this cycle they go over to the bonds of $p^{(2)}$. Consider first two permutations that differ from one another by only one transition cycle.

The preceding discussion showed that (3.10) holds if (3.11) holds where we replace $p^{(1)}$ and $p^{(2)}$, which do obey (2.3), by equivalent permutations $\bar{p}^{(1)}$ and $\bar{p}^{(2)}$ which do not obey (2.3). In particular, (3.11) will guarantee (3.10) if we replace $p^{(1)}$ and $p^{(2)}$ by those $\bar{p}^{(1)}$ and $\bar{p}^{(2)}$ which arrange the sites in a clockwise order as we go around the graph. For example, consider the transition cycle Fig. 4.4. The permutation $p^{(1)}$ obeying (2.3)

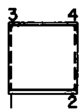


Fig. 4.4. A square transition cycle of four vertices.

which specifies the solid dimers is $|1,2|3,4|$ and the permutation $p^{(2)}$ obeying (2.3) which specifies the dashed dimers is $|1,3|2,4|$. However, a permutation $\bar{p}^{(1)}$ which arranges the sites of the configuration $p^{(1)}$ in clockwise order is $|2,1|3,4|$. Similarly a permutation $\bar{p}^{(2)}$ arranging the sites of $p^{(2)}$ in clockwise order is $|1,3|4,2|$. In general we see that if

$$\bar{p}^{(1)} = |\bar{p}_1^{(1)}, \bar{p}_2^{(1)}|\bar{p}_3^{(1)}, \bar{p}_4^{(1)}|\cdots|\bar{p}_{\mathcal{M}\mathcal{N}-1}^{(1)}, \bar{p}_{\mathcal{M}\mathcal{N}}^{(1)}|,$$

then

$$\bar{p}^{(2)} = |\bar{p}_2^{(1)}, \bar{p}_3^{(1)}|\bar{p}_4^{(1)}, \bar{p}_5^{(1)}|\cdots|\bar{p}_{\mathcal{M}\mathcal{N}}^{(1)}, \bar{p}_1^{(1)}|.$$

Clearly the shift from $\bar{p}^{(1)}$ to $\bar{p}^{(2)}$ is a cyclic permutation of one step of an even number of objects. Hence it involves an odd number of transpositions. Accordingly, if there is only one transition cycle,

$$\delta_{\bar{p}^{(1)}} = -\delta_{\bar{p}^{(2)}}. \tag{3.12}$$

In general, if there are t transition cycles, we apply this argument to one cycle at a time and find that

$$\delta_{\bar{p}^{(1)}} = (-1)^t\, \delta_{\bar{p}^{(2)}}. \tag{3.13}$$

Therefore the requirement that the terms associated with the two permutations $p^{(1)}$ and $p^{(2)}$ (or, equivalently, $\bar{p}^{(1)}$ and $\bar{p}^{(2)}$) have the same sign will be satisfied if for each transition cycle

$$\begin{aligned} & s(\bar{p}_1^{(1)}, \bar{p}_2^{(1)})s(\bar{p}_3^{(1)}, \bar{p}_4^{(1)})\cdots s(\bar{p}_{2N-1}^{(1)}, \bar{p}_{2N}^{(1)}) \\ & \qquad = -s(\bar{p}_2^{(1)}, \bar{p}_3^{(1)})s(\bar{p}_4^{(1)}, \bar{p}_5^{(1)})\cdots s(\bar{p}_{2N}^{(1)}, \bar{p}_1^{(1)}). \end{aligned} \tag{3.14}$$

or, in other words,

$$\prod_{k=1}^{2N} s(\bar{p}_k^{(1)}, \bar{p}_{k+1}^{(1)}) = -1, \tag{3.15}$$

where $\bar{p}_{2N+1}^{(1)} \equiv \bar{p}_1^{(1)}$.

We could attempt to satisfy (3.15) with complex $s(p_1, p_2)$. Indeed, if one wants to construct a matrix A which has the property that

$$a(j, k; j', k') = a(j + 1, k; j' + 1, k'),$$

$$1 \leq j \leq \mathcal{M} - 1, \; 1 \leq k \leq \mathcal{N},$$

and

$$a(j, k; j', k') = a(j, k + 1; j', k' + 1), \qquad 1 \leq j \leq \mathcal{M}, 1 \leq k \leq \mathcal{N} - 1, \tag{3.16}$$

it is mandatory that $s(p_1, p_2)$ be complex. However, to obtain the most direct geometric interpretation of $s(p_1, p_2)$ we must restrict $s(p_1, p_2)$ to take on only the values ± 1. As this geometric interpretation is exceedingly useful in the application of these considerations to the Ising model we shall so restrict s. Therefore (3.15) says that the number of minus signs coming from the functions $s(p_1, p_2)$ as we go around any transition cycle in a clockwise fashion must be odd.

The factors $s(p_1, p_2)$ are interpreted geometrically by drawing an arrow pointing from p_1 to p_2 if $s(p_1, p_2)$ is $+1$ and an arrow pointing from p_2 to p_1 if $s(p_1, p_2)$ is -1. This construction is clearly consistent with the antisymmetry of $a(p_1, p_2)$. A lattice on which these arrows are drawn will be called an oriented lattice.

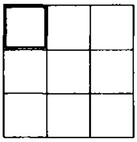
We define the orientation parity of a transition cycle to be $+1$ (-1) if, as we traverse this cycle in either direction the number of arrows pointing in the direction of motion is even (odd). The previous discussion therefore proves

Theorem A: If the orientation parity of every transition cycle is odd, all terms in the Pfaffian will have the same sign.

It is not possible to draw arrows on a general planar lattice so that the orientation parity of every polygon with an even number of sides is odd. However, not all polygons with an even number of sides are transition cycles.

To obtain a characterization of transition cycles on a lattice with free boundary conditions it is most useful to introduce the concept of inside and outside. For the square lattice drawn in its "natural" configuration (Fig. 4.5*a*) this concept is obvious. However, it must be pointed out that this "natural" configuration can be drawn in many topologically equivalent ways, as illustrated in Fig. 4.5*b*. These examples demonstrate that for our purposes the words inside and outside are not topologically invariant. Therefore when these words are used they always refer to a lattice drawn in the "natural" configuration of Fig. 4.5*a*.

With this intuitive (but nontechnical) definition of inside and outside we may easily characterize transition cycles. The only figures which make up transition graphs are double bonds or transition cycles. Each of



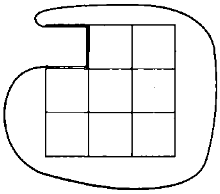


Fig. 4.5. (*a*) The square lattice in its "natural" configuration; the outlined square has no points or bonds of the lattice inside it. (*b*) A lattice which is topologically equivalent to the outlined square in (*a*) now has many lattice points and bonds in its interior.

these figures contains an even number of sites. Furthermore, these figures completely cover all sites of the lattice and no two figures can occupy the same site (see Fig. 4.3). Thus we have

Theorem B*:* The number of points contained within any transition cycle on a planar lattice is even.

To use the property of transition cycles given in Theorem B to choose a set of arrows on a planar lattice to satisfy the conditions of Theorem A we first define an elementary polygon. For the square lattice (drawn in the natural configuration) the elementary polygons are defined as each closed square consisting of 4 lattice sites and 4 bonds. More generally, an elementary polygon is a closed polygon drawn on the lattice in its natural configuration which has no bonds of the lattice (and hence no points of the lattice) on its interior.

If the number of arrows pointing in the clockwise direction on a polygon is odd (even) we say that the polygon is clockwise odd (even). Note that, in general, elementary polygons may have either an even or an odd number of sides, and thus an elementary polygon may be clockwise odd but counterclockwise even.

With these definitions we can prove

Theorem C*:* On any planar lattice (in its "natural" configuration) we may always choose an orientation of arrows such that every elementary polygon is clockwise odd.

However, instead of proving this theorem in general, it is sufficient

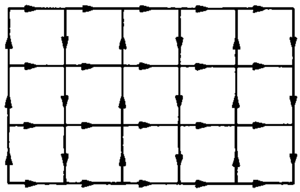


Fig. 4.6. An oriented square lattice with free boundary conditions corresponding to the matrix elements (3.9).

(and much easier) to draw a set of arrows on the lattice of interest and so verify Theorem C directly for the few special cases we are really interested in. In this chapter we are concentrating on the square lattice. It is immediately seen that the set of arrows shown in Fig. 4.6 satisfies the conclusion of Theorem C. The numbers $s(p_1, p_2)$ determined from this lattice combined with (3.7) give the matrix elements (3.9).

This set of arrows determined on elementary polygons satisfies the requirements of Theorem A for all transition cycles that are elementary polygons. To complete the proof that this specification of arrows satisfies the condition of Theorem A for all transition cycles on a planar lattice with free boundary conditions we prove

Theorem D*:* Once arrows have been specified so that every elementary polygon is clockwise odd, then for any polygon the number of clockwise bonds is odd if the number of enclosed lattice points is even and is even if the number of enclosed lattice points is odd.

In Fig. 4.7 we illustrate the elements of the proof of this theorem for the square lattice. However, the proof we give may be taken over word for word to the general case.

We prove this theorem by first remarking that any polygon on the lattice is made up of a number of elementary polygons and that Theorem C assures that Theorem D holds on these elementary polygons. Therefore the theorem will follow by induction if we assume it to be true on all polygons made up of n elementary polygons and prove that if Γ_n is one of those polygons then the theorem also holds on the polygon Γ_{n+1} obtained by enlarging Γ_n to include any adjacent elementary polygon Γ_1. Suppose that Γ_n surrounds p lattice points, contains a clockwise arrows, and has c arrows in common with Γ_1 (Fig. 4.7). Polygon Γ_1 contains a' clockwise arrows, whereby Theorem C, a' is odd. The number of clockwise arrows in Γ_{n+1} is the number of clockwise arrows in Γ_n, plus the number of clockwise arrows in Γ_1, minus the number of clockwise arrows lost from Γ_n by omitting the common arrows, minus the number of clockwise arrows lost from Γ_1 by omitting the common arrows. Now if an arrow on a common bond is clockwise for Γ_n it will be counterclockwise for Γ_1 because Γ_1 is outside of Γ_n. Therefore, the number of clockwise

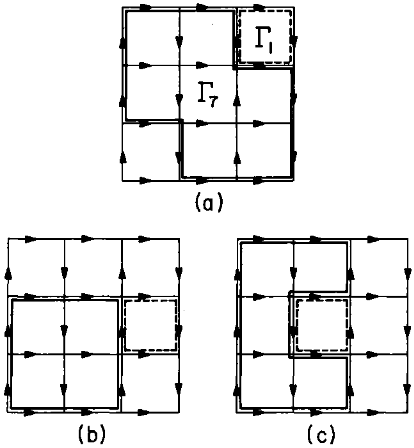


Fig. 4.7. (*a*) A special case of the proof of Theorem D. The dashed elementary polygon Γ_1 is added to the solid Γ_7 to form Γ_8; Γ_7 surrounds 2 ($= p$) lattice points, contains 7 ($= a$) clockwise arrows, and has 2 ($= c$) arrows in common with Γ_1; Γ_1 has 3 ($= a'$) clockwise arrows. We form Γ_8 by removing the 2 ($= c$) common bonds. This adds one new point to the interior so the number of points inside Γ_8 is 3. Furthermore, the number of clockwise arrows of Γ_8 is clearly $7 + 3 - 2 = a + a' - c = 8$. Therefore Theorem D holds. (*b*) and (*c*) Other geometric figures on which the reader is urged to verify Theorem D.

arrows in Γ_{n+1} is $a + a' - c$. Furthermore, the number of enclosed lattice points in Γ_{n+1} is $p + c - 1$, since when we omit c common bonds we must gain $c - 1$ new points in the interior. Now, by assumption, a is even (odd) if p is odd (even) and a' is odd. Therefore $a + a' - c$ must be even (odd) if $p + c - 1$ is odd (even). Hence, by induction, Theorem D follows.

We now may combine Theorem B with Theorem D to conclude that on the oriented lattice of Fig. 4.6 the orientation parity of every transition cycle is odd. Therefore, Theorem A proves that

$$Z^F_{\mathcal{M},\mathcal{N}} = \pm \operatorname{Pf} A_F, \tag{3.17}$$

where for the square lattice the nonzero matrix elements of one representation of A_F are given by (3.9). But the term in Pf A_F corresponding to the configuration C_0 surely has a positive sign. Therefore, we must choose the $+$ sign in (3.17) and obtain the desired result (3.8).

4. DIMER CONFIGURATIONS ON LATTICES WITH CYLINDRICAL BOUNDARY CONDITIONS

To discuss the extension of the considerations of the previous section that is needed to treat the square lattice with cylindrical boundary conditions, we must first decide if we are going to impose cyclic boundary conditions in the vertical or horizontal direction. Since, to insure that the total number of sites $\mathscr{M}\mathscr{N}$ be even, we have taken $\mathscr{N}$ to be even, there are several cases:

(1) Both $\mathscr{M}$ and $\mathscr{N}$ are even. In this case if we apply cyclic boundary conditions in one direction we can consider cyclic boundary conditions in the other direction by a simple relabeling.

(2) $\mathscr{M}$ odd and $\mathscr{N}$ (by definition) even. In this case there are two distinct subcases:

(*a*) Cyclic boundary conditions can be applied in the vertical direction. Then it is easily seen that the only allowed transition cycles are those considered in the previous section because it is not possible to have a transition cycle which loops the cylinder since this would require an odd number of bonds, whereas the number of bonds in a transition cycle must be even. Thus if we define $A_{c,v}$ by (3.9) and

$$a(\mathscr{M}, k; 1, k) = -a(1, k; \mathscr{M}, k) = (-1)^k z_2, \tag{4.1}$$

the conditions of Theorem A are satisfied and

$$Z^{c,v}_{\mathscr{M},\mathscr{N}} = \mathrm{Pf}\, A_{c,v}. \tag{4.2}$$

(*b*) Cyclic boundary conditions can be applied in the horizontal direction. In this case the simple argument leading to (4.1) will not hold. The remainder of this section is devoted to proving that for this case and for case (1)

$$Z^{c}_{\mathscr{M},\mathscr{N}} = \mathrm{Pf}\, A_c, \tag{4.3}$$

where A_c is determined from (3.9) and from

$$a(j, \mathscr{N}; j, 1) = -a(j, 1; j, \mathscr{N}) = -z_1. \tag{4.4}$$

In cases (1) and (2*b*) there are two distinct classes of transition cycles: (1) cycles which do not loop completely around the cylinder, and (2) cycles which do loop around the cylinder precisely once. One particularly simple class 2 transition cycle has no vertical bonds and is shown in Fig. 4.8. There are, in addition, $\mathscr{M} - 1$ transition cycles which differ from this one only by a vertical translation. These $\mathscr{M}$ transition cycles will be called elementary transition cycles of class 2.

To include in the Pfaffian terms corresponding to transition cycles of class 1 involving bonds between column $\mathscr{N}$ and column 1 we need to have for all j

$$a(j, \mathscr{N}; j, 1) = -a(j, 1; j, \mathscr{N}) = z_1 \tag{4.5a}$$

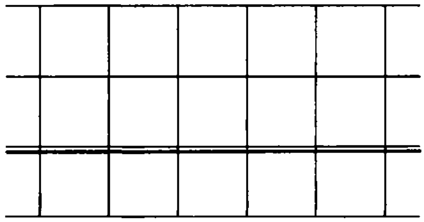


Fig. 4.8. An elementary class 2 transition cycle on a cylinder.

or

$$a(j, \mathcal{N}; j, 1) = -a(j, 1; j, \mathcal{N}) = -z_1. \tag{4.5b}$$

The arrows corresponding to these two choices of sign are shown in Fig. 4.9. Clearly for both choices of signs the orientation parity of every elementary polygon and, hence, of every transition cycle of class 1 is odd. Therefore the arguments of the last section demonstrate that for either choice of the sign (4.5) all transition cycles of class 1 are included in the Pfaffian with the same sign. However, if we consider the elementary transition cycles of class 2 we see that the orientation parity will be negative only with the choice of sign (4.5*b*). We therefore complete the proof of (4.3) and (4.4) by proving

Theorem E*:* If on the square lattice with cylindrical boundary conditions the orientation parity of the elementary class 2 transition cycles is

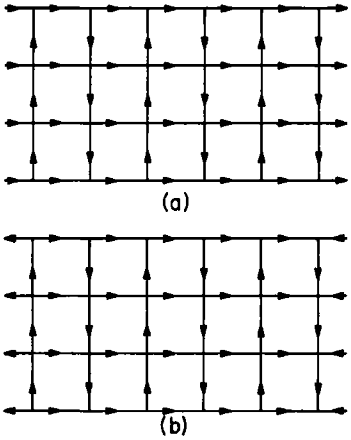


Fig. 4.9. (*a*) An oriented lattice corresponding to (4.5*a*). (*b*) An oriented lattice corresponding to (4.5*b*).

negative, the orientation parity of all class 2 transition cycles is negative.

To prove this we first remark that if we omit from the lattice all bonds and sites belonging to any class 2 transition cycle the cylinder is divided into two pieces. Since it must be possible to completely cover the lattice sites of each of these two pieces with double bonds, each piece contains an even number of sites.

Secondly, we remark that an arbitrary class 2 transition cycle may be considered to be made up of an elementary class 2 transition cycle and one or more closed polygons that do not loop the cylinder, each of which (*a*) has some bonds in common with the elementary class 2 transition cycle and (*b*) has the rest of its bonds on only one side of the elementary class 2 transition cycle (Fig. 4.10).

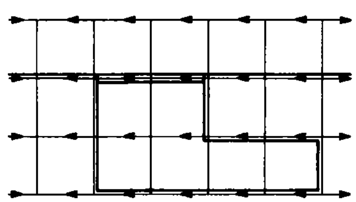


Fig. 4.10. A class 2 transition cycle considered as a superposition of an elementary class 2 transition cycle and a closed polygon. This figure is drawn on the oriented lattice of Fig. 4.9*b*.

With these two remarks the rest of the proof follows exactly along the lines of Theorem D of the previous section and is left as an exercise for the reader.

5. DIMER CONFIGURATIONS ON LATTICES WITH TOROIDAL BOUNDARY CONDITIONS

Our final extension of the dimer counting problem is to the square lattices with cyclic boundary conditions in both directions. Now, in addition to transition cycles which do not loop the torus or which loop the torus only once in the horizontal direction, there are transition cycles which loop the torus h times in the horizontal direction and v times in the vertical direction; for example, see Fig. 4.11.

It is a simple matter to extend the considerations of Section 3 to ensure that all dimer configurations connected by transition cycles with $h = v = 0$ contribute to the Pfaffian with the same sign. Indeed if we choose the signs of $a(j, k; j', k')$ as in (3.9) for all terms except those that refer to a horizontal bond from column $\mathcal{N}$ to column 1 or a vertical bond from row $\mathcal{M}$ to row 1, we may make the orientation parity of every elementary polygon, and hence of all transition cycles with

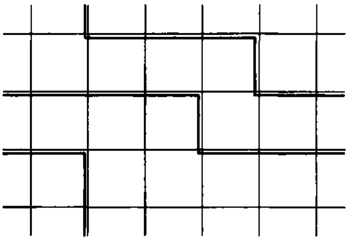


Fig. 4.11. A transition cycle that loops the torus twice in the horizontal direction and once in the vertical direction.

$h = v = 0$, negative with any of the 4 following assignments of signs to those remaining elements:

$$\begin{aligned}
&(1)\quad a_1(j, \mathcal{N}; j, 1) = -a_1(j, 1; j, \mathcal{N}) = z_1, && 1 \le j \le \mathcal{M}, \\
&\qquad a_1(\mathcal{M}, k; 1, k) = -a_1(1, k; \mathcal{M}, k) = (-1)^k z_2, && 1 \le k \le \mathcal{N}; \quad (5.1a)\\
&(2)\quad a_2(j, \mathcal{N}; j, 1) = -a_2(j, 1; j, \mathcal{N}) = z_1, && 1 \le j \le \mathcal{M}, \\
&\qquad a_2(\mathcal{M}, k; 1, k) = -a_2(1, k; \mathcal{M}, k) = -(-1)^k z_2, && 1 \le k \le \mathcal{N}; \quad (5.1b)\\
&(3)\quad a_3(j, \mathcal{N}; j, 1) = -a_3(j, 1; j, \mathcal{N}) = -z_1, && 1 \le j \le \mathcal{M}, \\
&\qquad a_3(\mathcal{M}, k; 1, k) = -a_3(1, k; \mathcal{M}, k) = (-1)^k z_2, && 1 \le k \le \mathcal{N}; \quad (5.1c)\\
&(4)\quad a_4(j, \mathcal{N}; j, 1) = -a_4(j, 1; j, \mathcal{N}) = -z_1, && 1 \le j \le \mathcal{M}, \\
&\qquad a_4(\mathcal{M}, k; 1, k) = -a_4(1, k; \mathcal{M}, k) = -(-1)^k z_2, && 1 \le k \le \mathcal{N}. \quad (5.1d)
\end{aligned}$$

The oriented lattices corresponding to these 4 sets of matrix elements are shown in Fig. 4.12.

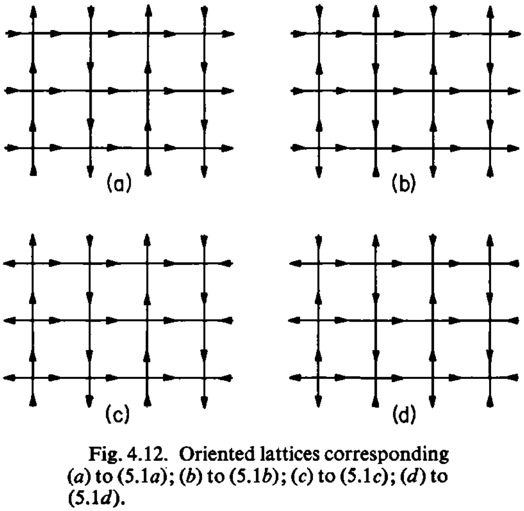


Fig. 4.12. Oriented lattices corresponding (*a*) to (5.1*a*); (*b*) to (5.1*b*); (*c*) to (5.1*c*); (*d*) to (5.1*d*).

DIMER STATISTICS

In the previous section it was possible to show that one of the several assignments of arrows for which the orientation parity of $v = h = 0$ transition cycles was odd had the property that the orientation parity of all transition cycles was odd. However, it is easily seen that no one assignment of signs in (5.1) can make the orientation parity of all three transition cycles in Fig. 4.13 odd simultaneously. To remedy this situation

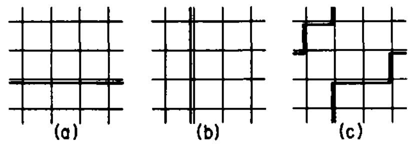


Fig. 4.13. Three transition cycles which together demonstrate that none of the four assignments of signs (5.1) will make the orientation parity of all transition cycles odd.

we will show that it is possible to find a suitable linear combination of the Pfaffians of the 4 matrices defined by (5.1) such that while each individual Pfaffian will include some class of terms with a sign opposite to the rest, the complete linear combination will include each dimer configuration exactly once. In particular, we will show that

$$Z^T_{\mathcal{M},\mathcal{N}} = \tfrac{1}{2}[-\mathrm{Pf}\,A_1 + \mathrm{Pf}\,A_2 + \mathrm{Pf}\,A_3 + \mathrm{Pf}\,A_4]. \tag{5.2}$$

Since no choice of signs in (5.1) allows the orientation parity of all transition cycles to be odd, it is necessary to have an efficient way of determining what the orientation parity of a given transition cycle will be. The most useful classification would be that for a given set of signs (5.1) the orientation parity depended only on v and h. Unfortunately, as the example of Fig. 4.14 shows, such a simple classification is not possible. However, our previous treatment has been much more general than it needs to be. In particular, we have used the fact that if the sign of any two terms in the Pfaffian is the same then all terms will be included in the Pfaffian with the same sign. We may replace this statement with the remark that if the sign of any dimer configuration is the same as one

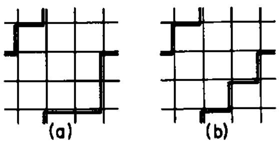


Fig. 4.14. Two transition cycles with $v = 1$ and $h = 1$ which have opposite orientation parity on any of the four oriented lattices specified by (5.1).

fixed dimer configuration then all dimer configurations occur in the Pfaffian with the same sign. A most convenient classification of transition cycles results if we choose this fixed dimer configuration to be the configuration C_0 defined by (3.3). We call a transition cycle made up of the configuration C_0 and an arbitrary configuration a C_0 transition cycle. Several examples of C_0 transition cycles are given in Fig. 4.15. Then Theorem A of Section 3 may be restated as

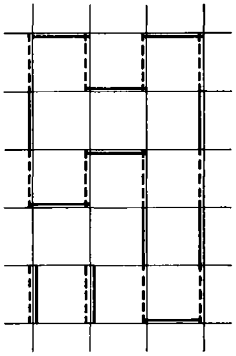


Fig. 4.15. A C_0 transition graph containing several C_0 transition cycles.

Theorem A′*:* If the orientation parity of every C_0 transition cycle is odd, all terms in the Pfaffian will have the same sign.

Each of the 4 sets of matrices specified by (3.9) and (5.1) satisfies the conditions of Theorem A for $v = h = 0$, so they must also satisfy Theorem A′. However, for each choice of sign in (5.1) the orientation parity of a C_0 transition cycle depends on v and h alone. This may be seen if we first define an elementary C_0 transition cycle to be a C_0 transition cycle for which v and h are not both zero and which may be traversed in such a fashion that on all the vertical bonds we always go from row j to row $j + 1$ and never from $j + 1$ to j (where $\mathscr{M} + 1$ is identified with 1). Elementary C_0 transition cycles with $h = 1, v = 0; h = 0, v = 1;$ and $h = 1, v = 1$ are shown in Fig. 4.16. It is clear from this figure that, with the possible exception of the arrows between row $\mathscr{M}$ and row 1, with every upward vertical arrow $\uparrow$ there is associated a horizontal arrow on a C_0 bond as $\uparrow\!\longrightarrow$. This configuration gives an even contribution to the orientation parity. Secondly, with the possible exception of the arrows between rows $\mathscr{M}$ and 1, with every downward vertical arrow $\downarrow$ is associated a horizontal arrow on a C_0 bond as $\longrightarrow\!\downarrow$. This configuration also gives an even contribution to the orientation parity. But every elementary C_0 transition consists of $v/2$ of each of these two types of corner

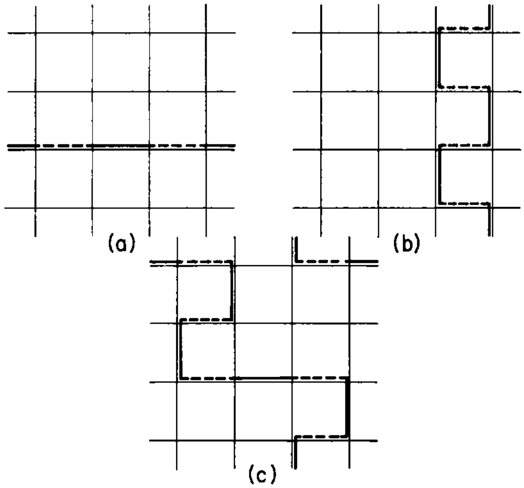


Fig. 4.16. Elementary C_0 transition cycles: (*a*) $h = 1, v = 0$; (*b*) $h = 0, v = 1$; (*c*) $h = 1$, $v = 1$.

plus horizontal bonds. Therefore, for the four sets of arrows determined from the assignment of signs in (5.1), the orientation parity of an elementary C_0 transition cycle in which either $h \neq 0$ or $v \neq 0$ is

$$(1) \quad 1, \tag{5.3a}$$

$$(2) \quad (-1)^{v}, \tag{5.3b}$$

$$(3) \quad (-1)^{h}, \tag{5.3c}$$

$$(4) \quad (-1)^{v+h}. \tag{5.3d}$$

We therefore will have determined the orientation parity of all C_0 transition cycles if we can prove

Theorem F: The orientation parity of any C_0 transition cycle with h horizontal loops and v vertical loops is the same as the orientation parity of an elementary C_0 transition cycle with the same values of h and v.

To prove this theorem, consider an arbitrary C_0 transition cycle to be a superposition of an elementary C_0 transition cycle and a number of closed polygons. A C_0 transition cycle has the property that if it occupies a site which is the endpoint of some C_0 bond it covers the entire C_0 bond as well. Therefore every lattice point in the interior of any of the closed polygons is connected to a neighboring interior point by a C_0 bond. Since only one C_0 bond may end at any point, we conclude that the number of points p enclosed by each closed polygon is even. Therefore, by Theorem D the orientation parity of each of these closed polygons is odd. Furthermore, as we traverse the C_0 transition cycle the last bond on the elementary C_0 transition cycle before we pass to a bond of one of the closed polygons must be a C_0 bond. Moreover, if we continue on around the C_0 transition cycle the first bond of the elementary C_0 transition cycle we cover after the closed polygon must also be a C_0 bond. Therefore, since C_0 and non-C_0 bonds alternate on all C_0 transition cycles, we conclude that the number of bonds c which the elementary C_0 transition cycle and the closed polygon have in common is odd. The change in orientation parity in forming a C_0 transition cycle by the addition of a closed polygon to an elementary C_0 transition cycle is the number of common bonds minus the number of clockwise (or counterclockwise) arrows in the closed polygon which has the same parity as $c + (p - 1)$. The foregoing arguments show that each term in this sum is odd. Therefore, the addition of this closed polygon does not change the orientation parity.

We now wish to find a suitable linear combination of the Pfaffians of the 4 matrices which will make each class of C_0 transition cycles specified by v and h appear exactly once. The sign with which the class determined by v and h will appear in the Pfaffian of each of the 4 separate matrices A_i defined by (5.1) and (3.9) is the negative of (5.3). These signs are tabulated in Table 1. Not only is there no single matrix A_i which includes

TABLE 1. Signs with which C_0 transition cycles are included in the Pfaffian of A_i.

(h, v)	A_1	A_2	A_3	A_4
(0, 0)	+	+	+	+
(odd, even)	−	−	+	+
(even, odd)	−	+	−	+
(odd, odd)	−	+	+	−
(even, even)	−	−	−	−

all (h, v) configurations with the same sign but, since in each A_i the term $v = 0$, $h = 0$ is included with a + sign, whereas $v =$ even, $h =$ even is included with a $-$ sign, there would appear to be no linear combination of the 4 Pfaffians which could count all configurations with the same sign. However, it may easily be seen that there are no transition cycles with $v =$ even and $h =$ even if $v \neq 0$. In fact we can prove

Theorem G: If a closed non-self-intersecting curve loops the torus v times in the vertical direction and h times in the horizontal direction, v and h can have no common divisor.

To prove this theorem, represent the torus as a rectangle with opposite edges identified. Indeed, it is geometrically useful to repeat this basic

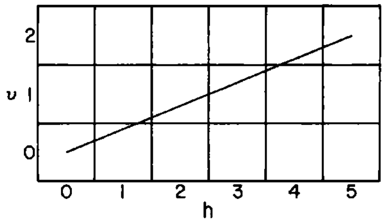


Fig. 4.17. Representation of a curve on a torus as a curve on a periodic array of squares. The curve of this example loops the torus twice in the vertical direction and five times in the horizontal direction.

lattice periodically in both the vertical and the horizontal directions (Fig. 4.17) and identify equivalent points in each rectangle. If a curve is drawn from a point in the (0, 0) rectangle to an equivalent point in the (h, v) rectangle, this curve corresponds to a curve that loops the torus h times in the horizontal direction and v times in the vertical direction. To see that h and v must have no common divisor it is sufficient to consider straight-line paths. But then it is clear that if h and v have a common divisor d the straight line already passes through a point equivalent to the starting point in the (0, 0) rectangle in the $(h/d, v/d)$ rectangle. Therefore if h and v have a common divisor it is not possible to draw the corresponding non-self-intersecting closed curve on the torus.

Theorem G allows us to ignore the last row in Table 1. Therefore the linear combination of the 4 Pfaffians $\mathrm{Pf}\, A_i$ which will include exactly once all classes of dimer configurations which are obtained from C_0 by one transition cycle is

$$\tfrac{1}{2}[-\mathrm{Pf}\, A_1 + \mathrm{Pf}\, A_2 + \mathrm{Pf}\, A_3 + \mathrm{Pf}\, A_4].$$

But if all configurations with one C_0 transition cycle are correctly counted then all configurations are correctly counted. Therefore (5.2) holds.

6. EVALUATION OF THE PFAFFIANS

The work of the three previous sections which relates the generating function for closest-packed dimer configurations to Pfaffians is useful only because the associated determinants may be evaluated. Many of these determinants have very simple structures which will occur again in the discussion of the Ising model of the next chapter. Therefore we will here explicitly evaluate all of the determinants we found in the three preceding sections. Finally we will determine the sign in the relation

$\operatorname{Pf} A = \pm [\det A]^{1/2}$ and will write out the final results for the partition functions.

It was easier to relate $Z^F_{\mathscr{M},\mathscr{N}}$ to $\operatorname{Pf} A_F$ than it was to relate $Z^T_{\mathscr{M},\mathscr{N}}$ to the linear combination (5.2). However, it is somewhat easier to evaluate the determinants related to the Pfaffians in $Z^T_{\mathscr{M},\mathscr{N}}$ than in $Z^F_{\mathscr{M},\mathscr{N}}$ and of the 4 determinants in (5.2) it is most straightforward to consider first $\det A_1$.

We may write A_i in a compact form if we define the $N \times N$ matrices

$$I_N = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}, \tag{6.1}$$

$$F_N = \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & -1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -1 \end{bmatrix} \text{(here N must be even)}, \tag{6.2}$$

and

$$J_N = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 0 & -1 \\ -1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 0 & \cdots & 0 & -1 & 0 \end{bmatrix}. \tag{6.3}$$

Then the $\mathscr{M}\mathscr{N} \times \mathscr{M}\mathscr{N}$ matrix A_1 is written in a direct-product notation as

$$A_1 = z_1 I_{\mathscr{M}} \otimes J_{\mathscr{N}} + z_2 J_{\mathscr{M}} \otimes F_{\mathscr{N}}, \tag{6.4}$$

where the labeling of the basis is such that

$$a_1(j, k; j', k') = z_1 [I_{\mathscr{M}}]_{j,j'} [J_{\mathscr{N}}]_{k,k'} + z_2 [J_{\mathscr{M}}]_{j,j'} [F_{\mathscr{N}}]_{k,k'}. \tag{6.5}$$

To compute $\det A_1$ it is convenient to define for even N the $N \times N$ matrix

$$T_N = \begin{bmatrix} i & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & i & 0 & \cdots & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 \end{bmatrix}. \tag{6.6}$$

Then if we multiply A_1 on the right by $I_{\mathcal{M}} \otimes T_{\mathcal{N}}$ and on the left by $I_{\mathcal{M}} \otimes (-iT_{\mathcal{N}})$ and note that

$$\det [I_{\mathcal{M}} \otimes T_{\mathcal{N}}] = (-i)^{\mathcal{M}\mathcal{N}/2} = i^{-\mathcal{M}\mathcal{N}/2} \tag{6.7a}$$

and

$$\det [I_{\mathcal{M}} \otimes (-iT_{\mathcal{N}})] = i^{\mathcal{M}\mathcal{N}/2}, \tag{6.7b}$$

we find that

$$\det A_1 = \det \bar{A}_1, \tag{6.8a}$$

where

$$\bar{A}_1 = z_1 I_{\mathcal{M}} \otimes J_{\mathcal{N}} + iz_2 J_{\mathcal{M}} \otimes I_{\mathcal{N}}. \tag{6.8b}$$

If $\lambda_l^{(N)}, l = 1, \cdots, N$, are the N eigenvalues of J_N, the $\mathcal{M}\mathcal{N}$ eigenvalues of $\bar{A}_1$ are $z_1\lambda_k^{(\mathcal{N})} + iz_2\lambda_j^{(\mathcal{M})}$, where $1 \leq j \leq \mathcal{M}$ and $1 \leq k \leq \mathcal{N}$. Then $\det A_1$ is calculated as

$$\det A_1 = \prod_{j=1}^{\mathcal{M}} \prod_{k=1}^{\mathcal{N}} [z_1\lambda_k^{(\mathcal{N})} + iz_2\lambda_j^{(\mathcal{M})}]. \tag{6.9}$$

Therefore we need to calculate the eigenvalues of J_N.

The matrix J_N has two important properties. First of all, the elements on each diagonal are equal, that is, the matrix elements are of the form

$$a_{l,l'} = a_{l-l'}. \tag{6.10}$$

Matrices of this form are known as Toeplitz matrices. Secondly, J_N has the property that if the first row is transposed to the bottom of the matrix and the first column is transposed to the extreme right of the matrix, the matrix is transformed into itself, that is, J_N is of the form

$$\begin{bmatrix} a_0 & a_{-1} & a_{-2} & \cdots & a_{-n+2} & a_{-n+1} \\ a_{-n+1} & a_0 & a_{-1} & \cdots & a_{-n+3} & a_{-n+2} \\ a_{-n+2} & a_{-n+1} & a_0 & \cdots & a_{-n+4} & a_{-n+3} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{-2} & a_{-3} & a_{-4} & \cdots & a_0 & a_{-1} \\ a_{-1} & a_{-2} & a_{-3} & \cdots & a_{-n+1} & a_0 \end{bmatrix}. \tag{6.11}$$

Toeplitz matrices of this form are called cyclic matrices. Cyclic matrices are important because their eigenvalues may be evaluated simply. Consider for example the specific case at hand, J_N. Its eigenvector equation,

$$J_N v = \lambda v, \tag{6.12}$$

is explicitly written out as

$$\begin{array}{lllllr} & v_2 & & & -v_N & = \lambda v_1, \\ -v_1 & & +v_3 & & & = \lambda v_2, \\ & -v_2 & & +v_4 & & = \lambda v_3, \\ & \vdots & & & & \vdots \\ v_1 & & & & -v_{N-1} & = \lambda v_N. \end{array} \tag{6.13}$$

We seek an eigenvector of the form

$$v_l = \alpha^l. \tag{6.14}$$

Then the second through the $(N-1)$th equations in (6.13) are all satisfied if one of them is, so the N equations of (6.13) reduce to the three equations

$$\begin{aligned} \alpha - \alpha^{N-1} &= \lambda(\alpha), \\ -\alpha^{-1} + \alpha &= \lambda(\alpha), \\ \alpha^{-N+1} - \alpha^{-1} &= \lambda(\alpha). \end{aligned} \tag{6.15}$$

These three equations will be identical if

$$\alpha^N = 1. \tag{6.16}$$

Therefore the N eigenvectors are

$$v_l^{(n)} = e^{2\pi i l/N}, \qquad 1 \leq n \leq N, \tag{6.17}$$

and the N corresponding eigenvalues are

$$\lambda_n^{(N)} = e^{2\pi i n/N} - e^{-2\pi i n/N} = 2i \sin(2\pi n/N). \tag{6.18}$$

In general, the N eigenvectors of (6.12) are given by (6.17) and the N corresponding eigenvalues are

$$\lambda_n^{(N)} = \sum_{l=1}^{N} a_l e^{2\pi i n l/N}. \tag{6.19}$$

These eigenvalues (6.18) may now be used in (6.9) and we obtain

$$\det A_1 = \prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}} \left[2iz_1 \sin\frac{2\pi k}{\mathscr{N}} - 2z_2 \sin\frac{2\pi j}{\mathscr{M}}\right]. \tag{6.20}$$

The term coming from $j = \mathscr{M}$, $k = \mathscr{N}$ is zero for all values of z_1 and z_2. Hence we conclude that

$$\mathrm{Pf}\, A_1 = (\det A_1)^{1/2} = 0. \tag{6.21}$$

The three remaining determinants related by (5.2) to the Pfaffians in $Z^T_{\mathscr{M},\mathscr{N}}$ may be evaluated almost as simply as was $\det A_1$. To compute them we define another $N \times N$ matrix,

$$J'_N = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 1 \\ -1 & 0 & 1 & \cdots & 0 & 0 \\ 0 & -1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -1 & 0 & 0 & \cdots & -1 & 0 \end{bmatrix}, \tag{6.22}$$

which differs from J_N only in the signs of the elements in the upper right-hand and lower left-hand corners. We then have

$$A_2 = z_1 I_{\mathscr{M}} \otimes J_{\mathscr{N}} + z_2 J'_{\mathscr{M}} \otimes F_{\mathscr{N}}, \tag{6.23a}$$

$$A_3 = z_1 I_{\mathscr{M}} \otimes J'_{\mathscr{N}} + z_2 J_{\mathscr{M}} \otimes F_{\mathscr{N}}, \tag{6.23b}$$

$$A_4 = z_1 I_{\mathscr{M}} \otimes J'_{\mathscr{N}} + z_2 J'_{\mathscr{M}} \otimes F_{\mathscr{N}}. \tag{6.23c}$$

We multiply each of these A_i on the right by $I_{\mathscr{M}} \otimes T_{\mathscr{N}}$ and on the left by $I_{\mathscr{M}} \otimes (-iT_{\mathscr{N}})$ and find that

$$\det A_i = \det \bar{A}_i, \qquad i = 2, 3, 4, \tag{6.24}$$

where

$$\bar{A}_2 = z_1 I_{\mathscr{M}} \otimes J_{\mathscr{N}} + iz_2 J'_{\mathscr{M}} \otimes I_{\mathscr{N}}, \tag{6.25a}$$

$$\bar{A}_3 = z_1 I_{\mathscr{M}} \otimes J'_{\mathscr{N}} + iz_2 J_{\mathscr{M}} \otimes I_{\mathscr{N}}, \tag{6.25b}$$

and

$$\bar{A}_4 = z_1 I_{\mathscr{M}} \otimes J'_{\mathscr{N}} + iz_2 J'_{\mathscr{M}} \otimes I_{\mathscr{N}}. \tag{6.25c}$$

Let $\lambda_n'^{(N)}$ be the N eigenvalues of J'_N and we find

$$\det A_2 = \prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}} (z_1 \lambda_k^{(\mathscr{N})} + iz_2 \lambda_j'^{(\mathscr{M})}), \tag{6.26a}$$

$$\det A_3 = \prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}} (z_1 \lambda_k'^{(\mathscr{N})} + iz_2 \lambda_j^{(\mathscr{M})}), \tag{6.26b}$$

and

$$\det A_4 = \prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}} (z_1 \lambda_k'^{(\mathscr{N})} + iz_2 \lambda_j'^{(\mathscr{M})}). \tag{6.26c}$$

The matrix J'_N is not cyclic but since it is "almost" cyclic it is referred to as a near-cyclic matrix. We may compute its eigenvalues exactly as we did for J_N by seeking eigenvectors of the form (6.14). The eigenvalue equation then reduces to the three equations

$$\begin{aligned} \alpha + \alpha^{N-1} &= \lambda(\alpha), \\ -\alpha^{-1} + \alpha &= \lambda(\alpha), \\ -\alpha^{-N+1} - \alpha^{-1} &= \lambda(\alpha). \end{aligned} \tag{6.27}$$

If

$$\alpha^N = -1, \tag{6.28}$$

these three equations are identical and thus we find the N eigenvalues $\lambda_n'^{(N)}$ are

$$\lambda_n'^{(N)} = 2i \sin [\pi(2n - 1)/N], \qquad 1 \leq n \leq N. \tag{6.29}$$

We may now combine (6.29) and (6.18) with (6.26) to evaluate the three remaining determinants:

$$\det A_2 = \prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}/2} \left[4z_1^2 \sin^2 \frac{2\pi k}{\mathscr{N}} + 4z_2^2 \sin^2 \frac{\pi(2j-1)}{\mathscr{M}}\right], \tag{6.30a}$$

$$\det A_3 = \prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}/2} \left[4z_1^2 \sin^2 \frac{\pi(2k-1)}{\mathscr{N}} + 4z_2^2 \sin^2 \frac{2\pi j}{\mathscr{M}}\right], \tag{6.30b}$$

$$\det A_4 = \prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}/2} \left[4z_1^2 \sin^2 \frac{\pi(2k-1)}{\mathscr{N}} + 4z_2^2 \sin^2 \frac{\pi(2j-1)}{\mathscr{M}}\right]. \tag{6.30c}$$

To use these determinants finally to evaluate $Z^T_{\mathscr{M},\mathscr{N}}$ we need to determine the sign in the relation $\operatorname{Pf} A_i = \pm(\det A_i)^{1/2}$. For this purpose we note that, though all three determinants are nonnegative,

$$\begin{aligned} &\det A_2 = 0 \qquad \text{if } z_2 = 0 \text{ or if } z_1 = 0 \text{ and } \mathscr{M} \text{ is odd,} \\ &\det A_3 = 0 \qquad \text{if } z_1 = 0, \end{aligned}$$

and

$$\det A_4 = 0 \qquad \text{if } z_1 = z_2 = 0 \text{ or if } z_1 = 0 \text{ and } \mathscr{M} \text{ is odd.} \tag{6.31}$$

Furthermore we may easily use the geometric considerations that were used to derive the matrices A_i in the first place to find that

$$\operatorname{Pf} A_2 = \begin{cases} (2z_2)^{\mathscr{M}\mathscr{N}/2} & \text{if } z_1 = 0 \text{ and } \mathscr{M} \text{ is even,} \\ 0 & \text{if } z_1 = 0 \text{ and } \mathscr{M} \text{ is odd;} \end{cases}$$

$$\operatorname{Pf} A_3 = (2z_1)^{\mathscr{M}\mathscr{N}/2} \qquad \text{if } z_2 = 0;$$

$$\operatorname{Pf} A_4 = \begin{cases} (2z_1)^{\mathscr{M}\mathscr{N}/2} & \text{if } z_2 = 0, \\ (2z_2)^{\mathscr{M}\mathscr{N}/2} & \text{if } z_1 = 0 \text{ and } \mathscr{M} \text{ is even,} \\ 0 & \text{if } z_1 = 0 \text{ and } \mathscr{M} \text{ is odd.} \end{cases} \tag{6.32}$$

We may determine the sign of $(\det A_i)^{1/2}$ by continuity from the special cases (6.32) as long as we do not encounter any of the zeroes given by (6.31). Accordingly, we obtain the result,

$$\begin{aligned} Z^T_{\mathscr{M},\mathscr{N}} = \frac{1}{2}\Bigg\{&\prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}/2} \left[4z_1^2 \sin^2 \frac{2\pi k}{\mathscr{N}} + 4z_2^2 \sin^2 \frac{\pi(2j-1)}{\mathscr{M}}\right]^{1/2} \\ &+ (2z_1)^{\mathscr{M}\mathscr{N}/2} \prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}/2} \left[\sin^2 \frac{\pi(2k-1)}{\mathscr{N}} + \left(\frac{z_2}{z_1}\right)^2 \sin^2 \frac{2\pi j}{\mathscr{M}}\right]^{1/2} \\ &+ \prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}/2} \left[4z_1^2 \sin^2 \frac{\pi(2k-1)}{\mathscr{N}} + 4z_2^2 \sin^2 \frac{\pi(2j-1)}{\mathscr{M}}\right]^{1/2}\Bigg\}. \end{aligned} \tag{6.33}$$

The evaluation of $Z^C_{\mathscr{M},\mathscr{N}}$ and $Z^F_{\mathscr{M},\mathscr{N}}$ requires the calculation of the eigenvalues of a matrix which is neither cyclic nor near-cyclic. Define the

$N \times N$ dimensional matrix J''_N by

$$J''_N = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 0 \\ -1 & 0 & 1 & \cdots & 0 & 0 \\ 0 & -1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & 0 & \cdots & -1 & 0 \end{bmatrix}, \tag{6.34}$$

which may be obtained from J_N or J'_N by replacing the elements in the upper right-hand and lower left-hand corners by zero. Then

$$A_c = z_1 I_{\mathscr{M}} \otimes J'_{\mathscr{N}} + z_2 J''_{\mathscr{M}} \otimes F_{\mathscr{N}} \tag{6.35}$$

and

$$A_F = z_1 I_{\mathscr{M}} \otimes J''_{\mathscr{N}} + z_2 J''_{\mathscr{M}} \otimes F_{\mathscr{N}}. \tag{6.36}$$

We again calculate determinants of these matrices by first multiplying on the right by $I_{\mathscr{M}} \otimes T_{\mathscr{N}}$ and on the left by $I_{\mathscr{M}} \otimes (-iT_{\mathscr{N}})$. Thus

$$\det A_c = \prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}} (z_1 \lambda_k'^{(\mathscr{N})} + iz_2 \lambda_j''^{(\mathscr{M})}) \tag{6.37}$$

and

$$\det A_F = \prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}} (z_1 \lambda_k''^{(\mathscr{N})} + iz_2 \lambda_j''^{(\mathscr{M})}), \tag{6.38}$$

where $\lambda_n''^{(N)}$ are the eigenvalues of J''_N. We determine these eigenvalues by considering the eigenvalue equation

$$\begin{aligned} v_2 \qquad\qquad\qquad &= \lambda v_1, \\ -v_1 \qquad + v_3 \qquad\qquad &= \lambda v_2, \\ -v_2 \qquad + v_4 \qquad &= \lambda v_3, \\ \vdots \qquad\qquad\qquad &\quad \vdots \\ -v_{N-1} &= \lambda v_N, \end{aligned} \tag{6.39}$$

which is equivalent to the difference equation

$$-v_{l-1} + v_{l+1} = \lambda v_l, \qquad 1 < l < N, \tag{6.40}$$

with the boundary conditions

$$v_0 = v_{N+1} = 0. \tag{6.41}$$

The most general solution of (6.40) is

$$v_l = A\alpha_+^l + B\alpha_-^l, \tag{6.42}$$

where α_+ and α_- satisfy

$$\alpha - \alpha^{-1} = \lambda. \tag{6.43}$$

Therefore

$$\alpha_{\pm} = \tfrac{1}{2}[\lambda \pm (\lambda^2 + 4)^{1/2}], \tag{6.44}$$

and, in particular,

$$\alpha_+\alpha_- = -1. \tag{6.45}$$

To satisfy the boundary conditions (6.41) we need

$$v_0 = A + B = 0 \tag{6.46a}$$

and

$$v_{N+1} = A\alpha_+^{N+1} + B\alpha_-^{N+1} = 0. \tag{6.46b}$$

Therefore we may combine (6.45) and (6.46) to obtain

$$\alpha_+ = \left.\begin{cases} -\exp\dfrac{-\pi i(2n-1)}{2(N+1)}, & N \text{ even} \\[2ex] -\exp\dfrac{-\pi i n}{N+1}, & N \text{ odd} \end{cases}\right\} 1 \le n \le 2(N+1); \tag{6.47a}$$

$$\alpha_- = \left.\begin{cases} \exp\dfrac{\pi i(2n-1)}{2(N+1)}, & N \text{ even} \\[2ex] \exp\dfrac{\pi i n}{N+1}, & N \text{ odd} \end{cases}\right\} 1 \le n \le 2(N+1), \tag{6.47b}$$

so that the eigenvalues $\lambda_n''^{(N)}$ are contained in the set

$$\left.\begin{matrix} 2i\sin\dfrac{\pi(2n-1)}{2(N+1)}, & N \text{ even} \\[1ex] 2i\sin \pi n/(N+1), & N \text{ odd} \end{matrix}\right\} 1 \le n \le 2(N+1). \tag{6.48}$$

From (6.44) we see that each $\lambda \neq 2i$ has two distinct eigenvectors. Each eigenvalue is counted twice in the set (6.48). Therefore we extract a nondegenerate set of eigenvalues by letting

$$\left.\begin{matrix} n = n' + \dfrac{N+2}{2}, & N \text{ even} \\[2ex] n = n' + \dfrac{N+1}{2}, & N \text{ odd} \end{matrix}\right\} 1 \le n' \le N+1. \tag{6.49}$$

However, if $n' = N + 1$, then $\lambda = -2i$. This value of λ has only the trivial eigenvector $v_l = 0$. Therefore we use (6.45) and find the desired result,

$$\lambda_n''^{(N)} = 2i\cos\frac{\pi n}{N+1}, \qquad 1 \le n \le N. \tag{6.50}$$

We may now combine (6.29) and (6.50) with (6.37) and (6.38) to obtain

$$\det A_c = \prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}/2} 4\left[z_1^2 \sin^2 \frac{\pi(2k-1)}{\mathscr{N}} + z_2^2 \cos^2 \frac{\pi j}{\mathscr{M}+1}\right] \tag{6.51}$$

and

$$\det A_F = \prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}/2} 4\left[z_1^2 \cos^2 \frac{\pi k}{\mathscr{N}+1} + z_2^2 \cos^2 \frac{\pi j}{\mathscr{M}+1}\right]. \tag{6.52}$$

It remains only to determine the sign in the relation $\operatorname{Pf} A = \pm(\det A)^{1/2}$. This is done exactly as it was for $\operatorname{Pf} A_t$ and we obtain the final results

$$Z^c_{\mathscr{M},\mathscr{N}} = (2z_1)^{\mathscr{M}\mathscr{N}/2} \prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}/2} \left[\sin^2 \frac{\pi(2k-1)}{\mathscr{N}} + \left(\frac{z_2}{z_1}\right)^2 \cos^2 \frac{\pi j}{\mathscr{M}+1}\right]^{1/2} \tag{6.53}$$

and

$$Z^F_{\mathscr{M},\mathscr{N}} = (2z_1)^{\mathscr{M}\mathscr{N}/2} \prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}/2} \left[\cos^2 \frac{\pi k}{\mathscr{N}+1} + \left(\frac{z_2}{z_1}\right)^2 \cos^2 \frac{\pi j}{\mathscr{M}+1}\right]^{1/2}. \tag{6.54}$$

7. THE THERMODYNAMIC LIMIT

For lattices of finite size, the evaluations of Z^F, Z^c, and Z^T of the previous section may be regarded as the final result. However, as discussed in Chapter II, our major interest in the Ising model is in the thermodynamic limit $\mathscr{M} \to \infty$ and $\mathscr{N} \to \infty$. Therefore, we will conclude this digression on dimer statistics by studying the behavior of $Z^F_{\mathscr{M},\mathscr{N}}$, $Z^c_{\mathscr{M},\mathscr{N}}$, and $Z^T_{\mathscr{M},\mathscr{N}}$ as $\mathscr{M} \to \infty$ and $\mathscr{N} \to \infty$.

When $\mathscr{M} \to \infty$ and $\mathscr{N} \to \infty$ we expect that boundary conditions should become, in some sense, irrelevant. More precisely, as $\mathscr{M} \to \infty$ and $\mathscr{N} \to \infty$ we expect that, though generating functions Z surely diverge, $\lim_{\mathscr{N}\to\infty}^{\mathscr{M}\to\infty} (\mathscr{M}\mathscr{N})^{-1} \ln Z$ should exist, and be the same for all boundary conditions. This limit is obtained from (6.33), (6.53), and (6.54) by using the definition of integrals, and we obtain

$$\begin{aligned}
&\lim_{\substack{\mathscr{M}\to\infty \\ \mathscr{N}\to\infty}} (\mathscr{M}\mathscr{N})^{-1} \ln Z^F_{\mathscr{M},\mathscr{N}} \\
&\qquad = \lim_{\substack{\mathscr{M}\to\infty \\ \mathscr{N}\to\infty}} (\mathscr{M}\mathscr{N})^{-1} \ln Z^c_{\mathscr{M},\mathscr{N}} = \lim_{\substack{\mathscr{M}\to\infty \\ \mathscr{N}\to\infty}} (\mathscr{M}\mathscr{N})^{-1} \ln Z^T_{\mathscr{M},\mathscr{N}} \\
&\qquad = \tfrac{1}{4}(2\pi)^{-2} \int_0^{2\pi} d\theta_1 \int_0^{2\pi} d\theta_2 \ln\left[4(z_1^2 \sin^2\theta_1 + z_2^2 \sin^2\theta_2)\right] \\
&\qquad = \tfrac{1}{4}(2\pi)^{-2} \int_0^{2\pi} d\theta_1 \int_0^{2\pi} d\theta_2 \ln\left[4(z_1^2 \cos^2\theta_1 + z_2^2 \cos^2\theta_2)\right],
\end{aligned} \tag{7.1}$$

where ln is defined to be real when z_1 and z_2 are positive.

CHAPTER V

Specific Heat of Onsager's Lattice in the Absence of a Magnetic Field

1. INTRODUCTION

The discussion of dimer statistics in the previous chapter is extremely useful for our treatment of the two-dimensional Ising model because, as we will show in the next section, the partition function for the two-dimensional Ising model in the absence of a magnetic field is very closely related to the generating function for closest-packed dimers on an appropriate lattice.[1] For this reason the partition function may be expressed in terms of the Pfaffian of a suitable matrix. However, the evaluation of the Pfaffian for an arbitrary lattice is a most complicated problem and in order to obtain explicit results we will confine our attention in this chapter to Onsager's lattice. (The lifting of this restriction in a nontrivial fashion will be studied in the last two chapters of this book.) Even the restriction to Onsager's lattice is not quite sufficient to obtain an explicit result for the partition function because it has not been possible to evaluate exactly the relevant Pfaffian when the boundary conditions are free in both directions. Therefore, in this chapter we will restrict our attention to Onsager's lattice with toroidal boundary conditions. In the following two chapters we will study the effects associated with cyclic boundary conditions in the horizontal direction and free boundary conditions in the vertical direction. For both boundary conditions we find that in the thermodynamic limit the free energy per site is the same. From this free energy we derive the specific heat c and demonstrate that there exists one, and only one, temperature, T_c, at which c fails to be an analytic function of T. At this "critical tem-

1. P. W. Kasteleyn, *J. Math. Phys.* **4**, 287 (1963).

perature" c behaves as

$$c \sim \text{const} \ln |T - T_c| + \text{const}'. \tag{1.1}$$

This remarkable logarithmic divergence of the specific heat of Onsager's lattice at zero magnetic field is the first indication that this system is undergoing a phase transition.

2. THE PARTITION FUNCTION FOR ONSAGER'S LATTICE

When we impose toroidal boundary conditions on Onsager's lattice with $H = 0$, the interaction energy may be explicitly written as

$$\mathscr{E} = -E_1 \sum_{j=1}^{\mathscr{M}} \sum_{k=1}^{\mathscr{N}} \sigma_{j,k}\sigma_{j,k+1} - E_2 \sum_{j=1}^{\mathscr{M}} \sum_{k=1}^{\mathscr{N}} \sigma_{j,k}\sigma_{j+1,k}, \tag{2.1}$$

where $j = \mathscr{M} + 1$ and $j = 1$ are identical and $k = \mathscr{N} + 1$ and $k = 1$ are identical. The partition function is then given as

$$\begin{aligned} Z &= \sum_{\sigma = \pm 1} e^{-\beta\mathscr{E}} \\ &= \sum_{\sigma = \pm 1} \exp\left[\beta E_1 \sum_{j=1}^{\mathscr{M}} \sum_{k=1}^{\mathscr{N}} \sigma_{j,k}\sigma_{j,k+1} + \beta E_2 \sum_{j=1}^{\mathscr{M}} \sum_{k=1}^{\mathscr{N}} \sigma_{j,k}\sigma_{j+1,k}\right] \\ &= \sum_{\sigma = \pm 1} \left[\prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}} \exp(\beta E_1 \sigma_{j,k}\sigma_{j,k+1})\right]\left[\prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}} \exp(\beta E_2 \sigma_{j,k}\sigma_{j+1,k})\right]. \end{aligned} \tag{2.2}$$

Now, σ may take on only the values ± 1, so that

$$\begin{aligned} e^{\beta E\sigma\sigma'} &= \begin{cases} e^{\beta E} & \text{if } \sigma = 1,\ \sigma' = 1 \\ & \text{or } \sigma = -1,\ \sigma' = -1 \\ e^{-\beta E} & \text{if } \sigma = 1,\ \sigma' = -1 \\ & \text{or } \sigma = -1,\ \sigma' = 1 \end{cases} \\ &= \cosh \beta E + \sigma\sigma' \sinh \beta E. \end{aligned} \tag{2.3}$$

Therefore, we may write Z as

$$\begin{aligned} Z = (\cosh \beta E_1 \cosh \beta E_2)^{\mathscr{M}\mathscr{N}} \sum_{\sigma = \pm 1} & \left[\prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}} (1 + z_1 \sigma_{j,k}\sigma_{j,k+1})\right] \\ \times & \left[\prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}} (1 + z_2 \sigma_{j,k}\sigma_{j+1,k})\right], \end{aligned} \tag{2.4}$$

where

$$z_1 = \tanh \beta E_1 \quad \text{and} \quad z_2 = \tanh \beta E_2. \tag{2.5}$$

We evaluate the sum over all $\sigma = \pm 1$ by expanding the products. Each term in this expansion contains a factor for every nearest-neighbor pair of sites α and α' which may be either 1 or $z\sigma_\alpha\sigma_{\alpha'}$ where z is the hyperbolic tangent of β times the energy of the bond between α and α'. Therefore, there are terms proportional to 1, σ_α, σ_α^2, σ_α^3, and σ_α^4. However, since σ_α can be only $+1$ or -1, all even powers of σ_α may be replaced by 1 whereas all terms containing σ_α or σ_α^3 give no contribution, since

$$\sum_{\sigma_\alpha = \pm 1} \sigma_\alpha = \sum_{\sigma_\alpha = \pm 1} \sigma_\alpha^3 = 0. \tag{2.6}$$

Furthermore,

$$\sum_{\text{all } \sigma = \pm 1} 1 = 2^{\mathcal{M}\mathcal{N}}. \tag{2.7}$$

Therefore we may obtain Z from the expansion of the products in (2.4) by omitting all terms where any σ_α appears an odd number of times, replacing every σ_α^2 and σ_α^4 by 1, and multiplying the resulting function of z_1, z_2 by $2^{\mathcal{M}\mathcal{N}}$. This procedure has a simple and useful graphical representation. Let N_{pq} be the number of figures that can be drawn on the lattice with the following properties: (i) each bond between nearest neighbors may be used, at most, once; (ii) an even number of bonds terminate at each vertex; (iii) the figure contains p horizontal and q vertical bonds. Several examples of figures with the properties (i) and (ii) are shown in Fig. 5.1. In terms of N_{pq},

$$Z = (2\cosh\beta E_1 \cosh\beta E_2)^{\mathcal{M}\mathcal{N}} \sum_{p,q} N_{pq} z_1^p z_2^q. \tag{2.8}$$

The problem of evaluating Z is therefore equivalent to the problem of finding the generating function for closed, and possibly intersecting,

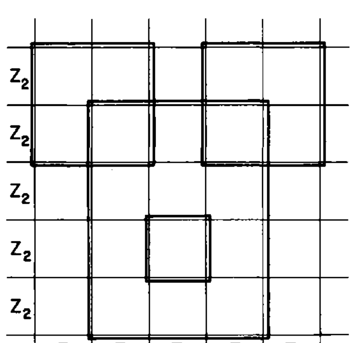


Fig. 5.1. Polygon figures on a portion of the square lattice with bonds z_1 and z_2.

polygons with p horizontal and q vertical sides on the square lattice, with the restriction that no two sides may overlap.[2] It is furthermore evident that, so far as this discussion is concerned, the restriction to Onsager's lattice is easily removed. For the most general Ising model, where E_1 and E_2 are functions of j and k, the partition function is given as

$$Z = 2^{\mathscr{M}\mathscr{N}} \prod_{j=1}^{\mathscr{M}} \prod_{k=1}^{\mathscr{N}} [\cosh \beta E_1(j, k) \cosh \beta E_2(j, k)]$$

$\times$ the weighted sum over all closed polygons satisfying properties (i) and (ii), where each bond of the polygon is given a weight of tanh β (the energy of the bond). (2.9)

There are several ways of relating the Ising-model problem of (2.8) [or (2.9)] to a problem of closest-packed dimers. Each method involves replacing each site on the Ising lattice with bonds z_i by a cluster of sites on a new "counting" lattice. One such cluster, which replaces one Ising vertex with six new vertices[3] is shown in Fig. 5.2. The eight possible configurations of bonds at any Ising vertex are in 1–1 correspondence with the ways one may draw closest-packed dimer configurations on this cluster as shown in Fig. 5.3. Therefore the sum in (2.8) is exactly the same as the generating function for closest-packed dimer configurations for the lattice of Fig. 5.4, where the three classes of bonds to be distinguished are: (1) horizontal bonds between clusters which have a weight of z_1, (2)

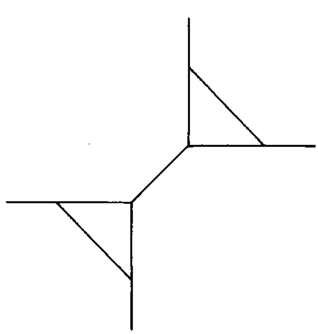


Fig. 5.2. A six-site cluster that may be used to convert the Ising problem into a dimer problem.

2. This construction was first made by B. L. van der Waerden, *Z. Physik* **118**, 473 (1941). It was first used in an exact evaluation of the partition function by M. Kac and J. C. Ward, *Phys. Rev.* **88**, 1332 (1952).
3. This construction was first made by M. E. Fisher, *J. Math. Phys.* **7**, 1776 (1966).

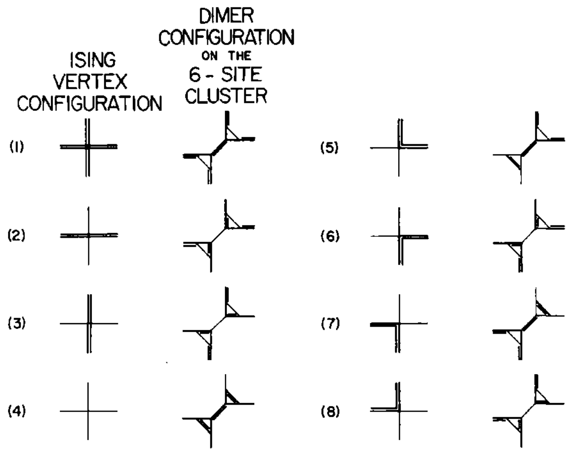


Fig. 5.3. The 1–1 equivalence of the Ising-model vertex configurations and dimer configurations on the six-site cluster.

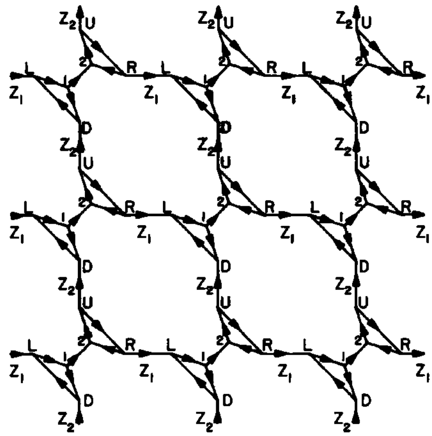


Fig. 5.4. A portion of the counting lattice with six-site clusters. All unmarked bonds in the clusters have a weight of 1. The arrows on this lattice and the notation labeling the six-site clusters corresponds to (2.10).

vertical bonds between clusters which have a weight of z_2, and (3) bonds within a cluster, all of which have a weight of 1.

If this counting lattice had free boundary conditions we could directly apply the results of Sec. 3 of the last chapter to construct an oriented lattice which allows us to represent the generating function as a Pfaffian. One such oriented lattice on which the orientation parity of all elementary polygons is clockwise odd is given in Fig. 5.4. In terms of the notation of that lattice we define the corresponding antisymmetric matrix as

$$\bar{A}(j,k;j,k) = \begin{array}{c} \\ R \\ L \\ U \\ D \\ 1 \\ 2 \end{array} \begin{array}{c} \begin{array}{cccccc} R & L & U & D & 1 & 2 \end{array} \\ \begin{bmatrix} 0 & 0 & -1 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 1 & 0 & 1 \\ -1 & 0 & 1 & 0 & -1 & 0 \end{bmatrix} \end{array}$$

$$\text{for } 1 \le j \le \mathscr{M},\ 1 \le k \le \mathscr{N}, \tag{2.10a}$$

$$\bar{A}(j,k;j,k+1) = -\bar{A}^T(j,k+1;j,k)$$

$$= \begin{array}{c} \\ R \\ L \\ U \\ D \\ 1 \\ 2 \end{array} \begin{array}{c} \begin{array}{cccccc} R & L & U & D & 1 & 2 \end{array} \\ \begin{bmatrix} 0 & z_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

$$1 \le j \le \mathscr{M},\ 1 \le k \le \mathscr{N} - 1, \tag{2.10b}$$

$$\bar{A}(j,k;j+1,k) = -\bar{A}^T(j+1,k;j,k)$$

$$= \begin{array}{c} \\ R \\ L \\ U \\ D \\ 1 \\ 2 \end{array} \begin{array}{c} \begin{array}{cccccc} R & L & U & D & 1 & 2 \end{array} \\ \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & z_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

$$1 \le j \le \mathscr{M} - 1,\ 1 \le k \le \mathscr{N}. \tag{2.10c}$$

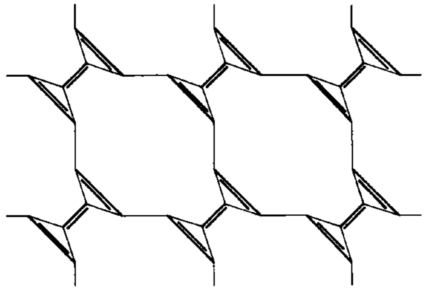


Fig. 5.5. A portion of the standard configuration C_0 for the six-site cluster Ising-model counting lattice.

To apply toroidal boundary conditions to this counting lattice we define a standard configuration C_0 as in Fig. 5.5. We may then use an argument identical to that of Sec. 5 of Chapter IV to show that if we define 4 matrices analogously to (IV.5.1) by (2.10) and by

$$\begin{aligned}(1)\quad &\bar{A}_1(j,\mathcal{N};j,1) = -\bar{A}_1^T(j,1;j,\mathcal{N}) = \bar{A}(j,1;j,2),\ 1 \le j \le \mathcal{M},\\ &\bar{A}_1(\mathcal{M},k;1,k) = -\bar{A}_1^T(1,k;\mathcal{M},k) = \bar{A}(1,k;2,k),\ 1 \le k \le \mathcal{N};\end{aligned} \tag{2.11a}$$

$$\begin{aligned}(2)\quad &\bar{A}_2(j,\mathcal{N};j,1) = -\bar{A}_2^T(j,1;j,\mathcal{N}) = \bar{A}(j,1;j,2),\ 1 \le j \le \mathcal{M},\\ &\bar{A}_2(\mathcal{M},k;1,k) = -\bar{A}_2^T(1,k;\mathcal{M},k) = -\bar{A}(1,k;2,k),\ 1 \le k \le \mathcal{N};\end{aligned} \tag{2.11b}$$

$$\begin{aligned}(3)\quad &\bar{A}_3(j,\mathcal{N};j,1) = -\bar{A}_3^T(j,1;j,\mathcal{N}) = -\bar{A}(j,1;j,2),\ 1 \le j \le \mathcal{M},\\ &\bar{A}_3(\mathcal{M},k;1,k) = -\bar{A}_3^T(1,k;\mathcal{M},k) = \bar{A}(1,k;2,k),\ 1 \le k \le \mathcal{N};\end{aligned} \tag{2.11c}$$

$$\begin{aligned}(4)\quad &\bar{A}_4(j,\mathcal{N};j,1) = -\bar{A}_4^T(j,1;j,\mathcal{N}) = -\bar{A}(j,1;j,2),\ 1 \le j \le \mathcal{M},\\ &\bar{A}_4(\mathcal{M},k;1,k) = -\bar{A}_4^T(1,k;\mathcal{M},k) = -\bar{A}(1,k;2,k),\ 1 \le k \le \mathcal{N},\end{aligned} \tag{2.11d}$$

then the partition function of Onsager's lattice with toroidal boundary conditions is

$$Z = \tfrac{1}{2}(2\cosh\beta E_1 \cosh\beta E_2)^{\mathcal{M}\mathcal{N}}\{-\operatorname{Pf}\bar{A}_1 + \operatorname{Pf}\bar{A}_2 + \operatorname{Pf}\bar{A}_3 + \operatorname{Pf}\bar{A}_4\}. \tag{2.12}$$

The Pfaffians which appear in (2.12) will be evaluated by means of the relation

$$\operatorname{Pf}\bar{A}_i = \pm(\det \bar{A}_i)^{1/2}. \tag{2.13}$$

The matrices occurring in this expression are of dimensions $6\mathcal{M}\mathcal{N}$. However, it is trivially possible to find $4\mathcal{M}\mathcal{N} \times 4\mathcal{M}\mathcal{N}$ matrices A_i such that

$$\operatorname{Pf}\bar{A}_i = \pm(\det A_i)^{1/2}. \tag{2.14}$$

This is done by noticing that if in every 6×6 submatrix $\bar{A}_i(j,k;j',k')$ we subtract column 1 from column R, add column 1 to column U, add column 2 to column L, and subtract column 2 from column D, we have

$$\det \bar{A}_l = \det A_l, \tag{2.15}$$

where

$$A_l(j,k;j,k) = \begin{array}{c} \\ R \\ L \\ U \\ D \end{array} \begin{array}{c} \begin{array}{cccc} R & L & U & D \end{array} \\ \begin{bmatrix} 0 & 1 & -1 & -1 \\ -1 & 0 & 1 & -1 \\ 1 & -1 & 0 & 1 \\ 1 & 1 & -1 & 0 \end{bmatrix} \end{array} \tag{2.16}$$

and all other $A_l(j,k;j',k')$ are identical to $\bar{A}_l(j,k;j',k')$ with the rows and columns labeled 1 and 2 removed.

The matrices A_l are antisymmetric and it might be expected that (2.16) can be given a geometric interpretation on a counting lattice obtained from the Ising lattice by replacing each Ising site by a cluster of 4 sites. Indeed, the matrices A_l do define oriented lattices and the oriented cluster which replaces a single Ising vertex is shown in Fig. 5.6. This

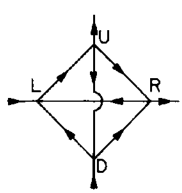


Fig. 5.6. An oriented four-site cluster which can replace an Ising-model vertex to construct the counting lattice related to the matrix A of (2.16).

cluster is not planar and therefore the arguments of the previous chapter do not apply. Nevertheless, a direct computation of $Z_{\mathscr{M},\mathscr{N}}$ in terms of the Pfaffians of A_l has been given.[4] However, the present derivation is more straightforward.

We now turn to the evaluation of $\det A_l$. Define the $n \times n$ matrices

$$H_n = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \end{bmatrix} \tag{2.17a}$$

4. Reference 1.

and

$$\tilde{H}_n = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ -1 & 0 & 0 & \cdots & 0 \end{bmatrix}. \tag{2.17b}$$

Then we may write the 4 matrices A_i in a direct-product notation as

$$\begin{aligned} A_i = & \begin{bmatrix} 0 & 1 & -1 & -1 \\ -1 & 0 & 1 & -1 \\ 1 & -1 & 0 & 1 \\ 1 & 1 & -1 & 0 \end{bmatrix} \otimes I_{\mathscr{M}} \otimes I_{\mathscr{N}} \\ & + \begin{bmatrix} 0 & z_1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \otimes I_{\mathscr{M}} \otimes \begin{cases} H_{\mathscr{N}} & \text{if } i = 1, 2 \\ \tilde{H}_{\mathscr{N}} & \text{if } i = 3, 4 \end{cases} \\ & + \begin{bmatrix} 0 & 0 & 0 & 0 \\ -z_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \otimes I_{\mathscr{M}} \otimes \begin{cases} H_{\mathscr{N}}^T & \text{if } i = 1, 2 \\ \tilde{H}_{\mathscr{N}}^T & \text{if } i = 3, 4 \end{cases} \\ & + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & z_2 \\ 0 & 0 & 0 & 0 \end{bmatrix} \otimes \left.\begin{cases} H_{\mathscr{M}} & \text{if } i = 1, 3 \\ \tilde{H}_{\mathscr{M}} & \text{if } i = 2, 4 \end{cases}\right\} \otimes I_{\mathscr{N}} \\ & + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -z_2 & 0 \end{bmatrix} \otimes \left.\begin{cases} H_{\mathscr{M}}^T & \text{if } i = 1, 3 \\ \tilde{H}_{\mathscr{M}}^T & \text{if } i = 2, 4 \end{cases}\right\} \otimes I_{\mathscr{N}}. \end{aligned} \tag{2.18}$$

Since $H_{\mathscr{N}}$ is a cyclic matrix, we find from (IV.6.19) that its eigenvalues are $e^{2\pi i n/\mathscr{N}}$, $n = 1, \ldots, \mathscr{N}$. Similarly, $\tilde{H}_{\mathscr{N}}$ is a near-cyclic matrix whose eigenvalues are $e^{\pi i(2n+1)/\mathscr{N}}$, $n = 1, \ldots, \mathscr{N}$. Furthermore, $H_{\mathscr{N}}$ and $\tilde{H}_{\mathscr{N}}$ are unitary:

$$H_{\mathscr{N}} H_{\mathscr{N}}^T = \tilde{H}_{\mathscr{N}} \tilde{H}_{\mathscr{N}}^T = 1. \tag{2.19}$$

Therefore if

$$UH_{\mathcal{N}}U^{-1} = \begin{bmatrix} e^{2\pi i/\mathcal{N}} & 0 & \cdots & 0 \\ 0 & e^{4\pi i/\mathcal{N}} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}, \tag{2.20a}$$

then

$$UH_{\mathcal{N}}^{T}U^{-1} = \begin{bmatrix} e^{-2\pi i/\mathcal{N}} & 0 & \cdots & 0 \\ 0 & e^{-4\pi i/\mathcal{N}} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}; \tag{2.20b}$$

and similarly, if

$$\tilde{U}\tilde{H}_{\mathcal{N}}\tilde{U}^{-1} = \begin{bmatrix} e^{\pi i/\mathcal{N}} & 0 & \cdots & 0 \\ 0 & e^{3\pi i/\mathcal{N}} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & -1 \end{bmatrix}, \tag{2.21a}$$

then

$$\tilde{U}\tilde{H}_{\mathcal{N}}^{T}\tilde{U}^{-1} = \begin{bmatrix} e^{-\pi i/\mathcal{N}} & 0 & \cdots & 0 \\ 0 & e^{-3\pi i/\mathcal{N}} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & -1 \end{bmatrix}. \tag{2.21b}$$

Therefore we may evaluate $\det A_i$ by first transforming $H_{\mathcal{N}}$ and $\tilde{H}_{\mathcal{N}}$ into diagonal form by a similarity transformation to obtain

$$\det A_i = \prod_{\theta_1}\prod_{\theta_2} \det \begin{bmatrix} 0 & 1 + z_1 e^{i\theta_1} & -1 & -1 \\ -1 - z_1 e^{-i\theta_1} & 0 & 1 & -1 \\ 1 & -1 & 0 & 1 + z_2 e^{i\theta_2} \\ 1 & 1 & -1 - z_2 e^{-i\theta_2} & 0 \end{bmatrix}, \tag{2.22}$$

where the product $\prod_{\theta_1}$ is over $\theta_1 = 2\pi n/\mathcal{N}$ if $i = 1, 2$ and is over $\theta_1 = \pi(2n - 1)/\mathcal{N}$ if $i = 3, 4$ $(n = 1, \ldots, \mathcal{N})$ and the product $\prod_{\theta_2}$ is over $\theta_2 = 2\pi n/\mathcal{M}$ if $i = 1, 3$ and is over $\theta_2 = \pi(2n - 1)/\mathcal{M}$ if $i = 2, 4$ $(n = 1, \ldots, \mathcal{M})$. The remaining 4×4 determinant may be evaluated and we find

$$\det A_i = \prod_{\theta_1}\prod_{\theta_2}[(1 + z_1^2)(1 + z_2^2) - 2z_1(1 - z_2^2)\cos\theta_1 - 2z_2(1 - z_1^2)\cos\theta_2]. \tag{2.23}$$

To obtain the final explicit expression for $Z_{\mathcal{M},\mathcal{N}}$, it remains to determine the signs in (2.14) and substitute the resulting expression into (2.12). The determination of these $\pm$ signs is a bit tedious since they depend on the temperature. However, these signs are irrelevant to the computation of the free energy in the thermodynamic limit and for that reason we defer their determination until Sec. 4. Therefore, as long as z_1 and z_2 are such that no factor in (2.23) vanishes, we may use (2.12), (2.14), (2.23) and the definition of integral to obtain the celebrated result[5] that the free energy in the thermodynamic limit of Onsager's lattice at $H = 0$ is

$$\begin{aligned}
F &= -\beta^{-1} \lim_{\substack{\mathcal{M}\to\infty \\ \mathcal{N}\to\infty}} (\mathcal{M}\mathcal{N})^{-1} \ln Z_{\mathcal{M},\mathcal{N}} \\
&= -\beta^{-1}\Big\{\ln (2\cosh\beta E_1 \cosh\beta E_2) \\
&\qquad + \tfrac{1}{2}(2\pi)^{-2}\int_0^{2\pi} d\theta_1 \int_0^{2\pi} d\theta_2 \ln [(1+z_1^2)(1+z_2^2) \\
&\qquad - 2z_1(1-z_2^2)\cos\theta_1 - 2z_2(1-z_1^2)\cos\theta_2]\Big\} \\
&= -\beta^{-1}\Big\{\ln 2 + \tfrac{1}{2}(2\pi)^{-2}\int_0^{2\pi} d\theta_1 \int_0^{2\pi} d\theta_2 \ln [\cosh 2\beta E_1 \cosh 2\beta E_2 \\
&\qquad - \sinh 2\beta E_1 \cos\theta_1 - \sinh 2\beta E_2 \cos\theta_2]\Big\}.
\end{aligned} \tag{2.24}$$

3. THE SPECIFIC HEAT OF ONSAGER'S LATTICE

The most interesting property of the free energy (2.24) is that there exists one temperature T_c at which it fails to be an analytic function of T. The existence of this T_c may be easily seen if we reduce the double integral in (2.24) to a single integral by explicitly integrating over (say) θ_2. To carry out this integration let

$$\zeta = e^{i\theta_2}. \tag{3.1}$$

In the ζ-plane the integrand of (2.24) has logarithmic branch points at $\zeta = 0, \infty$, and at the points $\alpha(\theta_1)$ and $\alpha^{-1}(\theta_1)$ where $\alpha(\theta)$ is the larger root in magnitude of the quadratic equation

$$(1+z_1^2)(1+z_2^2) - z_1(1-z_2^2)(e^{i\theta}+e^{-i\theta}) - z_2(1-z_1^2)(\alpha+\alpha^{-1}) = 0. \tag{3.2}$$

5. L. Onsager, *Phys. Rev.* **65**, 117 (1944). This result has been rederived by many authors. For example, see B. Kaufman, *Phys. Rev.* **76**, 1232 (1949), M. Kac and J. C. Ward, *Phys. Rev.* **88**, 1922 (1952), and C. A. Hurst and H. S. Green, *J. Chem. Phys.* **33**, 1059 (1960).

More explicitly, α is

$$\alpha^{\pm 1}(\theta) = \tfrac{1}{2}z_2^{-1}(1 - z_1^2)^{-1}\{(1 + z_1^2)(1 + z_2^2) - z_1(1 - z_2^2)(e^{i\theta} + e^{-i\theta}) \pm (1 - z_2^2)[(1 - \alpha_1 e^{i\theta})(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2^{-1}e^{i\theta}) \times (1 - \alpha_2^{-1}e^{-i\theta})]^{1/2}\}, \quad (3.3)$$

where

$$\alpha_1 = \frac{z_1(1 - |z_2|)}{1 + |z_2|} \quad (3.4a)$$

and

$$\alpha_2 = \frac{z_1^{-1}(1 - |z_2|)}{1 + |z_2|}. \quad (3.4b)$$

These branch points may be connected by branch cuts on the real axis running from 0 to α^{-1} and from α^{-1} to ∞ (Fig. 5.7). With the definition

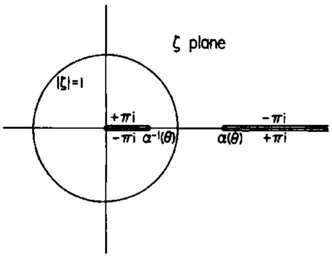


Fig. 5.7. The analyticity structure in the ζ-plane of the integrand of (2.24). The double lines represent logarithmic branch cuts and the values of the imaginary part of the logarithm on this branch cut are shown.

of α we have

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta_2 \ln[(1 + z_1^2)(1 + z_2^2) - 2z_1(1 - z_2^2)\cos\theta_1 - 2z_2(1 - z_1^2)\cos\theta_2]$$

$$= \frac{1}{2\pi}\int_0^{2\pi} d\theta_2 \ln[(e^{i\theta_2} - \alpha)(\alpha^{-1}e^{-i\theta_2} - 1)z_2(1 - z_1^2)]$$

$$= \frac{1}{2\pi i}\oint_{|\zeta|=1} \frac{d\zeta}{\zeta} \ln[(\alpha - \zeta)(\alpha^{-1} - \zeta)z_2(1 - z_1^2)], \quad (3.5)$$

where in the last line the logarithmic branch cuts are redefined as shown in Fig. 5.8. It is a simple matter to deform the contour of integration from

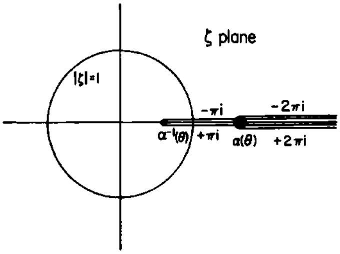


Fig. 5.8. The logarithmic branch cuts of the integrand of the last line in (3.5).

$|\zeta| = 1$ to the real axis from α^{-1} to 1 and evaluate (3.5). Thus we obtain

$$F = -\beta^{-1}\left\{\ln(2\cosh\beta E_1 \cosh\beta E_2) + (4\pi)^{-1}\int_0^{2\pi} d\theta \ln\left[z_2(1 - z_1^2)\alpha(\theta)\right]\right\}. \tag{3.6}$$

The analytic structure of the integrand in (3.6) is shown in Fig. 5.9.

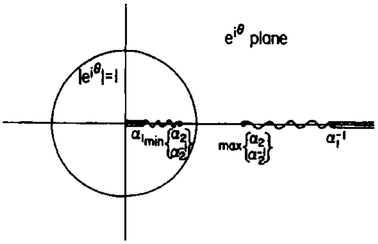


Fig. 5.9. The analytic structure of the integrand in (3.6). The double lines represent logarithmic branch cuts and wavy lines represent square-root branch cuts.

In particular we note that in the $\zeta = e^{i\theta}$ plane there are square-root branch points at $\zeta = \alpha_1,\ \alpha_1^{-1},\ \alpha_2,\ \alpha_2^{-1}$. These branch points may be connected pairwise by branch cuts on the real axis. The positions of these branch points depend on the temperature through (3.4). As long as T is confined to a region in which no two of these branch points coalesce on the contour of integration from opposite sides F will be an analytic function of T. It is easily seen from (3.4) that, for all $0 \le T \le \infty$,

$$-1 < \alpha_1 < 1, \tag{3.7}$$

so that α_1 and α_1^{-1} can never coalesce. However, it is also clear from (3.4) that

$$|\alpha_2| = 1 \tag{3.8}$$

if

$$|z_1| = \frac{1 - |z_2|}{1 + |z_2|}. \tag{3.9}$$

When (3.8) holds, the branch cuts which used to run from α_1 to min $(\alpha_2, \alpha_2^{-1})$ and from max $(\alpha_2, \alpha_2^{-1})$ to α_1^{-1} have coalesced to form one branch cut that runs from α_1 to α_1^{-1}. Such a branch cut runs directly through the contour of integration. This circumstance causes F to fail to be an analytic function of temperature when (3.9) holds, in a manner which will be made explicit shortly.

For a given value of E_1 and of E_2 there is precisely one value of T such that (3.9) holds. This value of T is defined as T_c and is called the critical temperature. All thermodynamic functions of Onsager's lattice at $H = 0$ will eventually be seen to be nonanalytic functions of T at T_c. In particular, we will see in Chapter X that for all temperatures below T_c Onsager's lattice possesses a spontaneous magnetization. Therefore a phase transition takes place at T_c.

The temperature T_c defined by (3.9) plays an enormous role in the theory of Onsager's lattice. Therefore it is useful to rewrite (3.9) in several ways. We may multiply (3.9) by $1 + |z_2|$ to find the symmetric formula

$$|z_1 z_2| + |z_1| + |z_2| = 1. \tag{3.10}$$

This curve is plotted in Fig. 5.10. We may also write (3.9) as

$$1 - |z_1 z_2| = |z_1| + |z_2|, \tag{3.11}$$

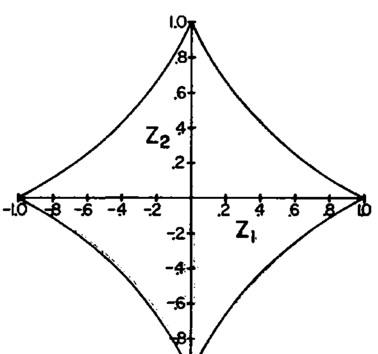


Fig. 5.10. Plot of the curve $|z_1 z_2| + |z_1| + |z_2| = 1$. Along this curve $T = T_c$.

which may be squared and rearranged to give

$$(1 - z_1^2)(1 - z_2^2) = 4|z_1 z_2|. \tag{3.12}$$

Finally, we note that

$$\tfrac{1}{2}z_k^{-1}(1 - z_k^2) = (\sinh 2\beta E_k)^{-1}, \qquad k = 1, 2, \tag{3.13}$$

and hence we find that (3.12) is equivalent to

$$1 = \sinh 2\beta|E_1| \sinh 2\beta|E_2|. \tag{3.14}$$

If $|E_1| = |E_2| = E$ this specializes to

$$1 = \sinh 2\beta E \tag{3.15}$$

from which we find

$$kT_c = 2E/\ln(1 + \sqrt{2}) = 2.26918531\ldots E. \tag{3.16}$$

If T_c is fixed and $E_2 \to 0$ we find that E_1 must go to ∞ as

$$|E_1| \sim -\tfrac{1}{2}kT_c \ln(|E_2|/kT_c). \tag{3.17}$$

If E_1 is fixed and $E_2 \to 0$, then T_c vanishes as

$$kT_c \sim -2|E_1|/\ln|E_2|. \tag{3.18}$$

In general, the contours in the E_1, E_2 plane along which T_c is a constant are plotted in Fig. 5.11.

We now must establish that, in fact, F does fail to be an analytic function of T at T_c. Indeed, we will not only establish the lack of analyticity at T_c but will be able to discover from (2.24) precisely how the internal energy u and the specific heat c behave near T_c. We will eventually study this lack of analyticity for the general case $E_1 \neq E_2$. However, the special case $E_1 = E_2$ has a simplifying feature which makes the analysis much

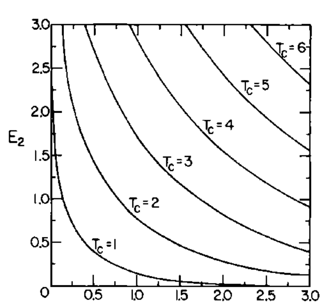


Fig. 5.11. Contours in the E_1, E_2-plane on which T_c is constant.

easier. Therefore we will present this simpler analysis before we embark on the general case.

Let

$$E_1 = E_2 = E \quad \text{and} \quad z_1 = z_2 = z. \tag{3.19}$$

Then (2.24) may be written as

$$F = -\beta^{-1}\Big\{\ln(2\cosh^2\beta E) + \ln(1+z^2) + \tfrac{1}{2}\pi^{-2}\int_0^\pi d\theta_1\int_0^\pi d\theta_2 \ln[1 - \tfrac{1}{2}k(\cos\theta_1 + \cos\theta_2)]\Big\}, \tag{3.20}$$

where

$$k = \frac{4z(1-z^2)}{(1+z^2)^2} = 2\,\frac{\sinh 2\beta E}{(\cosh 2\beta E)^2}. \tag{3.21}$$

It is clear from (3.15) that $k = 1$ if $T = T_c$.

Make the substitutions

$$\omega_1 = \tfrac{1}{2}(\theta_1 + \theta_2), \qquad \omega_2 = \tfrac{1}{2}(\theta_1 - \theta_2). \tag{3.22}$$

The region of integration of the double integral in (3.20) is the square

$$0 \le \theta_1 \le \pi, \qquad 0 \le \theta_2 \le \pi. \tag{3.23}$$

However, it is clear from the periodicity of the integrand that (3.20) is unchanged if we integrate over the rectangle

$$0 \le \omega_1 \le \pi, \qquad 0 \le \omega_2 \le \frac{\pi}{2}. \tag{3.24}$$

Therefore (3.20) becomes

$$F = -\beta^{-1}\Big\{\ln(2\cosh 2\beta E) + \pi^{-2}\int_0^{\pi/2} d\omega_2 \int_0^\pi d\omega_1 \ln[1 - k\cos\omega_1\cos\omega_2]\Big\}. \tag{3.25}$$

The integral over ω_1 is easily performed and we obtain

$$\begin{aligned} F &= -\beta^{-1}\Big\{\ln(\sqrt{2}\cosh 2\beta E) + \pi^{-1}\int_0^{\pi/2} d\omega \ln[1 + (1 - k^2\cos^2\omega)^{1/2}]\Big\} \\ &= -\beta^{-1}\Big\{\ln(\sqrt{2}\cosh 2\beta E) + \pi^{-1}\int_0^{\pi/2} d\omega \ln[1 + (1 - k^2\sin^2\omega)^{1/2}]\Big\}. \end{aligned} \tag{3.26}$$

This representation for F has the virtue that from it we obtain u and c directly in terms of the complete elliptic integral of the first kind,[6]

$$\mathbf{K}(k) = \int_0^{\pi/2} \frac{d\phi}{(1 - k^2 \sin^2 \phi)^{1/2}}, \tag{3.27}$$

and the complete elliptic integral of the second kind,

$$\mathbf{E}(k) = \int_0^{\pi/2} d\phi (1 - k^2 \sin^2 \phi)^{1/2}. \tag{3.28}$$

We first compute u:

$$u = \frac{\partial \beta F}{\partial \beta} = -2E \tanh 2\beta E + k \frac{dk}{d\beta} \pi^{-1} \int_0^{\pi/2} d\omega \frac{\sin^2 \omega}{\Delta(1 + \Delta)}, \tag{3.29}$$

where

$$\Delta \equiv \Delta(\omega, k) = (1 - k^2 \sin^2 \omega)^{1/2}. \tag{3.30}$$

However,

$$\frac{\sin^2 \omega}{\Delta(1 + \Delta)} = \frac{(1 - \Delta) \sin^2 \omega}{\Delta(1 - \Delta^2)} = k^{-2}\left(\frac{1}{\Delta} - 1\right). \tag{3.31}$$

Therefore, making use of definition (3.27), we obtain

$$u = -2E \tanh 2\beta E + \pi^{-1} k^{-1} \frac{dk}{d\beta}\left[\mathbf{K}(k) - \frac{\pi}{2}\right], \tag{3.32}$$

from which, if we note that

$$k^{-1} \frac{dk}{d\beta} = 2E \coth 2\beta E(1 - 2 \tanh^2 2\beta E), \tag{3.33}$$

we find the final expression for u when $E_1 = E_2 = E$, namely,

$$u = -E \coth 2\beta E[1 + 2\pi^{-1}(2 \tanh^2 2\beta E - 1)\mathbf{K}(k)]. \tag{3.34}$$

We next obtain the specific heat (k_0 = Boltzmann's const)

$$\begin{aligned} c = \frac{\partial u}{\partial T} &= -\frac{1}{k_0 T^2} \frac{\partial u}{\partial \beta} \\ &= \frac{E}{k_0 T^2}\Big\{-2E \operatorname{csch}^2 2\beta E[1 + 2\pi^{-1}(2 \tanh^2 2\beta E - 1)\mathbf{K}(k)] \\ &\qquad + 16\pi^{-1} E \operatorname{sech}^2 2\beta E \, \mathbf{K}(k) \\ &\qquad + 2\pi^{-1} \coth 2\beta E(2 \tanh^2 2\beta E - 1) \frac{dk}{d\beta} \frac{d\mathbf{K}(k)}{dk}\Big\}. \end{aligned} \tag{3.35}$$

6. We follow the standard notation as given, for example, in Bateman Manuscript Project, *Higher Transcendental Functions*, edited by Erdelyi (McGraw-Hill, New York, 1953), vol. 2, p. 317.

The derivative of $\mathbf{K}(k)$ may be expressed in terms of $\mathbf{E}(k)$ and $\mathbf{K}(k)$ if we first note that

$$\frac{d\mathbf{K}(k)}{dk} = k\int_0^{\pi/2} \frac{d\phi \sin^2\phi}{\Delta^3}, \tag{3.36}$$

which, since

$$\sin^2\phi = k^{-2}(1 - \Delta^2), \tag{3.37}$$

may be rewritten as

$$\frac{d\mathbf{K}(k)}{dk} = k^{-1}\int_0^{\pi/2} d\phi[\Delta^{-3} - \Delta^{-1}] = k^{-1}\int_0^{\pi/2} d\phi\Delta^{-3} - k^{-1}\mathbf{K}(k). \tag{3.38}$$

Now

$$\frac{d}{d\phi}\frac{\sin\phi\cos\phi}{\Delta} = \frac{1 - 2\sin^2\phi + k^2\sin^4\phi}{\Delta^3}, \tag{3.39}$$

or, equivalently,

$$\Delta^{-3} = k'^{-2}\Delta - k^2k'^{-2}\frac{d}{d\phi}\frac{\sin\phi\cos\phi}{\Delta}, \tag{3.40}$$

where

$$k'^2 = 1 - k^2. \tag{3.41}$$

Thus we obtain the well-known formula

$$\frac{d\mathbf{K}(k)}{dk} = \frac{1}{kk'^2}[\mathbf{E}(k) - k'^2\mathbf{K}(k)]. \tag{3.42}$$

This expression is now used in (3.35), and, noting that from (3.41) we may take

$$k' = 2\tanh^2 2\beta E - 1, \tag{3.43}$$

we obtain the final result[7] for $E_1 = E_2 = E$:

$$\begin{aligned} c = \frac{E^2}{k_0T^2}\{&-2\operatorname{csch}^2 2\beta E - 4\pi^{-1}\coth^2 2\beta E\,\mathbf{E}(k) \\ &- 4\pi^{-1}\coth^2 2\beta E[\operatorname{sech}^2 2\beta E(2\tanh^2 2\beta E - 1) \\ &- 4\tanh^2 2\beta E\operatorname{sech}^2 2\beta E - (2\tanh^2 2\beta E - 1)^2]\mathbf{K}(k)\} \\ = k_0(\beta E\coth 2\beta E)^2 2\pi^{-1}&\{2\mathbf{K}(k) - 2\mathbf{E}(k) - (1 - k')[\tfrac{1}{2}\pi + k'\mathbf{K}(k)]\}. \end{aligned} \tag{3.44}$$

7. Reference 5.

It now remains to approximate u and c when $T \sim T_c$. To carry out this approximation we need an expansion for $\mathbf{K}(k)$ and $\mathbf{E}(k)$ when $k \sim 1$. It is clear from (3.27) and (3.28) that, as $k \to 1$,

$$\mathbf{K}(k) \to \infty \tag{3.45}$$

but

$$\mathbf{E}(k) \to \mathbf{E}(1) = 1. \tag{3.46}$$

To discuss the manner in which $\mathbf{K}(k)$ diverges, we rewrite (3.27) as

$$\mathbf{K}(k) = \int_0^{\pi/2} \frac{d\phi}{(\cos^2 \phi + k'^2 \sin^2 \phi)^{1/2}}. \tag{3.47}$$

If $k \to 1$, then $k' \to 0$. We break the integrand in (3.47) into two pieces,

$$\mathbf{K}(k) = \int_{\pi/2-\varepsilon}^{\pi/2} \frac{d\phi}{(\cos^2 \phi + k'^2 \sin^2 \phi)^{1/2}} + \int_0^{\pi/2-\varepsilon} \frac{d\phi}{(\cos^2 \phi + k'^2 \sin^2 \phi)^{1/2}}, \tag{3.48}$$

where ϵ satisfies

$$\epsilon/|k'| \gg 1 \quad \text{and} \quad 1/\epsilon \gg 1. \tag{3.49}$$

In the first integral of (3.48) write $\phi = \frac{1}{2}\pi - t$. Then, since $\epsilon \ll 1$,

$$\int_{\pi/2-\varepsilon}^{\pi/2} \frac{d\phi}{(\cos^2 \phi + k'^2 \sin^2 \phi)^{1/2}} \sim \int_0^{\varepsilon} \frac{dt}{(k'^2 + k^2 t^2)^{1/2}} = \frac{1}{k} \ln \frac{k\epsilon + (k'^2 + k^2\epsilon^2)^{1/2}}{|k'|}, \tag{3.50}$$

which, since $\epsilon/|k'| \gg 1$, is approximately

$$\ln \frac{2\epsilon}{|k'|}. \tag{3.51}$$

In the second integral, $k' \sin \phi$ may be neglected in comparison with $\cos \phi$ because $\phi < \frac{1}{2}\pi - \epsilon$, so that

$$\int_0^{\pi/2-\varepsilon} \frac{d\phi}{(\cos^2 \phi + k'^2 \sin^2 \phi)^{1/2}} \sim \int_0^{\pi/2-\varepsilon} \frac{d\phi}{\cos \phi} = \ln [\sec(\tfrac{1}{2}\pi - \epsilon) + \tan(\tfrac{1}{2}\pi - \epsilon)] \sim \ln \frac{2}{\epsilon}. \tag{3.52}$$

Therefore we combine the approximations (3.51) and (3.52) to find that, as $k \to 1$,

$$\mathbf{K}(k) \sim \ln \frac{4}{|k'|}. \tag{3.53}$$

Somewhat more precisely, it can be shown[8] that, as $k \to 1$,

$$\mathbf{K}(k) = \ln \frac{4}{|k'|} + O(k'^2 \ln |k'|). \tag{3.54}$$

Approximations (3.46) and (3.54) may now be used to study u and c as $T \to T_c$. Near T_c,

$$k \sim 1 - 4\beta_c^2 E^2 \left(\frac{T}{T_c} - 1\right)^2 \tag{3.55}$$

and

$$k' \sim 2\sqrt{2}\beta_c E \left(\frac{T}{T_c} - 1\right). \tag{3.56}$$

Therefore from (3.34) we see that $u(T)$ is a continuous function of T even at T_c, where its value is

$$u(T_c) = -E \coth 2\beta_c E = -\sqrt{2}\, E. \tag{3.57}$$

From (3.44)

$$\begin{aligned} c/k_0 &\sim 8\pi^{-1}(\beta_c E)^2 \left\{ \ln \frac{4}{|k'|} - 1 - \frac{\pi}{4} \right\} \\ &= 2\pi^{-1}[\ln (1 + \sqrt{2})]^2 \left\{ -\ln \left| \frac{T}{T_c} - 1 \right| - 1 - \frac{\pi}{4} - \ln \left[\frac{\sqrt{2}}{4} \ln (1 + \sqrt{2}) \right] \right\}. \end{aligned} \tag{3.58}$$

In this form it is manifest that when $E_1 = E_2 = E$ the specific heat of Onsager's lattice has the logarithmic divergence shown in (1.1). It further should be noticed that the coefficient of the logarithm and the additive constant are the same for T above and below T_c.

We now turn our attention to the behavior of u and c in the general case $E_1 \neq E_2$. We will show that the qualitative conclusions about the continuity of u and the logarithmic divergence of c at T_c continue to be true in the general case. However, it is not possible to find expressions analogous to (3.34) and (3.44) which express u and c in terms of complete elliptic integrals of the first and second kinds. For the general case we are forced to introduce the complete elliptic integral of the third kind,[9]

$$\Pi_1(\nu, k) = \int_0^{\pi/2} d\phi (1 + \nu \sin^2 \phi)^{-1} (1 - k^2 \sin^2 \phi)^{-1/2}. \tag{3.59}$$

To analyze u and c in the general case it is desirable to make manifest the invariance of these functions under the interchange $E_1 \leftrightarrow E_2$. To obtain such a manifestly symmetric expression for u we return to the

8. Reference 6, p. 318.
9. Reference 6, p. 317.

expression of F as a double integral (2.24) and find

$$u = \frac{\partial \beta F}{\partial \beta} = -E_1 \tanh \beta E_1 - E_2 \tanh \beta E_2$$

$$- \left[E_1(1 - z_1^2) \frac{\partial}{\partial z_1} + E_2(1 - z_2^2) \frac{\partial}{\partial z_2} \right]$$

$$\times \tfrac{1}{2}(2\pi)^{-2} \int_0^{2\pi} d\theta_1 \int_0^{2\pi} d\theta_2 \ln [(1 + z_1^2)(1 + z_2^2)$$

$$- 2z_1(1 - z_2^2) \cos \theta_1 - 2z_2(1 - z_1^2) \cos \theta_2]$$

$$= -E_1 \left[z_1 + (1 - z_1^2)(2\pi)^{-2} \int_0^{2\pi} d\theta_1 \int_0^{2\pi} d\theta_2 \right.$$

$$\left. \times \frac{z_1(1 + z_2^2) - (1 - z_2^2) \cos \theta_1 + 2z_1 z_2 \cos \theta_2}{(1 + z_1^2)(1 + z_2^2) - 2z_1(1 - z_2^2) \cos \theta_1 - 2z_2(1 - z_1^2) \cos \theta_2} \right]$$

$$+ \text{ the same form with } 1 \leftrightarrow 2. \tag{3.60}$$

In the term proportional to E_1 we evaluate the integral over θ_2 and in the term proportional to E_2 we evaluate the integral over θ_1, to find

$$u = -\frac{E_1}{2\pi} \int_0^{2\pi} d\theta \frac{1 + \alpha_1\alpha_2 - \frac{1}{2}(\alpha_1 + \alpha_2)(e^{i\theta} + e^{-i\theta})}{[(1 - \alpha_1 e^{i\theta})(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{i\theta})(1 - \alpha_2 e^{-i\theta})]^{1/2}}$$

$$+ (E_1 \leftrightarrow E_2), \tag{3.61}$$

where the square root is defined to be positive at $\theta = \pi$. Then if we write

$$1 + \alpha_1\alpha_2 - \tfrac{1}{2}(\alpha_1 + \alpha_2)(e^{i\theta} + e^{-i\theta})$$

$$= \tfrac{1}{2}[(1 - \alpha_1 e^{i\theta})(1 - \alpha_2 e^{-i\theta}) + (1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{i\theta})], \tag{3.62}$$

we obtain

$$u = -\frac{E_1}{2\pi} \int_{-\pi}^{\pi} d\theta \left[\frac{(1 - \alpha_1 e^{i\theta})(1 - \alpha_2 e^{-i\theta})}{(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{i\theta})} \right]^{1/2} + (E_1 \leftrightarrow E_2). \tag{3.63}$$

There are several ways in which (3.63) may be reduced to complete elliptic integrals. The most straightforward reduction of (3.63) is to write

$$u = -\frac{E_1}{2\pi} \int_0^{2\pi} d\theta \frac{1 + \alpha_1\alpha_2 - (\alpha_1 + \alpha_2)e^{i\theta}}{[(1 - \alpha_1 e^{i\theta})(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{i\theta})(1 - \alpha_2 e^{-i\theta})]^{1/2}}$$

$$+ (E_1 \leftrightarrow E_2)$$

$$= -\frac{E_1}{\pi} \int_{\alpha_1}^{\alpha_2} d\zeta \frac{1 + \alpha_1\alpha_2 - (\alpha_1 + \alpha_2)\zeta}{[(1 - \alpha_1\zeta)(\zeta - \alpha_1)(1 - \alpha_2\zeta)(\alpha_2 - \zeta)]^{1/2}}$$

$$+ (E_1 \leftrightarrow E_2). \tag{3.64}$$

Then, if $T < T_c$ ($\alpha_2 < 1$), we may make, in the term proportional to E_1, the substitution

$$\zeta = \frac{\alpha_1(\alpha_1^{-1} - \alpha_2) + \alpha_1^{-1}(\alpha_2 - \alpha_1)\sin^2\phi}{\alpha_1^{-1} - \alpha_2 + (\alpha_2 - \alpha_1)\sin^2\phi}, \tag{3.65}$$

and we find that

$$\frac{d\zeta}{[(1-\alpha_1\zeta)(\zeta-\alpha_1)(1-\alpha_2\zeta)(\alpha_2-\zeta)]^{1/2}} = \frac{2d\phi}{(1-\alpha_1\alpha_2)(1-k_<^2\sin^2\phi)^{1/2}}, \tag{3.66}$$

with

$$k_< = \frac{\alpha_2 - \alpha_1}{1 - \alpha_1\alpha_2} = (\sinh 2\beta E_1 \sinh 2\beta E_2)^{-1} \tag{3.67}$$

and obtain

$$\begin{aligned} u = &-\frac{2E_1}{\pi}(\alpha_1 - \alpha_1^{-1})(\alpha_2^{-1} - \alpha_1)^{-1} \\ &\times \int_0^{\pi/2} d\phi \left[1 - \frac{1 + \alpha_1\alpha_2^{-1}}{1 + (\alpha_2 - \alpha_1)(\alpha_1^{-1} - \alpha_2)^{-1}\sin^2\phi}\right] \\ &\times (1 - k_<^2 \sin^2\phi)^{-1/2} + (E_1 \leftrightarrow E_2) \\ = &-\frac{2E_1}{\pi}(\alpha_1 - \alpha_1^{-1})(\alpha_2^{-1} - \alpha_1)^{-1}[\mathbf{K}(k_<) - (1 + \alpha_1\alpha_2^{-1})\Pi_1(\alpha_1 k_<, k_<)] \\ &+ (E_1 \leftrightarrow E_2). \end{aligned} \tag{3.68}$$

Similarly, when $T > T_c$ ($\alpha_2 > 1$), we may use the substitution

$$\zeta = \frac{\alpha_1(\alpha_1^{-1} - \alpha_2^{-1}) + \alpha_1^{-1}(\alpha_2^{-1} - \alpha_1)\sin^2\phi}{\alpha_1^{-1} - \alpha_2^{-1} + (\alpha_2^{-1} - \alpha_1)\sin^2\phi}, \tag{3.69}$$

and find

$$\begin{aligned} u = &-\frac{2E_1}{\pi}(\alpha_1 - \alpha_1^{-1})\alpha_2(1 - \alpha_1\alpha_2^{-1})^{-1} \\ &\times [\mathbf{K}(k_>) - (1 + \alpha_1\alpha_2^{-1})\Pi_1(\alpha_1 k_>, k_>)] + (E_1 \leftrightarrow E_2), \end{aligned} \tag{3.70}$$

where

$$k_> = \frac{\alpha_2^{-1} - \alpha_1}{1 - \alpha_1\alpha_2^{-1}} = k_<^{-1} = \sinh 2\beta E_1 \sinh 2\beta E_2. \tag{3.71}$$

We could continue an analysis just as we did for the case $E_1 = E_2$, by developing formulas for $\partial\Pi_1/\partial\nu$ and $\partial\Pi_1/\partial k$ which can be used in (3.68) and (3.70) to obtain expressions for c in terms of $\mathbf{E}$, $\mathbf{K}$, and Π_1. Then for $T \sim T_c$ it remains to develop an approximation to $\Pi_1(\nu, k)$ when $k \sim 1$, to study the continuity of u and the logarithmic divergence of c.

We choose not to pursue this line of analysis for two reasons. First, the resulting expression for the specific heat contains a forest of hyperbolic functions. Secondly, the expressions (3.68) and (3.70), which involve elliptic integrals of the third kind, do not manifestly reduce to (3.34) when $E_1 = E_2$. Therefore, to make the simplification for $E_1 = E_2$ more apparent and to obtain a more compact form of the final answer, we will present the method of reduction of u to elliptic integrals which was originally used by Onsager.

Our starting point is (3.63). We consider first $T > T_c$. The square root is defined to be $+1$ when $\theta = \pi$ and, for $T > T_c$, it is easily seen that when $\theta = 0$ the integrand is -1. Furthermore, when $\theta \to -\theta$ the integrand (which is in general complex) goes into its reciprocal. Therefore, we can rewrite the coefficient of E_1 in (3.63) as

$$-\pi^{-1}\int_0^{\pi} d\theta \cos \psi(\theta), \tag{3.72}$$

where

$$\cos \psi = \frac{1}{2}\left\{\left[\frac{(1-\alpha_1 e^{i\theta})(1-\alpha_2 e^{-i\theta})}{(1-\alpha_1 e^{-i\theta})(1-\alpha_2 e^{i\theta})}\right]^{1/2} + \left[\frac{(1-\alpha_1 e^{-i\theta})(1-\alpha_2 e^{i\theta})}{(1-\alpha_1 e^{i\theta})(1-\alpha_2 e^{-i\theta})}\right]^{1/2}\right\} \tag{3.73}$$

and in particular

$$\psi(0) = \pi, \qquad \psi(\pi) = 0. \tag{3.74}$$

We achieve a reduction to a complete elliptic integral by considering ψ as the independent variable instead of θ. Therefore,

$$\int_0^{\pi} d\theta \cos \psi(\theta) = \int_0^{\pi} d\psi \left|\frac{\partial \theta}{\partial \psi}\right| \cos \psi. \tag{3.75}$$

For (3.75) to be useful, we must be able to compute $\partial\theta/\partial\psi$ explicitly as a function of ψ alone. To do this, we first use the definition of α_1 and α_2 in (3.73) to find

$$\begin{aligned} \cos \psi = {} & (\sinh 2\beta E_1 \cosh 2\beta E_2 - \cosh 2\beta E_1 \cos \theta) \\ & \times \{[\cosh 2\beta E_1 \cosh 2\beta E_2 - \sinh 2\beta E_1 \cos \theta - \sinh 2\beta E_2] \\ & \times [\cosh 2\beta E_1 \cosh 2\beta E_2 - \sinh 2\beta E_1 \cos \theta + \sinh 2\beta E_2]\}^{-1/2}. \end{aligned} \tag{3.76}$$

This equation may be solved for $\cos \theta$, giving

$$-\cos \theta = \frac{\cosh 2\beta E_1 \cos \psi - k_> \coth 2\beta E_2 (1 - k_>^2 \sin^2 \psi)^{1/2}}{\cosh 2\beta E_1 (1 - k_>^2 \sin^2 \psi)^{1/2} - k_> \coth 2\beta E_2 \cos \psi}. \tag{3.77}$$

From this we easily obtain

$$\begin{aligned} \sin \theta &= (1 - \cos^2 \theta)^{1/2} \\ &= \frac{(1 - k_>^2) \sin \psi}{\cosh 2\beta E_1 (1 - k_>^2 \sin^2 \psi)^{1/2} - k_> \coth 2\beta E_2 \cos \psi}. \end{aligned} \tag{3.78}$$

Then if we differentiate (3.78) and use (3.77), we find

$$-\frac{\partial\theta}{\partial\psi} = (1 - k_>^2)(1 - k_>^2 \sin^2\psi)^{-1/2} \times [\cosh 2\beta E_1(1 - k_>^2 \sin^2\psi)^{1/2} - k_> \coth 2\beta E_2 \cos\psi]^{-1}. \tag{3.79}$$

This may now be used in (3.75) and, if we note that

$$[\cosh 2\beta E_1(1 - k_>^2 \sin^2\psi)^{1/2} - k_> \coth 2\beta E_2 \cos\psi]^{-1} = [\cosh 2\beta E_1(1 - k_>^2 \sin^2\psi)^{1/2} + k_> \coth 2\beta E_2 \cos\psi](1 - k_>^2)^{-1} \times (1 + \sinh^2 2\beta E_1 \sin^2\psi)^{-1}, \tag{3.80}$$

we obtain

$$\begin{aligned}\int_0^\pi d\theta \cos\psi(\theta) &= \int_0^\pi d\psi \left|\frac{\partial\theta}{\partial\psi}\right| \cos\psi \\ &= \int_0^\pi d\psi \frac{k_> \coth 2\beta E_2 \cos^2\psi}{(1 + \sinh^2 2\beta E_1 \sin^2\psi)(1 - k_>^2 \sin^2\psi)^{1/2}} \\ &= 2 \coth 2\beta E_1 \cosh 2\beta E_1 \cosh 2\beta E_2\, \Pi_1(\sinh^2 2\beta E_1, k_>) \\ &\quad - 2 \operatorname{csch} 2\beta E_1 \cosh 2\beta E_2\, \mathbf{K}(k_>).\end{aligned} \tag{3.81}$$

Therefore, when $T > T_c$,

$$\begin{aligned}u = &-(2/\pi)E_1 \coth 2\beta E_1 \cosh 2\beta E_1 \cosh 2\beta E_2 \\ &\times [\Pi_1(\sinh^2 2\beta E_1, k_>) - \operatorname{sech}^2 2\beta E_1\, \mathbf{K}(k_>)] \\ &- (2/\pi)E_2 \coth 2\beta E_2 \cosh 2\beta E_1 \cosh 2\beta E_2 \\ &\times [\Pi_1(\sinh^2 2\beta E_2, k_>) - \operatorname{sech}^2 2\beta E_2\, \mathbf{K}(k_>)].\end{aligned} \tag{3.82}$$

From this expression for u we may regain (3.34) by the application of a few identities from the theory of elliptic integrals. In particular, $\Pi_1(\nu, k)$ satisfies the relation[10]

$$\Pi_1(\nu, k) + \Pi_1\left(\frac{k^2}{\nu}, k\right) = \mathbf{K}(k) + \frac{\pi}{2}\left[(1 + \nu)\left(1 + \frac{k^2}{\nu}\right)\right]^{-1/2}. \tag{3.83}$$

It is evident from (3.71) and (3.82) that when $E_1 = E_2 = E$

$$k_> = \sinh^2 2\beta E \tag{3.84}$$

and

$$u = -4\pi^{-1}E \coth 2\beta E \cosh^2 2\beta E[\Pi_1(k_>, k_>) - \operatorname{sech}^2 2\beta E\, \mathbf{K}(k_>)]. \tag{3.85}$$

10. See, for example, A. Cayley, *An Elementary Treatise on Elliptic Functions*, (Dover Publication, New York, 1961), p. 120.

But from (3.83) we find

$$\Pi_1(k_>, k_>) = \frac{1}{2}\mathrm{K}(k_>) + \frac{\pi}{4}\operatorname{sech}^2 2\beta E. \tag{3.86}$$

Therefore

$$u = -E\coth 2\beta E[1 + 2\pi^{-1}\cosh^2 2\beta E(2\tanh^2 2\beta E - 1)\mathrm{K}(k_>)]. \tag{3.87}$$

This is not quite yet of the form (3.34). However, if we transform the integral (3.27) which defines $\mathrm{K}(k_>)$ by making the quadratic Landen substitution

$$\sin\phi' = \frac{(1 + k_>)\sin\phi}{1 + k_>\sin^2\phi}, \tag{3.88}$$

we find that

$$\mathrm{K}(k_>) = \frac{1}{1 + k_>}\mathrm{K}\left(\frac{2k_>^{1/2}}{1 + k_>}\right). \tag{3.89}$$

But

$$\frac{2k_>^{1/2}}{1 + k_>} = \frac{2\sinh 2\beta E}{(\cosh 2\beta E)^2}, \tag{3.90}$$

and therefore (3.87) reduces to (3.34).

A similar reduction procedure may be carried out when $T < T_c$. However, in this case, the expression on the right-hand side of (3.77) does not go monotonically from -1 to 1 as θ goes from 0 to π. Instead it goes from 1 when θ is π through some minimum value and then increases again so that it is again 1 when $\theta = 0$. Therefore the substitution (3.73) is no longer appropriate. To find what substitution should be used instead, we consider

$$\frac{1}{2}\left\{\left[\frac{(1 - \alpha_1 e^{i\theta})(1 - \alpha_2 e^{-i\theta})}{(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{i\theta})}\right]^{1/2} - \left[\frac{(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{i\theta})}{(1 - \alpha_1 e^{i\theta})(1 - \alpha_2 e^{-i\theta})}\right]^{1/2}\right\}, \tag{3.91}$$

which, if we use the definitions of α_1 and α_2 from (3.4), is equal to

$$\sin\theta[(\cosh 2\beta E_1\cosh 2\beta E_2 - \sinh 2\beta E_1\cos\theta)^2 - \sinh^2 2\beta E_2]^{-1/2}. \tag{3.92}$$

Since $T < T_c$, it is straightforward to show that the value of θ lying in the range 0 to π at which (3.92) reaches its maximum is given by

$$\cos\theta_m = \coth 2\beta E_1 \operatorname{sech} 2\beta E_2 \tag{3.93}$$

and that the value of this maximum is $k_<$. Therefore the substitution which is analogous to (3.73) or (3.77) is

$$k_<\sin\psi$$
$$= \frac{2}{1}\left\{\left[\frac{(1 - \alpha_1 e^{i\theta})(1 - \alpha_2 e^{-i\theta})}{(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{i\theta})}\right]^{1/2} - \left[\frac{(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{i\theta})}{(1 - \alpha_1 e^{i\theta})(1 - \alpha_2 e^{-i\theta})}\right]^{1/2}\right\}. \tag{3.94}$$

Using this substitution we have

$$(1 - k_<^2 \sin^2 \psi)^{1/2}$$
$$= \frac{1}{2}\left\{\left[\frac{(1 - \alpha_1 e^{i\theta})(1 - \alpha_2 e^{-i\theta})}{(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{i\theta})}\right]^{1/2} + \left[\frac{(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{i\theta})}{(1 - \alpha_1 e^{i\theta})(1 - \alpha_2 e^{-i\theta})}\right]^{1/2}\right\}. \quad (3.95)$$

Therefore we obtain

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta \left[\frac{(1 - \alpha_1 e^{i\theta})(1 - \alpha_2 e^{-i\theta})}{(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{i\theta})}\right]^{1/2} = \frac{1}{\pi}\int_0^{\pi} d\psi \left|\frac{\partial \theta}{\partial \psi}\right| (1 - k_<^2 \sin^2 \psi)^{1/2}. \quad (3.96)$$

The reduction now is entirely similar to the case $T > T_c$. We solve (3.94) for $\cos \theta$ to find

$$-\cos \theta = \frac{\coth 2\beta E_2 \cos \psi - k_< \cosh 2\beta E_1 (1 - k_<^2 \sin^2 \psi)^{1/2}}{\coth 2\beta E_2 (1 - k_<^2 \sin^2 \psi)^{1/2} - k_< \cosh 2\beta E_1 \cos \psi} \quad (3.97)$$

and

$$\sin \theta = \frac{(1 - k_<^2) \sin \psi}{\coth 2\beta E_2 (1 - k_<^2 \sin^2 \psi)^{1/2} - k_< \cosh 2\beta E_1 \cos \psi}. \quad (3.98)$$

From these we obtain

$$-\frac{\partial \theta}{\partial \psi}$$
$$= \frac{1 - k_<^2}{[\coth 2\beta E_2 (1 - k_<^2 \sin^2 \psi)^{1/2} - k_< \cosh 2\beta E_1 \cos \psi](1 - k_<^2 \sin^2 \psi)^{1/2}}, \quad (3.99)$$

which we use to show that the right-hand side of (3.96) is explicitly written as

$$\frac{1}{\pi}\int_0^{\pi} d\psi \frac{1 - k_<^2}{\coth 2\beta E_2 (1 - k_<^2 \sin^2 \psi)^{1/2} - k_< \cosh 2\beta E_1 \cos \psi}. \quad (3.100)$$

We further note that

$$[\coth 2\beta E_2 (1 - k_<^2 \sin^2 \psi)^{1/2} - k_< \cosh 2\beta E_1 \cos \psi]^{-1}$$
$$= [\coth 2\beta E_2 (1 - k_<^2 \sin^2 \psi)^{1/2} + k_< \cosh 2\beta E_1 \cos \psi]$$
$$\times [(1 - k_<^2)(1 + \operatorname{csch}^2 2\beta E_2 \sin^2 \psi)]^{-1}. \quad (3.101)$$

With this identity (3.100) reduces to

$$\frac{1}{\pi}\int_0^{\pi} d\psi \frac{\coth 2\beta E_2 (1 - k_<^2 \sin^2 \psi)^{1/2}}{1 + \operatorname{csch}^2 2\beta E_2 \sin^2 \psi}$$
$$= \frac{2}{\pi} \coth 2\beta E_2 \coth^2 2\beta E_1 [\Pi_1(\operatorname{csch}^2 2\beta E_2, k_<) - \operatorname{sech}^2 2\beta E_1 \, \mathbf{K}(k_<)]. \quad (3.102)$$

Therefore, when $T < T_c$ we have the desired result:

$$u = -\frac{2E_1}{\pi}\coth 2\beta E_2 \coth^2 2\beta E_1[\Pi_1(\operatorname{csch}^2 2\beta E_2, k_<) - \operatorname{sech}^2 2\beta E_1\, \mathbf{K}(k_<)]$$

$$-\frac{2E_2}{\pi}\coth 2\beta E_1 \coth^2 2\beta E_2[\Pi_1(\operatorname{csch}^2 2\beta E_1, k_<) - \operatorname{sech}^2 2\beta E_2\, \mathbf{K}(k_<)]. \quad (3.103)$$

As was the case with (3.82), we find that, as expected when $E_1 = E_2$, the use of (3.84) and the Landen transformation (3.88) reduces (3.103) to (3.34).

We now compute the specific heat by differentiating u with respect to T. To do this we need to differentiate $\Pi_1(\nu, k)$ with respect to ν and k. Consider first

$$\frac{\partial \Pi_1(\nu, k)}{\partial k} = k\int_0^{\pi/2} d\phi \frac{\sin^2\phi}{(1 + \nu\sin^2\phi)(1 - k^2\sin^2\phi)\Delta}. \quad (3.104)$$

Using

$$\frac{\sin^2\phi}{(1 + \nu\sin^2\phi)(1 - k^2\sin^2\phi)} = \frac{1}{\nu + k^2}\left(\frac{1}{1 - k^2\sin^2\phi} - \frac{1}{1 + \nu\sin^2\phi}\right), \quad (3.105)$$

we find

$$\frac{\partial \Pi_1(\nu, k)}{\partial k} = \frac{k}{\nu + k^2}\left[\int_0^{\pi/2} d\phi\Delta^{-3} - \Pi_1(\nu, k)\right], \quad (3.106)$$

from which, with the aid of (3.40), we obtain

$$\frac{\partial \Pi_1(\nu, k)}{\partial k} = \frac{k}{\nu + k^2}[k'^{-2}\mathbf{E}(k) - \Pi_1(\nu, k)]. \quad (3.107)$$

It is only slightly more difficult to compute $\partial\Pi_1(\nu, k)/\partial\nu$. From the definition (3.59),

$$\frac{\partial \Pi_1(\nu, k)}{\partial \nu} = -\int_0^{\pi/2} \frac{\sin^2\phi\, d\phi}{(1 + \nu\sin^2\phi)^2\Delta}$$

$$= \frac{1}{\nu}\int_0^{\pi/2}\frac{d\phi}{(1 + \nu\sin^2\phi)^2\Delta} - \frac{1}{\nu}\Pi_1(\nu, k). \quad (3.108)$$

By directly carrying out the differentiation we verify that

$$\frac{d}{d\phi}\frac{\Delta\sin\phi\cos\phi}{1 + \nu\sin^2\phi} = 2(1 + \nu^{-1})(1 + k^2\nu^{-1})(1 + \nu\sin^2\phi)^{-2}\Delta^{-1}$$

$$- [1 + 2\nu^{-1}(1 + k^2) + 3k^2\nu^{-2}](1 + \nu\sin^2\phi)^{-1}\Delta^{-1}$$

$$+ k^2\nu^{-2}(1 + \nu\sin^2\phi)\Delta^{-1}. \quad (3.109)$$

Therefore

$$
\begin{aligned}
2(1+\nu^{-1})\left(1+\frac{k^2}{\nu}\right)\int_0^{\pi/2} \frac{d\phi}{(1+\nu\sin^2\phi)^2\Delta} \\
= \left[1+\frac{2}{\nu}(1+k^2)+\frac{3k^2}{\nu^2}\right]\int_0^{\pi/2}\frac{d\phi}{(1+\nu\sin^2\phi)\Delta} \\
-\frac{k^2}{\nu^2}\int_0^{\pi/2} d\phi(1+\nu\sin^2\phi)\Delta^{-1}.
\end{aligned}
\tag{3.110}
$$

However,

$$
k^2\int_0^{\pi/2} d\phi(1+\nu\sin^2\phi)\Delta^{-1} = (k^2+\nu)\mathbf{K}(k) - \nu\mathbf{E}(k),
\tag{3.111}
$$

and hence we obtain

$$
\begin{aligned}
\frac{\partial\Pi_1(\nu,k)}{\partial\nu} &= \frac{1}{2(1+\nu)(1+k^2\nu^{-1})} \\
&\times\left[\left(\frac{k^2}{\nu^2}-1\right)\Pi_1(\nu,k) - \frac{1}{\nu^2}(k^2+\nu)\mathbf{K}(k) + \frac{1}{\nu}\mathbf{E}(k)\right].
\end{aligned}
\tag{3.112}
$$

With the aid of (3.42), (3.107), and (3.112) it is completely straightforward to differentiate the expressions for u given by (3.82) and (3.103) to obtain the desired results that when $T > T_c$

$$
\begin{aligned}
\frac{c}{k_0} = \frac{4\beta^2}{\pi}\Bigg\{&\left(\frac{E_1}{\sinh 2\beta E_1}\right)^2 \cosh 2\beta E_1 \cosh 2\beta E_2 \\
&\times [\mathbf{K}(k_>) - \Pi_1(\sinh^2 2\beta E_1, k_>)] \\
&+ \left(\frac{E_2}{\sinh 2\beta E_2}\right)^2 \cosh 2\beta E_1 \cosh 2\beta E_2 \\
&\times [\mathbf{K}(k_>) - \Pi_1(\sinh^2 2\beta E_2, k_>)] \\
&+ 2\frac{E_1E_2}{\sinh 2\beta E_1 \sinh 2\beta E_2}[\mathbf{K}(k_>) - \mathbf{E}(k_>)]\Bigg\},
\end{aligned}
\tag{3.113}
$$

and if $T < T_c$

$$
\begin{aligned}
\frac{c}{k_0} = \frac{4\beta^2}{\pi}\Bigg\{&\left(\frac{E_1}{\sinh 2\beta E_1}\right)^2 \coth 2\beta E_1 \coth 2\beta E_2 \\
&\times [\mathbf{K}(k_<) - \Pi_1(\operatorname{csch}^2 2\beta E_2, k_<)] \\
&+ \left(\frac{E_2}{\sinh 2\beta E_2}\right)^2 \coth 2\beta E_1 \coth 2\beta E_2 \\
&\times [\mathbf{K}(k_<) - \Pi_1(\operatorname{csch}^2 2\beta E_1, k_<)] \\
&+ 2E_1E_2[\mathbf{K}(k_<) - \mathbf{E}(k_<)]\Bigg\}.
\end{aligned}
\tag{3.114}
$$

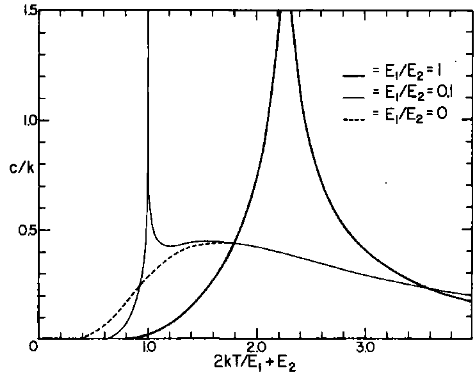


Fig. 5.12. Specific heat of Onsager's lattice for $E_2/E_1 = 1$, $E_2/E_1 = 0.01$, and $E_2/E_1 = 0$. The abscissa of the graph is $2kT/(E_1 + E_2)$, which ensures that the areas under all the curves are the same.

Using these formulas we plot the specific heat in Fig. 5.12 for several values of E_1/E_2.

It remains only to demonstrate that the critical behavior of u and c in this general case is the same as was previously found when $E_1 = E_2$. To study this behavior we need, in addition to the expansion for $\mathbf{K}(k)$ and $\mathbf{E}(k)$ obtained in (3.46) and (3.53), an approximation for $\Pi_1(\nu, k)$ when $k \sim 1$. This approximation is obtained if we write

$$\begin{aligned}\Pi_1(\nu, k) &= \int_0^{\pi/2} \frac{d\phi}{(1+\nu)(1 - k^2 \sin^2\phi)^{1/2}} \\ &\quad + \int_0^{\pi/2} \frac{d\phi}{(1 - k^2\sin^2\phi)^{1/2}} \left(\frac{1}{1+\nu\sin^2\phi} - \frac{1}{1+\nu}\right) \\ &= \frac{1}{1+\nu}\mathbf{K}(k) + \frac{\nu}{1+\nu}\int_0^{\pi/2} d\phi \frac{\cos^2\phi}{(1+\nu\sin^2\phi)(1-k^2\sin^2\phi)^{1/2}}. \qquad (3.115)\end{aligned}$$

In the first term we use the expansion of $\mathbf{K}(k)$ (3.53) and in the second term we set $k = 1$ and find that for $k \sim 1$

$$\Pi_1(\nu, k) \sim \frac{1}{1+\nu}\ln\frac{4}{|k'|} + \frac{\nu^{1/2}}{1+\nu}\arctan \nu^{1/2}. \qquad (3.116)$$

With these approximations for $\mathbf{K}$, $\mathbf{E}$, and Π_1 we can easily study u and c near T_c. By substituting the approximation (3.53) and (3.116) in (3.82) and (3.103) [or into (3.68) and (3.70)], we find that $u(T)$ is continuous at T_c and that

$$u(T_c) = -\frac{2}{\pi}(E_1 \coth 2\beta_c E_1 \operatorname{gd} 2\beta_c E_1 + E_2 \coth 2\beta_c E_2 \operatorname{gd} 2\beta_c E_2), \qquad (3.117)$$

where

$$\operatorname{gd} x = \arctan \sinh x \tag{3.118}$$

is the Gudermannian of x. Furthermore we substitute (3.46), (3.53), and (3.116) in (3.113) and (3.114) and find that near T_c

$$\begin{aligned}\frac{c}{k_0} \sim \frac{2\beta_c^2}{\pi} \{ &(E_1^2 \sinh^2 2\beta_c E_2 + 2E_1E_2 + E_2^2 \sinh^2 2\beta_c E_1) \\ &\times [-\ln|1 - T/T_c| - \ln \tfrac{1}{4}\beta_c(E_1 \coth 2\beta_c E_1 + E_2 \coth 2\beta_c E_2)] \\ &- 2(E_1^2 \sinh^2 2\beta_c E_2 \operatorname{gd} 2\beta_c E_1 + 2E_1E_2 + E_2^2 \sinh^2 2\beta_c E_1 \operatorname{gd} 2\beta_c E_2)\}.\end{aligned} \tag{3.119}$$

Therefore, as in the special case $E_1 = E_2$, the specific heat has a logarithmic singularity at T_c. Furthermore, as in (3.58), the coefficient of the logarithm and the additive constant are the same for T above and below T_c.

This completes the analysis of the specfiic heat of Onsager's lattice in the thermodynamic limit. However, it may be asked how these results are related to the case of a lattice that is large but finite, since for such a lattice the specific heat must be an analytic (and hence bounded) function of temperature for all T. This question was studied by Onsager in his original paper[11] for the special case where $\mathcal{N} \to \infty$ but $\mathcal{M}$ is finite and was studied in great detail for the general case of $\mathcal{M}$ and $\mathcal{N}$ both large but $\mathcal{M}/\mathcal{N}$ of order one by Ferdinand and Fisher.[12] We could reproduce the results of these papers if we carried out a detailed analysis of the partition function of a finite lattice given by (2.12). However, as our primary interest is in the case $\mathcal{M} \to \infty$ and $\mathcal{N} \to \infty$ and as the computations are somewhat involved we will not pursue this topic in detail. Instead we will be content with the following remarks.

When $\mathcal{M}$ and $\mathcal{N}$ are large and $\mathcal{M}/\mathcal{N}$ is of order one, the specific heat deviates appreciably from the specific heat of the infinite lattice only when $(1 - T/T_c) \sim \mathcal{M}^{-1}$. The maximum of the specific heat of the finite lattice in general does not occur at T_c but at some other value which depends on $\mathcal{M}/\mathcal{N}$, and the height of this maximum grows as $\mathcal{M} \to \infty$ as $\ln \mathcal{M}$. In the case considered by Onsager $\mathcal{N} \to \infty$ and $\mathcal{M}$ finite the deviation of the position of the maximum from T_c is proportional to $\mathcal{M}^{-2} \ln \mathcal{M}$; and the value of the specific heat at this maximum is approximately given as

$$\begin{aligned}\frac{c}{k_0} \sim \frac{2\beta_c^2}{\pi} \{ &(E_1^2 \sinh 2\beta_c E_2 + 2E_1E_2 + E_2^2 \sinh 2\beta_c E_1) \\ &\times [\ln \mathcal{M} + \ln(8\pi^{-1} \operatorname{sech} 2\beta_c E_1) + \gamma] \\ &+ E_1^2 \sinh 2\beta_c E_2 - 2E_1E_2 + E_2^2 \sinh 2\beta_c E_1 \\ &- 2E_1^2 \sinh^2 2\beta_c E_2 \operatorname{gd} 2\beta_c E_1 - E_2^2 \sinh^2 2\beta_c E_1 \operatorname{gd} 2\beta_c E_2\},\end{aligned} \tag{3.120}$$

11. Reference 5.
12. A. E. Ferdinand and M. E. Fisher, *Phys. Rev.* **185**, 832 (1969).

where γ stands for Euler's constant and has the approximate value 0.577215.

4. THE ANTIFERROMAGNETIC SEAM

We close this chapter by returning to the one point in the calculation of $Z_{\mathcal{M},\mathcal{N}}$ which was not completed in Sec. 2, namely, the determination of the signs in (2.14). These signs are important because there is more than one term on the right-hand side of (2.12).

A straightforward method of determining these signs is to use (2.23) and (2.14) in (2.12) and then to adjust the signs to make the value of $Z_{\mathcal{M},\mathcal{N}}$ so obtained agree for certain special values of z_1 and z_2 with values of $Z_{\mathcal{M},\mathcal{N}}$ which may be independently computed. Then for values of z_1 and z_2 which may be joined to the special values by a path along which $\det A_i \neq 0$ the sign of $\det A_i$ will be fixed by the requirement that $\det A_i$ be a continuous function of z_1 and z_2. It is easily seen from (2.23) that $\det A_i = 0$ can occur only if

$$(1 + z_1^2)(1 + z_2^2) - 2|z_1|(1 - z_2^2) - 2|z_2|(1 - z_1^2) = 0. \tag{4.1}$$

When (4.1) is satisfied, $T = T_c$ and we have the following cases:

(1) if $E_1 > 0$ and $E_2 > 0$, then $\det A_1 = 0$;

(2) If $E_1 < 0$ and $E_2 > 0$, then $\det A_1 = 0$ when $\mathcal{N}$ is even and $\det A_3 = 0$ when $\mathcal{N}$ is odd;

(3) If $E_1 > 0$ and $E_2 < 0$, then $\det A_1 = 0$ when $\mathcal{M}$ is even and $\det A_2 = 0$ when $\mathcal{M}$ is odd; and

(4) if $E_1 < 0$ and $E_2 < 0$, then $\det A_1 = 0$ when $\mathcal{N}$ and $\mathcal{M}$ are both even, $\det A_2 = 0$ when $\mathcal{N}$ is even and $\mathcal{M}$ is odd, $\det A_3 = 0$ when $\mathcal{N}$ is odd and $\mathcal{M}$ is even, and $\det A_4 = 0$ when $\mathcal{N}$ and $\mathcal{M}$ are both odd.

From this list it is clear that, if z_1 and z_2 are suitably small so that (4.1) does not hold, then the signs of $(\det A_i)^{1/2}$ may be determined by continuity from the cases $z_1 = 0$ or $z_2 = 0$. However, for any value of $z_1 \neq 0$, if $|z_2|$ is made large enough (4.1) will eventually hold and the sign of one of the $(\det A_i)^{1/2}$ may change. For values of z_1 and z_2 in this region the sign of that $(\det A_i)^{1/2}$ which could change will be determined by continuity from $T = 0$. Therefore we consider several special cases.

(A) Here z_1 and z_2 are inside the curve in the z_1, z_2-plane specified by (4.1) (that is, $T > T_c$). If $z_2 = 0$,

$$\det A_1 = \det A_2 = \prod_{k=1}^{\mathcal{N}} \left(1 + z_1^2 - 2z_1 \cos \frac{2\pi k}{\mathcal{N}}\right)^{\mathcal{M}}$$

$$= \prod_{k=1}^{\mathcal{N}} |1 - z_1 e^{i\pi 2k/\mathcal{N}}|^{2\mathcal{M}} = (1 - z_1^{\mathcal{N}})^{2\mathcal{M}} \tag{4.2a}$$

and

$$\det A_3 = \det A_4 = \prod_{k=1}^{\mathscr{N}} \left[1 + z_1^2 - 2z_1 \cos \frac{\pi(2k-1)}{\mathscr{N}}\right]^{\mathscr{M}}$$

$$= \prod_{k=1}^{\mathscr{N}} |1 - z_1 e^{i\pi(2k-1)/\mathscr{N}}|^{2\mathscr{M}} = (1 + z_1^{\mathscr{N}})^{2\mathscr{M}}. \tag{4.2b}$$

Similarly, if $z_1 = 0$

$$\det A_1 = \det A_3 = (1 - z_2^{\mathscr{M}})^{2\mathscr{N}} \tag{4.2c}$$

and

$$\det A_2 = \det A_4 = (1 + z_2^{\mathscr{M}})^{2\mathscr{N}}. \tag{4.2d}$$

We know from (III.2.15) that if $z_2 = 0$

$$Z_{\mathscr{M},\mathscr{N}} = (2 \cosh \beta E_1)^{\mathscr{M}\mathscr{N}}(1 + z_1^{\mathscr{N}})^{\mathscr{M}}, \tag{4.3a}$$

and if $z_1 = 0$

$$Z_{\mathscr{M},\mathscr{N}} = (2 \cosh \beta E_2)^{\mathscr{M}\mathscr{N}}(1 + z_2^{\mathscr{M}})^{\mathscr{N}}. \tag{4.3b}$$

Therefore, combining (4.3) and (4.2) with (2.12) and (2.14), we conclude in this case that

$$Z_{\mathscr{M},\mathscr{N}} = \tfrac{1}{2}(2 \cosh \beta E_1 \cosh \beta E_2)^{\mathscr{M}\mathscr{N}} \times [-(\det A_1)^{1/2} + (\det A_2)^{1/2} + (\det A_3)^{1/2} + (\det A_4)^{1/2}]. \tag{4.4}$$

(*B*) In this case z_1 and z_2 are outside the curve in the z_1,z_2-plane specified by (4.1) ($T < T_c$). Now the signs in (2.14) are determined by continuity from $T = 0$. There are 3 subcases to consider:

(i) $E_1 > 0$, $E_2 > 0$ and $\mathscr{M}$ and $\mathscr{N}$ unrestricted; $E_1 > 0$, $E_2 < 0$, $\mathscr{N}$ even; $E_1 < 0$, $E_2 > 0$, $\mathscr{M}$ even; or $E_1 < 0$, $E_2 < 0$, $\mathscr{N}$ and $\mathscr{M}$ both even. Thus $\det A_1 = 0$ when (4.1) is satisfied. In this case the ground-state energy is

$$\mathscr{E}_{\min}(\sigma) = -\mathscr{M}\mathscr{N}(|E_1| + |E_2|). \tag{4.5}$$

This state is doubly degenerate. Therefore for $T \sim 0$

$$Z_{\mathscr{M},\mathscr{N}} \sim 2e^{\beta\mathscr{M}\mathscr{N}(|E_1|+|E_2|)}. \tag{4.6}$$

From (2.23) we see that as $T \to 0$

$$\det A_i \to 4^{\mathscr{M}\mathscr{N}}. \tag{4.7}$$

Thus, combining (4.7), (4.6), and (2.12) with (2.14) we conclude that

$$Z_{\mathscr{M},\mathscr{N}} = \tfrac{1}{2}(2 \cosh \beta E_1 \cosh \beta E_2)^{\mathscr{M}\mathscr{N}} \times [(\det A_1)^{1/2} + (\det A_2)^{1/2} + (\det A_3)^{1/2} + (\det A_4)^{1/2}]. \tag{4.8}$$

(ii) $E_1 < 0$, and E_2 unrestricted, with $\mathscr{N}$ odd and $\mathscr{M}$ even. Thus $\det A_3 = 0$ when (4.1) is satisfied. (The case E_1 unrestricted, $E_2 < 0$ with $\mathscr{M}$ odd and $\mathscr{N}$ even is obviously obtained from this case if $E_1 \leftrightarrow E_2$, $\mathscr{N} \leftrightarrow \mathscr{M}$.) One of the ground states for this case is shown in Fig. 5.13.

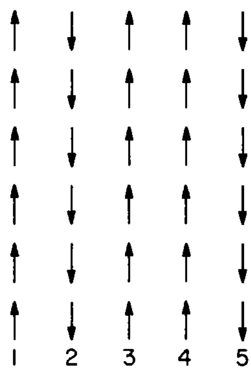


Fig. 5.13. One of the $2\mathscr{N}$ ground states of an $\mathscr{M} \times \mathscr{N}$ lattice ($\mathscr{N}$ odd) with an antiferromagnetic seam running in the vertical direction. The spins at opposite ends of the lattice are joined by cyclic boundary conditions. The antiferromagnetic seam is between columns 3 and 4.

This ground state deviates from a periodic up-down arrangement of spins in the horizontal direction by the necessity, due to the fact that $\mathscr{N}$ is odd, of having one column of bonds connecting spins pointing in the same direction. This column of mismatched spins is an antiferromagnetic seam such as we encountered in the ground state of the one-dimensional Ising model. The energy of this ground state is

$$\mathscr{E}_{\min}(\sigma) = -\mathscr{M}(\mathscr{N} - 2)|E_1| - \mathscr{M}\mathscr{N}|E_2| \tag{4.9}$$

and its degeneracy is $2\mathscr{N}$. Therefore, for $T \sim 0$,

$$Z_{\mathscr{M},\mathscr{N}} \sim 2\mathscr{N} e^{\beta\mathscr{M}[(\mathscr{N}-2)|E_1|+\mathscr{N}|E_2|]}. \tag{4.10}$$

By (4.7), $Z_{\mathscr{M},\mathscr{N}}$ must be given by (4.4), except that $(\det A_3)^{1/2}$ cannot have the same sign it had in (4.4), since otherwise (4.10) will surely fail. Therefore, we surmise that

$$Z_{\mathscr{M},\mathscr{N}} = \tfrac{1}{2}(2\cosh\beta E_1 \cosh\beta E_2)^{\mathscr{M}\mathscr{N}} \times [-(\det A_1)^{1/2} + (\det A_2)^{1/2} - (\det A_3)^{1/2} + (\det A_4)^{1/2}]. \tag{4.11}$$

To verify that (4.11) is indeed correct, we use an identity which is obtainable from (4.2):

$$\prod_{j=1}^{\mathcal{M}}\left(A - B\cos\frac{\pi 2j}{\mathcal{M}}\right)$$
$$= \{[\tfrac{1}{2}(A + \sqrt{A^2 - B^2})]^{\mathcal{M}/2} - [\tfrac{1}{2}(A - \sqrt{A^2 - B^2})]^{\mathcal{M}/2}\}^2 \tag{4.12a}$$

and

$$\prod_{j=1}^{\mathcal{M}}\left(A - B\cos\frac{\pi(2j-1)}{\mathcal{M}}\right)$$
$$= \{[\tfrac{1}{2}(A + \sqrt{A^2 - B^2})]^{\mathcal{M}/2} + [\tfrac{1}{2}(A - \sqrt{A^2 - B^2})]^{\mathcal{M}/2}\}^2. \tag{4.12b}$$

Then we find that as $T \to 0$

$$(\det A_2)^{1/2} - (\det A_1)^{1/2}$$
$$\sim \prod_{k=1}^{\mathcal{N}}\left[\frac{A(2k) + \sqrt{A^2(2k) - B^2}}{2}\right]^{\mathcal{M}/2-} + \mathcal{N}[z_2(1 - z_1^2)]^{\mathcal{M}}4^{-\mathcal{M}}2^{\mathcal{M}\mathcal{N}}$$
$$- \prod_{k=1}^{\mathcal{N}}\left[\frac{A(2k) + \sqrt{A^2(2k) - B^2}}{2}\right]^{\mathcal{M}/2} - \mathcal{N}[z_2(1 - z_1^2)]^{\mathcal{M}}4^{-\mathcal{M}}2^{\mathcal{M}\mathcal{N}}$$
$$\sim 2^{\mathcal{M}\mathcal{N}+1}4^{-\mathcal{M}}\mathcal{N}[z_2(1 - z_1^2)]^{\mathcal{M}}$$
$$\sim 2^{\mathcal{M}\mathcal{N}+1}\mathcal{N}e^{-\beta 2\mathcal{M}|E_1|}, \tag{4.13}$$

where

$$A(k) = (1 + z_1^2)(1 + z_2^2) - 2z_1(1 - z_2^2)\cos\frac{\pi k}{\mathcal{N}}. \tag{4.14}$$

Similarly

$$(\det A_3)^{1/2} - (\det A_4)^{1/2} \sim 2^{\mathcal{M}\mathcal{N}+1}\mathcal{N}e^{-2\beta\mathcal{M}|E_1|}. \tag{4.15}$$

Hence, it follows that (4.11) reduces to (4.10) as $T \to 0$.

(iii) $E_1 < 0$, $E_2 < 0$ with $\mathcal{M}$ and $\mathcal{N}$ odd. Thus $\det A_4 = 0$ when (4.1) is satisfied. In this case at $T = 0$ there will be two antiferromagnetic seams, one in the vertical and one in the horizontal directions. The energy of this ground state is

$$\mathcal{E}_{\min}(\sigma) = -\mathcal{M}(\mathcal{N} - 2)|E_1| - (\mathcal{M} - 2)\mathcal{N}|E_2|, \tag{4.16}$$

and its degeneracy is $(2\mathcal{M})(2\mathcal{N})$. Therefore, it may be verified by a slight extension of the previous procedure that

$$Z_{\mathcal{M},\mathcal{N}} = \tfrac{1}{2}(2\cosh\beta E_1\cosh\beta E_2)^{\mathcal{M}\mathcal{N}}$$
$$\times [-(\det A_1)^{1/2} + (\det A_2)^{1/2} + (\det A_3)^{1/2} - (\det A_4)^{1/2}]. \tag{4.17}$$

The skeptic may now argue with the somewhat cavalier manner with which we obtained the free energy per site in the thermodynamic limit from $Z_{\mathscr{M},\mathscr{N}}$ in Sec. 2. There we simply took the logarithm of $(\det A_i)^{1/2}$ and converted the resulting sum to an integral by the use of the definition of integral. In other words, we made the approximation

$$(\det A_i)^{1/2} \sim \exp\left\{\mathscr{M}\mathscr{N}(2\pi)^{-2}\int_0^{2\pi} d\theta_1 \int_0^{2\pi} d\theta_2 \ln\left[(1+z_1^2)(1+z_2^2) - 2z_1(1-z_2^2)\cos\theta_1 - 2z_2(1-z_1^2)\cos\theta_2\right]\right\}. \tag{4.18}$$

This approximation is the same for $i = 1, 2, 3$, and 4. Therefore, if $T > T_c$ we may use (4.4) to find

$$Z_{\mathscr{M},\mathscr{N}} \sim e^{\mathscr{M}\mathscr{N}\beta F}, \tag{4.19}$$

and, if $T < T_c$ and the conditions of (B, i) hold so that there is no antiferromagnetic seam, we use (4.8) to find

$$Z_{\mathscr{M},\mathscr{N}} \sim 2e^{-\mathscr{M}\mathscr{N}\beta F}. \tag{4.20}$$

However, if $T < T_c$ and the conditions of (B, ii) or (B, iii) hold, so that there is (at least) one antiferromagnetic seam, the use of the approximation (4.18) in (4.11) or (4.17) yields

$$Z_{\mathscr{M},\mathscr{N}} \sim 0\cdot e^{-\mathscr{M}\mathscr{N}\beta F} = 0. \tag{4.21}$$

To demonstrate that this "vanishing" of the partition function does not invalidate the previous calculation and analysis of the free energy, we will present a more precise approximation for $Z_{\mathscr{M},\mathscr{N}}$ under the conditions of (B, ii) than that given by (4.21). We first use the exact evaluations (4.12) in (4.11) to write

$$\begin{aligned}
Z_{\mathscr{M},\mathscr{N}} = \tfrac{1}{2}(2\cosh\beta E_1 \cosh\beta E_2) \times \Bigg[&- \prod_{k=1}^{\mathscr{N}} \{[\tfrac{1}{2}(A(2k) + \sqrt{A^2(2k) - B^2})]^{\mathscr{M}/2} \\
&- [\tfrac{1}{2}(A(2k) - \sqrt{A^2(2k) - B^2})]^{\mathscr{M}/2}\} \\
&+ \prod_{k=1}^{\mathscr{N}} \{[\tfrac{1}{2}(A(2k) + \sqrt{A^2(2k) - B^2})]^{\mathscr{M}/2} \\
&+ [\tfrac{1}{2}(A(2k) - \sqrt{A^2(2k) - B^2})]^{\mathscr{M}/2}\} \\
&- \prod_{k=1}^{\mathscr{N}} \{[\tfrac{1}{2}(A(2k-1) + \sqrt{A^2(2k-1) - B^2})]^{\mathscr{M}/2} \\
&- [\tfrac{1}{2}(A(2k-1) - \sqrt{A^2(2k-1) - B^2})]^{\mathscr{M}/2}\} \\
&+ \prod_{k=1}^{\mathscr{N}} \{[\tfrac{1}{2}(A(2k-1) + \sqrt{A^2(2k-1) - B^2})]^{\mathscr{M}/2} \\
&+ [\tfrac{1}{2}(A(2k-1) - \sqrt{A^2(2k-1) - B^2})]^{\mathscr{M}/2}\}\Bigg]
\end{aligned} \tag{4.22}$$

when $B = 2z_2(1 - z_1^2)$. The factors in each product are the sums of two terms, the second of which is exponentially smaller than the first when $\mathscr{M} \to \infty$. Approximation (4.21) is obtained by omitting these terms. Since this approximation vanishes, we must continue to the next order of approximation. Thus we find

$$Z_{\mathscr{M},\mathscr{N}} \sim e^{-\mathscr{M}\mathscr{N}\beta F} \sum_{k=1}^{2\mathscr{N}} \left[\frac{A(k) - \sqrt{A^2(k) - B^2}}{A(k) + \sqrt{A^2(k) - B^2}}\right]^{\mathscr{M}/2}. \tag{4.23}$$

The first factor in this approximation is independent of shape and gives the free energy per site discussed in Sec. 2. The second factor, however, is more complicated. If $T \to 0$ it is approximated by

$$2\mathscr{N} e^{-2\beta|E_1|\mathscr{M}}, \tag{4.24}$$

which is in conformity with (4.10). On the other hand, if $0 < T < T_c$ and $\mathscr{M} \gg \mathscr{N}$, then the sum is well approximated by its largest term. This term is easily seen to come from $k = \mathscr{N}$ and we have

$$Z_{\mathscr{M},\mathscr{N}} \sim \alpha(\pi)^{-\mathscr{M}} e^{\mathscr{M}\mathscr{N}\beta F}, \tag{4.25}$$

where we have used the α of (3.3); more specifically, we note that

$$\alpha(\pi)^{-1} = |z_2|^{-1}\left(\frac{1 - |z_1|}{1 + |z_1|}\right). \tag{4.26}$$

If we now let $T \to 0$ in (4.25) we obtain

$$Z_{\mathscr{M},\mathscr{N}} \sim e^{-\beta\mathscr{M}[(\mathscr{N}-1)|E_1| + |E_2|]}. \tag{4.27}$$

This does not agree with (4.10) since it lacks the factor $2\mathscr{N}$. Therefore, as far as the sum in (4.23) is concerned, the approximations which are valid for $\mathscr{M} \gg 1$ and $\mathscr{N} \gg 1$ with T fixed and positive fail in the $T \to 0$ limit.

The significance of the sum in (4.23) may be made clearer if we write

$$\sum_{k=1}^{2\mathscr{N}} \left[\frac{A(k) - \sqrt{A^2(k) - B^2}}{A(k) + \sqrt{A^2(k) - B^2}}\right]^{\mathscr{M}/2} = \alpha(\pi)^{-\mathscr{M}} \sum_{k=1}^{2\mathscr{N}} \left(\frac{\alpha(\theta_k)}{\alpha(\pi)}\right)^{-\mathscr{M}}. \tag{4.28}$$

Because $\alpha(\theta_k)/\alpha(\pi)$ has the minimum value of 1, the sum does not depend exponentially on $\mathscr{M}$. However, the value of the sum will depend on the manner in which $\mathscr{M} \to \infty$ and $\mathscr{N} \to \infty$. In particular, if $0 < T < T_c$ we may consider evaluating the sum by a steepest-descent method. Only the values of θ_k near π contribute and we may write

$$\alpha(\theta_k) \sim \alpha(\pi) + \tfrac{1}{2}[\theta_k - \pi]^2\alpha''(\pi). \tag{4.29}$$

Thus

$$\alpha(\pi)^{-\mathscr{M}} \sum_{k=1}^{2\mathscr{N}} \left(\frac{\alpha(\theta_k)}{\alpha(\pi)}\right)^{-\mathscr{M}} \sim \alpha(\pi)^{-\mathscr{M}} \sum_{k=0}^{\mathscr{N}} \left[1 + \frac{1}{2}\frac{\alpha''(\pi)}{\alpha(\pi)}\left(\frac{\pi k}{\mathscr{N}}\right)^2\right]^{-\mathscr{M}}, \tag{4.30}$$

and, if $\mathcal{N}$ is large and $\mathcal{M}/\mathcal{N}$ does not vanish as $\mathcal{N} \to \infty$, this is well approximated by

$$\alpha(\pi)^{-\mathcal{M}} \sum_{k=0}^{\infty} \exp - \frac{1}{2} \frac{\alpha''(\pi)}{\alpha(\pi)} \frac{\pi^2 k^2}{\mathcal{N}} \left(\frac{\mathcal{M}}{\mathcal{N}}\right). \tag{4.31}$$

We may consider how this sum behaves for various relations between $\mathcal{M}$ and $\mathcal{N}$. For example, if $\mathcal{M} = K\mathcal{N}$ as $\mathcal{N} \to \infty$, then (4.31) becomes

$$c(K)\alpha(\pi)^{-\mathcal{M}}\mathcal{N}^{1/2}, \tag{4.32}$$

where $c(K)$ depends on K alone and not on $\mathcal{M}$ or $\mathcal{N}$ separately. If $\mathcal{M} = K_1\mathcal{N}^2$ as $\mathcal{N} \to \infty$, then (4.31) becomes

$$c_1(K_1)\alpha(\pi)^{-\mathcal{M}}, \tag{4.33}$$

where, again, $c_1(K_1)$ depends only on K_1 and not on $\mathcal{M}$ or $\mathcal{N}$. In all cases the logarithm of the sum in (4.30) will vanish if we divide by $\mathcal{M}$ and let $\mathcal{M} \to \infty$, no matter how $\mathcal{M}$ and $\mathcal{N}$ are related. Therefore we conclude that if $\mathcal{M}$ and $\mathcal{N}$ are large

$$\ln Z_{\mathcal{M},\mathcal{N}} = -\mathcal{M}\mathcal{N}\beta F + \mathcal{M} \ln |z_2|^{-1}\left(\frac{1 - |z_1|}{1 + |z_1|}\right) + o(\mathcal{M}). \tag{4.34}$$

The first term in (4.34) gives the free energy per site of Sec. 2. The second term is proportional to $\mathcal{M}$ and exists only for the case in which an antiferromagnetic seam is present at $T = 0$. Accordingly, for $0 \leq T \leq T_c$, we follow Onsager[13] and interpret

$$\beta^{-1} \ln |z_2|^{-1}\left(\frac{1 - |z_1|}{1 + |z_1|}\right) \tag{4.35}$$

as the additional free energy per row in a lattice with an antiferromagnetic seam. In contrast to the one-dimensional case, this additional free energy does not vanish as soon as T becomes sensibly different from zero but remains nonzero until $T = T_c$. This reflects the not unexpected fact that the antiferromagnetic order which is present in one dimension only at $T = 0$ persists in two dimensions until $T = T_c$. However, it would be more satisfying if (4.35) could be computed directly from a knowledge of the antiferromagnetic order. Unfortunately, even though in Chapters X–XII we will learn a great deal about both ferromagnetic and antiferromagnetic order in Onsager's lattice, such a direct calculation of (4.35) has not been found.

13. Reference 5.

CHAPTER VI
Boundary Specific Heat and Magnetization

1. INTRODUCTION

The specific heat of Onsager's lattice at $H = 0$ computed in the last chapter is only the first of several quantities which we will study. More specifically, we will later concern ourselves with the spontaneous magnetization and the spin-spin correlation functions of Onsager's lattice. Unfortunately, the study of these quantities requires the introduction of additional mathematical machinery, in particular, the theory of Wiener-Hopf sum equations. This machinery will be developed in detail in Chapter IX. However, even with these techniques, it has not yet proved possible to compute the free energy, to say nothing of the spin-spin correlation functions, of the Onsager lattice in the presence of a magnetic field. Therefore complete information about magnetic properties of Onsager's lattice is not available. For example, we do not possess analytic expressions for the behavior of the magnetization at $T = T_c$ near $H = 0$. In other words, the one-dimensional Ising model can be completely solved but shows no phase transition, while the two-dimensional Ising model discussed in the last chapter cannot yet be solved exactly in the presence of a magnetic field.

We therefore look for a model somewhere intermediate between the one-dimensional and the two-dimensional Ising models. This model must have a phase transition in the absence of a magnetic field and still be exactly solvable for all values of the magnetic field. In this chapter we shall show that the boundary behavior of the two-dimensional Ising model has these two properties. More precisely, we impose on the Onsager lattice a cyclic boundary condition in the horizontal direction only and let a magnetic field $\mathfrak{H}$ interact with one of the two horizontal boundary rows of spins. Fortunately, in this case, the partition function can be studied exactly by the Pfaffian method of the last chapter, and we find that the logarithm of this partition function may be written

$$\mathcal{M}\mathcal{N}F + 2\mathcal{N}\mathfrak{F}_0 + \mathcal{N}\mathfrak{F}(\mathfrak{H}). \tag{1.1}$$

The term $\mathcal{M}\mathcal{N}F$ is the bulk free energy we obtained in the previous chapter. The terms $2\mathcal{N}\mathfrak{F}_0$ and $\mathcal{N}\mathfrak{F}(\mathfrak{H})$ are additional contributions coming from the existence of the free boundary which interacts with the magnetic field. Both $\mathfrak{F}_0$ and $\mathfrak{F}(\mathfrak{H})$, together with a number of other properties such as the spin-spin correlation function, can be computed exactly in the limit of the infinite lattice. This chapter is devoted to the study of these boundary contributions to the free energy,[1] while the correlation function of two spins on the boundary is the subject of the next chapter.

2. FORMULATION OF THE PROBLEM

The system to be studied in this chapter and the next is the Onsager lattice with cyclic boundary conditions imposed in the horizontal direction only. The lattice has $2\mathcal{M}$ rows and $2\mathcal{N}$ columns[2] and it interacts with a magnetic field $\mathfrak{H}$ applied to one of the two boundary rows (defined to be the first row). We use German letters to denote quantities pertaining to the boundary. The interaction energy for this system is

$$\begin{aligned}\mathscr{E} = -E_1 \sum_{j=1}^{2\mathcal{M}} \sum_{k=-\mathcal{N}+1}^{\mathcal{N}} \sigma_{j,k}\sigma_{j,k+1} \\ - E_2 \sum_{j=1}^{2\mathcal{M}-1} \sum_{k=-\mathcal{N}+1}^{\mathcal{N}} \sigma_{j,k}\sigma_{j+1,k} - \mathfrak{H} \sum_{k=-\mathcal{N}+1}^{\mathcal{N}} \sigma_{1,k},\end{aligned} \tag{2.1}$$

with $k = \mathcal{N} + 1$ identified with $k = -\mathcal{N} + 1$. The first row does *not* interact with the $2\mathcal{M}$th row. In (2.1), the magnetic-moment factor for the spins on the first row has been absorbed in $\mathfrak{H}$. We shall be interested in the limit $\mathcal{M} \to \infty$ and $\mathcal{N} \to \infty$ where the cylinder becomes a semi-infinite half-plane; only in this limit will a phase transition occur.

1. The material of this chapter and the next is taken from B. M. McCoy and T. T. Wu, *Phys. Rev.* **162**, 436 (1967). For an alternative derivation of some of the results of Sec. 4 see M. E. Fisher and A. E. Ferdinand, *Phys. Rev. Letters* **19**, 169 (1967).

2. We choose the number of columns and the number of rows to be both even to avoid all problems connected with a possible antiferromagnetic seam.

With (2.1), the partition function is

$$
\begin{aligned}
Z &= \sum_{\sigma=\pm 1} e^{-\beta\mathscr{E}} \\
&= \sum_{\sigma=\pm 1} \exp\left[\sum_{j=1}^{2\mathscr{M}} \sum_{k=-\mathscr{N}+1}^{\mathscr{N}} \beta E_1 \sigma_{j,k}\sigma_{j,k+1} \right. \\
&\qquad \left. + \sum_{j=1}^{2\mathscr{M}-1} \sum_{k=-\mathscr{N}+1}^{\mathscr{N}} \beta E_2 \sigma_{j,k}\sigma_{j+1,k} + \sum_{k=-\mathscr{N}+1}^{\mathscr{N}} \beta\mathfrak{H}\sigma_{1,k}\right] \\
&= (\cosh\beta E_1)^{4\mathscr{M}\mathscr{N}}(\cosh\beta E_2)^{2\mathscr{N}(2\mathscr{M}-1)}(\cosh\beta\mathfrak{H})^{2\mathscr{N}} \\
&\quad \times \sum_{\sigma=\pm 1}\left\{\left[\prod_{j=1}^{2\mathscr{M}} \prod_{k=-\mathscr{N}+1}^{\mathscr{N}} (1 + z_1\sigma_{j,k}\sigma_{j,k+1})\right]\right. \\
&\qquad \times \left[\prod_{j=1}^{2\mathscr{M}-1} \prod_{k=-\mathscr{N}+1}^{\mathscr{N}} (1 + z_2\sigma_{j,k}\sigma_{j+1,k})\right] \\
&\qquad \left. \times \left[\prod_{k=-\mathscr{N}+1}^{\mathscr{N}} (1 + z\sigma_{1,k})\right]\right\},
\end{aligned}
\tag{2.2}
$$

where

$$z = \tanh\beta\mathfrak{H}. \tag{2.3}$$

If the sum over $\sigma = \pm 1$ is carried out, the result is

$$Z = (2\cosh\beta E_1)^{4\mathscr{M}\mathscr{N}}(\cosh\beta E_2)^{2\mathscr{N}(2\mathscr{M}-1)}(\cosh\beta\mathfrak{H})^{2\mathscr{N}} \sum_{p,q,r} z_1^p z_2^q z^r N_{pqr}, \tag{2.4}$$

where N_{pqr} is the number of figures that can be drawn on the lattice with the following properties. First, each bond between nearest neighbors may be used, at most, once. Secondly, the figure contains p horizontal bonds and q vertical bonds. Thirdly, let e_{jk} be the number of bonds with the site (j, k) as one end; then, for $j > 1$, e_{jk} is even, that is, $e_{jk} = 0, 2$, or 4. And lastly, r is the number of e_{1k} which is odd. An example with $p = 12$, $q = 14$, and $r = 4$ is shown in Fig. 6.1(a).

We wish to express the sum in (2.4) in terms of an appropriate Pfaffian. To do so, we first note that if z is zero, then in the sum it is sufficient to keep only the terms with N_{pq0}, which is the number of *closed* polygons with p horizontal bonds and q vertical bonds. The factor $z_1^p z_2^q$ is taken into account by associating a factor z_1 with each horizontal bond and a factor z_2 with each vertical bond, as shown in Fig. 6.2. This procedure may also be followed for the case of general z by adding a zeroth row of sites connected to the first row of sites by vertical bonds of weight z. The sites in this zeroth row are also connected to each other by bonds of weight 1 between nearest neighbors, as shown in Fig. 6.3(a). Each figure on the original lattice counted in N_{pqr} corresponds, because of the cyclic

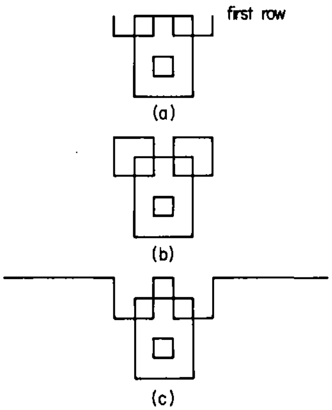


Fig. 6.1. An example of a figure with $p = 12, q = 14$, and $r = 4$.

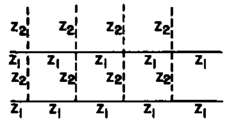


Fig. 6.2. Lattice with weights z_1 and z_2.

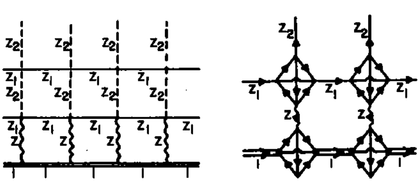


Fig. 6.3. (*a*) Lattice representing a half-plane of Ising spins interacting with a magnetic field applied to the boundary row; (*b*) oriented half-plane lattice used to compute the matrix A.

boundary condition in the horizontal direction, to *two* closed polygons on the lattice in Fig. 6.3(a). These polygons that correspond to the example of Fig. 6.1(a) are shown in Figs. 6.1(b) and 6.1(c). Each of the closed polygons has p horizontal bonds, not including those on the zeroth row, and $p + r$ vertical bonds, of which r are between the zeroth row and the first row. That there are two closed polygons is clear from the example of Fig. 6.1; in case $r = 0$, either all the bonds on the zeroth row are used or none is used. We have thus reduced the problem of evaluating (2.4) to that of finding the generating function for closed polygons on the lattice of Fig. 6.3(a). By the methods of the previous chapter, the solution is immediately given in terms of the Pfaffian for the counting lattice of Fig. 6.3(b). More explicitly,

$$Z = \tfrac{1}{2}(2\cosh\beta E_1)^{4\mathcal{M}\mathcal{N}}(\cosh\beta E_2)^{2\mathcal{N}(2\mathcal{M}-1)}(\cosh\beta\mathfrak{H})^{2\mathcal{N}}\,\mathrm{Pf}\,A, \tag{2.5}$$

where the antisymmetric matrix A is given by

$$A(j,k;j,k) = \begin{array}{c c} & \begin{array}{cccc} R & L & U & D \end{array} \\ \begin{array}{c} R \\ L \\ U \\ D \end{array} & \begin{bmatrix} 0 & 1 & -1 & -1 \\ -1 & 0 & 1 & -1 \\ 1 & -1 & 0 & 1 \\ 1 & 1 & -1 & 0 \end{bmatrix} \end{array} \tag{2.6a}$$

for $0 \le j \le 2\mathcal{M}$ and $-\mathcal{N}+1 \le k \le \mathcal{N}$,

$$A(j,k;j,k+1) = -A^T(j,k+1;j,k) = \begin{bmatrix} 0 & z_1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{2.6b}$$

for $1 \le j \le 2\mathcal{M}$ and $-\mathcal{N}+1 \le k \le \mathcal{N}-1$,

$$A(0,k;0,k+1) = -A^T(0,k+1;0,k) = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{2.6c}$$

for $-\mathcal{N}+1 \le k \le \mathcal{N}-1$,

$$A(j,\mathcal{N};j,-\mathcal{N}+1) = -A^T(j,-\mathcal{N}+1;j,\mathcal{N}) = -A(j,0;j,1) \tag{2.6d}$$

for $0 \le j \le 2\mathcal{M}$,

$$A(j,k;j+1,k) = -A^T(j+1,k;j,k) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & z_2 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{2.6e}$$

for $1 \le j \le 2\mathcal{M}-1$ and $-\mathcal{N}+1 \le k \le \mathcal{N}$,

$$A(0,k;1,k) = -A^T(1,k;0,k) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & z \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{2.6f}$$

for $-\mathcal{N} + 1 \le k \le \mathcal{N}$, and all the other elements of A are zero. In (2.6d), an extra minus sign is introduced in the weight for the bonds between the $(-\mathcal{N} + 1)$th column and the $\mathcal{N}$th column, as was discussed in Chapter IV, in order that all transition cycles which loop the lattice once may be correctly counted. Using the connection (IV.2.7) between Pfaffians and determinants, we finally obtain

$$Z^2 = \tfrac{1}{4}(2\cosh\beta E_1)^{8\mathcal{M}\mathcal{N}}(\cosh\beta E_2)^{4\mathcal{N}(2\mathcal{M}-1)}(\cosh\beta\mathfrak{H})^{4\mathcal{N}} \det A. \tag{2.7}$$

3. PARTITION FUNCTION

This section is devoted to the evaluation of det A, which appears on the right-hand side of (2.7). We first note that A is nearly cyclic in the horizontal direction; accordingly, we use the procedure of Sec. 6 of Chapter IV to find

$$\det A = \Pi_\theta \det B(\theta), \tag{3.1}$$

where the product is over the values

$$\theta = \frac{\pi(2n-1)}{2\mathcal{N}}, \tag{3.2}$$

with $n = 1, 2, 3, \ldots, 2\mathcal{N}$, and $B(\theta)$ is a $4(2\mathcal{M} + 1) \times 4(2\mathcal{M} + 1)$ matrix defined by

$$B_{j,j}(\theta) = \begin{array}{c} \\ R \\ L \\ U \\ D \end{array} \begin{array}{c} \begin{array}{cccc} R & L & U & D \end{array} \\ \begin{bmatrix} 0 & 1 + z_1 e^{i\theta} & -1 & -1 \\ -1 - z_1 e^{-i\theta} & 0 & 1 & -1 \\ 1 & -1 & 0 & 1 \\ 1 & 1 & -1 & 0 \end{bmatrix} \end{array} \tag{3.3a}$$

for $1 \le j \le 2\mathcal{M}$,

$$B_{0,0}(\theta) = \begin{bmatrix} 0 & 1 + e^{i\theta} & -1 & -1 \\ -1 - e^{-i\theta} & 0 & 1 & -1 \\ 1 & -1 & 0 & 1 \\ 1 & 1 & -1 & 0 \end{bmatrix}, \tag{3.3b}$$

$$B_{j,j+1}(\theta) = -B^T_{j+1,j}(\theta) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & z_2 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{3.3c}$$

for $1 \leq j \leq 2\mathcal{M} - 1$,

$$B_{0,1}(\theta) = -B^T_{1,0}(\theta) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & z \\ 0 & 0 & 0 & 0 \end{bmatrix}, \tag{3.3d}$$

and all the other matrix elements are zero. It is convenient to eliminate all rows and columns labeled by R and L in $B(\theta)$. For this purpose, let $T(\theta)$ be the $4(2\mathcal{M} + 1) \times 4(2\mathcal{M} + 1)$ matrix with

$$T_{j,j}(\theta) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ (1 + z_1 e^{i\theta})^{-1} & (1 + z_1 e^{-i\theta})^{-1} & 1 & 0 \\ -(1 + z_1 e^{i\theta})^{-1} & (1 + z_1 e^{-i\theta})^{-1} & 0 & 1 \end{bmatrix} \tag{3.4a}$$

for $1 \leq j \leq 2\mathcal{M}$,

$$T_{0,0}(\theta) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ (1 + e^{i\theta})^{-1} & (1 + e^{-i\theta})^{-1} & 1 & 0 \\ -(1 + e^{i\theta})^{-1} & (1 + e^{-i\theta})^{-1} & 0 & 1 \end{bmatrix}, \tag{3.4b}$$

and all the other matrix elements are zero. Let

$$B'(\theta) = T(\theta)B(\theta); \tag{3.5}$$

then, by (3.3) and (3.4), $B'(\theta)$ is given by

$$B'_{j,j}(\theta) = \begin{bmatrix} 0 & 1 + z_1 e^{i\theta} & -1 & -1 \\ -1 - z_1 e^{-i\theta} & 0 & 1 & -1 \\ 0 & 0 & 2iz_1 \sin\theta |1 + z_1 e^{i\theta}|^{-2} & -(1 - z_1^2)|1 + z_1 e^{i\theta}|^{-2} \\ 0 & 0 & (1 - z_1^2)|1 + z_1 e^{i\theta}|^{-2} & -2iz_1 \sin\theta |1 + z_1 e^{i\theta}|^{-2} \end{bmatrix} \tag{3.6a}$$

for $1 \leq j \leq 2\mathcal{M}$,

$$B'_{0,0}(\theta) = \begin{bmatrix} 0 & 1 + e^{i\theta} & -1 & -1 \\ -1 - e^{-i\theta} & 0 & 1 & -1 \\ 0 & 0 & 2i \sin\theta |1 + e^{i\theta}|^{-2} & 0 \\ 0 & 0 & 0 & -2i \sin\theta |1 + e^{i\theta}|^{-2} \end{bmatrix}, \tag{3.6b}$$

and all the other matrix elements are identical to those of $B(\theta)$. Because of (3.6), it is convenient to introduce the symbols

$$\mathfrak{a} = 2iz_1 \sin\theta |1 + z_1 e^{i\theta}|^{-2}, \tag{3.7a}$$

$$\mathfrak{b} = (1 - z_1^2)|1 + z_1 e^{i\theta}|^{-2}, \tag{3.7b}$$

$$\mathfrak{c} = 2i \sin\theta |1 + e^{i\theta}|^{-2}, \tag{3.7c}$$

and the $2(2\mathscr{M} + 1) \times 2(2\mathscr{M} + 1)$ matrix $\mathfrak{G}(\theta)$ defined by

$$\mathfrak{C}_{j,j}(\theta) = \begin{array}{c c} & \begin{array}{cc} D & U \end{array} \\ \begin{array}{c} D \\ U \end{array} & \begin{bmatrix} -\mathfrak{a} & \mathfrak{b} \\ -\mathfrak{b} & \mathfrak{a} \end{bmatrix} \end{array} \tag{3.8a}$$

for $1 \leq j \leq 2\mathscr{M}$,

$$\mathfrak{C}_{0,0}(\theta) = \begin{bmatrix} -\mathfrak{c} & 0 \\ 0 & \mathfrak{c} \end{bmatrix}, \tag{3.8b}$$

$$\mathfrak{C}_{j,j+1}(\theta) = -\mathfrak{C}^T_{j+1,j}(\theta) = \begin{bmatrix} 0 & 0 \\ z_2 & 0 \end{bmatrix} \tag{3.8c}$$

for $1 \leq j \leq 2\mathscr{M} - 1$,

$$\mathfrak{C}_{0,1}(\theta) = -\mathfrak{C}^T_{1,0}(\theta) = \begin{bmatrix} 0 & 0 \\ z & 0 \end{bmatrix}, \tag{3.8d}$$

and again all the other elements are zero. More explicitly, the matrix $\mathfrak{G}(\theta)$ is of the following form:

$$\begin{bmatrix} -\mathfrak{c} & 0 & & & & & & & & \\ 0 & \mathfrak{c} & z & & & & & & & \\ & -z & -\mathfrak{a} & \mathfrak{b} & & & & & & \\ & & -\mathfrak{b} & \mathfrak{a} & z_2 & & & & & \\ & & & -z_2 & -\mathfrak{a} & \mathfrak{b} & & & & \\ & & & & -\mathfrak{b} & \mathfrak{a} & z_2 & & & \\ & & & & & -z_2 & \cdot & \cdot & & \\ & & & & & & \cdot & \cdot & \cdot & \\ & & & & & & & \cdot & -\mathfrak{a} & \mathfrak{b} \\ & & & & & & & & -\mathfrak{b} & \mathfrak{a} \end{bmatrix} \tag{3.9}$$

and $\det A$ is given by

$$\det A = \Pi_\theta [|1 + e^{i\theta}|^2 |1 + z_1 e^{i\theta}|^{4\mathscr{M}} \det \mathfrak{C}(\theta)]. \tag{3.10}$$

Let $\mathfrak{C}_n(\theta)$ be the determinant of the $2(n + 1) \times 2(n + 1)$ matrix of the form (3.9) and $\mathfrak{D}_n(\theta)$ be the corresponding $(2n+1)\times(2n+1)$ determinant with the last row and last column removed; then

$$\det \mathfrak{C}(\theta) = \mathfrak{C}_{2\mathscr{M}}(\theta). \tag{3.11}$$

The recurrence relations for $\mathfrak{C}_n(\theta)$ and $\mathfrak{D}_n(\theta)$ are

$$\begin{bmatrix} \mathfrak{C}_n(\theta) \\ z_2\mathfrak{D}_n(\theta) \end{bmatrix} = \begin{bmatrix} -\mathfrak{a}^2 + \mathfrak{b}^2 & \mathfrak{a}z_2 \\ -\mathfrak{a}z_2 & z_2^2 \end{bmatrix} \begin{bmatrix} \mathfrak{C}_{n-1}(\theta) \\ z_2\mathfrak{D}_{n-1}(\theta) \end{bmatrix} \tag{3.12a}$$

for $n > 1$, and

$$\begin{bmatrix} \mathfrak{C}_1(\theta) \\ z_2\mathfrak{D}_1(\theta) \end{bmatrix} = \begin{bmatrix} -\mathfrak{a}^2 + \mathfrak{b}^2 & \mathfrak{a}z_2 \\ -\mathfrak{a}z_2 & z_2^2 \end{bmatrix} \begin{bmatrix} \mathfrak{C}_0(\theta) \\ z^2 z_2^{-1}\mathfrak{D}_0(\theta) \end{bmatrix}, \tag{3.12b}$$

together with the boundary conditions

$$\mathfrak{C}_0(\theta) = -\mathfrak{c}^2 \quad \text{and} \quad \mathfrak{D}_0(\theta) = -\mathfrak{c}. \tag{3.13}$$

The 2×2 matrix that appears in (3.12) is Hermitian with the eigenvalues

$$\lambda = \frac{z_2(1-z_1^2)\alpha}{|1+z_1e^{i\theta}|^2}, \qquad \lambda' = \frac{z_2(1-z_1^2)}{|1+z_1e^{i\theta}|^2\alpha}, \tag{3.14}$$

where α is the larger root in magnitude of the quadratic equation

$$(1+z_1^2)(1+z_2^2) - z_1(1-z_2^2)(e^{i\theta}+e^{-i\theta}) - z_2(1-z_1^2)(\alpha+\alpha^{-1}) = 0. \tag{3.15}$$

More explicitly, we recall from (V.3.3) and (V.3.4) that

$$\begin{aligned} \alpha = {} & \frac{1}{2z_2(1-z_2^1)} \\ & \times \Bigg\{(1+z_1^2)(1+z_2^2) - z_1(1-z_2^2)(e^{i\theta}+e^{-i\theta}) \\ & \quad + (1-z_2^2)\left[(1-\alpha_1e^{i\theta})(1-\alpha_1e^{-i\theta})\left(1-\frac{e^{i\theta}}{\alpha_2}\right)\left(1-\frac{e^{-i\theta}}{\alpha_2}\right)\right]^{1/2}\Bigg\}, \end{aligned} \tag{3.16}$$

where, as in (V.3.4),

$$\alpha_1 = \frac{z_1(1-|z_2|)}{1+|z_2|} \quad \text{and} \quad \alpha_2 = \frac{z_1^{-1}(1-|z_2|)}{1+|z_2|}. \tag{3.17}$$

The normalized eigenvector with the eigenvalue λ of (3.14) is

$$\begin{bmatrix} v \\ iv' \end{bmatrix} \tag{3.18a}$$

and that with the eigenvalue λ' is

$$\begin{bmatrix} iv' \\ v \end{bmatrix}, \tag{3.18b}$$

where

$$v = \left[\frac{1}{2}\left(1 + \frac{z_2^2 + \mathfrak{a}^2 - \mathfrak{b}^2}{\lambda' - \lambda}\right)\right]^{1/2}$$

and (3.19)

$$v' = \left[\frac{1}{2}\left(1 - \frac{z_2^2 + \mathfrak{a}^2 - \mathfrak{b}^2}{\lambda' - \lambda}\right)\right]^{1/2} \operatorname{sgn}(i\alpha z_2).$$

Note that

$$\frac{v}{v'} = \frac{i(z_2^2 - \lambda)}{\alpha z_2} = \frac{i\alpha z_2}{z_2^2 - \lambda'}. \tag{3.20}$$

With (3.18)–(3.20), the equations (3.12) with the boundary condition (3.13) can be solved to give explicitly, for $n \geq 0$,

$$\mathfrak{C}_n(\theta) = -\lambda^n v^2\left(\mathfrak{c}^2 - \frac{iz^2}{z_2}\mathfrak{c}\frac{v'}{v}\right) - \lambda'^n v'^2\left(\mathfrak{c}^2 + \frac{iz^2}{z_2}\mathfrak{c}\frac{v}{v'}\right), \tag{3.21}$$

and for $n \geq 1$,

$$z_2\mathfrak{D}_n(\theta) = -i\lambda^n v'^2\left(\mathfrak{c}^2\frac{v}{v'} - \frac{iz^2}{z_2}\mathfrak{c}\right) + i\lambda'^n v^2\left(\mathfrak{c}^2\frac{v'}{v} + \frac{iz^2}{z_2}\mathfrak{c}\right). \tag{3.22}$$

The substitution of (3.21) and (3.11) into (3.10) gives

$$\det A = \Pi_\theta\left\{4|1 + e^{i\theta}|^{-2}\sin^2\theta|1 + z_1e^{i\theta}|^{4\mathscr{M}}\lambda^{2\mathscr{M}}\right.$$
$$\left.\times\left[v^2\left(1 - \frac{iz^2}{z_2\mathfrak{c}}\frac{v'}{v}\right) + \alpha^{-4\mathscr{M}}v'^2\left(1 + \frac{iz^2}{z_2\mathfrak{c}}\frac{v}{v'}\right)\right]\right\}. \tag{3.23}$$

Since

$$\Pi_\theta|1 + e^{i\theta}| = 2 \tag{3.24}$$

and

$$\Pi_\theta|2\sin\theta| = 4, \tag{3.25}$$

(3.23) can be simplified and the substitution into (2.7) gives

$$Z^2 = (2\cosh\beta E_1)^{8\mathscr{M}\mathscr{N}}(\cosh\beta E_2)^{4\mathscr{N}(2\mathscr{M}-1)}(\cosh\beta\mathfrak{H})^{4\mathscr{N}}$$
$$\times\,\Pi_\theta\left\{|1 + z_1e^{i\theta}|^{4\mathscr{M}}\lambda^{2\mathscr{M}}\left[v^2\left(1 - \frac{iz^2}{z_2\mathfrak{c}}\frac{v'}{v}\right) + \alpha^{-4\mathscr{M}}v'^2\left(1 + \frac{iz^2}{z_2\mathfrak{c}}\frac{v}{v'}\right)\right]\right\}. \tag{3.26}$$

So far, the calculation is valid for any $\mathscr{M}$ and $\mathscr{N}$. We now take the limit of large $\mathscr{M}$ and large $\mathscr{N}$ for fixed $T \neq T_c$. We can therefore drop the term proportional to $\alpha^{-4\mathscr{M}}$ in (3.26) and Z is given approximately by

$$-\frac{1}{\beta}\ln Z \sim 4\mathscr{N}\mathscr{M}F + 4\mathscr{N}\mathfrak{F}_0 + 2\mathscr{N}\mathfrak{F}(\mathfrak{H}), \tag{3.27}$$

where

$$F = -\frac{1}{\beta}\left\{\ln(2\cosh\beta E_1\cosh\beta E_2) + \frac{1}{4\pi}\int_{-\pi}^{\pi} d\theta \ln[|1 + z_1 e^{i\theta}|^2\lambda(\theta)]\right\}, \tag{3.28}$$

and

$$2\mathfrak{F}_0 + \mathfrak{F}(\mathfrak{H}) = -\frac{1}{\beta}\left\{-\ln\cosh\beta E_2 + \ln\cosh\beta\mathfrak{H} + \frac{1}{4\pi}\int_{-\pi}^{\pi} d\theta \ln\left[v^2\left(1 - \frac{iz^2}{z_2 \mathfrak{c}}\frac{v'}{v}\right)\right]\right\}. \tag{3.29}$$

Physically, F is the bulk free energy per site, $\mathfrak{F}_0$ is the boundary free energy per boundary site in the absence of the magnetic field, and $\mathfrak{F}(\mathfrak{H})$ is the increase in boundary free energy per boundary site interacting with the magnetic field. Thus, $\mathfrak{F}_0$ is independent of $\mathfrak{H}$ and $\mathfrak{F}(0)$ is zero. Accordingly,

$$\mathfrak{F}_0 = -\frac{1}{2\beta}\left[-\ln\cosh\beta E_2 + \frac{1}{4\pi}\int_{-\pi}^{\pi} d\theta \ln v^2\right] \tag{3.30}$$

and

$$\mathfrak{F}(\mathfrak{H}) = -\frac{1}{\beta}\left[\ln\cosh\beta\mathfrak{H} + \frac{1}{4\pi}\int_{-\pi}^{\pi} d\theta \ln\left(1 - \frac{iz^2}{z_2\mathfrak{c}}\frac{v'}{v}\right)\right]. \tag{3.31}$$

By (3.19), (3.7), and (3.14), Eq. (3.30) is more explicitly

$$\mathfrak{F}_0 = -\frac{1}{2\beta}\Bigg(-\ln\cosh\beta E_2 + \frac{1}{4\pi}\int_{-\pi}^{\pi} d\theta \ln\frac{1}{2}\bigg\{1 + \frac{1}{z_2(1-z_1^2)(\alpha-\alpha^{-1})} \times [(1+z_1^2)(1-z_2^2) - 2z_1(1+z_2^2)\cos\theta]\bigg\}\Bigg). \tag{3.32}$$

Similarly, by (3.20), (3.7), (3.14), and (3.15), Eq. (3.31) is

$$\mathfrak{F}(\mathfrak{H}) = -\frac{1}{\beta}\left\{\ln\cosh\beta\mathfrak{H} + \frac{1}{4\pi}\int_{-\pi}^{\pi} d\theta \ln\left[1 - \frac{z^2 z_1|1+e^{i\theta}|^2}{z_2} \times \frac{1}{z_2(1+z_1^2+2z_1\cos\theta) - (1-z_1^2)\alpha}\right]\right\}. \tag{3.33}$$

The free energy $\mathfrak{F}_0$ in the absence of a magnetic field is considered in detail in the next section; the quantity $\mathfrak{F}(\mathfrak{H})$, or more precisely $\mathfrak{F}'(\mathfrak{H})$, is studied in Sec. 5.

4. BOUNDARY FREE ENERGY AND SPECIFIC HEAT ($\mathfrak{H} = 0$)

In this section we discuss the thermodynamics of the boundary in the absence of a magnetic field; more specifically, we study the boundary free energy as given by (3.32) together with the boundary entropy and boundary specific heat, both of which are essentially derivatives of $\mathfrak{F}_0$ with respect to the temperature T. The interesting features are to be found in the vicinity of the critical temperature T_c; there the boundary entropy is unbounded while the boundary specific heat has a singularity of the form $(T_c - T)^{-1}$. These features are not possible for the corresponding bulk properties, and remind us very strongly that we are dealing with boundary effects.

Equation (3.32) can be simplified by using (3.16) and (3.17):

$$\begin{aligned}\mathfrak{F}_0 = -\frac{1}{2\beta}\Bigg(&-\ln\cosh\beta E_2 \\ &+\frac{1}{4\pi}\int_{-\pi}^{\pi} d\theta \ln\frac{1}{2}\left\{1+\left[1+\frac{\alpha_1}{\alpha_2}-\left(\alpha_1+\frac{1}{\alpha_2}\right)\cos\theta\right]\right. \\ &\qquad\left.\times\left[(1-\alpha_1e^{i\theta})(1-\alpha_1e^{-i\theta})\left(1-\frac{e^{i\theta}}{\alpha_2}\right)\left(1-\frac{e^{-i\theta}}{\alpha_2}\right)\right]^{-1/2}\right\}\Bigg) \\ = -\frac{1}{2\beta}\Bigg\{&-\ln\cosh\beta E_2+\frac{1}{4\pi}\int_{-\pi}^{\pi} d\theta\ln\tfrac{1}{4}[2+\phi(\theta)+\phi^{-1}(\theta)]\Bigg\},\end{aligned} \tag{4.1}$$

where

$$\phi(\theta) = \left[\frac{(1-\alpha_1e^{i\theta})(1-e^{-i\theta}/\alpha_2)}{(1-\alpha_1e^{-i\theta})(1-e^{i\theta}/\alpha_2)}\right]^{1/2} \tag{4.2}$$

is defined to be positive at $\theta = \pi$ if $z_1 \geq 0$ and at $\theta = 0$ if $z_1 \leq 0$. Since

$$\phi(\theta)\phi(-\theta) = 1, \tag{4.3}$$

it follows from (4.1) that

$$\mathfrak{F}_0 = \frac{1}{2\beta}\left\{\ln\cosh\beta E_2 - \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta\ln\tfrac{1}{2}[1+\phi(\theta)]\right\}. \tag{4.4}$$

Equation (4.4) is the desired result.

We begin with a qualitative discussion of $\mathfrak{F}_0$ as given by (4.4). First, as may be expected, $\mathfrak{F}_0$ is finite, nonnegative, and independent of the signs of E_1 and E_2. The behavior of $\mathfrak{F}_0$ in some simple limiting cases is as follows.

(*a*) $T \to 0$ for fixed E_1 and E_2: In this case,

$$z_1 \to \operatorname{sgn} E_1, \tag{4.5}$$

$$z_2 \to \operatorname{sgn} E_2, \tag{4.6}$$

$$\alpha_1 \to 0, \tag{4.7}$$

$$\alpha_2 \to 0, \tag{4.8}$$

$$\phi(\theta) \to -e^{i\theta}\operatorname{sgn} E_1, \tag{4.9}$$

and

$$\mathfrak{F}_0 \to \tfrac{1}{2}|E_2|. \tag{4.10}$$

(*b*) $T \to \infty$ for fixed E_1 and E_2: In this case, $\beta \to 0$,

$$\oint(\theta) = 1 + O(\beta), \tag{4.11}$$

and

$$\mathfrak{F}_0 \to 0. \tag{4.12}$$

(*c*) $E_1 \to \infty$ for fixed E_2 and T: Here $z_1 \to 1$,

$$\alpha_1 \sim \alpha_2 < 1, \tag{4.13}$$

$$\oint(\theta) \to -e^{-i\theta}\frac{1 - \alpha_1 e^{i\theta}}{1 - \alpha_1 e^{-i\theta}}, \tag{4.14}$$

and

$$\mathfrak{F}_0 \to \tfrac{1}{2}\beta^{-1}[\ln\cosh\beta E_2 - \ln\tfrac{1}{2}(1 + \alpha_1)] = \tfrac{1}{2}|E_2|. \tag{4.15}$$

(*d*) $E_2 \to \infty$ for fixed E_1 and T: This case is very similar to (*a*); in particular, (4.6)–(4.10) hold.

(*e*) $E_1 \to 0$ for fixed E_2 and T: In this case, $z_1 \to 0$, $\alpha_1 \to 0$, $1/\alpha_2 \to 0$,

$$\oint(\theta) \to 1, \tag{4.16}$$

and

$$\mathfrak{F}_0 \to \frac{1}{2\beta}\ln\cosh\beta E_2. \tag{4.17}$$

This is the result for the one-dimensional Ising model, and may indeed be written down without calculation.

(*f*) $E_2 \to 0$ for fixed E_1 and T: In this case, $z_2 \to 0$,

$$\alpha_1 = \frac{1}{\alpha_2} = z_1, \tag{4.18}$$

and (4.16) and (4.17) hold, that is, $\mathfrak{F}_0 \to 0$.

The rest of this section is devoted to an analysis of the behavior of $\mathfrak{F}_0$ when T is near T_c. Since there is no magnetic field, $\mathfrak{F}_0$ depends only on the magnitudes of E_1 and E_2, but not on their signs. Therefore, without loss of generality, we assume both E_1 and E_2 to be positive. With this convention, $\alpha_2 = 1$ when $T = T_c$. An inspection of (4.4) with (4.2) then indicates that the expansion of $\mathfrak{F}_0$ for α_2 near 1 may contain terms proportional to the following: 1, $(1 - \alpha_2)\ln|1 - \alpha_2|$, $1 - \alpha_2$, $(1 - \alpha_2)^2 \cdot \ln|1 - \alpha_2|$, $(1 - \alpha_2)^2$, and so forth. We are only interested in the terms containing the logarithms, since they are responsible for the singularities in the boundary entropy

$$\mathfrak{S} = -\frac{\partial\mathfrak{F}_0}{\partial T} \tag{4.19}$$

and the specific heat

$$c_v = -\frac{T\partial^2\mathfrak{F}_0}{\partial T^2}. \tag{4.20}$$

The computation of these required terms is rather complicated.[3] The first step is to change the variable of integration to

$$\omega = \frac{e^{i\theta} - 1}{e^{i\theta} + 1}, \tag{4.21}$$

so that the path of integration is changed from the unit circle to the imaginary axis. The result is

$$\mathfrak{F}_0 = \frac{1}{2\beta}\left\{\ln\cosh\beta E_2 + \frac{i}{\pi}\int_{-i\infty}^{i\infty}\frac{d\omega}{1-\omega^2}\ln\frac{1}{2}\left[1 + \left(\frac{\tau_1 - \omega}{\tau_1 + \omega}\frac{\tau_2 - \omega}{\tau_2 + \omega}\right)^{1/2}\right]\right\}, \tag{4.22}$$

where

$$\tau_i = \frac{1 - \alpha_i}{1 + \alpha_i} \tag{4.23}$$

for $i = 1, 2$. In (4.22), the square root is equal to 1 as $\omega \to \pm i\infty$. It is convenient to redefine the square root by the value at $\omega = 0$. Thus

$$\mathfrak{F}_0 = \frac{1}{2\beta}\left\{\ln\cosh\beta E_2 + \frac{i}{\pi}\int_{-i\infty}^{i\infty}\frac{d\omega}{1-\omega^2}\ln\frac{1}{2}\left[1 + \left(\frac{\tau_1 - \omega}{\tau_1 + \omega}\frac{\tau + \omega}{\tau - \omega}\right)^{1/2}\right]\right\} \tag{4.24a}$$

for $T > T_c$, and

$$\mathfrak{F}_0 = \frac{1}{2\beta}\left\{\ln\cosh\beta E_2 + \frac{i}{\pi}\int_{-i\infty}^{i\infty}\frac{d\omega}{1-\omega^2}\ln\frac{1}{2}\left[1 - \left(\frac{\tau_1 - \omega}{\tau_1 + \omega}\frac{\tau - \omega}{\tau + \omega}\right)^{1/2}\right]\right\} \tag{4.24b}$$

for $T < T_c$. In (4.24), the square roots are defined to be 1 at $\omega = 0$, and

$$\tau = \tau_2 \operatorname{sgn}(T_c - T). \tag{4.25}$$

The second step is to continue analytically in τ, taken to be a complex variable. Define disc $\mathfrak{F}_0$ by

$$\operatorname{disc}\mathfrak{F}_0 = \mathfrak{F}_0(\tau e^{2\pi i}) - \mathfrak{F}_0(\tau). \tag{4.26}$$

We consider the case $T > T_c$ first. Both $\mathfrak{F}_0(\tau)$ and $\mathfrak{F}_0(\tau e^{2\pi i})$ are given by (4.24a) with the contours of integration shown in Fig. 6.4(a) and Fig. 6.4(b), respectively. Accordingly,

$$\operatorname{disc}\mathfrak{F}_0 = \frac{i}{2\beta\pi}\int\frac{d\omega}{1-\omega^2}\ln\left[1 + \left(\frac{\tau_1 - \omega}{\tau_1 + \omega}\frac{\tau + \omega}{\tau - \omega}\right)^{1/2}\right], \tag{4.27}$$

where the contour of integration is shown in Fig. 6.4(c), which was first

3. We could proceed by reducing $\mathfrak{F}_0$ to elliptic integrals much as we did in the previous chapter. However, since we are only interested in the singularities of $\mathfrak{F}_0$ it is more convenient to proceed directly.

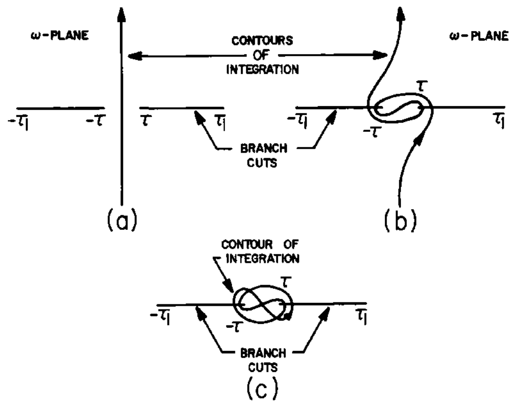


Fig. 6.4. The contours of integration for $\mathfrak{F}_0(\tau)$, $\mathfrak{F}_0(\tau e^{2\pi i})$, and disc $\mathfrak{F}_0$.

used by Pochammer nearly a century ago. It follows immediately from (4.27) that

$$\operatorname{disc}\mathfrak{F}_0 = \frac{i}{\beta\pi}\int_{-\tau}^{\tau} d\omega\left\{\ln\left[1 + \left(\frac{\tau_1-\omega}{\tau_1+\omega}\frac{\tau+\omega}{\tau-\omega}\right)^{1/2}\right] - \ln\left|1 - \left(\frac{\tau_1-\omega}{\tau_1+\omega}\frac{\tau+\omega}{\tau-\omega}\right)^{1/2}\right|\right\}. \tag{4.28}$$

In the form (4.28), it is straightforward to expand in a power series in τ; the two leading terms are

$$\begin{aligned}\operatorname{disc}\mathfrak{F}_0 = \frac{i\tau}{\beta\pi}\Bigg(&\int_{-1}^{1} dx\left\{\ln\left[1 + \left(\frac{1+x}{1-x}\right)^{1/2}\right] - \ln\left|1 - \left(\frac{1+x}{1-x}\right)^{1/2}\right|\right\}\\ &- \frac{\tau}{\tau_1}\int_{-1}^{1} dx\left\{x\left(\frac{1+x}{1-x}\right)^{1/2}\left[1 + \left(\frac{1+x}{1-x}\right)^{1/2}\right]^{-1}\right.\\ &\left.+ x\left(\frac{1+x}{1-x}\right)^{1/2}\left[1 - \left(\frac{1+x}{1-x}\right)^{1/2}\right]^{-1}\right\} + O(\tau^2)\Bigg).\end{aligned} \tag{4.29}$$

The integrals on the right-hand side of (4.29) are easily evaluated; the first one is found to be π and the second one is $-\frac{1}{2}\pi$. Therefore

$$\operatorname{disc}\mathfrak{F}_0 = \frac{i}{\beta}\left[\tau + \frac{\tau^2}{2\tau_1} + O(\tau^3)\right] \tag{4.30}$$

for $T > T_c$. This implies that, for small positive τ, $\mathfrak{F}_0$ is of the form

$$\mathfrak{F}_0 = \text{Taylor series in } \tau + \frac{1}{2\pi\beta}\left[\tau + \frac{\tau^2}{2\tau_1} + O(\tau^3)\right]\ln\tau. \tag{4.31}$$

To obtain the corresponding result for $T < T_c$, it is convenient to introduce the function

$$\mathfrak{F}_0^- = \frac{1}{2\beta}\left\{\ln\cosh\beta E_2 + \frac{i}{\pi}\int_{-i\infty}^{i\infty}\frac{d\omega}{1-\omega^2}\ln\frac{1}{2}\left[1+\left(\frac{\tau_1-\omega}{\tau_1+\omega}\frac{\tau-\omega}{\tau+\omega}\right)^{1/2}\right]\right\}, \tag{4.32}$$

which differs from $\mathfrak{F}_0$ of (4.24*b*) only in the sign of the square root. It is easily verified that $\mathfrak{F}_0 + \mathfrak{F}_0^-$ is analytic in τ for sufficiently small τ. Therefore, it follows from

$$\mathfrak{F}_0^- = \text{Taylor series in } \tau + \frac{1}{2\pi\beta}\left[\tau - \frac{\tau^2}{2\tau_1} + O(\tau^3)\right]\ln\tau \tag{4.33}$$

that

$$\mathfrak{F}_0 = \text{Taylor series in } \tau - \frac{1}{2\pi\beta}\left[\tau - \frac{\tau^2}{2\tau_1} + O(\tau^3)\right]\ln\tau \tag{4.34}$$

for $T < T_c$. Note that the imaginary part of each of the logarithms in (4.24) and (4.32) has been taken to be less than π in magnitude. By (4.25), Eqs. (4.31) and (4.34) can be combined in the form

$$\mathfrak{F}_0 = \text{Taylor series in } \tau_2 - \frac{1}{2\pi\beta}\left[\tau_2 - \frac{\tau_2^2}{2\tau_1} + O(\tau_2^3)\right]\ln|\tau_2| \tag{4.35}$$

for both $T > T_c$ and $T < T_c$. Note that the Taylor series to be used in (4.35) may be different for $T > T_c$ and for $T < T_c$. We shall return to this point later in this section.

It remains to substitute (4.35) into (4.19) and (4.20). Let z_{1c} and z_{2c} be the values of z_1 and z_2 at $T = T_c$, so that by (V.3.11)

$$1 - z_{1c} - z_{2c} - z_{1c}z_{2c} = 0. \tag{4.36}$$

Then it is easily verified that, for T near T_c,

$$\tau_2 = \left(\frac{1}{kT}-\frac{1}{kT_c}\right)\left[\mathcal{E}_1 - E_1^2\frac{(1-z_{1c})(z_{1c}+z_{2c})}{(1-z_{2c})^2}\left(\frac{1}{kT}-\frac{1}{kT_c}\right)\right] + O[(T-T_c)^3], \tag{4.37}$$

where

$$\mathcal{E}_1 = (1-z_{2c})^{-1}[E_1(1-z_{1c}) + E_2(1-z_{2c})]. \tag{4.38}$$

Accordingly, since at $T = T_c$

$$\tau_1 = \frac{1-z_{1c}}{z_{1c}+z_{2c}}, \tag{4.39}$$

$$\frac{1}{\beta}\left(\tau_2 - \frac{\tau_2^2}{2\tau_1}\right) = \left(1-\frac{T}{T_c}\right)\left\{\mathcal{E}_1 - \frac{1}{2}\mathcal{E}_2\left(1-\frac{T}{T_c}\right) + O[(T-T_c)^2]\right\}, \tag{4.40}$$

where

$$\mathfrak{s}_2 = \frac{z_{1c} + z_{2c}}{kT_c(1 - z_{2c})^2}\left[3E_1^2(1 - z_{1c}) + 2E_1E_2(1 - z_{2c}) + E_2^2\frac{(1 - z_{2c})^2}{1 - z_{1c}}\right]. \tag{4.41}$$

The results for the entropy and the specific heat are thus

$$\mathfrak{S} = -\frac{\mathfrak{s}_1}{2\pi T_c}\ln\left|1 - \frac{T}{T_c}\right| + O(1), \tag{4.42}$$

and

$$\mathfrak{c}_v = -\frac{1}{2\pi}\left[\frac{\mathfrak{s}_1}{T - T_c} + \frac{\mathfrak{s}_2}{T_c}\ln\left|1 - \frac{T}{T_c}\right|\right] + O(1). \tag{4.43}$$

Note that $\mathfrak{s}_1$ is positive so that $\mathfrak{S}$ is unbounded from above for T near T_c. This and the singularity of $\mathfrak{c}_v$ have already been discussed at the beginning of this section.

We write down more explicitly the singularities of $\mathfrak{S}$ and $\mathfrak{c}_v$ for the special case $E_1 = E_2$:

$$\mathfrak{S} = -\frac{k}{2\pi}[\ln(1 + \sqrt{2})]\left[\ln\left|1 - \frac{T}{T_c}\right| + O(1)\right], \tag{4.44}$$

$$\mathfrak{c}_v = \frac{k}{2\pi}[\ln(1 + \sqrt{2})] \times\left\{\left(1 - \frac{T}{T_c}\right)^{-1} - \frac{3}{\sqrt{2}}[\ln(1 + \sqrt{2})]\left[\ln\left|1 - \frac{T}{T_c}\right|\right] + O(1)\right\}. \tag{4.45}$$

Equation (4.42) does not quite tell the whole story. It should be supplemented by

$$\lim_{\delta T\to 0}[\mathfrak{S}(T_c + \delta T) - \mathfrak{S}(T_c - \delta T)] = -\frac{1}{2}\frac{\mathfrak{s}_1}{T_c}, \tag{4.46}$$

which may be derived by considering $\mathfrak{F}_0(\tau e^{\pi i}) - \mathfrak{F}_0^-(\tau)$. This "latent heat" is not understood by the authors.

In spite of the peculiarities of the boundary entropy exhibited in this section, we will proceed to a discussion of the boundary magnetization and hysteresis.

5. BOUNDARY MAGNETIZATION

Attention is next focused on the additional boundary free energy due to the presence of a magnetic field, as given by (3.33). More precisely, we shall consider the magnetization $\mathfrak{M}_1$ of the first row. The substitution of (3.33) and (3.27) in (II.5.10) gives that

$$\begin{aligned}
\mathfrak{M}_1 &= -\mathfrak{F}'(\mathfrak{H}) \\
&= z + \frac{1 - z^2}{4\pi}\frac{\partial}{\partial z} \\
&\quad \times \int_{-\pi}^{\pi} d\theta \ln\Big\{1 - \frac{z^2 z_1}{z_2}|1 + e^{i\theta}|^2 \\
&\qquad\qquad \times [z_2(1 + z_1^2 + 2z_1\cos\theta) - (1 - z_1^2)\alpha]^{-1}\Big\} \\
&= z + \frac{1 - z^2}{2\pi} z z_1 \int_{-\pi}^{\pi} d\theta |1 + e^{i\theta}|^2 \\
&\quad \times [z^2 z_1|1 + e^{i\theta}|^2 - z_2^2(1 + z_1^2 + 2z_1\cos\theta) + z_2(1 - z_1^2)\alpha]^{-1}.
\end{aligned} \tag{5.1}$$

Clearly, $\mathfrak{M}_1 \to 1$ as $\mathfrak{H} \to \infty$.

It is useful to rewrite (5.1) in the following two ways. First, by (3.15),

$$\begin{aligned}
\mathfrak{M}_1 &= z + \frac{1 - z^2}{2\pi} z \int_{-\pi}^{\pi} d\theta[-z_2(1 - z_1)\alpha + (1 + z_1)] \\
&\quad \times [z_2(1 - z_1)(1 - z^2)\alpha - (1 + z_1)(z_2^2 - z^2)]^{-1}.
\end{aligned} \tag{5.2}$$

Thus the integrand is singular if and only if

$$\alpha = \frac{(1 + z_1)(z_2^2 - z^2)}{z_2(1 - z_1)(1 - z^2)}. \tag{5.3}$$

Alternatively, α as given by (3.16) may be substituted into (5.1), to give

$$\begin{aligned}
\mathfrak{M}_1 &= z + \frac{1 - z^2}{2\pi} z z_1 \int_{-\pi}^{\pi} d\theta |1 + e^{i\theta}|^2 \\
&\quad \times (z^2 z_1|1 + e^{i\theta}|^2 - \tfrac{1}{4}z_1(1 + |z_2|)^2 \\
&\qquad \times \{(1 + \alpha_1\alpha_2)(e^{i\theta} + e^{-i\theta}) - 2(\alpha_1 + \alpha_2) \\
&\qquad\quad - 2[(1 - \alpha_1 e^{i\theta})(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{i\theta})(1 - \alpha_2 e^{-i\theta})]^{1/2}\})^{-1}.
\end{aligned} \tag{5.4}$$

At least when $T < T_c$, that is, $|\alpha_1| < 1$ and $|\alpha_2| < 1$, the last factor in (5.4) can be further factored to give

$$\mathfrak{M}_1 = z + \frac{1 - z^2}{2\pi} 4z \int_{-\pi}^{\pi} \frac{d\theta|1 + e^{i\theta}|^2}{s_1 s_2}, \tag{5.5}$$

where

$$\begin{aligned}
s_1 &= 2z(1 + e^{i\theta}) - (1 + |z_2|) \\
&\quad \times \{[(1 - \alpha_1 e^{i\theta})(1 - \alpha_2 e^{i\theta})]^{1/2} - e^{i\theta}[(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{-i\theta})]^{1/2}\}
\end{aligned} \tag{5.6}$$

and

$$s_2 = 2z(1 + e^{-i\theta}) - (1 + |z_2|)$$
$$\times \{[(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{-i\theta})]^{1/2} - e^{-i\theta}[(1 - \alpha_1 e^{i\theta})(1 - \alpha_2 e^{i\theta})]^{1/2}\}, \quad (5.7)$$

with both square roots defined to be positive at $\theta = 0$ and π. The right-hand side of (5.5) may be expressed as a partial fraction,

$$\mathfrak{M}_1 = z + \frac{1 - z^2}{2\pi} \int_{-\pi}^{\pi} d\theta \left(\frac{1 + e^{i\theta}}{s_1} + \frac{1 + e^{-i\theta}}{s_2} \right). \quad (5.8)$$

This form is needed for purposes of analytical continuation.

We study in some detail the location of the singularity of the integrand as given by (5.3). Let r be the value of $e^{\pm i\theta}$ such that (3.15) and (5.3) are both satisfied. Therefore

$$r + \frac{1}{r} = \frac{(1 + z_1^2)(1 + z_2^2)}{z_1(1 - z_2^2)} - \frac{(1 + z_1)^2(z_2^2 - z^2)}{z_1(1 - z_2^2)(1 - z^2)} - \frac{z_2^2(1 - z_1)^2(1 - z^2)}{z_1(1 - z_2^2)(z_2^2 - z^2)}$$
$$= 2\frac{(1 - \alpha_1\alpha_2)^2 - 2(\alpha_1 + \alpha_2)\alpha_3^2 - \alpha_3^4}{(1 - \alpha_1\alpha_2)^2 - 2(1 + \alpha_1\alpha_2)\alpha_3^2 + \alpha_3^4}, \quad (5.9)$$

where

$$\alpha_3 = \frac{2z}{1 + |z_2|}. \quad (5.10)$$

With the additional condition $|r| < 1$, (5.9) gives,

$$r = [(1 - \alpha_1\alpha_2)^2 - 2(1 + \alpha_1\alpha_2)\alpha_3^2 - \alpha_3^4]^{-1}$$
$$\times \{(1 - \alpha_1\alpha_2)^2 - 2(\alpha_1 + \alpha_2)\alpha_3^2 - \alpha_3^4$$
$$- 2[\![\alpha_3^2[\alpha_3^2 - (1 - \alpha_1)(1 - \alpha_2)][(1 + \alpha_1)(1 + \alpha_2)\alpha_3^2 - (1 - \alpha_1\alpha_2)^2]]\!]^{1/2}\} \quad (5.11)$$

The qualitative motion of r is of interest. In the $e^{i\theta}$-plane, α has four branch points, at α_1, $1/\alpha_1$, α_2, and $1/\alpha_2$. We define the cut plane for $e^{i\theta}$ by joining these branch points pairwise along the real axis; thus the unit circle does not intersect the branch cuts unless $|\alpha_2| = 1$. In this cut plane, $|\alpha| \geq 1$. Therefore, by (5.3), there is a pair of singular points at r and $1/r$ in the cut plane if and only if

$$\left| \frac{(1 + z_1)(z_2^2 - z^2)}{z_2(1 - z_1)(1 - z^2)} \right| \geq 1. \quad (5.12)$$

Since $|z| \leq 1$, (5.12) holds if and only if either

$$z^2 \geq |z_2| \frac{1 - \alpha_1}{1 + \alpha_1} \quad (5.13)$$

or

$$T \leq T_c, \qquad E_1 \geq 0,$$

and

$$z^2 \leq |z_2| \frac{1 - \alpha_2}{1 + \alpha_2}. \tag{5.14}$$

Accordingly, in the cut plane, r is real; moreover,

$$0 \leq \frac{r}{\alpha_1} \leq 1 \tag{5.15}$$

when (5.13) holds and

$$0 \leq \alpha_2 \leq r \leq 1 \tag{5.16}$$

when (5.14) holds. In (5.16), $r = 1$ if $z = 0$.

With this information on r it is clear that $\mathfrak{M}_1$ is an analytic function of $\mathfrak{H}$ except when $T \leq T_c$ and $\mathfrak{H} = 0$. We proceed to study the behavior of $\mathfrak{M}_1$ near $\mathfrak{H} = 0$ and also the analytic continuation of $\mathfrak{M}_1$ as a function of $\mathfrak{H}$.

A. Spontaneous Magnetization

The boundary spontaneous magnetization is defined to be

$$\mathfrak{M}_1(0^+) = \lim_{\mathfrak{H}\to 0^+} \mathfrak{M}_1(\mathfrak{H}). \tag{5.17}$$

By (5.1), it is zero unless $r \to 1$ in this limit. That is, by (5.16), it is zero unless $T < T_c$ and $E_1 > 0$. We consider only this case. Expansion about $\theta = 0$ gives

$$\alpha \sim z_2 \frac{1 + z_1}{1 - z_1} \left\{ 1 + \frac{z_1(1 - z_2^2)}{z_2^2(1 + z_1)^2 - (1 - z_1)^2} \theta^2 \right\} \tag{5.18}$$

from (3.15) or (3.16), and hence

$$\begin{aligned} \mathfrak{M}_1(0^+) &= \lim_{z\to 0} \frac{z}{2\pi} \int_{-\infty}^{\infty} \frac{d\theta}{z^2 + z_1 z_2^2 [z_2^2(1 + z_1)^2 - (1 - z_1)^2]^{-1} \theta^2} \\ &= \frac{1}{2|z_2|} \left[\frac{z_2^2(1 + z_1)^2 - (1 - z_1)^2}{z_1} \right]^{1/2}. \end{aligned} \tag{5.19}$$

This is the desired result. In terms of E_1 and E_2, (5.19) is

$$\mathfrak{M}_1(0^+) = \left[\frac{\cosh 2\beta E_2 - \coth 2\beta E_1}{\cosh 2\beta E_2 - 1} \right]^{1/2}. \tag{5.20}$$

This vanishes at the critical temperature as $(T_c - T)^{1/2}$, and is plotted in Fig. 6.5 for the case $E_1 = E_2$.

The magnetization (5.1) is computed in the thermodynamic limit $\mathscr{M} \to \infty$, $\mathscr{N} \to \infty$. Only in this limiting case can the spontaneous magnetization (5.17) be different from zero. On the other hand, we

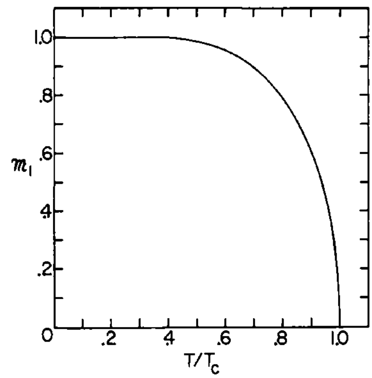


Fig. 6.5. The boundary magnetization for $E_1 = E_2$ as a function of temperature.

expect that, if $\mathscr{M}$ and $\mathscr{N}$ are large but are not both infinite, the magnetization, even though it vanishes when $\mathfrak{H} = 0$, should in some sense be well approximated by (5.1). The sense of this approximation can be made more precise by considering the boundary magnetization of the finite strip in which $\mathscr{N}$ is infinite but $\mathscr{M}$, while large, is finite. We thus must retain the term proportional to $\alpha^{-4\mathscr{M}}$ in (3.26) and find

$$\mathfrak{F}(\mathfrak{H}) = -\frac{1}{\beta}\left\{\ln\cosh\beta\mathfrak{H} + \frac{1}{4\pi}\int_{-\pi}^{\pi} d\theta \ln\left[\left(1 - \frac{iz^2}{z_2\mathfrak{c}}\frac{v'}{v}\right) + \alpha^{-4\mathscr{M}}\left(\frac{v'}{v}\right)^2\left(1 + \frac{iz^2}{z_2\mathfrak{c}}\frac{v}{v'}\right)\right]\right\}. \tag{5.21}$$

Then, using (3.20), we find

$$\begin{aligned}\mathfrak{M}_1(\mathfrak{H}) &= -\frac{\partial\mathfrak{F}(\mathfrak{H})}{\partial\mathfrak{H}}\\ &= z + \frac{(1 - z^2)zz_1}{2\pi}\int_{-\pi}^{\pi} d\theta(1 - \alpha^{-4\mathscr{M}})|1 + e^{i\theta}|^2\\ &\quad\times \{z^2z_1|1 + e^{i\theta}|^2 - z_2^2|1 + z_1e^{i\theta}|^2 + z_2(1 - z_1^2)\alpha\\ &\quad + \alpha^{-4\mathscr{M}}[z_2^2|1 + z_1e^{i\theta}|^2 - z_2(1 - z_1^2)\alpha^{-1} - z^2z_1|1 + e^{i\theta}|^2]\}^{-1}.\end{aligned} \tag{5.22}$$

If we let $\mathscr{M} \to \infty$, we recover (5.1). In that case, when $T < T_c$, $E_1 > 0$, and $z \to 0$, the integral multiplying z diverges as $1/z$ and spontaneous magnetization occurs. If we keep $\mathscr{M}$ finite, however, when $T < T_c$, $E_1 > 0$, and $z \to 0$, the integral multiplying z is finite, so $\mathfrak{M}_1 \to 0$. When z is not zero, then when $\mathscr{M}$ is large enough that

$$z^2 \gg \frac{1}{4z_1}\left[\frac{(1 - z_1)}{z_2(1 + z_1)}\right]^{4\mathscr{M}}[z_2^2(1 + z_1)^2 - (1 - z_1)^2], \tag{5.23}$$

the terms proportional to $\alpha^{-4\mathscr{M}}$ may be neglected and the boundary magnetization for the finite strip becomes identical with the boundary magnetization of the half-plane. Only very near $\mathfrak{H} = 0$ will the boundary magnetization of the strip be sensibly different from the boundary magnetization of the half-plane.

We are interested in seeing in detail how spontaneous magnetization arises when $T < T_c$ as $\mathscr{M} \to \infty$. We may compute this behavior from (5.22) for large $\mathscr{M}$ by expanding the integrand about $\theta = 0$ and keeping the lowest-order terms. Using (5.18) we obtain

$$\begin{aligned}\mathfrak{M}_1 \sim z + (1 - z^2)z \frac{z_2^2(1 + z_1)^2 - (1 - z_1)^2}{z_1 z_2^2} \frac{1}{2\pi} \\ \times \int_{-\infty}^{\infty} d\theta \{[z_2^2(1 + z_1)^2 - (1 - z_1)^2] z_2^2 z_1^{-1} \\ \times (z^2 + \tfrac{1}{4} z_1^{-1}[z_2(1 + z_1)(1 - z_1)^{-1}]^{-4} \\ \times [z_2^2(1 + z_1)^2 - (1 - z_1)^2]) + \theta^2\}^{-1},\end{aligned} \tag{5.24}$$

so that when z is small and $\mathscr{M}$ is large,

$$\begin{aligned}\mathfrak{M}_1 \sim z + \frac{1}{2} \frac{1 - z^2}{z_1^{1/2}|z_2|} [z_2^2(1 + z_1)^2 - (1 - z_1)^2]^{1/2} z \\ \times \left\{z^2 + \frac{1}{4z_1}\left[\frac{z_2(1 + z_1)}{1 - z_1}\right]^{-4\mathscr{M}} [z_2^2(1 + z_1)^2 - (1 - z_1)^2]\right\}^{-1/2}.\end{aligned} \tag{5.25}$$

If $\mathscr{M} \to \infty$ and then $z \to 0$, $\mathfrak{M}_1$ clearly goes to the value of the spontaneous magnetization given by (5.19). On the other hand, if $\mathscr{M}$ is finite and $z \to 0$, $\mathfrak{M}_1$ does vanish. From (5.25) we find that the susceptibility at zero field for a large finite strip is

$$\left.\frac{\partial \mathfrak{M}_1}{\partial \mathfrak{H}}\right|_{\mathfrak{H}=0} = \beta\left\{1 + \frac{1}{|z_2|}\left[\frac{z_2(1 + z_1)}{1 - z_1}\right]^{2\mathscr{M}}\right\}, \tag{5.26}$$

which becomes exponentially large as $\mathscr{M} \to \infty$.

B. Behavior Near Critical Temperature

We apply essentially the same procedure which we used to compute $\mathfrak{M}_1(0^+)$ to study the behavior of $\mathfrak{M}_1$ when T is near T_c and $\mathfrak{H}$ is positive and small. We consider first the ferromagnetic case where $E_1 > 0$. The basic idea is still to expand about $\theta = 0$, but the actual computation is somewhat less straightforward than that of spontaneous magnetization. Consider first $T < T_c$; we neglect throughout terms in $\mathfrak{M}_1$ of order z. Then it follows from (5.4) that

$$\mathfrak{M}_1 \sim \mathfrak{M}_1^{(1)} + \mathfrak{M}_1^{(2)}, \tag{5.27}$$

where

$$\mathfrak{M}_1^{(1)} = \frac{zz_1}{2\pi}\int_{-\pi}^{\pi} d\theta|1 + e^{i\theta}|^2 2z_1^{-1}(1 + |z_2|)^{-2} \tag{5.28}$$
$$\times [(1 - \alpha_1 e^{i\theta})(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{i\theta})(1 - \alpha_2 e^{-i\theta})]^{-1/2}$$

and

$$\mathfrak{M}_1^{(2)} = \frac{zz_1}{2\pi}\int_{-\pi}^{\pi} d\theta|1 + e^{i\theta}|^2$$
$$\times \Big[(z^2 z_1|1 + e^{i\theta}|^2 - \tfrac{1}{4}z_1(1 + |z_2|)^2\{(1 + \alpha_1\alpha_2)(e^{i\theta} + e^{-i\theta})$$
$$- 2(\alpha_1 + \alpha_2) - 2[(1 - \alpha_1 e^{i\theta})(1 - \alpha_1 e^{-i\theta})$$
$$\times (1 - \alpha_2 e^{i\theta})(1 - \alpha_2 e^{-i\theta})]^{1/2}\})^{-1}$$
$$- \{\tfrac{1}{2}z_1(1 + |z_2|)^2[(1 - \alpha_1 e^{i\theta})(1 - \alpha_1 e^{-i\theta})$$
$$\times (1 - \alpha_2 e^{i\theta})(1 - \alpha_2 e^{-i\theta})]^{1/2}\}^{-1}\Big]. \tag{5.29}$$

These two parts are to be approximated differently. Since α_2 is close to 1 and α_1 is close to z_1^2,

$$\mathfrak{M}_1^{(1)} \sim \frac{8z}{\pi(1 + |z_2|)^2(1 - z_1^2)}\int_0^{\pi} \frac{d\theta}{[(1 - \alpha_2 e^{i\theta})(1 - \alpha_2 e^{-i\theta})]^{1/2}}$$
$$= \frac{16z}{\pi(1 + |z_2|)^2(1 - z_1^2)(1 + z_1^2)}\mathbf{K}\left[\frac{2\alpha_2^{1/2}}{1 + \alpha_2}\right]$$
$$\sim -\frac{2z}{\pi z_2}\ln(1 - \alpha_2), \tag{5.30}$$

where $\mathbf{K}$ denotes the complete elliptic integral of the first kind as given by (V.3.27). In order to compute $\mathfrak{M}_1^{(2)}$ approximately, we expand all $e^{i\theta}$ in power series for small θ:

$$\mathfrak{M}_1^{(2)} \sim \frac{2z}{\pi}\int_{-\infty}^{\infty} d\theta$$
$$\times \left\{\frac{1}{4z^2 - \frac{1}{2}(1 + |z_2|)^2\{(1 - \alpha_1)(1 - \alpha_2) - (1 - \alpha_1)[(1 - \alpha_2)^2 + \theta^2]^{1/2}\}}\right.$$
$$\left. - \frac{1}{\frac{1}{2}(1 + |z_2|)^2(1 - \alpha_1)[(1 - \alpha_2)^2 + \theta^2]^{1/2}}\right\}. \tag{5.31}$$

A change of variable reduces the right-hand side of (5.31) to

$$\mathfrak{M}_1^{(2)} \sim \frac{2z}{\pi|z_2|}(1 - p)\int_0^{\infty} \frac{d\theta}{p - 1 + \cosh\theta}, \tag{5.32}$$

where

$$p = \frac{2z^2}{|z_2|(1 - \alpha_2)}. \tag{5.33}$$

Note that p can take any real positive value. The integral in (5.32) can be approximately evaluated:

$$(1 - p)\int_0^\infty d\theta(p - 1 + \cosh\theta)^{-1} = \frac{\pi}{(2p)^{1/2}} - \ln\left[1 + \tfrac{1}{2}|z_2|p\right] + O(1). \tag{5.34}$$

In (5.34), the coefficient of p in the logarithm is arbitrary; it has been chosen to make (5.35) below simple. The desired result follows immediately from Eqs. (5.27), (5.30), and (5.32)–(5.34):

$$\mathfrak{M}_1 \sim \frac{(1 - \alpha_2)^{1/2}}{|z_2|^{1/2}}\operatorname{sgn} z - \frac{2z}{\pi|z_2|}\ln(1 - \alpha_2 + z^2) \tag{5.35}$$

for $T < T_c$. The computation is virtually identical in the case $T > T_c$. Equations (5.27)–(5.29) hold without modification, and (5.30) is also valid if α_2 is replaced by $1/\alpha_2$. So far as $\mathfrak{M}_1^{(2)}$ is concerned, the main change is the appearance of $1 + \cosh\theta$ instead of $-1 + \cosh\theta$. The result is

$$\mathfrak{M}_1 \sim -\frac{2z}{\pi|z_2|}\ln\left(1 - \frac{1}{\alpha_2} + z^2\right) \tag{5.36}$$

for $T > T_c$.

As $z \to 0^+$, (5.35) agrees with (5.19) and exhibits the square-root behavior explicitly. At $T = T_c$, it follows from either (5.35) or (5.36) that

$$\mathfrak{M}_1 \sim -\frac{4z}{\pi|z_2|}\ln|z|. \tag{5.37}$$

Thus the boundary magnetic susceptibility is not finite at $T = T_c$. More generally, we get from (5.35) and (5.36) that

$$\left.\frac{\partial\mathfrak{M}_1}{\partial\mathfrak{H}}\right|_{\mathfrak{H}=0} = -\frac{2\beta}{\pi}\coth\beta E_2\ln|1 - \alpha_2| + O(1) \tag{5.38}$$

both above and below the critical temperature. In other words, the boundary magnetic susceptibility at zero field has a logarithmic singularity at the critical temperature.

It is also necessary to determine the behavior near T_c for two remaining cases: (i) $E_1 > 0$ with $\mathfrak{H}$ away from zero and (ii) $E_1 < 0$. This can be easily done by means of the devices of analytic continuation and Pochammer's contour. In this manner we obtain for case (i)

$$\mathfrak{M}_1(\mathfrak{H}) = \text{Taylor series in } \tau_2 + \left[\frac{|z_2|(1 - z^2)\tau_2^2}{\pi z^2} + O(\tau_2^3)\right]\ln|\tau_2| \tag{5.39}$$

and for case (ii)

$$\mathfrak{M}_1(\mathfrak{H}) = \text{Taylor series in } \frac{1}{\tau_2} + \left[\frac{(1-z^2)z}{\pi|z_2|\tau_2^2} + O\left(\frac{1}{\tau_2^3}\right)\right] \ln|1/\tau_2|. \tag{5.40}$$

In both cases the Taylor series above T_c are the same as those below T_c.

C. Hysteresis

We return once more to the ferromagnetic case below critical temperature, that is, $T < T_c$ and $E_1 > 0$. As seen above, $\mathfrak{M}_1$ is an analytic function of $\mathfrak{H}$ for all $\mathfrak{H} \neq 0$, and $\mathfrak{M}_1$ is discontinuous at $\mathfrak{H} = 0$. We discuss here the analytic continuation of $\mathfrak{M}_1$; since $\mathfrak{M}_1$ is odd, it is sufficient to consider the continuation of $\mathfrak{M}_1$ for $\mathfrak{H} > 0$ to negative values of $\mathfrak{H}$. Let $\mathfrak{M}_1^c$, defined for some nonpositive $\mathfrak{H}$, be such that $\mathfrak{M}_1(\mathfrak{H})$ with $\mathfrak{H} > 0$ and $\mathfrak{M}_1^c(\mathfrak{H})$ with $\mathfrak{H} \leq 0$ taken together are analytic at $\mathfrak{H} = 0$. That this analytic continuation is possible can be most easily seen from (5.8), where s_1 and s_2 each has at most one zero in the cut $e^{i\theta}$-plane. For $\mathfrak{H}$ small, s_1 has a zero inside the unit circle, namely, the r of (5.11), and s_2 has a zero outside the unit circle, namely, $1/r$. After analytic continuation to negative small values of $\mathfrak{H}$,

$$r > 1, \tag{5.41}$$

and, still as before,

$$s_1(r) = s_2(1/r) = 0. \tag{5.42}$$

For $\mathfrak{H} < 0$, the difference between $\mathfrak{M}_1$ and $\mathfrak{M}_1^c$ is due to the residues at r and $1/r$; more explicitly,

$$\mathfrak{M}_1^c(\mathfrak{H}) - \mathfrak{M}_1(\mathfrak{H}) = \frac{2z}{(1/r - r)(1 - z^2)z_1(z_2^2 - z^2)^2} \times [(1 + z_1)^2(z_2^2 - z^2)^2 - z_2^2(1 - z_1)^2(1 - z^2)^2]. \tag{5.43}$$

When $-\mathfrak{H}$ is small, the right-hand side of (5.43) is positive and decreases with decreasing $\mathfrak{H}$. It reaches zero, as seen from (5.12) and (5.14), at

$$z^2 = |z_2| \frac{1 - \alpha_2}{1 + \alpha_2}. \tag{5.44}$$

The situation is thus as shown in Fig. 6.6.

It is natural to interpret this figure as a hysteresis loop. From (5.44), this loop shrinks to the single point $\mathfrak{H} = \mathfrak{M} = 0$ as $T \to T_c^-$. As $T \to 0$, $|z_2|$ is close to 1, and hence by (3.17)

$$2\alpha_2 \sim 1 - |z_2|. \tag{5.45}$$

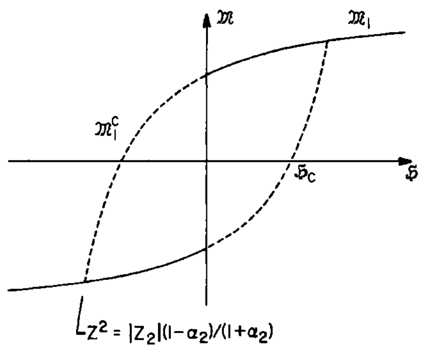


Fig. 6.6. Hysteresis loop for the magnetization of the first row for $E_1 = E_2$ at $T/T_c = 0.9$. The solid curve is $\mathfrak{M}_1$; the dotted curve shows its analytic continuation.

Substitution in (5.44) then gives

$$|z| \sim |z_2|. \tag{5.46}$$

Thus, in this limit of zero temperature, the hysteresis loop becomes a square, as shown in Fig. 6.7. Note that the limit $T \to 0$ of the analytic continuation of $\mathfrak{M}_1(\mathfrak{H})$ is different from the analytic continuation of

$$\lim_{T\to 0} \mathfrak{M}_1(\mathfrak{H}).$$

It is possible to make this interpretation of the analytic continuation much more precise by (1) studying the magnetization in rows other than the first and (2) computing the probability distribution function for the average spin in row 1. However, we will delay their presentation until Chapter XIII.

D. Numerical Results

We conclude this discussion of the boundary magnetization by presenting in graphical form the results of numerical evaluations of $\mathfrak{M}_1(\mathfrak{H})$.

In Fig. 6.8, we plot $\mathfrak{M}_1$ versus $\mathfrak{H}$ for $E_1 = E_2 = 1$ (all energies on the scale $k = 1$) for several values of T. For comparison, we also plot the one-dimensional case $E_1 = 1$, $E_2 = 0$ at $T = 2.498$, which corresponds to $T/T_c = 1.1$ when $E_1 = E_2$. In Fig. 6.9, we plot $\mathfrak{M}_1$ versus T/T_c for $E_1 = E_2 = 1$ at $\mathfrak{H} = 0, 0.3$, and 1 and we particularly note the smooth appearance of the latter two curves at $T = T_c$. In Fig. 6.10, we plot the susceptibility $\chi = \partial\mathfrak{M}_1(\mathfrak{H})/\partial\mathfrak{H}$ versus T and in particular note how the logarithmic divergence in χ for $\mathfrak{H} = 0$ at $T = T_c$ becomes a maximum

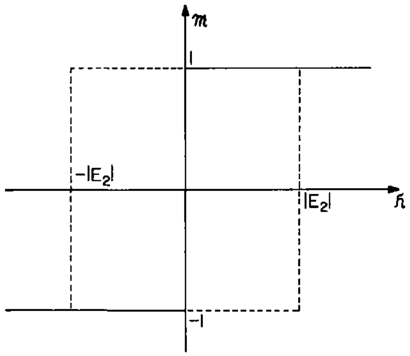


Fig. 6.7. Hysteresis loop at zero temperature.

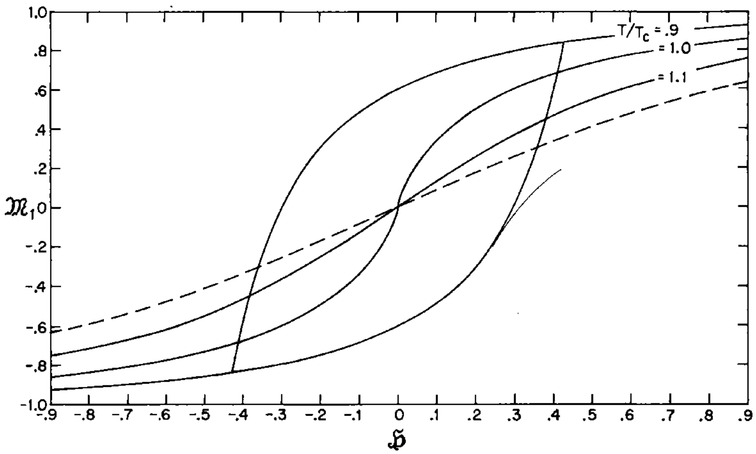


Fig. 6.8. $\mathfrak{M}_1$ versus $\mathfrak{H}$ for $E_1/k = E_2/k = 1$ (ferromagnetic) at various values of T/T_c. The broken line is the one-dimensional ($E_1/k = 1$, $E_2 = 0$) magnetization at the same temperature as $T/T_c = 1.1$.

which occurs at $T > T_c$ for $\mathfrak{H} \neq 0$. In Fig. 6.11, we show $\mathfrak{M}_1$ in the antiferromagnetic ($E_1 = -E_2 = -1$) case versus T and finally, in Fig. 6.12, we plot χ in the antiferromagnetic case versus T. In this last case, the shallow maximum which occurs slightly above T_c at $\mathfrak{H} = 0$ moves below T_c as $\mathfrak{H}$ is increased and will become a divergence at $T = 0$ when $\mathfrak{H} = 3$. All of these curves look perfectly smooth at $T = T_c$, even though they have infinite second derivatives there.

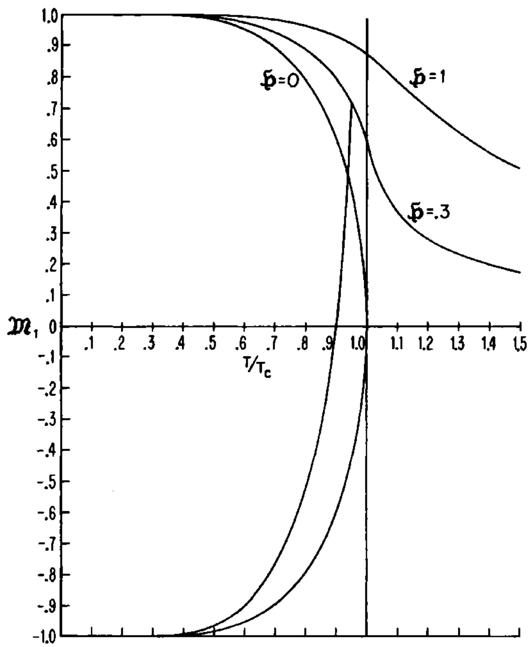


Fig. 6.9. **Boundary magnetization versus temperature for $E_1/k = E_2/k = 1$ at various values of $\mathfrak{H}$.**

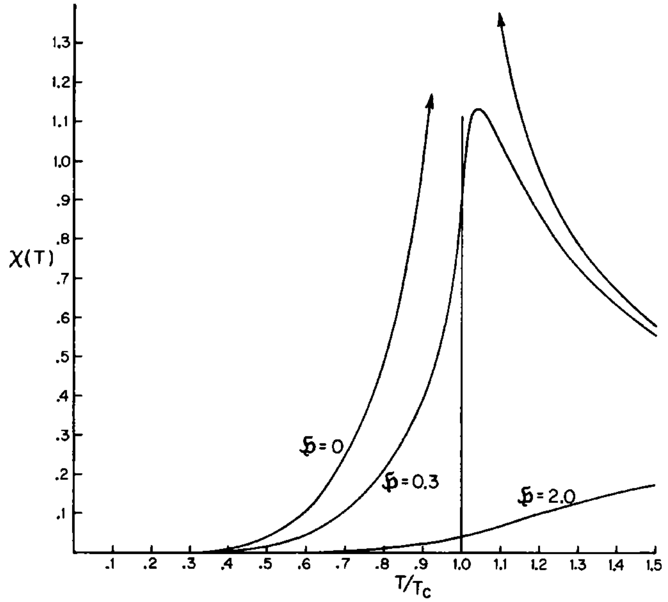


Fig. 6.10. **Boundary susceptibility versus temperature for $E_1/k = E_2/k = 1$ at various values of $\mathfrak{H}$.**

BOUNDARY HEAT AND MAGNETIZATION

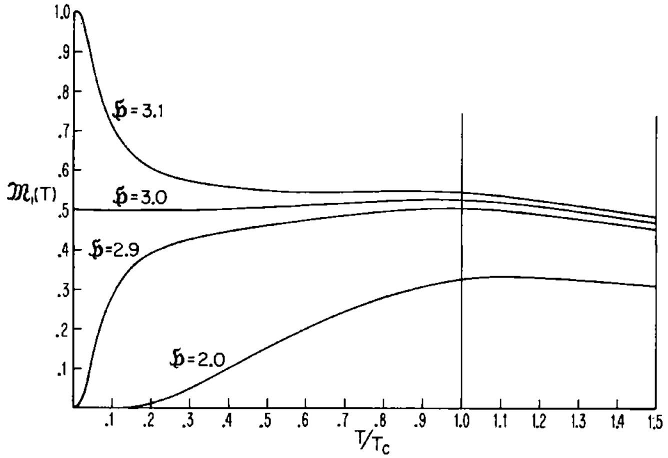


Fig. 6.11. Boundary magnetization versus temperature for $E_1/k = -E_2/k = -1$ (antiferromagnetic) at various values of $\mathfrak{H}$.

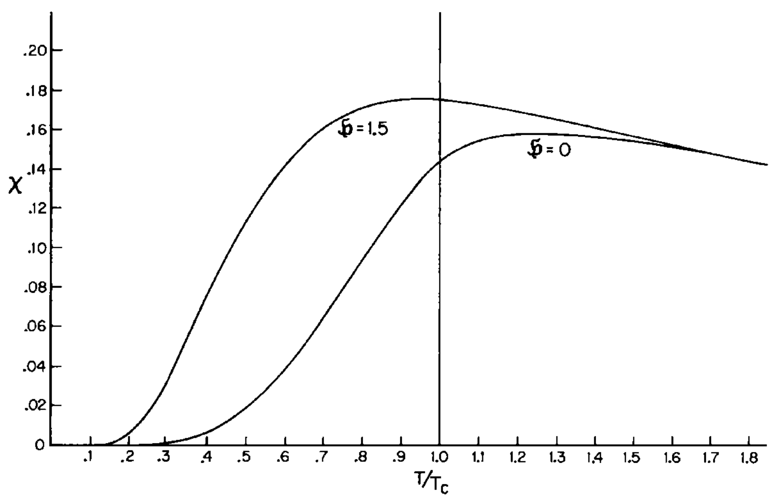


Fig. 6.12. Boundary susceptibility versus temperature for $E_1/k = -E_2/k = -1$ at various values of $\mathfrak{H}$.

CHAPTER VII
Boundary Spin-Spin Correlation Functions

1. INTRODUCTION

In this chapter[1] we will discuss the spin-spin correlation function of two spins in the boundary row [see (II.5.30)],

$$\mathfrak{S}_{1,1}(N, \mathfrak{H}) = \langle \sigma_{1,0}\sigma_{1,N} \rangle. \tag{1.1}$$

By a modest extension of the previous techniques we will be able to obtain a closed expression for $\mathfrak{S}_{1,1}(N, \mathfrak{H})$ with arbitrary $\mathfrak{H}$ as a sum of three terms each of which involves a product of two integrals. When $\mathfrak{H} = 0$ this result simplifies to a single integral. Therefore, though our result is more complicated than the corresponding one-dimensional result (III.3.5), it is a great deal simpler than the corresponding result for the bulk which involves an $N \times N$ determinant of integrals.

When $N \to \infty$ we know from (II.5.43) that, at least if $E_1 > 0$,

$$\lim_{N \to \infty} \mathfrak{S}_{1,1}(N, \mathfrak{H}) = \mathfrak{M}_1^2(\mathfrak{H}); \tag{1.2}$$

$\mathfrak{M}_1(\mathfrak{H})$ was studied in the last chapter and seen to have very different behavior near $\mathfrak{H} = 0$, depending upon whether $T < T_c$, $T > T_c$, or $T = T_c$. In this chapter we will study in detail the approach of $\mathfrak{S}_{1,1}(N, \mathfrak{H})$ to this limiting value. The manner of this approach is quite dependent on whether $T < T_c$, $T > T_c$, or $T = T_c$ and whether $\mathfrak{H} = 0$ or $\mathfrak{H} \neq 0$. Fortunately the exact form for $\mathfrak{S}_{1,1}(N, \mathfrak{H})$ is sufficiently simple that explicit asymptotic expansion may be made in each of these various regions and, furthermore, uniform expansions may be found which allow us to connect the various regions together. Moreover, this is the

1. The material of this chapter is taken from B. M. McCoy and T. T. Wu, *Phys. Rev.* **162**, 436 (1967).

only example of a correlation function for which all of these $N \gg 1$ expansions may be explicitly exhibited near T_c. Therefore in this chapter we will present the asymptotic analysis of $\mathfrak{S}_{1,1}(N, \mathfrak{H})$ in complete detail so that for the more complicated situations of the bulk, where it has so far proved impossible to obtain complete results, we will have some framework against which the incomplete results may be compared.

The expansions of this chapter are not technically very difficult to carry out, but there are a great many cases to consider. Furthermore, we have been unable to find any elegant method for doing the expansions and the final results tend to look rather formidable, particularly since most of the expansions are carried out to at least two terms. Therefore, before we present the details of the calculations, it is extremely useful to summarize the various ways in which $\mathfrak{S}_{1,1}(N, \mathfrak{H})$ may approach its limiting behavior at infinite N and explain how this behavior depends on $T - T_c$, $\mathfrak{H}$, and the sign of E_1.

When $\mathfrak{H} = 0$, Onsager's lattice possesses a symmetry that allows us to simply compute a spin-spin correlation function $\langle \sigma_{j,k}\sigma_{j',k'} \rangle$ for $E_1 < 0$ in terms of the value this correlation has for $E_1 > 0$. In the one-dimension model this symmetry has already been discussed in Sec. 3 of Chapter III. In the present case it is evident that the interaction energy

$$\mathscr{E} = -E_1 \sum_j \sum_k \sigma_{j,k}\sigma_{j,k+1} - E_2 \sum_j \sum_k \sigma_{j,k}\sigma_{j+1,k} \tag{1.3}$$

is invariant if $E_1 \to -E_1$ and $\sigma_{j,k}$ is replaced by $(-1)^k \sigma_{j,k}$ (see Fig. 7.1). Therefore when $\mathfrak{H} = 0$

$$\langle \sigma_{j,k}\sigma_{j',k'} \rangle|_{-E_1} = (-1)^{k+k'} \langle \sigma_{j,k}\sigma_{j',k'} \rangle|_{E_1}, \tag{1.4}$$

so that without loss of generality we may restrict our considerations to the ferromagnetic case $E_1 > 0$. When $\mathfrak{H} \neq 0$, of course, there is no such symmetry and both $E_1 > 0$ and $E_1 < 0$ must be separately investigated.

The simplest way to summarize the asymptotic behavior of $\mathfrak{S}_{1,1}(N, \mathfrak{H}) - \mathfrak{M}_1^2(\mathfrak{H})$ at $\mathfrak{H} = 0$ is by means of Fig. 7.2. There we see that there are

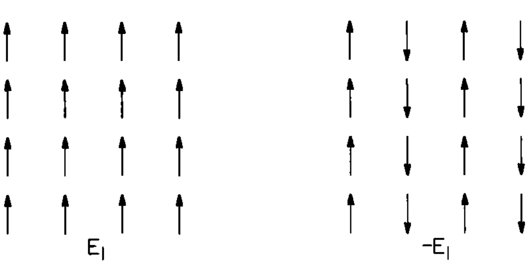


Fig. 7.1. The redefinition of spins associated with the replacement $E_1 \to -E_1$ when $\mathfrak{H} = 0$.

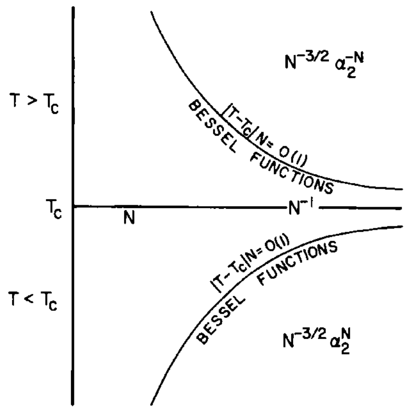


Fig. 7.2. Summary of the various types of behavior of $\mathfrak{S}_{1,1}(N, \mathfrak{H}) - \mathfrak{M}_1^2(\mathfrak{H})$ for $N \gg 1$ when $\mathfrak{H} = 0$ and $E_1 > 0$.

several forms for the asymptotic expansion. When T is fixed and $N \to \infty$, $\mathfrak{S}_{1,1}(N, 0) - \mathfrak{M}_1^2(0)$ behaves as $N^{-3/2}\alpha_2^{-N}$ if $T > T_c$ and as $N^{-3/2}\alpha_2^N$ if $T < T_c$. However, it is not possible to obtain the $T = T_c$ expansion from these expansions simply by setting $T = T_c$ because the second term in the asymptotic series becomes larger than the first when $|T - T_c|N \sim 1$. When $T = T_c$ and $N \gg 1$ we must approximate $\mathfrak{S}_{1,1}(N, 0)$ differently and find that $\mathfrak{S}_{1,1}(N, 0)$ behaves as N^{-1}. These three regions of relatively simple asymptotic behavior are connected by two transition regions in which $|T - T_c| \ll 1$ and $N \gg 1$ in such a fashion that

$$t = (T - T_c)N \tag{1.5}$$

is of order 1. In this region $\mathfrak{S}_{1,1}(N)$ is asymptotically expressed as a power series in N^{-1} whose coefficients are explicitly determined as modified Bessel functions or certain integrals of modified Bessel functions. When $t \to 0$, $\mathfrak{S}_{1,1}(N)$ approaches the $T = T_c$ asymptotic value and when $t \to \pm\infty$, $\mathfrak{S}_{1,1}(N)$ approaches the form that would be obtained by letting $T \to T_c$ in the asymptotic expansion obtained for the case $T \neq T_c$ fixed as $N \to \infty$.

When $T = T_c$ and $E_1 < 0$, $\mathfrak{S}_{1,1}(N, \mathfrak{H}) - \mathfrak{M}_1^2(\mathfrak{H})$ behaves asymptotically for all $\mathfrak{H}$ as $(-1)^N N^{-1}$. The ferromagnetic case $E_1 > 0$, however, is more complicated, and it is useful to summarize the behavior of $\mathfrak{S}_{1,1}(N, \mathfrak{H})$ for $N \gg 1$ when $T = T_c$ in terms of the diagram of Fig. 7.3. There are two regions of simple asymptotic behavior: (1) $\mathfrak{H} \neq 0$ fixed and $N \gg 1$, where $\mathfrak{S}_{1,1}(N, \mathfrak{H})$ behaves as N^{-4}; and (2) the previously discussed case of $\mathfrak{H} = 0$ where $\mathfrak{S}_{1,1}(N, 0)$ behaves as N^{-1}. There is a

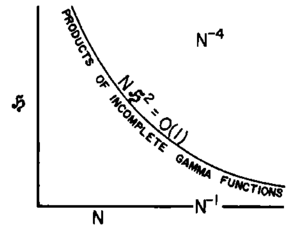


Fig. 7.3. Summary of the various types of behavior of $\mathfrak{S}_{1,1}(N, \mathfrak{H}) - \mathfrak{M}_1^2(\mathfrak{H})$ for $N \gg 1$ when $T = T_c$ and $E_1 > 0$.

transition region between these two simple cases that occurs when $\mathfrak{H}^2 N = u$ is of order 1. In this region $\mathfrak{S}_{1,1}(N, \mathfrak{H})$ is expressed as a power series in N^{-1} whose coefficients are functions of u alone and involve products of incomplete gamma functions. When $u \to 0$, this result reduces to the expansion of region 2 and when $u \to \infty$ it reduces to the $\mathfrak{H} \to 0$ form of the expansion of region 1.

We finally note that when $T \neq T_c$ and $\mathfrak{H} \neq 0$, $\mathfrak{S}_{1,1}(N, \mathfrak{H})$ approaches its $N \to \infty$ behavior exponentially rapidly. When $T < T_c$ and $E_1 > 0$, the rate of this exponential fall-off depends on $\mathfrak{H}$ if $|\mathfrak{H}|$ is smaller than the value at which the analytic continuation of $\mathfrak{M}_1$ meets $\mathfrak{M}_1$ itself. However, when $|\mathfrak{H}|$ is larger than this value the rate of fall-off depends on $T - T_c$ alone and not on $\mathfrak{H}$. For $\mathfrak{H}$ in this regime the asymptotic behavior of $\mathfrak{S}_{1,1}(N, \mathfrak{H}) - \mathfrak{M}_1^2(\mathfrak{H})$ is quite different from the case $\mathfrak{H} = 0$ and is summarized in Fig. 7.4.

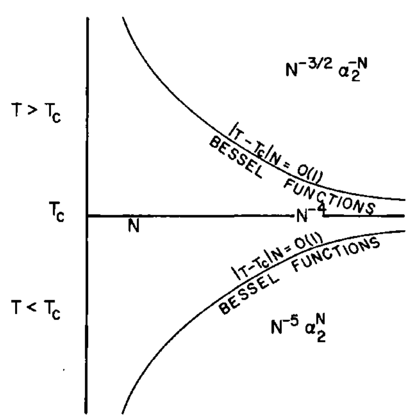


Fig. 7.4. Summary of the various types of behavior of $\mathfrak{S}_{1,1}(N, \mathfrak{H}) - \mathfrak{M}_1^2(\mathfrak{H})$ for $N \gg 1$ when $\mathfrak{H}$ is fixed and sufficiently large and $E_1 > 0$.

We have so far discussed the ferromagnetic case and shall now summarize qualitatively the situation with the antiferromagnetic case. When $T < T_c$, $\mathfrak{S}_{1,1}(N, \mathfrak{H}) - \mathfrak{M}_1^2(\mathfrak{H})$ does not approach a limit as $N \to \infty$ but rather oscillates as const. $(-1)^N$. The approach to this oscillatory behavior, however, is the same as the approach of $\mathfrak{S}_{1,1}(N, 0)$ to $(-1)^N \mathfrak{M}_1^2(0)$ and Fig. 7.2 therefore applies for arbitrary $\mathfrak{H}$.

2. FORMULATION OF THE PROBLEM

The correlation function between two spins in the boundary row is given as

$$\mathfrak{S}_{1,1}(N, \mathfrak{H}) = \langle \sigma_{1,0}\sigma_{1,N} \rangle = Z^{-1} \sum_{\sigma = \pm 1} \sigma_{1,0}\sigma_{1,N} e^{-\beta \mathscr{E}}. \tag{2.1}$$

To evaluate this we expand $e^{-\beta\mathscr{E}}$ as was done in (VI.2.2) to find

$$\begin{aligned} \mathfrak{S}_{1,1}(N, \mathfrak{H}) = {} & Z^{-1}(\cosh \beta E_1)^{4\mathscr{M}\mathscr{N}}(\cosh \beta E_2)^{2\mathscr{N}(2\mathscr{M}-1)}(\cosh \beta \mathfrak{H})^{2\mathscr{N}} \\ & \times \sum_{\sigma = \pm 1} \sigma_{1,0}\sigma_{1,N} \left[\prod_{j=1}^{2\mathscr{M}} \prod_{k=-\mathscr{N}+1}^{\mathscr{N}} (1 + z_1 \sigma_{j,k}\sigma_{j,k+1}) \right] \\ & \times \left[\prod_{j=1}^{2\mathscr{M}-1} \prod_{k=-\mathscr{N}+1}^{\mathscr{N}} (1 + z_2 \sigma_{j,k}\sigma_{j+1,k}) \right] \left[\prod_{k=-\mathscr{N}+1}^{\mathscr{N}} (1 + z\sigma_{1,k}) \right]. \end{aligned} \tag{2.2}$$

Now

$$\sigma_{1,0}(1 + z\sigma_{1,0}) = z(1 + z^{-1}\sigma_{1,0}). \tag{2.3}$$

Then we may rewrite $\mathfrak{S}_{1,1}(N, \mathfrak{H})$ as

$$\begin{aligned} \mathfrak{S}_{1,1}(N, \mathfrak{H}) = {} & Z^{-1}z^2(\cosh \beta E_1)^{4\mathscr{M}\mathscr{N}}(\cosh \beta E_2)^{2\mathscr{N}(2\mathscr{M}-1)}(\cosh \beta \mathfrak{H})^{2\mathscr{N}} \\ & \times \sum_{\sigma = \pm 1} \left[\prod_{j=1}^{2\mathscr{M}} \prod_{k=-\mathscr{N}+1}^{\mathscr{N}} (1 + z_1 \sigma_{j,k}\sigma_{j,k+1}) \right] \\ & \times \left[\prod_{j=1}^{2\mathscr{M}-1} \prod_{k=-\mathscr{N}+1}^{\mathscr{N}} (1 + z_2 \sigma_{j,k}\sigma_{j+1,k}) \right] \\ & \times \left[(1 + z^{-1}\sigma_{1,0})(1 + z^{-1}\sigma_{1,N}) \prod_{\substack{k=-\mathscr{N}+1 \\ k \neq 0,N}}^{\mathscr{N}} (1 + z\sigma_{1,k}) \right]. \end{aligned} \tag{2.4}$$

The summation $\sum_{\sigma=\pm 1}$ is of exactly the same type as was considered in the last chapter in the evaluation of the partition function. The only difference is that the lattice of Fig. 6.3(a) is replaced by the lattice of Fig. 7.5. We may compute the partition function for this lattice in terms

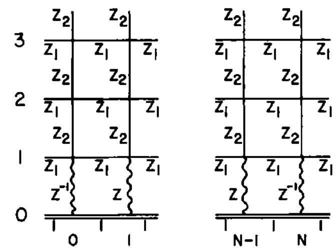


Fig. 7.5. Modified lattice used for computing $\langle\sigma_{1,0}\sigma_{1,N}\rangle$.

of the Pfaffian of a matrix A' where $A' - A = \delta$ has the following nonzero elements:

$$\delta(0, 0; 1, 0) = \delta(0, N; 1, N) = -\delta^T(1, 0; 0, 0) = -\delta^T(1, N; 0, N)$$

$$= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & z^{-1} - z \\ 0 & 0 & 0 & 0 \end{bmatrix}, \tag{2.5}$$

and the matrix A was defined by (VI.2.6). Therefore, since from (VI.2.7)

$$Z = \tfrac{1}{2}(2 \cosh \beta E_1)^{4\mathcal{M}\mathcal{N}}(\cosh \beta E_2)^{2\mathcal{N}(2\mathcal{M}-1)}(\cosh \beta\mathfrak{H})^{2\mathcal{N}} \operatorname{Pf} A, \tag{2.6}$$

the $\sum_{\sigma=\pm 1}$ summation in (2.2) is given by $\frac{1}{2} \operatorname{Pf} A'$ and

$$\mathfrak{S}_{1,1}(N, \mathfrak{H}) = z^2 \frac{\operatorname{Pf} A'}{\operatorname{Pf} A} = z^2 \frac{\operatorname{Pf}(A + \delta)}{\operatorname{Pf} A}, \tag{2.7}$$

which may be squared to give

$$\mathfrak{S}^2_{1,1}(N, \mathfrak{H}) = z^4 \frac{\det (A + \delta)}{\det A} = z^4 \det (1 + A^{-1}\delta). \tag{2.8}$$

Define y to be the nonzero submatrix of δ. Explicitly,

$$y = \begin{array}{ll} & \\ & \\ 10 & D \\ 1N & D \\ 00 & U \\ 0N & U \end{array} \begin{array}{c} \begin{array}{cccc} 10 & 1N & 00 & 0N \\ D & D & U & U \end{array} \\ \begin{bmatrix} 0 & 0 & -(z^{-1} - z) & 0 \\ 0 & 0 & 0 & -(z^{-1} - z) \\ z^{-1} - z & 0 & 0 & 0 \\ 0 & z^{-1} - z & 0 & 0 \end{bmatrix} \end{array}. \tag{2.9}$$

Define Q to be the submatrix of A^{-1} in the subspace defined by y.

Explicitly,

$$Q = \begin{bmatrix} 0 & A^{-1}(1,0;1,N)_{DD} & A^{-1}(1,0;0,0)_{DU} & A^{-1}(1,0;0,N)_{DU} \\ A^{-1}(1,N;1,0)_{DD} & 0 & A^{-1}(1,N;0,0)_{DU} & A^{-1}(1,N;0,N)_{DU} \\ A^{-1}(0,0;1,0)_{UD} & A^{-1}(0,0;1,N)_{UD} & 0 & A^{-1}(0,0;0,N)_{UU} \\ A^{-1}(0,N;1,0)_{UD} & A^{-1}(0,N;1,N)_{UD} & A^{-1}(0,N;0,0)_{UU} & 0 \end{bmatrix}, \tag{2.10}$$

Therefore we may rewrite (2.8) as

$$\mathfrak{S}_{1,1}^2(N, \mathfrak{H}) = z^4 \det(1 + Qy) = z^4 \det y \det(y^{-1} + Q). \tag{2.11}$$

Since

$$\det y = (z^{-1} - z)^4, \tag{2.12}$$

and since

$$y^{-1} = \begin{bmatrix} 0 & 0 & (z^{-1}-z)^{-1} & 0 \\ 0 & 0 & 0 & (z^{-1}-z)^{-1} \\ -(z^{-1}-z)^{-1} & 0 & 0 & 0 \\ 0 & -(z^{-1}-z)^{-1} & 0 & 0 \end{bmatrix} \tag{2.13}$$

is antisymmetric, we find

$$\begin{aligned} \mathfrak{S}_{1,1}(N, \mathfrak{H}) &= \pm(1 - z^2)^2 \operatorname{Pf}[y^{-1} + Q] \\ &= \pm(1 - z^2)^2\{[A^{-1}(1,0;0,0)_{DU} + (z^{-1} - z)^{-1}] \\ &\qquad \times [A^{-1}(1,N;0,N)_{DU} + (z^{-1} - z)^{-1}] \\ &\qquad - A^{-1}(1,0;1,N)_{DD}A^{-1}(0,0;0,N)_{UU} \\ &\qquad - A^{-1}(1,N;0,0)_{DU}A^{-1}(1,0;0,N)_{DU}\}, \end{aligned} \tag{2.14}$$

where the $\pm$ sign must be appropriately chosen. Thus we have a complete expression for $\mathfrak{S}_{1,1}(N, \mathfrak{H})$ if we can evaluate the inverse matrix elements of A.

3. THE INVERSE OF A

The matrix A may be explicitly written in a direct-product notation as

$$A = \begin{bmatrix} 0 & 1 & -1 & -1 \\ -1 & 0 & 1 & -1 \\ 1 & -1 & 0 & 1 \\ 1 & 1 & -1 & 0 \end{bmatrix} \otimes I_{2\mathscr{M}+1} \otimes I_{2\mathscr{N}}$$

$$
\begin{aligned}
&+\begin{bmatrix} 0 & z_1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \otimes I^{(z)}_{2\mathscr{M}+1} \otimes \tilde{H}_{2\mathscr{N}} \\
&+\begin{bmatrix} 0 & 0 & 0 & 0 \\ -z_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \otimes I^{(z)}_{2\mathscr{M}+1} \otimes \tilde{H}^{T}_{2\mathscr{N}} \\
&+\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & z_2 \\ 0 & 0 & 0 & 0 \end{bmatrix} \otimes \tilde{H}^{(z)}_{2\mathscr{M}+1} \otimes I_{2\mathscr{N}} \\
&+\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -z_2 & 0 \end{bmatrix} \otimes \tilde{H}^{(z)T}_{2\mathscr{M}+1} \otimes I_{2\mathscr{N}},
\end{aligned} \tag{3.1}
$$

where the $(2\mathscr{M} + 1) \times (2\mathscr{M} + 1)$-dimensional matrix $I^{(z)}_{2\mathscr{M}+1}$ is defined as

$$
\begin{aligned}
[I^{(z)}_{2\mathscr{M}+1}]_{0,0} &= z_1^{-1} \\
[I^{(z)}_{2\mathscr{M}+1}]_{j,j} &= 1 \qquad \text{if } 1 \le j \le 2\mathscr{M}
\end{aligned} \tag{3.2}
$$

and all other elements are zero, $\tilde{H}_{2\mathscr{N}}$ is the nearly cyclic matrix defined by (V.2.17b), and $\tilde{H}^{(z)}_{2\mathscr{M}+1}$ is the $(2\mathscr{M} + 1) \times (2\mathscr{M} + 1)$-dimensional matrix defined by

$$
\begin{aligned}
[\tilde{H}^{(z)}_{2\mathscr{M}+1}]_{0,1} &= \frac{z}{z_2}; \\
[\tilde{H}^{(z)}_{2\mathscr{M}+1}]_{j,j+1} &= 1 \qquad \text{if } 1 \le j \le 2\mathscr{M} - 1
\end{aligned} \tag{3.3}
$$

and all other matrix elements are zero. We know from Chapter V that because $\tilde{H}_{2\mathscr{N}}$ is a near-cyclic matrix its $2\mathscr{N}$ eigenvectors are $v_l^{(n)} = e^{\pi i(2n-1)l/2\mathscr{N}}$ and that if we define the $2\mathscr{N} \times 2\mathscr{N}$ matrix u as

$$
u_{ln} = v_l^{(n)} = e^{\pi i(2n-1)l/2\mathscr{N}} \tag{3.4}
$$

we have

$$
u^{-1}\tilde{H}_{2\mathscr{N}}u = \begin{bmatrix} e^{\pi i/2\mathscr{N}} & & & & \\ & e^{3\pi i/2\mathscr{N}} & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & \cdot \\ & & & & & e^{(2n-1)\pi i/2\mathscr{N}} \end{bmatrix}, \tag{3.5}
$$

where

$$u_{ln}^{-1} = (2\mathcal{N})^{-1} e^{\pi i(2l-1)n/2\mathcal{N}}. \tag{3.6}$$

Therefore we find

$$\sum_{l,l'} u_{kl}^{-1} A(j, l; j', l') u_{l'k'} = B_{j,j'}[\pi(2k - 1)/2\mathcal{N}]\delta_{k,k'}, \tag{3.7}$$

where the 4×4 matrices $B_{j,j'}$ are defined by (VI.3.3).

It is now an easy matter to compute A^{-1} in terms of the $4(2\mathcal{M} + 1) \times 4(2\mathcal{M} + 1)$ matrix B^{-1}. We take the inverse of both sides of (3.7) to find

$$[u^{-1}A^{-1}u]_{j,k;j',k'} = [B^{-1}(\pi(2k - 1)/2\mathcal{N})]_{j,j'}\delta_{k,k'}, \tag{3.8}$$

from which, if we multiply by u on the left and u^{-1} on the right, we obtain

$$\begin{aligned} A^{-1}(j, k; j', k') &= \sum_{l,l'} u_{kl}\delta_{l,l'} u_{l'k'}^{-1}[B^{-1}(\pi(2k - 1)/2\mathcal{N})]_{j,j'} \\ &= (2\mathcal{N})^{-1} \sum_{\theta} e^{i\theta(k-k')}[B^{-1}(\theta)]_{j,j'}, \end{aligned} \tag{3.9}$$

where the sum over θ is over $\theta = \pi(2n - 1)/2\mathcal{N}$ with $n = 1, \ldots, 2\mathcal{N}$.

We may easily find the elements of B^{-1} in the U, D subspace by relating these elements to the elements of $\mathfrak{C}^{-1}$ [$\mathfrak{C}$ given by (VI.3.9)]. We first remark that if we rearrange the rows and columns of B', B, and T (as defined in Sec. 3 of Chapter VI) so that all R, L rows (columns) precede all U, D rows (columns) and call the resulting $4(2\mathcal{M} + 1) \times 4(2\mathcal{M} + 1)$ matrices,

$$\begin{bmatrix} b'_{11} & b'_{12} \\ 0 & b'_{22} \end{bmatrix}, \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}, \text{ and } \begin{bmatrix} 1 & 0 \\ t_{21} & 1 \end{bmatrix}, \tag{3.10}$$

where each entry is a $2(2\mathcal{M} + 1) \times 2(2\mathcal{M} + 1)$ matrix, then we may write, using (VI.3.5),

$$\begin{aligned} \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}^{-1} &= \begin{bmatrix} b'_{11} & b'_{12} \\ 0 & b'_{22} \end{bmatrix}^{-1} \begin{bmatrix} 1 & 0 \\ t_{21} & 1 \end{bmatrix} \\ &= \begin{bmatrix} b'^{-1}_{11} & -b'^{-1}_{11} b'_{12} b'^{-1}_{22} \\ 0 & b'^{-1}_{22} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ t_{21} & 1 \end{bmatrix}. \end{aligned} \tag{3.11}$$

The matrix $\mathfrak{C}$ is just b'_{22} with U and D interchanged, so we have from (3.11) the relation

$$[B^{-1}]_{jl,j'l'} = [\mathfrak{C}^{-1}]_{jl,j'l'}, \qquad l = U, D, \qquad l' = U, D. \tag{3.12}$$

We now compute $\mathfrak{C}^{-1}$ from the formula

$$[\mathfrak{C}^{-1}]_{jl,j'l'} = \text{cofactor } \mathfrak{C}_{j'l',jl}/\det \mathfrak{C}. \tag{3.13}$$

To evaluate these cofactors, we define the $2n \times 2n$ determinant $\mathfrak{C}_n$ to be the determinant obtained from $\mathfrak{C}_n$ by striking out the first two rows and columns. Similarly, we define $\bar{\mathfrak{D}}_n$ to be the $(2n - 1) \times (2n - 1)$ determinant obtained from $\mathfrak{D}_n$ by striking out the first two rows and columns, and $\bar{\bar{\mathfrak{D}}}_n$ to be the $(2n - 1) \times (2n - 1)$ determinant obtained from $\mathfrak{C}_n$ by striking out the first three rows and columns. We evaluate $\bar{\mathfrak{C}}_n$, $\bar{\mathfrak{D}}_n$, and $\bar{\bar{\mathfrak{D}}}_n$ exactly as we did in Chapter VI and find

$$\bar{\mathfrak{C}}_n = v^2\lambda^n + v'^2\lambda'^n, \tag{3.14a}$$

$$\bar{\mathfrak{D}}_n = z_2^{-1} iv'v(\lambda^n - \lambda'^n), \tag{3.14b}$$

and

$$\bar{\bar{\mathfrak{D}}}_n = -\bar{\mathfrak{D}}_n. \tag{3.14c}$$

Because $\mathfrak{C}$ has only three nonvanishing diagonals, we find for $j \geq j' \geq 1$,

$$[B^{-1}]_{jD,j'D} = -[B^{-1}]^*_{j'D,jD} = -z_2^{j-j'}\mathfrak{b}^{j-j'}\bar{\mathfrak{D}}_{2\mathscr{M}-j+1}\mathfrak{C}_{j'-1}/\mathfrak{C}_{2\mathscr{M}}, \tag{3.15a}$$

$$[B^{-1}]_{jU,j'U} = -[B^{-1}]^*_{j'U,jU} = z_2^{j-j'}\mathfrak{b}^{j-j'}\bar{\mathfrak{C}}_{2\mathscr{M}-j}\mathfrak{D}_{j'}/\mathfrak{C}_{2\mathscr{M}}, \tag{3.15b}$$

$$[B^{-1}]_{jU,j'D} = -[B^{-1}]^*_{j'D,jU} = z_2^{j-j'}\mathfrak{b}^{j-j'+1}\bar{\mathfrak{C}}_{2\mathscr{M}-j}\mathfrak{C}_{j'-1}/\mathfrak{C}_{2\mathscr{M}}; \tag{3.15c}$$

for $j > j' \geq 1$,

$$[B^{-1}]_{jD,j'U} = -[B^{-1}]^*_{j'U,jD} = -z_2^{j-j'}\mathfrak{b}^{j-j'-1}\bar{\bar{\mathfrak{D}}}_{2\mathscr{M}-j+1}\mathfrak{D}_{j'}/\mathfrak{C}_{2\mathscr{M}}; \tag{3.15d}$$

for $j > 0$

$$[B^{-1}]_{jD,0U} = -[B^{-1}]^*_{0U,jD} = z\mathfrak{c}\mathfrak{b}^{j-1}z_2^{j-1}\bar{\mathfrak{D}}_{2\mathscr{M}-j+1}/\mathfrak{C}_{2\mathscr{M}}, \tag{3.15e}$$

$$[B^{-1}]_{jU,0U} = -[B^{-1}]^*_{0U,jU} = -z\mathfrak{c}\mathfrak{b}^{j}z_2^{j-1}\mathfrak{C}_{2\mathscr{M}-j}/\mathfrak{C}_{2\mathscr{M}}, \tag{3.15f}$$

$$[B^{-1}]_{0U,0U} = -\mathfrak{c}\bar{\mathfrak{C}}_{2\mathscr{M}}/\mathfrak{C}_{2\mathscr{M}}, \tag{3.15g}$$

$$[B^{-1}]_{jD,0D} = 0, \tag{3.15h}$$

$$[B^{-1}]_{0D,0D} = -\mathfrak{c}^{-1}; \tag{3.15i}$$

and for all j,

$$[B^{-1}]_{jU,0D} = 0. \tag{3.15j}$$

For fixed j, k, j', and k' as $\mathscr{M} \to \infty$ and $\mathscr{N} \to \infty$, we have for $j \geq j' \geq 1$,

$$\begin{aligned} &A^{-1}(j,k;j',k')_{DD} \\ &\quad = -A^{-1}(j',k';j,k)_{DD} \\ &\quad = -\frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta e^{i\theta(k-k')}\,\frac{\alpha^{j'-j}z_1}{z_2(1-z_1^2)}\,\frac{e^{i\theta}-e^{-i\theta}}{\alpha^{-1}-\alpha} \\ &\qquad \times\left[1+\frac{(v'/v)^2}{\alpha^{2(j'-1)}}\left(\frac{(e^{i\theta}-1)/(e^{i\theta}+1)+iz^2z_2^{-1}v/v'}{(e^{i\theta}-1)/(e^{i\theta}+1)-iz^2z_2^{-1}v'/v}\right)\right], \end{aligned} \tag{3.16a}$$

$$A^{-1}(j,k;j',k')_{UU} = -A^{-1}(j',k';j,k)_{UU}$$
$$= \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta e^{i\theta(k-k')} \frac{\alpha^{j'-j}z_1}{z_2(1-z_1^2)} \frac{e^{i\theta}-e^{-i\theta}}{\alpha^{-1}-\alpha}$$
$$\times \left[1 - \frac{1}{\alpha^{2j'}}\left(\frac{(e^{i\theta}-1)/(e^{i\theta}+1) + iz^2z_2^{-1}v/v'}{(e^{i\theta}-1)/(e^{i\theta}+1) - iz^2z_2^{-1}v'/v}\right)\right], \tag{3.16b}$$

$$A^{-1}(j,k;j',k')_{UD}$$
$$= -A^{-1}(j',k';j,k)_{DU}$$
$$= \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta e^{i\theta(k-k')} \frac{\alpha^{j'-j}}{z_2(1-z_1^2)(\alpha^{-1}-\alpha)}[-1+z_1^2+\alpha^{-1}z_2|1+z_1e^{i\theta}|^2]$$
$$\times \left[1 + \frac{(v'/v)^2}{\alpha^{2(j'-1)}}\left(\frac{(e^{i\theta}-1)/(e^{i\theta}+1) + iz^2z_2^{-1}v/v'}{(e^{i\theta}-1)/(e^{i\theta}+1) - iz^2z_2^{-1}v'/v}\right)\right]; \tag{3.16c}$$

for $j > j' \geq 1$,

$$A^{-1}(j,k;j',k')_{DU}$$
$$= -A^{-1}(j',k';j,k)_{UD}$$
$$= \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta e^{i\theta(k-k')} \frac{\alpha^{j'-j}}{z_2(1-z_1^2)(\alpha^{-1}-\alpha)}[1-z_1^2-z_2\alpha|1+z_1e^{i\theta}|^2]$$
$$\times \left[1 - \frac{1}{\alpha^{2j'}}\left(\frac{(e^{i\theta}-1)/(e^{i\theta}+1) + iz^2z_2^{-1}v/v'}{(e^{i\theta}-1)/(e^{i\theta}+1) - iz^2z_2^{-1}v'/v}\right)\right]; \tag{3.16d}$$

for $j \geq 1$,

$$A^{-1}(j,k;0,k')_{DU} = -A^{-1}(0,k';j,k)_{UD}$$
$$= -\frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta e^{i\theta(k-k')} \frac{iz}{\alpha^{j-1}}\left(z_2\frac{e^{i\theta}-1}{e^{i\theta}+1}\frac{v}{v'} - iz^2\right)^{-1}, \tag{3.16e}$$

$$A^{-1}(j,k;0,k')_{UU} = -A^{-1}(0,k';j,k)_{UU}$$
$$= \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta e^{i\theta(k-k')} \frac{z}{z_2\alpha^j}\left(\frac{e^{i\theta}-1}{e^{i\theta}+1} - \frac{iz^2}{z_2}\frac{v'}{v}\right)^{-1}, \tag{3.16f}$$

$$A^{-1}(0,k;0,k')_{UU} = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta e^{i\theta(k-k')}\left(\frac{e^{i\theta}-1}{e^{i\theta}+1} - \frac{iz^2}{z_2}\frac{v'}{v}\right)^{-1}, \tag{3.16g}$$

$$A^{-1}(j,k;0,k')_{DD} = 0, \tag{3.16h}$$

$$A^{-1}(0,k;0,k')_{DD} = -\frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta e^{i\theta(k-k')}\frac{e^{i\theta}+1}{e^{i\theta}-1}; \tag{3.16i}$$

for all $j \geq 0$,

$$A^{-1}(j,k;0,k')_{UD} = 0. \tag{3.16j}$$

In the foregoing equations, v'/v is given by (VI.3.20). Furthermore, note that

$$A^{-1}(j,k;j',k)_{DD} = A^{-1}(j,k;j',k)_{UU} = 0. \tag{3.17}$$

4. GENERAL CONSIDERATIONS

We now use in (2.14) the explicit forms for the matrix elements of A^{-1} found in the last section and obtain

$$\begin{aligned}
&\pm \mathfrak{S}_{1,1}(N,\mathfrak{H})\\
&\quad=(1-z^2)^2\{[A^{-1}(1,0;0,0)_{DU}+(z^{-1}-z)^{-1}]^2-A^{-1}(1,0;1,N)_{DD}\\
&\qquad\qquad\times A^{-1}(0,0;0,N)_{UU}-[A^{-1}(1,N;0,0)_{DU}]^2\}\\
&\quad=\left[\frac{z(1-z^2)}{2\pi}z_1\int_{-\pi}^{\pi}d\theta\,\frac{|1+e^{i\theta}|^2}{z_2^2|1+z_1e^{i\theta}|^2-z^2z_1|1+e^{i\theta}|^2-z_2(1-z_1^2)\alpha}-z\right]^2\\
&\qquad-(1-z^2)^2\left\{\left[\frac{z}{2\pi}\int_{-\pi}^{\pi}d\theta\,\frac{e^{iN\theta}|1+e^{i\theta}|^2z_1}{z_2^2|1+z_1e^{i\theta}|^2-z^2z_1|1+e^{i\theta}|^2-z_2(1-z_1^2)\alpha}\right]^2\right.\\
&\qquad\qquad-\left[\frac{1}{2\pi}\int_{-\pi}^{\pi}d\theta\,\frac{e^{iN\theta}z_1(e^{i\theta}-1)(e^{-i\theta}+1)}{z_2^2|1+z_1e^{i\theta}|^2-z^2z_1|1+e^{i\theta}|^2-z_2(1-z_1^2)\alpha}\right]\\
&\qquad\qquad\times\frac{1}{2\pi}\int_{-\pi}^{\pi}d\theta e^{iN\theta}\,\frac{e^{i\theta}+1}{e^{i\theta}-1}\\
&\qquad\qquad\left.\times\left[1+\frac{z_1z^2|1+e^{i\theta}|^2}{z_2^2|1+z_1e^{i\theta}|^2-z^2z_1|1+e^{i\theta}|^2-z_2(1-z_1^2)\alpha}\right]\right\},
\end{aligned}\tag{4.1}$$

where the first term is recognized as $\mathfrak{M}_1^2$. If $\mathfrak{H}\to\infty$, the right-hand side of (4.1) goes to 1; so, since we know that $\mathfrak{S}_{1,1}(N,\mathfrak{H})$ must go to 1 when $\mathfrak{H}\to\infty$, the plus sign must be chosen in (4.1) when $\mathfrak{H}$ is large. Because $\mathfrak{S}_{1,1}(N,\mathfrak{H})$ is a continuous function of $\mathfrak{H}$, this consideration determines the correct sign in (4.1) for all $\mathfrak{H}$ unless there is an $\mathfrak{H}$ for which $\mathfrak{S}_{1,1}(N,\mathfrak{H})$ vanishes. This only occurs at fixed N when the lattice is antiferromagnetic and $T<T_c$. In this case, when $\mathfrak{H}$ is small, $\mathfrak{S}_{1,1}$ tends to alternate in sign. The plus sign in (4.1) still holds but now we will determine it by continuity from $T=0$, where $\mathfrak{S}_{1,1}(N,\mathfrak{H})=(-1)^N$, as is explicitly shown later.

Before we consider asymptotic expansions, it is instructive to look at a number of simple limiting cases. To do this in a systematic fashion, and also because it clearly exhibits the several types of exponential behavior as $N\to\infty$, we will shift the contours of integration of the integrals with a term $e^{iN\theta}$ in the integrand from the unit circle to the contour Γ which goes around the branch cuts of α inside the unit circle. In doing this, we pick up contributions from the poles at $e^{i\theta}=1$, -1, and r. The form of

$\mathfrak{S}_{1,1}$ now depends on whether or not r is in the cut $e^{i\theta}$-plane as determined by (VI.5.13) and (VI.5.14). We also rationalize the denominators in (4.1) and obtain the following forms for the correlation where $\zeta = e^{i\theta}$ and we use the following notation:

$$\Xi_1 = z_2(1 - z_1^2)\frac{2}{\pi i}\int_\Gamma d\zeta \frac{\zeta^{N-1}}{(\zeta^{-1}r^{-1} - 1)(\zeta^2 - 1)}\left(\frac{\zeta}{r} - 1\right)\alpha^{-1}, \tag{4.2a}$$

$$\Xi_2 = z_2(1 - z_1^2)\frac{1}{2\pi i}\int_\Gamma d\zeta\left(\frac{\zeta - 1}{\zeta + 1}\right)\zeta^{N-1}\frac{\alpha^{-1}}{(\zeta - r)(\zeta^{-1}r^{-1} - 1)}, \tag{4.2b}$$

$$\begin{aligned}\Xi_3 = 4z_2^2\frac{(1 - z_1^2)^2z^2}{z_1^2(z_2^2 - z^2)^2}\Bigg\{&\left[\frac{1}{2\pi i}\int_\Gamma d\zeta\frac{\zeta^{N+1}}{(\zeta^2 - 1)(\zeta - r)}\frac{\alpha^{-1}}{(r^{-1}\zeta^{-1} - 1)}\right]\\ &\times\left[\frac{1}{2\pi i}\int_\Gamma d\zeta'\frac{\zeta'^{N-1}}{(\zeta'^2 - 1)(\zeta' - r)}\frac{\alpha^{-1}}{(r^{-1}\zeta'^{-1} - 1)}\right]\\ &-\left[\frac{1}{2\pi i}\int_\Gamma d\zeta\frac{\zeta^{N}}{(\zeta^2 - 1)(\zeta - r)}\frac{\alpha^{-1}}{(r^{-1}\zeta^{-1} - 1)}\right]^2\Bigg\},\end{aligned} \tag{4.2c}$$

$$\Xi_4 = z_2(1 - z_1^2)\frac{1}{2\pi i}\int_\Gamma d\zeta\frac{\zeta^{N-1}}{(\zeta - r)}\frac{\alpha^{-1}}{(r^{-1}\zeta^{-1} - 1)}\frac{\zeta + 1}{\zeta - 1}; \tag{4.2d}$$

if $T > T_c$ and $z^2 \geq |z_2|(1 - \alpha_1)/(1 + \alpha_1)$,

$$\begin{aligned}\mathfrak{S}_{1,1}(N, \mathfrak{H}) = \mathfrak{M}_1^2 &+ r^Nz^2\frac{(1 + z_1)^2(z^2 - z_2^2)^2 - z_2^2(1 - z_1)^2(1 - z^2)^2}{z_1^2(1 - z^2)(z^2 - z_2^2)^3(r^{-1} - r)^2}\\ &\times[(1 - z_1)^2 - z_2^2(1 + z_1)^2 - \Xi_1]\\ &+ z^2\frac{(1 - z_1)^2 - z_2^2(1 + z_1)^2}{z_1^2(z_2^2 - z^2)^2(r - 1)(r^{-1} - 1)^2}\Xi_2 + \Xi_3;\end{aligned} \tag{4.3}$$

if $T < T_c$, $E_1 > 0$, and either $z^2 \geq |z_2|(1 - \alpha_1)/(1 + \alpha_1)$ or $z^2 \leq |z_2|(1 - \alpha_2)/(1 + \alpha_2)$,

$$\mathfrak{S}_{1,1}(N, \mathfrak{H}) = \mathfrak{M}_1^2 - r^Nz^2r^2\frac{(1+z_1)^2(z^2-z_2^2)^2-z_2^2(1-z_1)^2(1-z^2)^2}{z_1^2(1-z^2)(z^2-z_2^2)^3(1-r^2)^2}\Xi_1 + \Xi_3; \tag{4.4}$$

if $T > T_c$ and $z^2 \leq |z_2|(1 - \alpha_1)/(1 + \alpha_1)$,

$$\mathfrak{S}_{1,1}(N, \mathfrak{H}) = \mathfrak{M}_1^2 - z^2r\frac{(1 - z_1)^2 - z_2^2(1 + z_1)^2}{(r - 1)^2(z_2^2 - z^2)^2z_1^2}\Xi_2 + \Xi_3; \tag{4.5}$$

if $T < T_c$, $E_1 > 0$, and $|z_2|(1 - \alpha_2)/(1 + \alpha_2) \leq z^2 \leq |z_2|(1 - \alpha_1)/(1 + \alpha_1)$,

$$\mathfrak{S}_{1,1}(N, \mathfrak{H}) = \mathfrak{M}_1^2 + \Xi_3; \tag{4.6}$$

if $T < T_c$, $E_1 < 0$, and $z^2 \geq |z_2|(1 - \alpha_1)/(1 + \alpha_1)$,

$$\begin{aligned}
&\mathfrak{S}_{1,1}(N, \mathfrak{H}) \\
&\quad = \mathfrak{M}_1^2 - z^2(-1)^N r \frac{z_2^2(1-z_1)^2-(1+z_1)^2}{(z_2^2-z^2)^2 z_1^2 (r+1)^2} \\
&\qquad \times \left\{ \frac{-r}{(r-1)^2} \left[(1-z_1)^2 - z_2^2(1+z_1)^2 \right.\right. \\
&\qquad\qquad \left.\left. - r^N \frac{(z_2^2-z^2)^2(1+z_1)^2 - z_2^2(1-z^2)^2(1-z_1)^2}{(1-z^2)(z_2^2-z^2)} \right] + \Xi_4 \right\} \\
&\qquad + r^N z^2 \frac{(1+z_1^2)(z^2-z_2^2)^2 - z_2^2(1-z_1)^2(1-z^2)^2}{z_1^2(1-z^2)(z^2-z_2^2)^3(r^{-1}-r)^2} \\
&\qquad \times [(1-z_1)^2 - z_2^2(1+z_1)^2 - \Xi_1] - z^2 r \frac{(1-z_1)^2 - z_2^2(1+z_1)^2}{(r-1)^2 z_1^2 (z_2^2-z^2)^2} \Xi_2 + \Xi_3;
\end{aligned} \tag{4.7}$$

and if $T < T_c$, $E_1 < 0$, and $z^2 < |z_2|(1 - \alpha_1)/(1 + \alpha_1)$,

$$\begin{aligned}
\mathfrak{S}_{1,1}(N, \mathfrak{H}) = \mathfrak{M}_1^2 &+ z^2(-1)^N r \frac{z_2^2(1 - z_1)^2 - (1 + z_1)^2}{(z_2^2 - z^2)^2 z_1^2 (r + 1)^2} \\
&\times \left\{ r \frac{(1 - z_1)^2 - z_2^2(1 + z_1)^2}{(r - 1)^2} - \Xi_4 \right\} \\
&- z^2 r \frac{(1 - z_1)^2 - z_2^2(1 + z_1)^2}{(r - 1)^2 (z_2^2 - z^2)^2 z_1^2} \Xi_2 + \Xi_3,
\end{aligned} \tag{4.8}$$

where it is convenient to note that

$$\begin{aligned}
(r - 1)(r^{-1} - 1)&z_1(1 - z^2)(z^2 - z_2^2) \\
&= -z^2[(1 - z_1)^2 - z_2^2(1 + z_1)^2 + 4z_1 z^2]
\end{aligned} \tag{4.9a}$$

and

$$\begin{aligned}
(r + 1)(r^{-1} + 1)&z_1(1 - z^2)(z^2 - z_2^2) \\
&= z^2(1 + z_1)^2 - z^2 z_2^2(1 - z_1)^2 - 4z_1 z_2^2.
\end{aligned} \tag{4.9b}$$

We now consider several limiting cases.

(i) $E_1 \to \infty$. In this case, $T < T_c$ and $\alpha_1 = \alpha_2 > 0$. Therefore, (4.4) holds and, using (VI.5.1) for $\mathfrak{M}_1$, we see that

$$\lim_{E_1 \to \infty} \mathfrak{S}_{1,1}(N, \mathfrak{H}) = 1. \tag{4.10}$$

(ii) $E_1 \to -\infty$. In this case, $T < T_c$ and $\alpha_1 = -(1 - |z_2|)/(1 + |z_2|)$. Therefore, (4.8) always holds and we have

$$\lim_{E \to -\infty} \mathfrak{S}_{1,1}(N, \mathfrak{H}) = (-1)^N. \tag{4.11}$$

(iii) $E_2 \to \pm\infty$. In this case, $T < T_c$, $\alpha_1 = \alpha_2 = 0$, and

$$r = (1 - |z|)/(1 + |z|).$$

If $E_1 > 0$, (4.4) holds and

$$\lim_{E_2 \to \pm\infty} \mathfrak{S}_{1,1}(N, \mathfrak{H}) = 1. \tag{4.12a}$$

If $E_1 < 0$, (4.8) holds and

$$\lim_{E_2 \to \pm\infty} \mathfrak{S}_{1,1}(N, \mathfrak{H}) = (-1)^N. \tag{4.12b}$$

(iv) $E_1 \to 0$. For this limit, it is easier to use (4.1) directly to see that

$$\lim_{E_1 \to 0} \mathfrak{S}_{1,1}(N, \mathfrak{H}) = z^2. \tag{4.13}$$

(v) $T \to 0$. In this limit, $r \to 0$ and $\alpha_1 \sim \alpha_2 = 0$. If $E_1 > 0$, then (4.4) holds, none of the integrals contributes, and $\mathfrak{S}_{1,1}(N, \mathfrak{H}) = 1$. If $E_1 < 0$, and if $|\mathfrak{H}| > 2|E_1| + E_2$, then $\lim_{T\to 0} (z^2 - z_2^2)/r = \infty$ and $\mathfrak{S}_{1,1}(N, \mathfrak{H}) = 1$; if $|\mathfrak{H}| < 2|E_1| + E_2$, then $\lim_{T\to 0} (z^2 - z_2^2)/r = 4$ and $\mathfrak{S}_{1,1}(N, \mathfrak{H}) = (-1)^N$; if $|\mathfrak{H}| = 2|E_1| + E_2$, then $\lim_{T\to 0} (z^2 - z_2^2)/r = 8$ and $\mathfrak{S}_{1,1}(N, \mathfrak{H}) = \frac{1}{4}(1 + (-1)^N)$.

(vi) $E_2 \to 0$. In this limit, we have reduced the vertical bond strength to zero, $T > T_c$, $\alpha_1 = 1/\alpha_2 = z_1$, and (4.3) holds. The integrals vanish and we have

$$\lim_{E_2 \to 0} \mathfrak{S}_{1,1}(N, \mathfrak{H}) = \frac{(1 - z^2)(1 + z_1)^2}{4z^2 z_1 + (1 - z_1)^2}\left[\frac{z^2}{1 - z^2} + r^N\left(\frac{1 - z_1}{1 + z_1}\right)^2\right]. \tag{4.14}$$

This is the spin-spin correlation function for the one-dimensional Ising model. It agrees with the one-dimensional calculation of (III.3.5) if we note that

$$\lim_{E_2 \to 0} r = \frac{\lambda_-}{\lambda_+}, \tag{4.15}$$

where λ_+, λ_- are defined by (III.2.10).

(vii) $\mathfrak{H} \to 0$. The behavior of $\mathfrak{M}_1(\mathfrak{H})$ in this limit has already been obtained in (VI.5.19). Therefore,

(a) if $T > T_c$, (4.5) holds and

$$\mathfrak{S}_{1,1}(N, 0) = -\frac{1 - z_1^2}{z_1 z_2}\frac{1}{2\pi i}\int_\Gamma d\zeta\, \frac{\zeta^N}{(\zeta^2 - 1)\alpha}; \tag{4.16a}$$

(b) if $T < T_c$ and $E_1 > 0$, (4.4) holds and

$$\mathfrak{S}_{1,1}(N, 0) = \frac{1}{4}\frac{z_2^2(1 + z_1)^2 - (1 - z_1)^2}{z_1 z_2^2} - \frac{1 - z_1^2}{z_1 z_2}\frac{1}{2\pi i}\int_\Gamma d\zeta\, \frac{\zeta^N}{(\zeta^2 - 1)\alpha}; \tag{4.16b}$$

(c) if $T < T_c$ and $E_1 < 0$, (4.8) holds and

$$\mathfrak{S}_{1,1}(N, 0) = -(-1)^N \frac{1}{4} \frac{(1 - z_1)^2 z_2^2 - (1 + z_1)^2}{z_1 z_2^2} - \frac{1 - z_1^2}{z_1 z_2} \frac{1}{2\pi i} \int_\Gamma d\zeta \frac{\zeta^N}{(\zeta^2 - 1)\alpha}. \tag{4.16c}$$

We now turn to the question of the behavior of $\mathfrak{S}_{1,1}(N, \mathfrak{H})$ for large N. We first consider the regions in which

$$N|1 - T/T_c| \gg 1 \tag{4.17}$$

and

$$N\left|1 - z^2 \frac{1 + \alpha_2}{(1 - \alpha_2)|z_2|}\right| \gg 1. \tag{4.18}$$

In this region, as the expressions (4.3)–(4.8) show, the correlation function approaches its limiting value exponentially rapidly. We will compute the asymptotic series multiplying the exponential for the several regions (4.3)–(4.8) and explicitly exhibit the first few terms. We then will consider the region where T is near T_c but where (4.18) still holds by assuming that N is such that $N|1 - T/T_c|$ is *fixed* and of order 1. In this case, the correlation functions do not approach their limiting value exponentially but only as an inverse power of N. The coefficients of the first few powers of N will be evaluated as functions of $N|1 - T/T_c|$. We next examine the case where $\mathfrak{H} = 0$ and $N|1 - T/T_c|$ is of order 1. Here, we obtain approximations to the simpler expressions (4.16). Finally, we consider the case where $T = T_c$ and Nz^2 is fixed and of order 1.

5. $T > T_c$, $N|1 - T/T_c| \gg 1$

From (VI.5.15), when r is in the cut $e^{i\theta}$-plane, $|r| \le |\alpha_1|$. Furthermore, $0 \le |\alpha_1| \le |\alpha_2^{-1}| \le 1$, so that each integral in (4.3) and (4.5) is of order α_2^{-N}. Thus, for all values of $\mathfrak{H}$, we have

$$\begin{aligned}\mathfrak{S}_{1,1}(N, \mathfrak{H}) \doteqdot \mathfrak{M}_1^2 &+ \frac{z^2[(1 - z_1)^2 - z_2^2(1 + z_1)^2](1 - z_2^2)}{z_1^2(r - 1)(r^{-1} - 1)(z_2^2 - z^2)^2} \\ &\times \frac{1}{2\pi} \int_{\alpha_1}^{\alpha_2^{-1}} d\zeta \zeta^N \left(\frac{\zeta - 1}{\zeta + 1}\right) \frac{r}{(\zeta - r)(1 - \zeta r)} \\ &\times [(1 - \alpha_1\zeta)(1 - \alpha_1\zeta^{-1})(1 - \alpha_2^{-1}\zeta)(\alpha_2^{-1}\zeta^{-1} - 1)]^{1/2},\end{aligned} \tag{5.1}$$

where $\doteqdot$ means that the right-hand side and the left-hand side have the same asymptotic expansion as $N \to \infty$. We now call

$$\zeta_1 = \alpha_2 \zeta \tag{5.2}$$

and write

$$\frac{1}{2\pi}\int_{\alpha_1}^{\alpha_2^{-1}} d\zeta\zeta^N\left(\frac{\zeta-1}{\zeta+1}\right)\frac{r}{(\zeta-r)(1-\zeta r)}$$
$$\times\,[(1-\alpha_1\zeta)(1-\alpha_1\zeta^{-1})(1-\alpha_2^{-1}\zeta)(\alpha_2^{-1}\zeta^{-1}-1)]^{1/2}$$
$$=\tfrac{1}{2}\alpha_2^{-N}\pi^{-1}\int_{\alpha_1\alpha_2}^{1} d\zeta_1\frac{\zeta_1^N(\alpha_2^{-1}\zeta_1-1)}{(\alpha_2^{-1}\zeta_1+1)(\alpha_2^{-1}\zeta_1-r)(\alpha_2 r^{-1}-\zeta_1)}$$
$$\times\,[(1-\alpha_1\alpha_2^{-1}\zeta_1)(1-\alpha_1\alpha_2\zeta_1^{-1})(1-\alpha_2^{-2}\zeta_1)(\zeta_1^{-1}-1)]^{1/2}. \quad (5.3)$$

Define

$$x_1=\frac{1+\alpha_1/\alpha_2}{1-\alpha_1/\alpha_2}=\cosh 2\beta E_1, \quad (5.4)$$

$$x_2=\frac{1+\alpha_1\alpha_2}{1-\alpha_1\alpha_2}=\coth 2\beta|E_2|, \quad (5.5)$$

$$x_3=\frac{\alpha_2^2+1}{\alpha_2^2-1}. \quad (5.6)$$

These three x's are related by

$$x_1x_2+x_1x_3-x_2x_3=1. \quad (5.7)$$

We further define

$$x_4=\frac{\alpha_2+1}{\alpha_2-1}, \quad (5.8)$$

$$x_5=\frac{1+\alpha_2 r}{1-\alpha_2 r}, \quad (5.9)$$

and

$$x_6=\frac{1+\alpha_2/r}{1-\alpha_2/r}. \quad (5.10)$$

We use these six x's in (5.3); for example,

$$(1-\zeta_1\alpha_1/\alpha_2)^{1/2}=\left(\frac{1+\zeta_1}{1+x_1}\right)^{1/2}\left[1+x_1\frac{1-\zeta_1}{1+\zeta_1}\right]^{1/2}. \quad (5.11)$$

Then we may write the right-hand side of (5.3) as

$$\frac{1}{2\pi}\alpha_2^{-N-1}\frac{(x_5-1)(x_6-1)}{x_4(x_1+1)^{1/2}(x_2+1)^{1/2}(x_3+1)^{1/2}}$$
$$\times\int_{\alpha_1\alpha_2}^{1} d\zeta_1\zeta_1^{N-1}\left(\frac{1-\zeta_1}{1+\zeta_1}\right)^{1/2}A_>\left(\frac{1-\zeta_1}{1+\zeta_1}\right). \quad (5.12)$$

where

$$A_>(\eta)=\frac{1+x_4\eta}{(1+\eta/x_4)(1-x_5\eta)(1-x_6\eta)}[(1+x_1\eta)(1-x_2\eta)(1+x_3\eta)]^{1/2}. \quad (5.13)$$

We will be able to reduce many of our asymptotic expressions to forms similar to (5.12). It is thus convenient to consider the following generalization:

$$\int^{1} d\zeta_1 \zeta_1^{N'} \frac{(1-\zeta_1)^q}{(1+\zeta_1)^p} R\left(\frac{1-\zeta_1}{1+\zeta_1}\right). \tag{5.14}$$

We expand $R(\eta)$ in a power series as

$$R(\eta) = \sum_{n=0}^{\infty} R_n \eta^n, \tag{5.15}$$

which we substitute into (5.14). The lower limit of integration in (5.14), if it is not 1, may always be extended to zero without altering the asymptotic series. Integrating term by term, we obtain

$$\int_0^{1} d\zeta_1 \zeta_1^{N'} \frac{(1-\zeta_1)^q}{(1+\zeta_1)^p} R\left(\frac{1-\zeta_1}{1+\zeta_1}\right) \doteqdot \sum_{n=0}^{\infty} R_n \frac{\Gamma(N'+1)\Gamma(n+q+1)}{\Gamma(n+q+2+N')} \frac{1}{2^{n+p}} \times F(n+p, n+q+1; N'+n+q+2; \tfrac{1}{2}). \tag{5.16}$$

In (5.16), the sum over n is to be interpreted in the sense of an asymptotic series and we have used Euler's integral representation of the hypergeometric function F:

$$F(a,b;c;z) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \frac{1}{(1-z)^a} \times \int_0^1 ds s^{c-b-1}(1-s)^{b-1}\left[1 - \frac{sz}{z-1}\right]^{-a} \tag{5.17}$$

$$= \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 dt t^{b-1}(1-t)^{c-b-1} \frac{1}{(1-tz)^a}, \tag{5.18}$$

where (5.18) is obtained by letting $s = 1 - t$. To obtain an explicit asymptotic expansion we expand F as a power series in z by expanding $(1-tz)^{-a}$ in (5.18) and integrating term by term, to find

$$F(a,b;c;z) = \Gamma(c)[\Gamma(a)\Gamma(b)]^{-1} \sum_{n=0}^{\infty} \frac{\Gamma(a+n)\Gamma(b+n)z^n}{\Gamma(c+n)n!}. \tag{5.19}$$

We may now use this series representation for F in (5.16), to find

$$\int^{1} d\zeta_1 \zeta_1^{N'} \frac{(1-\zeta_1)^q}{(1+\zeta_1)^p} R\left(\frac{1-\zeta_1}{1+\zeta_1}\right)$$

$$\doteqdot \sum_{n=0}^{\infty} R_n \frac{\Gamma(N'+1)}{\Gamma(n+p)} \frac{1}{2^{n+p}} \sum_{m=0}^{\infty} \frac{\Gamma(m+n+p)\Gamma(m+n+q+1)}{\Gamma(N'+m+n+q+2)m!} 2^{-m}$$

$$= N'! \sum_{m=0}^{\infty} \frac{1}{2^{m+p}} \frac{\Gamma(m+p)\Gamma(m+q+1)}{\Gamma(N'+m+q+2)} \sum_{n=0}^{m} \frac{R_n}{\Gamma(p+n)(m-n)!}, \tag{5.20}$$

where the final form is obtained by a trivial rearrangement of the double infinite series.

In the present case, we define $A_{n>}$ by

$$A_{>}(\eta) = \sum_{n=0}^{\infty} A_{n>}\eta^n, \tag{5.21}$$

where the first few terms are

$$A_{0>} = 1, \tag{5.22}$$

$$A_{1>} = x_4 - x_4^{-1} + x_5 + x_6 + \tfrac{1}{2}(x_1 - x_2 + x_3), \tag{5.23}$$

$$\begin{aligned} A_{2>} = {} & x_4^{-2} + x_5^2 + x_6^2 - \tfrac{1}{8}(x_1^2 + x_2^2 + x_3^2) - 1 + (x_4 - x_4^{-1})(x_5 + x_6) \\ & + x_5x_6 + \tfrac{1}{2}(x_4 - x_4^{-1} + x_5 + x_6)(x_1 - x_2 + x_3) \\ & - \tfrac{1}{4}(x_1x_2 - x_1x_3 + x_2x_3). \end{aligned} \tag{5.24}$$

We now may specialize (5.20) to (5.12) and obtain

$$\begin{aligned} \mathfrak{S}_{1,1}(N, \mathfrak{H}) \doteqdot {} & \mathfrak{M}_1^2 + \frac{z^2[(1 - z_1)^2 - z_2^2(1 + z_1)^2](1 - z_2^2)}{z_1^2(r - 1)(r^{-1} - 1)(z_2^2 - z^2)^2} \\ & \times \alpha_2^{-N-1} \frac{(x_5 - 1)(x_6 - 1)}{2^{3/2}\pi x_4(x_1 + 1)^{1/2}(x_2 + 1)^{1/2}(x_3 + 1)^{1/2}} \\ & \times (N - 1)! \sum_{m=0}^{\infty} \frac{\Gamma(m + \frac{1}{2})\Gamma(m + \frac{3}{2})}{\Gamma(N + \frac{3}{2} + m)2^m} \sum_{n=0}^{m} \frac{A_{n>}}{(m - n)!\,\Gamma(n + \frac{1}{2})}. \end{aligned} \tag{5.25}$$

This is the desired asymptotic expansion for $T > T_c$. For completeness, we write down the first three terms as $N \to \infty$:

$$\begin{aligned} \mathfrak{S}_{1,1}(N, \mathfrak{H}) \sim {} & \mathfrak{M}_1^2 + \frac{z^2[(1 - z_1)^2 - z_2^2(1 + z_1)^2](1 - z_2^2)}{z_1^2(r - 1)(r^{-1} - 1)(z_2^2 - z^2)^2} \\ & \times \frac{(x_5 - 1)(x_6 - 1)}{2^{5/2}\pi^{1/2}x_4(x_1 + 1)^{1/2}(x_2 + 1)^{1/2}(x_3 + 1)^{1/2}}\, \alpha_2^{-N-1}N^{-3/2} \\ & \times \left\{1 + \frac{3}{4N}A_{1>} + \frac{5}{32N^2}(6A_{2>} - 1) + O(N^{-3})\right\}. \end{aligned} \tag{5.26}$$

For this asymptotic series to be valid, we must have $N \gg A_{1>}$ which implies the restrictions

$$N \gg x_3 \tag{5.27}$$

and

$$N \gg |x_5 + x_6| = |2(1 - \alpha_2^2)(1 - \alpha_2 r)^{-1}(1 - \alpha_2 r^{-1})^{-1}|. \tag{5.28}$$

For all values of $\mathfrak{H}$, both of these requirements are satisfied if N is much larger than $(T/T_c - 1)^{-1}$. We may therefore let $\mathfrak{H} \to 0$ and find

$$\begin{aligned}\mathfrak{S}_{1,1}(N, 0) \sim\ & z_1^{-1} z_2^{-2}(1 - z_2^2)2^{-3/2}\pi^{-1/2} \\ & \times (x_1 + 1)^{-1/2}(x_2 + 1)^{-1/2}(x_3 + 1)^{1/2}\alpha_2^{-N-1}N^{-3/2} \\ & \times [1 + N^{-1}\tfrac{3}{4}A_{1>} + N^{-2}\tfrac{5}{32}(6A_{2>} - 1) + O(N^{-3})]. \end{aligned} \tag{5.29}$$

6. $T < T_c$, $E_1 > 0$, $N[1 - T/T_c] \gg 1$

When $T < T_c$ and $E_1 > 0$, there are two cases. If

$$z^2 < |z_2|(1 - \alpha_2)/(1 + \alpha_2),$$

then (4.4) holds. By (VI.5.16) we see that r is real and $0 \le \alpha_2 \le r < 1$. Therefore, we retain the leading exponential terms to find

$$\begin{aligned}\mathfrak{S}_{1,1}(N, \mathfrak{H}) \doteqdot\ & \mathfrak{M}_1^2 - 4r^N(r^{-1} - r)^{-2}(1 - z^2)^{-1}(z^2 - z_2^2)^{-3}z^2(z_1^{-2} - 1)z_2 \\ & \times [(1 + z_1)^2(z^2 - z_2^2)^2 - z_2^2(1 - z_1)^2(1 - z^2)^2] \\ & \times \frac{1}{2\pi i}\int_\Gamma d\zeta\zeta^{N-1}(\zeta^2 - 1)^{-1}(\zeta^{-1}r^{-1} - 1)^{-1}(\zeta r^{-1} - 1)\alpha^{-1}. \end{aligned} \tag{6.1}$$

We proceed as in the previous section to obtain an asymptotic expansion to the integral

$$\begin{aligned} & \frac{1}{2\pi i}\int_\Gamma d\zeta\zeta^N \frac{\zeta - r}{(1 - \zeta r)(\zeta^2 - 1)}\alpha^{-1} \\ & = -\frac{1}{2\pi}\frac{1 - z_2^2}{z_2(1 - z_1^2)x_4}\alpha_2^N \frac{(x_4 - 1)^2(x_5 - 1)}{(x_1 + 1)^{1/2}(x_2 + 1)^{1/2}(-x_3 - 1)^{1/2}(x_6 + 1)} \\ & \quad \times \int_{\alpha_1/\alpha_2}^1 d\zeta_1\zeta_1^{N-1}\left(\frac{1 - \zeta_1}{1 + \zeta_1}\right)^{1/2} A_<^{(1)}\left(\frac{1 - \zeta_1}{1 + \zeta_1}\right). \end{aligned} \tag{6.2}$$

where $\zeta_1 = \alpha_2^{-1}\zeta$ and

$$A_<^{(1)}(\eta) = \frac{(1 + x_6\eta)\{(1 + x_2\eta)(1 - x_1\eta)(1 - x_3\eta)\}^{1/2}}{(1 - x_4\eta)(1 - x_4^{-1}\eta)(1 + x_5\eta)}. \tag{6.3}$$

Expand $A_<^{(1)}(\eta)$ as

$$A_<^{(1)}(\eta) = \sum_{n=0}^{\infty} A_{n<}^{(1)}\eta^n, \tag{6.4}$$

where the first few terms are

$$A_{0<}^{(1)} = 1, \tag{6.5}$$

$$A_{1<}^{(1)} = \tfrac{1}{2}(x_2 - x_1 - x_3) + x_4 + x_4^{-1} - x_5 + x_6, \tag{6.6}$$

$$\begin{aligned} A_{2<}^{(1)} =\ & x_4^2 + x_4^{-2} + x_5^2 - \tfrac{1}{8}(x_2^2 + x_1^2 + x_3^2) + 1 + (x_4 + x_4^{-1})(x_6 - x_5) \\ & - x_5x_6 + (x_4 + x_4^{-1} - x_5 + x_6)\tfrac{1}{2}(x_2 - x_1 - x_3) \\ & - \tfrac{1}{4}(x_1x_2 + x_2x_3 - x_1x_3). \end{aligned} \tag{6.7}$$

We then use (5.20) to obtain

$$\mathfrak{S}_{1,1}(N, \mathfrak{H})$$
$$\doteqdot \mathfrak{M}_1^2 + \frac{\sqrt{2}\,\alpha_2^N r^N z^2(1 - z_2^2)[(1 + z_1)^2(z^2 - z_2^2)^2 - z_2^2(1 - z_1)^2(1 - z^2)^2]}{\pi z_1^2(r^{-1} - r)^2(1 - z^2)(z^2 - z_2^2)^3[(x_1 + 1)(x_2 + 1)(-x_3 - 1)]^{1/2}}$$
$$\times \frac{(1 - x_4)^2(x_5 - 1)}{x_4(x_6 + 1)}(N - 1)! \sum_{m=0}^{\infty} \frac{\Gamma(m + \frac{1}{2})\Gamma(m + \frac{3}{2})}{2^m\Gamma(N + \frac{3}{2} + m)}$$
$$\times \sum_{n=0}^{m} \frac{A_{n<}^{(1)}}{\Gamma(\frac{1}{2} + n)(m - n)!}. \tag{6.8}$$

Explicitly, for large N, this becomes

$$\mathfrak{S}_{1,1}(N, \mathfrak{H})$$
$$\sim \mathfrak{M}_1^2 + \frac{\alpha_2^N r^N z^2(1 - z_2^2)[(1 + z_1)^2(z^2 - z_2^2)^2 - z_2^2(1 - z_1)^2(1 - z^2)^2]}{z_1^2(r^{-1} - r)^2(1 - z^2)(z^2 - z_2^2)^3[2\pi(x_1 + 1)(x_2 + 1)(-x_3 - 1)]^{1/2}}$$
$$\times \frac{(1 - x_4)^2(x_5 - 1)}{x_4(x_6 + 1)} N^{-3/2}$$
$$\times \left\{1 + \frac{3}{4N}A_{1<}^{(1)} + \frac{5}{32N^2}(6A_{2<}^{(1)} - 1) + O(N^{-3})\right\}. \tag{6.9}$$

For this asymptotic expansion to be valid, we must have

$$N \gg |x_3| \quad \text{and} \quad N \gg x_6, \tag{6.10}$$

which hold if (4.17) and (4.18) are obeyed.

We may let $\mathfrak{H} \to 0^+$ without violating (6.10), and find

$$\mathfrak{S}_{1,1}(N, 0) \sim \mathfrak{M}_1^2(0^+) + \frac{\alpha_2^{N-1}(1 - z_2^2)|x_3 + 1|^{1/2}}{2z_1 z_2^2[2\pi(x_1 + 1)(x_2 + 1)]^{1/2}} N^{-3/2}$$
$$\times \left\{1 + \frac{3}{4N}A_{1<}^{(1)} + \frac{5}{32N^2}(6A_{2<}^{(1)} - 1) + O(N^{-3})\right\}. \tag{6.11}$$

If $z^2 > |z_2|(1 - \alpha_2)/(1 + \alpha_2)$, then (4.4) or (4.6) holds. In either case, the terms of leading exponential order are given by

$$\mathfrak{S}_{1,1}(N, \mathfrak{H}) \doteqdot \mathfrak{M}_1^2 + \frac{4z_2^2 z^2(z_1^{-1} - z_1)^2}{(z_2^2 - z^2)^2}$$
$$\times \left\{\left[\frac{1}{2\pi i}\int_\Gamma \frac{d\zeta\,\zeta^{N+1}\alpha^{-1}}{(\zeta^2 - 1)(\zeta - r)(r^{-1}\zeta^{-1} - 1)}\right]\right.$$
$$\times \left[\frac{1}{2\pi i}\int_\Gamma \frac{d\zeta'\,\zeta'^{N-1}\alpha^{-1}}{(\zeta'^2 - 1)(\zeta' - r)(r^{-1}\zeta'^{-1} - 1)}\right]$$
$$\left. - \left[\frac{1}{2\pi i}\int_\Gamma \frac{d\zeta\,\zeta^N\alpha^{-1}}{(\zeta^2 - 1)(\zeta - r)(r^{-1}\zeta^{-1} - 1)}\right]^2\right\}. \tag{6.12}$$

The three integrals in (6.12) differ only in the power of ζ in the integrand and clearly all have the same leading-order term. To display the cancellation that occurs, we first write

$$\frac{1}{2\pi i}\int_{\Gamma}\frac{d\zeta\zeta^{N}\alpha^{-1}}{(\zeta^{2}-1)(\zeta-r)(r^{-1}\zeta^{-1}-1)}$$
$$=\frac{-\alpha_{2}^{N+2}(1-z_{2}^{2})(x_{4}-1)^{2}(x_{5}+1)(x_{6}+1)}{2\pi z_{2}(1-z_{1}^{2})x_{4}[(x_{1}+1)(x_{2}+1)(-x_{3}-1)]^{1/2}}$$
$$\times\int_{\alpha_{1}\alpha_{2}^{-1}}^{1}\frac{d\zeta_{1}\zeta_{1}^{N}(1-\zeta_{1})^{1/2}A_{<}^{(2)}[(1-\zeta_{1})/(1+\zeta_{1})]}{(\zeta_{1}+1)^{5/2}},\tag{6.13}$$

where

$$A_{<}^{(2)}(\eta)=\frac{[(1+x_{2}\eta)(1-x_{1}\eta)(1-x_{3}\eta)]^{1/2}}{(1-x_{4}\eta)(1-x_{4}^{-1}\eta)(1+x_{5}\eta)(1+x_{6}\eta)}.\tag{6.14}$$

We now write

$$\zeta^{N+1}=[1-(1-\zeta)]\zeta^{N}\tag{6.15}$$

and

$$\zeta^{N-1}=\zeta^{N}[1+(1-\zeta)+(1-\zeta)^{2}\zeta^{-1}].\tag{6.16}$$

Using (6.13), (6.15), and (6.16), we are able to write (6.12) as

$$\mathfrak{S}_{1,1}(N,\mathfrak{H})\doteqdot\mathfrak{M}_{1}^{2}+\frac{\alpha_{2}^{2N+4}z^{2}(1-z_{2}^{2})^{2}(x_{4}-1)^{4}(x_{5}+1)^{2}(x_{6}+1)^{2}}{\pi^{2}z_{1}^{2}(z_{2}^{2}-z^{2})^{2}x_{4}^{2}(x_{1}+1)(x_{2}+1)(-x_{3}-1)}$$
$$\times\left\{\left[\int_{\alpha_{1}/\alpha_{2}}^{1}d\zeta_{1}\zeta_{1}^{N-1}\left[\frac{1-\zeta_{1}}{1+\zeta_{1}}\right]^{5/2}A_{<}^{(2)}\left(\frac{1-\zeta_{1}}{1+\zeta_{1}}\right)\right]\right.$$
$$\times\left[\int_{\alpha_{1}/\alpha_{2}}^{1}d\zeta\zeta^{N}\frac{(1-\zeta)^{1/2}}{(1+\zeta)^{5/2}}A_{<}^{(2)}\left(\frac{1-\zeta}{1+\zeta}\right)\right]$$
$$-\left[\int_{\alpha_{1}/\alpha_{2}}^{1}d\zeta_{1}\zeta_{1}^{N-1}\frac{(1-\zeta_{1})^{3/2}}{(1+\zeta_{1})^{5/2}}A_{<}^{(2)}\left(\frac{1-\zeta_{1}}{1+\zeta_{1}}\right)\right]$$
$$\left.\times\left[\int_{\alpha_{1}/\alpha_{2}}^{1}d\zeta\zeta^{N}\frac{(1-\zeta)^{3/2}}{(1+\zeta)^{5/2}}A_{<}^{(2)}\left(\frac{1-\zeta}{1+\zeta}\right)\right]\right\}.\tag{6.17}$$

We now expand $A_{<}^{(2)}(\eta)$ as

$$A_{<}^{(2)}(\eta)=\sum_{n=0}^{\infty}A_{n<}^{(2)}\eta^{n},\tag{6.18}$$

where the first few coefficients are

$$A_{0<}^{(2)}=1,\tag{6.19}$$

$$A_{1<}^{(2)}=x_{4}+x_{4}^{-1}-x_{5}-x_{6}+\tfrac{1}{2}(x_{2}-x_{1}-x_{3}),\tag{6.20}$$

and

$$\begin{aligned} A^{(2)}_{2<} &= x_4^2 + x_4^{-2} + x_5^2 + x_6^2 - \tfrac{1}{8}(x_1^2 + x_2^2 + x_3^2) \\ &\quad + 1 - (x_4 + x_4^{-1})(x_5 + x_6) + x_5 x_6 \\ &\quad + (x_4 + x_4^{-1} - x_5 - x_6)\tfrac{1}{2}(x_2 - x_1 - x_3) \\ &\quad - \tfrac{1}{4}(x_1 x_2 + x_2 x_3 - x_1 x_3). \end{aligned} \tag{6.21}$$

We may now apply (5.20) and obtain

$$\begin{aligned} &\mathfrak{S}_{1,1}(N, \mathfrak{H}) \\ &\sim \mathfrak{M}_1^2 + \frac{\alpha_2^{2N+4} z^2 (1 - z_2^2)^2 (x_4 - 1)^4 (x_5 + 1)^2 (x_6 + 1)^2}{2^5 \pi^2 z_1^2 (z_2^2 - z^2)^2 x_4^2 (x_1 + 1)(x_2 + 1)(-x_3 - 1)} \\ &\quad \times \left\{ \left[(N-1)! \sum_{m=0}^{\infty} \frac{\Gamma(m + \frac{5}{2})\Gamma(m + \frac{7}{2})}{2^m \Gamma(N + m + \frac{7}{2})} \sum_{n=0}^{m} \frac{A^{(2)}_{n<}}{(m-n)!\,\Gamma(\frac{5}{2} + n)} \right] \right. \\ &\quad \times \left[N! \sum_{m=0}^{\infty} \frac{\Gamma(m + \frac{5}{2})\Gamma(m + \frac{3}{2})}{2^m \Gamma(N + m + \frac{5}{2})} \sum_{n=0}^{m} \frac{A^{(2)}_{n<}}{(m-n)!\,\Gamma(\frac{5}{2} + n)} \right] \\ &\quad - \left[(N-1)! \sum_{m=0}^{\infty} \frac{\Gamma^2(m + \frac{5}{2})}{2^m \Gamma(N + m + \frac{5}{2})} \sum_{n=0}^{m} \frac{A^{(2)}_{n<}}{(m-n)!\,\Gamma(\frac{5}{2} + n)} \right] \\ &\quad \left. \times \left[N! \sum_{m=0}^{\infty} \frac{\Gamma^2(m + \frac{5}{2})}{2^m \Gamma(N + m + \frac{7}{2})} \sum_{n=0}^{m} \frac{A^{(2)}_{n<}}{(m-n)!\,\Gamma(\frac{5}{2} + n)} \right] \right\}. \end{aligned} \tag{6.22}$$

For large N, the first two terms of this expansion explicitly are

$$\begin{aligned} \mathfrak{S}_{1,1}(N, \mathfrak{H}) &\sim \mathfrak{M}_1^2 + \frac{\alpha_2^{2N+4} z^2 (1 - z_2^2)^2 (x_4 - 1)^4 (x_5 + 1)^2 (x_6 + 1)^2}{\pi 2^9 z_1^2 (z_2^2 - z^2)^2 x_4^2 (x_1 + 1)(x_2 + 1)(-x_3 - 1)} \\ &\quad \times 3N^{-5}\{2 + 5N^{-1} A^{(2)}_{1<} + O(N^{-2})\}. \end{aligned} \tag{6.23}$$

7. $T < T_c$, $E_1 < 0$

In this case, (4.7) or (4.8) holds, depending on the strength of $\mathfrak{H}$. For both cases, the terms of leading exponential order are given by

$$\begin{aligned} \mathfrak{S}_{1,1}(N, \mathfrak{H}) &\doteqdot \mathfrak{M}_1^2 - (-1)^N \frac{z^2[z_2^2(1 - z_1)^2 - (1 + z_1)^2]}{z_1^2(z_2^2 - z^2)^2 (r + 1)(r^{-1} + 1)} \\ &\quad \times \left\{ \frac{(1 - z_1)^2 - z_2^2(1 + z_1)^2}{(r - 1)(r^{-1} - 1)} \right. \\ &\quad\quad \left. + \frac{z_2(1 - z_1^2)}{2\pi i} \int_\Gamma \frac{d\zeta\, \zeta^{N-1}(\zeta + 1)\alpha^{-1}}{(\zeta - r)(r^{-1}\zeta^{-1} - 1)(\zeta - 1)} \right\} \\ &\quad + \frac{z^2 z_2 (z_1^{-2} - 1)[(1 - z_1)^2 - z_2^2(1 + z_1)^2]}{(r - 1)(r^{-1} - 1)(z_2^2 - z^2)^2} \\ &\quad \times \frac{1}{2\pi i} \int_\Gamma d\zeta \frac{\zeta^{N-1}(\zeta - 1)\alpha^{-1}}{(\zeta + 1)(\zeta - r)(\zeta^{-1} r^{-1} - 1)}. \end{aligned} \tag{7.1}$$

We obtain asymptotic expansions to the two integrals exactly as in the ferromagnetic cases, to obtain

$$
\begin{aligned}
&\mathfrak{S}_{1,1}(N, \mathfrak{H}) \\
&= \mathfrak{M}_1^2 - \frac{z^2(-1)^N[z_2^2(1-z_1)^2-(1+z_1)^2]}{z_1^2(z_2^2-z^2)^2(r+1)(r^{-1}+1)} \\
&\quad \times \left\{\frac{(1-z_1)^2-z_2^2(1+z_1)^2}{(r-1)(r^{-1}-1)} + \frac{\alpha_2^{N+1}(1-z_2^2)x_4(x_5+1)(x_6+1)}{2^{3/2}\pi[(x_1+1)(x_2+1)(-x_3-1)]^{1/2}}\right. \\
&\quad \left. \times (N-1)! \sum_{m=0}^{\infty} \frac{\Gamma(m+\frac{1}{2})\Gamma(m+\frac{3}{2})}{2^m\Gamma(N+\frac{3}{2}+m)} \sum_{n=0}^{m} \frac{B_{n<}^{(1)}}{(m-n)!\,\Gamma(\frac{1}{2}+n)}\right\} \\
&\quad + \frac{\alpha_2^{N+1}z^2(1-z_2^2)[(1-z_1)^2-z_2^2(1+z_1)^2](x_5+1)(x_6+1)}{2^{3/2}\pi z_1^2(z_2^2-z^2)^2(r-1)(r^{-1}-1)x_4[(x_1+1)(x_2+1)(-x_3-1)]^{1/2}} \\
&\quad \times (N-1)! \sum_{m=0}^{\infty} \frac{\Gamma(m+\frac{1}{2})\Gamma(m+\frac{3}{2})}{2^m\Gamma(N+\frac{3}{2}+m)} \sum_{n=0}^{m} \frac{B_{n<}^{(2)}}{(m-n)!\,\Gamma(\frac{1}{2}+n)}, \qquad (7.2)
\end{aligned}
$$

where

$$
\begin{aligned}
B_<^{(1)}(\eta) &= \frac{[(1+x_2\eta)(1-x_1\eta)(1-x_3\eta)]^{1/2}(1-\eta/x_4)}{(1-x_4\eta)(1+x_5\eta)(1+x_6\eta)} \\
&= \sum_{n=0}^{\infty} B_{n<}^{(1)}\eta^n \qquad (7.3a)
\end{aligned}
$$

and

$$
\begin{aligned}
B_<^{(2)}(\eta) &= \frac{[(1+x_2\eta)(1-x_1\eta)(1-x_3\eta)]^{1/2}(1-x_4\eta)}{(1-\eta/x_4)(1+x_5\eta)(1+x_6\eta)} \\
&= \sum_{n=0}^{\infty} B_{n<}^{(2)}\eta^n. \qquad (7.3b)
\end{aligned}
$$

In particular,

$$B_{0<}^{(1)} = 1, \qquad (7.4a)$$

$$B_{1<}^{(1)} = -x_4^{-1} + x_4 - x_5 - x_6 + \tfrac{1}{2}(x_2 - x_1 - x_3), \qquad (7.4b)$$

$$
\begin{aligned}
B_{2<}^{(1)} &= x_4^2 + x_5^2 + x_6^2 - \tfrac{1}{8}(x_2^2 + x_1^2 + x_3^2) \\
&\quad - 1 - (x_4 - x_4^{-1})(x_5 + x_6) + x_5x_6 \\
&\quad + \tfrac{1}{2}(x_4 - x_4^{-1} - x_5 - x_6)(x_2 - x_1 - x_3) \\
&\quad - \tfrac{1}{4}(x_1x_2 + x_2x_3 - x_1x_3), \qquad (7.4c)
\end{aligned}
$$

$$B_{0<}^{(2)} = 1, \qquad (7.4d)$$

$$B_{1<}^{(2)} = x_4^{-1} - x_4 - x_5 - x_6 + \tfrac{1}{2}(x_2 - x_1 - x_3), \qquad (7.4e)$$

and

$$B_{2<}^{(2)} = x_4^{-2} + x_5^2 + x_6^2 - \tfrac{1}{8}(x_2^2 + x_1^2 + x_3^2)$$
$$- 1 + (x_4 - x_4^{-1})(x_5 + x_6) + x_5 x_6$$
$$+ (x_4^{-1} - x_4 - x_5 - x_6)\tfrac{1}{2}(x_2 - x_1 - x_3)$$
$$- \tfrac{1}{4}(x_1 x_2 + x_2 x_3 - x_1 x_3). \tag{7.4f}$$

The two series to be expanded in (7.2) are each of the form of the series expanded in (5.25), so we immediately find that the first three terms of the asymptotic series are

$$\mathfrak{S}_{1,1}(N, \mathfrak{H})$$
$$\sim \mathfrak{M}_1^2 - \frac{(-1)^N z^2[z_2^2(1 - z_1)^2 - (1 + z_1)^2]}{z_1^2(z_2^2 - z^2)^2(r + 1)(r^{-1} + 1)}$$
$$\times \left\{\frac{(1 - z_1)^2 - z_2^2(1 + z_1)^2}{(r - 1)(r^{-1} - 1)} + \frac{\alpha_2^{N+1}(1 - z_2^2)x_4(x_5 + 1)(x_6 + 1)}{4[2\pi(x_1 + 1)(x_2 + 1)(-x_3 - 1)]^{1/2}}\right.$$
$$\left.\times N^{-3/2}\left[1 + \frac{3}{4N} B_{1<}^{(1)} + \frac{5}{32N^2}(6B_{2<}^{(1)} - 1)\right]\right\}$$
$$+ \frac{\alpha_2^{N+1} z^2(1 - z_2^2)[(1 - z_1)^2 - z_2^2(1 + z_1)^2](x_5 + 1)(x_6 + 1)}{4(r - 1)(r^{-1} - 1)z_1^2(z_2^2 - z^2)^2 x_4[2\pi(x_1 + 1)(x_2 + 1)(-x_3 - 1)]^{1/2}}$$
$$\times N^{-3/2}\left[1 + \frac{3}{4N} B_{1<}^{(2)} + \frac{5}{32N^2}(6B_{2<}^{(2)} - 1)\right]. \tag{7.5}$$

This series is valid under the restriction (4.17).

8. T NEAR T_c

(A) $T < T_c$, $E_1 > 0$, $\mathfrak{H} \neq 0$

All of the asymptotic series found so far are valid only when $N \gg |1 - T/T_c|^{-1}$. We now consider the limit that $T \to T_c$, such that $N|1 - T/T_c|$ remains fixed and of order 1. For $E_1 > 0$, $\alpha_2 = 1$ and $\alpha_1 = z_{1c}^2$ at T_c. We first consider $T < T_c$. Then (4.6) or (4.4) holds. We consider only the case in which $z^2 \geq |z_2|(1 - \alpha_2)/(1 + \alpha_2)$. Then the term involving r^N in (4.4) is exponentially small compared with the other terms, and may be dropped. Therefore, both (4.4) and (4.6) reduce to (6.12), which, with (6.15) and (6.16), may be written

$$
\begin{aligned}
&\mathfrak{S}_{1,1}(N, \mathfrak{H}) \\
&= \mathfrak{M}_1^2 + \frac{z^2(1-z_2^2)^2}{\pi^2 z_1^2(z_2^2-z^2)^2} \\
&\times\left\{\left[\int_{\alpha_1}^{\alpha_2} d\zeta\, \frac{\zeta^N[(1-\alpha_1\zeta)(1-\alpha_1\zeta^{-1})(1-\alpha_2^{-1}\zeta)(\alpha_2^{-1}\zeta^{-1}-1)]^{1/2}}{(\zeta^2-1)(\zeta-r)(r^{-1}\zeta^{-1}-1)}\right]\right. \\
&\times\left[\int_{\alpha_1}^{\alpha_2} d\zeta_1\, \frac{\zeta_1^{N-1}(\zeta_1-1)[(1-\alpha_1\zeta_1)(1-\alpha_1\zeta_1^{-1})(1-\alpha_2^{-1}\zeta_1)(\alpha_2^{-1}\zeta_1^{-1}-1)]^{1/2}}{(\zeta_1+1)(\zeta_1-r)(r^{-1}\zeta_1^{-1}-1)}\right] \\
&-\left[\int_{\alpha_1}^{\alpha_2} d\zeta\, \frac{\zeta^N[(1-\alpha_1\zeta)(1-\alpha_1\zeta^{-1})(1-\alpha_2^{-1}\zeta)(\alpha_2^{-1}\zeta^{-1}-1)]^{1/2}}{(\zeta+1)(\zeta-r)(r^{-1}\zeta^{-1}-1)}\right] \\
&\times\left.\left[\int_{\alpha_1}^{\alpha_2} d\zeta_1\, \frac{\zeta_1^{N-1}[(1-\alpha_1\zeta_1)(1-\alpha_1\zeta_1^{-1})(1-\alpha_2^{-1}\zeta_1)(\alpha_2^{-1}\zeta_1^{-1}-1)]^{1/2}}{(\zeta_1+1)(\zeta_1-r)(r^{-1}\zeta_1^{-1}-1)}\right]\right\}. \qquad (8.1)
\end{aligned}
$$

All integrals in this expression are of the form

$$
I_n(N) = \int_{\alpha_1}^{\alpha_2} d\zeta\, \frac{\zeta^N(\zeta-1)^n[(1-\alpha_1\zeta)(1-\alpha_1\zeta^{-1})(1-\alpha_2^{-1}\zeta)(\alpha_2^{-1}\zeta^{-1}-1)]^{1/2}}{(\zeta+1)(\zeta-r)(r^{-1}\zeta^{-1}-1)}. \qquad (8.2)
$$

To approximate this integral, make the change of variables

$$
\xi = \frac{1-\zeta}{1-\alpha_2}. \qquad (8.3)
$$

Then (8.2) becomes

$$
\begin{aligned}
I_n(N) &= \alpha_2^{-1}(\alpha_2-1)^{n+2}\int_1^{(1-\alpha_1)/(1-\alpha_2)} d\xi\, \frac{[1-(1-\alpha_2)\xi]^N\xi^n(1-\alpha_1)}{2(1-r)(r^{-1}-1)} \\
&\times \frac{\left\{(\xi-1)(1+\alpha_2\xi)\left[1+\xi\alpha_1\dfrac{1+\alpha_2}{1-\alpha_1}\right]\left[1-\xi\dfrac{1-\alpha_2}{1-\alpha_1}\right]\right\}^{1/2}}{[1-\frac{1}{2}\xi(1-\alpha_2)]\left[1-\xi\dfrac{1-\alpha_2}{1-r}\right]\left[1+\xi\dfrac{1-\alpha_2}{r^{-1}-1}\right]}. \qquad (8.4)
\end{aligned}
$$

Define

$$
t = (1-\alpha_2)N, \qquad (8.5)
$$

which is the fixed quantity of order 1. Then, correct to terms of second order, we have

$$
[1-(1-\alpha_2)\xi]^N \sim e^{-t\xi}[1-\tfrac{1}{2}t^2\xi^2N^{-1}]. \qquad (8.6)
$$

If we require $|1-r| > 1-\alpha_2$, we may expand the rest of the integrand as a power series in $(1-\alpha_2)$ to obtain

$$
\begin{aligned}
I_n(N) &= \alpha_2^{-1}(\alpha_2-1)^{n+2}\tfrac{1}{2}(1-r)^{-1}(r^{-1}-1)^{-1}(1-\alpha_1) \\
&\times \int_1^{(1-\alpha_1)/(1-\alpha_2)} d\xi\,\xi^n e^{-t\xi}(\xi^2-1)^{1/2} \\
&\times \{1+(1-\alpha_2)\xi-\tfrac{1}{2}t^2\xi^2N^{-1}+\tfrac{1}{2}(\alpha_2-1)\xi(\xi+1)^{-1}+O[(\alpha_2-1)^2]\}. \qquad (8.7)
\end{aligned}
$$

We may replace the upper limit by infinity without changing the asymptotic expansion. The integrals may then be evaluated as Bessel functions.

The modified Bessel function of the third kind of order ν, $K_\nu(z)$, has an integral representation of

$$K_\nu(z) = \pi^{1/2}[\Gamma(\tfrac{1}{2} - \nu)]^{-1}(\tfrac{1}{2}z)^{-\nu}\int_1^\infty d\xi e^{-z\xi}(\xi^2 - 1)^{-\nu-1/2}. \tag{8.8}$$

Furthermore, modified Bessel functions have the well-known properties[2]

(i) $$K_\nu(z) = K_{-\nu}(z), \tag{8.9}$$

(ii) $$\left(\frac{\partial}{z\partial z}\right)^m [z^{-\nu}K_\nu(z)] = (-1)^m z^{-\nu-m}K_{\nu+m}(z), \tag{8.10}$$

(iii) $$K_{\nu-1}(z) - K_{\nu+1}(z) = -2\nu z^{-1}K_\nu(z), \tag{8.11}$$

and

(iv) $$K_{\nu-1}(z) + K_{\nu+1}(z) = -2\frac{\partial}{\partial z}K_\nu(z). \tag{8.12}$$

Then we may evaluate the following integrals:

(1) $$\int_1^\infty d\xi e^{-t\xi}(\xi^2 - 1)^{1/2} = t^{-1}K_1(t), \tag{8.13}$$

(2) $$\int_1^\infty d\xi e^{-t\xi}\xi^{-1}(\xi^2 - 1)^{1/2} = \int_t^\infty d\xi \xi^{-1}K_1(\xi), \tag{8.14}$$

(3) $$\begin{aligned}\int_1^\infty d\xi e^{-t\xi}\xi(\xi^2 - 1)^{1/2} &= -\frac{\partial}{\partial t}t^{-1}K_1(t)\\ &= t^{-1}K_2(t),\end{aligned} \tag{8.15}$$

(4) $$\begin{aligned}\int_1^\infty d\xi e^{-t\xi}\xi^2(\xi^2 - 1)^{1/2} &= \int_1^\infty d\xi e^{-t\xi}[(\xi^2 - 1)^{3/2} + (\xi^2 - 1)^{1/2}]\\ &= 3t^{-2}K_2(t) + t^{-1}K_1(t),\end{aligned} \tag{8.16}$$

(5) $$\begin{aligned}\int_1^\infty d\xi e^{-t\xi}\xi^3(\xi^2 - 1)^{1/2} &= -\frac{\partial}{\partial t}[3t^{-2}K_2(t) + t^{-1}K_1(t)]\\ &= 3t^{-2}K_3(t) + t^{-1}K_2(t),\end{aligned} \tag{8.17}$$

(6) $$\begin{aligned}\int_1^\infty d\xi e^{-t\xi}(\xi + 1)^{-1}(\xi^2 - 1)^{1/2} &= \int_1^\infty d\xi e^{-t\xi}(\xi - 1)(\xi^2 - 1)^{-1/2}\\ &= -\frac{\partial}{\partial t}K_0(t) - K_0(t)\\ &= K_1(t) - K_0(t),\end{aligned} \tag{8.18}$$

2. A. Erdelyi, ed., *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), vol. II, chap. 7.

$$(7)\quad \int_1^\infty d\xi e^{-t\xi}\xi(\xi+1)^{-1}(\xi^2-1)^{1/2} = \int_1^\infty d\xi e^{-t\xi}[1-(\xi+1)^{-1}] \times (\xi^2-1)^{1/2} = t^{-1}K_1(t) - K_1(t) + K_0(t), \tag{8.19}$$

and finally

$$(8)\quad \int_1^\infty d\xi e^{-t\xi}\xi^2(\xi+1)^{-1}(\xi^2-1)^{1/2} = \int_1^\infty d\xi e^{-t\xi} \times [\xi - 1 + (\xi+1)^{-1}](\xi^2-1)^{1/2} = t^{-1}K_2(t) - t^{-1}K_1(t) + K_1(t) - K_0(t). \tag{8.20}$$

With the aid of these eight integrals and the four identities (8.9)–(8.12), it is now a simple matter to evaluate the first two terms in the expansion of the required integrals $I_n(N)$ of (8.2). In particular

$$I_{-1}(N) \sim -\frac{(1-\alpha_1)t}{2\alpha_2(1-r)(r^{-1}-1)} N^{-1}\left\{\int_t^\infty d\xi \frac{K_1(\xi)}{\xi} - \tfrac{1}{2}N^{-1}tK_1(t)\right\}, \tag{8.21}$$

$$I_0(N) \sim \frac{(1-\alpha_1)t^2}{2\alpha_2(1-r)(r^{-1}-1)} N^{-2} \times \{t^{-1}K_1(t) - \tfrac{1}{2}N^{-1}[K_2(t) + K_1(t) + tK_0(t)]\}, \tag{8.22}$$

$$I_0(N-1) \sim \frac{(1-\alpha_1)t^2}{2\alpha_2(1-r)(r^{-1}-1)} N^{-2} \times \{t^{-1}K_1(t) + \tfrac{1}{2}N^{-1}[K_2(t) - K_1(t) - tK_0(t)]\}, \tag{8.23}$$

$$I_1(N-1) \sim -\frac{(1-\alpha_1)t^3}{2\alpha_2(1-r)(r^{-1}-1)} N^{-3} \times \{t^{-1}K_2(t) - \tfrac{1}{2}N^{-1}[K_2(t) + tK_1(t)]\}. \tag{8.24}$$

Combining these expressions we find that the first two terms in the asymptotic expansion for $\mathfrak{S}_{1,1}(N, \mathfrak{H})$ are

$$\begin{aligned}\mathfrak{S}_{1,1}(N,\mathfrak{H}) &= \mathfrak{M}_1^2 + \frac{z^2(1-z_2^2)^2}{\pi^2 z_1^2(z_2^2-z^2)^2}\{I_{-1}(N)I_1(N-1) - I_0(N)I_0(N-1)\} \\ &\sim \mathfrak{M}_1^2 + \frac{z^2(1-z_2^2)^2(1-\alpha_1)^2}{4\pi^2\alpha_2^2 z_1^2(z_2^2-z^2)^2(1-r)^2(r^{-1}-1)^2} t^4 N^{-4} \\ &\quad \times \left\{\left[\int_t^\infty d\xi \xi^{-1}K_1(\xi) - \tfrac{1}{2}N^{-1}tK_1(t)\right]\right. \\ &\quad \times \{t^{-1}K_2(t) - \tfrac{1}{2}N^{-1}[K_2(t) + tK_1(t)]\} \\ &\quad - \{t^{-1}K_1(t) - \tfrac{1}{2}N^{-1}[K_2(t) + K_1(t) + tK_0(t)]\} \\ &\quad \left.\times \{t^{-1}K_1(t) + \tfrac{1}{2}N^{-1}[K_2(t) - K_1(t) - tK_0(t)]\}\right\}.\end{aligned} \tag{8.25}$$

We may eliminate α_2^{-2} in favor of N and t, using

$$\alpha_2^{-2} \sim 1 + 2tN^{-1}, \tag{8.26}$$

and thus obtain the final explicit answer

$$\begin{aligned}
&\mathfrak{S}_{1,1}(N, \mathfrak{H}) \\
&\sim \mathfrak{M}_1^2 + \frac{z^2(1 - z_2^2)^2}{4\pi^2 z_1^2(z_2^2 - z^2)^2(1 - r)^2(r^{-1} - 1)^2} \\
&\quad \times (1 - \alpha_1)^2 N^{-4}\left\{t^3 K_2(t)\int_t^\infty d\xi\xi^{-1}K_1(\xi) - t^2 K_1^2(t) + N^{-1}t^4\right. \\
&\quad \times \left.\left[\tfrac{1}{2}[3K_2(t) - tK_1(t)]\int_t^\infty d\xi\xi^{-1}K_1(\xi) - \tfrac{1}{2}K_1(t)[4t^{-1}K_1(t) - K_0(t)]\right]\right\} \\
&\qquad + O(N^{-2}).
\end{aligned} \tag{8.27}$$

For this expansion to hold, we need $N > |1 - r|^{-1}$.

We make contact with the expansion (6.23) which is valid for $\mathfrak{H}$ and T fixed ($T < T_c$) if we use the asymptotic expansion valid for large t,

$$K_n(t) \sim \left(\frac{\pi}{2t}\right)^{1/2} e^{-t}\{1 + (4n^2 - 1)(8t)^{-1} + \tfrac{1}{2}(4n^2 - 1)(4n^2 - 9)(8t)^{-2}\}, \tag{8.28}$$

to find

$$\int_t^\infty d\xi\xi^{-1}K_1(\xi) \sim \left(\frac{\pi}{2}\right)^{1/2} e^{-t}t^{-3/2}\left\{1 - \frac{9}{8t} + \frac{15\cdot 23}{128t^2}\right\}. \tag{8.29}$$

Therefore, if we also note that as $t \to \infty, e^{-t} \sim \alpha_2^N$, the leading terms of (8.27) are

$$\mathfrak{M}_1^2 + \frac{3z^2(1 - z_2^2)^2(1 - \alpha_1)^2}{16\pi z_1^2(z_2^2 - z^2)^2(1 - r)^2(r^{-1} - 1)^2}\,\frac{1}{1 - \alpha_2}\,\alpha_2^{2N}N^{-5}, \tag{8.30}$$

which agrees with the leading term of (6.23) when $\alpha_2 \to 1$.

We may also obtain the $T = T_c$ behavior from (8.27) if we note that when $t \sim 0$

$$K_2(t) \sim 2t^{-2} + O(t^{-1}), \tag{8.31a}$$

$$K_1(t) \sim t^{-1} + O(1), \tag{8.31b}$$

$$K_0(t) \sim -\ln t + O(1). \tag{8.31c}$$

Therefore, if we further use the identity

$$|z_{1c}|^{-1}|z_{2c}|^{-1}(1 - z_{2c}^2)(1 - z_{1c}^2) = 4, \tag{8.32}$$

we obtain the result that may be simply found by directly setting $\alpha_2 = 1$ in (8.1), namely

$$\mathfrak{S}_{1,1}(N, \mathfrak{H}) \sim \mathfrak{M}_1^2 + \frac{4z^2 z_{2c}^2}{\pi^2(z_{2c}^2 - z^2)^2(1 - r)^2(r^{-1} - 1)^2}[N^{-4} + O(N^{-6})]. \tag{8.33}$$

(*B*) $T > T_c$, $E_1 > 0$, $\mathfrak{H} \neq 0$

In this case (4.3) or (4.5) holds. The terms with r^N are exponentially small and may be neglected. Since $E_1 > 0$,

$$(1 - z_1)^2 - z_2^2(1 + z_1)^2 = (1 - z_1)^2(1 - \alpha_2^{-2}); \tag{8.34}$$

we see that the remaining terms in (4.3) or (4.5) have a leading-order term of N^{-4} and all must be retained. Define

$$t' = N(1 - \alpha_2^{-1}). \tag{8.35}$$

In terms of this variable and the change of variable

$$\xi' = (1 - \zeta)(1 - \alpha_2^{-1})^{-1}, \tag{8.36}$$

the calculation is almost identical with the case for $T < T_c$. In particular, (8.7) holds if we omit the first factor α_2^{-1} and replace α_2 by α_2^{-1}. Therefore,

$$\begin{aligned}
&\mathfrak{S}_{1,1}(N, \mathfrak{H}) \\
&\sim \mathfrak{M}_1^2 + \frac{z^2(1 - z_1)^2(1 - z_2^2)(1 - \alpha_1)}{2\pi z_1^2(r - 1)^2(r^{-1} - 1)^2(z_2^2 - z^2)^2} \\
&\quad \times N^{-4}\{t'^3K_2(t') - N^{-1}t'^4[K_2(t') + \tfrac{1}{2}t'K_1(t')] + O(N^{-2})\} \\
&\quad + \pi^{-2}z_1^{-2}(1 - z_2^2)^2z^2(z_2^2 - z^2)^{-2}\tfrac{1}{4}(1 - r)^{-2}(r^{-1} - 1)^{-2}(1 - \alpha_1)^2 \\
&\quad \times N^{-4}\Big\{t'^3K_2(t')\int_{t'}^{\infty} d\xi\xi^{-1}K_1(\xi) - t'^2K_1^2(t') + N^{-1}t'^4 \\
&\qquad \times \Big[-\tfrac{1}{4}[t'K_1(t') + K_2(t')]\int_{t'}^{\infty} d\xi\xi^{-1}K_1(\xi) + \tfrac{1}{2}K_1(t')K_0(t')\Big] \\
&\qquad + O(N^{-2})\Big\}.
\end{aligned} \tag{8.37}$$

When $t' \to \infty$ this expansion behaves as

$$\mathfrak{M}_1^2 + \frac{z^2(1 - z_1^2)(1 - z_2^2)(1 - \alpha_1)(\alpha_2 - 1)^{5/2}}{z_1^2\pi^{1/2}2^{3/2}(r - 1)^2(r^{-1} - 1)^2(z_2^2 - z^2)^2}\alpha_2^{-N}N^{-3/2}, \tag{8.38}$$

which agrees with the $T \to T_c^+$ behavior of (5.26). When $T = T_c$ ($t' = 0$), the second term in (8.37) vanishes and we obtain the same limit as we attained from below T_c. We note that in both the leading-order term is N^{-4}. This is to be compared with the result to be obtained when $\mathfrak{H} = 0$.

(*C*) $\mathfrak{H} = 0$, ($E_1 > 0$)

When $\mathfrak{H} = 0$, the correlation functions reduce to the expressions (4.16). We expand these for the ferromagnetic case near T_c. When $T > T_c$, we have

$$\mathfrak{S}_{1,1}(N, 0) = -(2\pi)^{-1}z_2^{-2}(1 - z_2^2)z_1^{-1}\int_{\alpha_1}^{\alpha_2^{-1}} d\zeta\zeta^N(\zeta^2 - 1)^{-1}$$
$$\times [(1 - \alpha_1\zeta)(1 - \alpha_1\zeta^{-1})(1 - \alpha_2^{-1}\zeta)(\alpha_2^{-1}\zeta^{-1} - 1)]^{1/2}. \qquad (8.39)$$

The substitution (8.35) reduces (8.39) to an integral similar to I_{-1} of (8.2). Then

$$\mathfrak{S}_{1,1}(N, 0) = (4\pi)^{-1}(1 - z_2^2)z_1^{-1}z_2^{-2}(1 - \alpha_1)N^{-1}$$
$$\times \left[t'\int_{t'}^{\infty} d\xi K_1(\xi)\xi^{-1} - N^{-1}\tfrac{1}{2}t'^2K_1(t') + O(N^{-2})\right]. \qquad (8.40)$$

When $T < T_c$, an analogous calculation gives

$$\mathfrak{S}_{1,1}(N, 0) = \tfrac{1}{4}z_2^{-2}z_1^{-1}[z_2^2(1 + z_1)^2 - (1 - z_1)^2]$$
$$+ (4\pi)^{-1}z_2^{-2}(1 - z_2^2)z_1^{-1}(1 - \alpha_1)N^{-1}$$
$$\times \left\{t\int_t^{\infty} d\xi\xi^{-1}K_1(\xi)\right.$$
$$\left. + N^{-1}\left[t^2\int_t^{\infty} d\xi\xi^{-1}K_1(\xi) - \tfrac{1}{2}tK_1(t)\right] + O(N^{-2})\right\}. \qquad (8.41)$$

If $t' \to \infty$, (8.40) agrees with the $T \to T_c^+$ behavior of (5.29), whereas if $t \to \infty$, (8.41) agrees with the $T \to T_c^-$ behavior of (6.11). In either (8.40) or (8.41) we may let $T = T_c$ and obtain

$$\mathfrak{S}_{1,1}(N, 0) = \pi^{-1}|z_{2c}|^{-1}N^{-1} + O(N^{-3}). \qquad (8.42)$$

Therefore, at T_c, $\mathfrak{S}_{1,1}(N, \mathfrak{H})$ approaches its $N \to \infty$ limit much more rapidly when $\mathfrak{H} \neq 0$ than when $\mathfrak{H} = 0$.

(D) $T = T_c$, $\mathfrak{H}$ near zero, $E_1 > 0$

Our final remark about the ferromagnetic spin-spin correlation functions will be to find the asymptotic behavior when $T = T_c$ and z is near zero, so that

$$u = 2Nz^2|z_{2c}|^{-1} \qquad (8.43)$$

is a constant of order 1. We may approach this case from either (4.5) or (4.6). In either case, we have only the product-of-integrals term (8.1), which with $\alpha_2 = 1$ specializes to

$$\mathfrak{S}_{1,1}(N, \mathfrak{H}) = \mathfrak{M}_1^2 + \frac{z^2(1 - z_{2c}^2)^2}{\pi^2 z_{1c}^2(z_{2c}^2 - z^2)^2} \times \left\{ \left[\int_{z_{1c}^2}^1 d\zeta \zeta^N \frac{[(1 - z_{1c}^2\zeta)(\zeta - z_{1c}^2)]^{1/2}}{(\zeta + 1)(\zeta - r)(r^{-1} - \zeta)} \right] \times \left[\int_{z_{1c}^2}^1 d\zeta \zeta^{N-1} \frac{(\zeta - 1)^2[(1 - z_{1c}^2\zeta)(\zeta - z_{1c}^2)]^{1/2}}{(\zeta + 1)(\zeta - r)(r^{-1} - \zeta)} \right] - \left[\int_{z_{1c}^2}^1 d\zeta \zeta^N \frac{(1 - \zeta)[(1 - z_{1c}^2\zeta)(\zeta - z_{1c}^2)]^{1/2}}{(\zeta + 1)(\zeta - r)(r^{-1} - \zeta)} \right] \times \left[\int_{z_{1c}^2}^1 d\zeta \zeta^{N-1} \frac{(1 - \zeta)[(1 - z_{1c}^2\zeta)(\zeta - z_{1c}^2)]^{1/2}}{(\zeta + 1)(\zeta - r)(r^{-1} - \zeta)} \right] \right\}. \tag{8.44}$$

When $\mathfrak{H}$ is near zero,

$$r \approx 1 + 2z^2 z_{2c}^{-1} i. \tag{8.45}$$

We obtain the leading asymptotic term if we approximate all of the integrand that varies slowly near $\zeta = 1$ by its value at $\zeta = 1$. Therefore,

$$\mathfrak{S}_{1,1}(N, \mathfrak{H}) \sim \mathfrak{M}_1^2 + \frac{z^2(1 - z_{2c}^2)^2(1 - z_{1c}^2)^2}{4\pi^2 z_{1c}^2(z_{2c}^2 - z^2)^2} \times \left\{ \left[\int_{z_{1c}^2}^1 d\zeta \frac{\zeta^N}{(\zeta - 1 - 2iz^2/z_{2c})(1 - \zeta - 2iz^2/z_{2c})} \right] \times \left[\int_{z_{1c}^2}^1 d\zeta \frac{\zeta^N(\zeta - 1)^2}{(\zeta - 1 - 2iz^2/z_{2c})(1 - \zeta - 2iz^2/z_{2c})} \right] - \left[\int_{z_{1c}^2}^1 d\zeta \frac{\zeta^N(\zeta - 1)}{(\zeta - 1 - 2iz^2/z_{2c})(1 - \zeta - 2iz^2/z_{2c})} \right]^2 \right\}. \tag{8.46}$$

We make the change of variables

$$\xi = \tfrac{1}{2} z^{-2} |z_{2c}| (1 - \zeta) \tag{8.47}$$

and use (8.43) to obtain

$$\mathfrak{S}_{1,1}(N, \mathfrak{H}) \sim \mathfrak{M}_1^2 + \pi^{-2} z_{1c}^{-2}(1 - z_{2c}^2)^2 |z_{2c}|^{-3}(1 - z_{1c}^2)^2 \tfrac{1}{8} u N^{-1} \times \left\{ \left[\int_0^{(1/2)|z_{2c}|(1 - z_{1c}^2)/z^2} d\xi e^{-\xi u}(\xi^2 + 1)^{-1} \right] \times \left[\int_0^{(1/2)|z_{2c}|(1 - z_{1c}^2)/z^2} d\xi \xi^2 e^{-\xi u}(\xi^2 + 1)^{-1} \right] - \left[\int_0^{(1/2)|z_{2c}|(1 - z_{1c}^2)/z^2} d\xi \xi e^{-\xi u}(\xi^2 + 1)^{-1} \right]^2 \right\}. \tag{8.48}$$

We may replace the upper limit by infinity and use the identity (8.32) to obtain

$$\begin{aligned}\mathfrak{S}_{1,1}(N, \mathfrak{H}) \sim \mathfrak{M}_1^2 &+ 2\pi^{-2}|z_{2c}|^{-1}uN^{-1} \\ &\times \left\{\left[\int_0^\infty d\xi e^{-\xi u}(\xi^2+1)^{-1}\right]\left[u^{-1} - \int_0^\infty d\xi e^{-\xi u}(\xi^2+1)^{-1}\right]\right. \\ &\left. - \left[\int_0^\infty d\xi \xi e^{-\xi u}(\xi^2+1)^{-1}\right]^2\right\}. \end{aligned} \tag{8.49}$$

The integrals in (8.49) may be expressed in terms of the sine and cosine integrals which are defined as[3]

$$\mathrm{si}\, z = -\int_z^\infty dt \frac{\sin t}{t} \tag{8.50}$$

and

$$\mathrm{Ci}\, z = -\int_z^\infty dt \frac{\cos t}{t}. \tag{8.51}$$

For example,

$$\int_0^\infty d\xi e^{-\xi u}(\xi^2+1)^{-1} = -\mathrm{Im} \int_0^\infty d\xi e^{-\xi u}(\xi + i)^{-1}. \tag{8.52}$$

We now rotate the contour of integration to the positive imaginary ξ-axis and let $\xi = i(\xi' u^{-1} - 1)$, to find

$$\int_0^\infty d\xi e^{-\xi u}(\xi^2+1)^{-1} = \sin u\, \mathrm{Ci}\, u - \cos u\, \mathrm{si}\, u. \tag{8.53}$$

Similarly,

$$\begin{aligned}\int_0^\infty d\xi \xi e^{-\xi u}(\xi^2+1)^{-1} &= \mathrm{Re}\int_0^\infty d\xi e^{-\xi u}(\xi + i)^{-1} \\ &= -\cos u\, \mathrm{Ci}\, u - \sin u\, \mathrm{si}\, u. \end{aligned} \tag{8.54}$$

Therefore, we obtain the desired result

$$\begin{aligned}\mathfrak{S}_{1,1}(N, \mathfrak{H}) \sim \mathfrak{M}_1^2 &+ 2\pi^{-2}|z_{2c}|^{-1}N^{-1} \\ &\times [\sin u\, \mathrm{Ci}\, u - \cos u\, \mathrm{si}\, u - u(\sin u\, \mathrm{Ci}\, u - \cos u\, \mathrm{si}\, u)^2 \\ &\quad - u(\cos u\, \mathrm{Ci}\, u + \sin u\, \mathrm{si}\, u)^2]. \end{aligned} \tag{8.55}$$

When $\mathfrak{H} \to 0$, $u \to 0$. Therefore, since[3] for $u \to 0$

$$\mathrm{Ci}\, u = \ln u + O(1) \tag{8.56}$$

3. Reference 2, pp. 145–146.

and

$$\operatorname{si} u = -\frac{\pi}{2} + O(u), \tag{8.57}$$

we find

$$\mathfrak{S}_{1,1}(N, 0) \sim \frac{1}{\pi |z_{2c}| N}, \tag{8.58}$$

which agrees with (8.42). Furthermore,[3] as $u \to \infty$,

$$\operatorname{Ci} u \sim \frac{\sin u}{u} - \frac{\cos u}{u^2} - \frac{2 \sin u}{u^3} \tag{8.59}$$

and

$$\operatorname{si} u \sim -\frac{\cos u}{u} - \frac{\sin u}{u^2} + \frac{2 \cos u}{u^3}. \tag{8.60}$$

Therefore, for u large,

$$\mathfrak{S}_{1,1}(N, \mathfrak{H}) \sim \mathfrak{M}_1^2 + 2\pi^{-2}|z_{2c}|^{-1}N^{-1}u^{-3} = \mathfrak{M}_1^2 + \tfrac{1}{4}\pi^{-2}z_{2c}^2 z^{-6} N^{-4}, \tag{8.61}$$

which is the same as the $z \to 0$ behavior of (8.33).

(*E*) $T \sim T_c$, $E_1 < 0$

We close this section by studying the antiferromagnetic case T near T_c and $\mathfrak{H}$ arbitrary. At T_c, $\alpha_2 = -1$ and $\alpha_1 = -z_{1c}^2$. When $T > T_c$, $\mathfrak{S}_{1,1}$ is given by (4.3) or (4.5). However, since $|r| < |\alpha_2|$, the term involving r does not contribute to the asymptotic expansion. Therefore, for all $\mathfrak{H}$,

$$\mathfrak{S}_{1,1}(N, \mathfrak{H}) \doteq \mathfrak{M}_1^2 + \frac{z^2[(1 - z_1)^2 - z_2^2(1 + z_1)^2]}{z_1^2(r - 1)(r^{-1} - 1)(z_2^2 - z^2)^2} \Xi_2 + \Xi_3. \tag{8.62}$$

To obtain the desired expansion, define

$$t'_- = (1 + \alpha_2^{-1})N = (1 - |\alpha_2|^{-1})N \tag{8.63}$$

and

$$\xi' = (\zeta + 1)/(1 + \alpha_2^{-1}) = (\zeta + 1)/(1 - |\alpha_2|^{-1}). \tag{8.64}$$

We then proceed exactly as in the corresponding ferromagnetic case. It is seen that to $O(N^{-2})$ we may omit Ξ_3 and obtain

$$\begin{aligned} \mathfrak{S}_{1,1}(N, \mathfrak{H}) \sim \mathfrak{M}_1^2 &+ (-1)^N \frac{z^2[z_2^2(1 - |z_1|)^2 - (1 + |z_1|)^2](1 - |\alpha_1|)(1 - z_2^2)}{z_1^2\pi(r^2 - 1)(r^{-2} - 1)(z_2^2 - z^2)^2} \\ &\times N^{-1}\left\{t'_- \int_{t'_-}^{\infty} d\xi\xi^{-1}K_1(\xi) - N^{-1}\tfrac{1}{2}t'^2_- K_1(t') + O(N^{-2})\right\}. \end{aligned} \tag{8.65}$$

The $t'_- \to \infty$ limit of this expansion agrees with the $T \to T_c^+$, $\alpha_2 \to -1$ behavior of (5.26), and, when $T = T_c$, (8.65) simplifies to

$$\mathfrak{S}_{1,1}(N, \mathfrak{H}) \sim \mathfrak{M}_1^2 + (-1)^N \frac{4z^2|z_{2c}|[z_{2c}^2(1 - |z_{1c}|)^2 - (1 + |z_{1c}|)^2]}{\pi|z_{1c}|(r^2 - 1)(r^{-2} - 1)(z_{2c}^2 - z^2)^2} \times N^{-1}[1 + O(N^{-2})]. \tag{8.66}$$

If $T < T_c$, $\mathfrak{S}_{1,1}(N, \mathfrak{H})$ is given by (4.7) or (4.8). The term containing r^N does not contribute to the asymptotic behavior. Furthermore, if we define

$$t_- = (1 + \alpha_2)N = (1 - |\alpha_2|)N \tag{8.67}$$

and

$$\xi' = (\zeta + 1)/(1 + \alpha_2) = (\zeta + 1)/(1 - |\alpha_2|), \tag{8.68}$$

it is easily seen that to $O(N^{-2})$ both Ξ_3 and Ξ_4 may be omitted, and we therefore obtain

$$\begin{aligned}
&\mathfrak{S}_{1,1}(N, \mathfrak{H})\\
&\quad \sim \mathfrak{M}_1^2 + (-1)^N\\
&\qquad \times \frac{z^2[z_2^2(1 + |z_1|)^2 + (1 - |z_1|)^2][z_2^2(1 - |z_1|)^2 - (1 + |z_1|)^2]}{(z_2^2 - z^2)^2(r^2 - 1)(r^{-2} - 1)}\\
&\qquad + (-1)^N \frac{z^2[z_2^2(1 - |z_1|)^2 - (1 + |z_1|)^2](1 - |\alpha_1|)}{(r^2 - 1)(r^{-2} - 1)(z_2^2 - z^2)^2(1 - z_2^2)}\\
&\qquad \times N^{-1}\Big\{t_- \int_{t_-}^{\infty} d\xi \xi^{-1} K_1(\xi)\\
&\qquad\qquad + N^{-1}\Big(t^2 \int_{t_-}^{\infty} d\xi \xi^{-1} K_1(\xi) - \tfrac{1}{2}K_1(t)\Big) + O(N^{-2})\Big\}.
\end{aligned} \tag{8.69}$$

If $t_- \to \infty$, this agrees with the $T \to T_c^-$ behavior of (7.5); when $t_- \to 0$ we regain (8.66).

Both expansions (8.65) and (8.69) are valid without restriction on $\mathfrak{H}$. We therefore may set $\mathfrak{H} = 0$ and compare (8.65) and (8.69) with (8.40) and (8.41) respectively, to find that, as expected from (1.4), if we replace E_1 by $-E_1$,

$$\mathfrak{S}_{1,1}(N, 0) \to (-1)^N \mathfrak{S}_{1,1}(N, 0). \tag{8.70}$$

CHAPTER VIII

The Correlation Functions $\langle \sigma_{0,0}\sigma_{0,N} \rangle$ and $\langle \sigma_{0,0}\sigma_{N,N} \rangle$

1. INTRODUCTION

The aim of this and the next four chapters is the discussion of the magnetization and the spin-spin correlation functions of Onsager's lattice. When the spins involved were in the boundary row we were able to make a complete study of these quantities. However, the interest here is in the bulk, where the calculations are more difficult and such a complete study does not exist. Indeed, we can make progress only in the absence of the magnetic field. Therefore, unlike the situation in the boundary row, it is not possible to compute the magnetization $M(H)$ simply by differentiating the free energy with respect to H. Likewise, it is not possible to compute the susceptibility $\chi(H)$ even at $H = 0$ by differentiating $M(H)$ with respect to H. In particular, no calculation of $\chi(0)$ exists, although we shall see in Chapter XII that important information about its behavior near $T = T_c$ may be obtained from a study of $\langle \sigma_{0,0}\sigma_{M,N} \rangle$ in the asymptotic region where $M^2 + N^2$ is large.

Since we are restricted to $H = 0$, we can use (VII.1.4) to relate the case of negative E_1 to that of positive E_1. Since this remark also applies to E_2, we shall without loss of generality assume both E_1 and E_2 to be positive throughout the rest of this book, unless the contrary is explicitly stated.

It is possible to compute the spontaneous magnetization

$$M = \lim_{H \to 0^+} \lim_{\substack{\mathcal{M} \to \infty \\ \mathcal{N} \to \infty}} (\mathcal{M}\mathcal{N})^{-1} \sum_{j=1}^{\mathcal{M}} \sum_{k=1}^{\mathcal{N}} \langle \sigma_{j,k} \rangle_{\mathcal{M},\mathcal{N}} \tag{1.1}$$

by making use of the connection between M and the spin-spin correlation function for two spins in the same row.[1] We have

$$M^2 = \lim_{N\to\infty} S_N, \tag{1.2}$$

where

$$S_N = \lim_{\substack{\mathscr{M}\to\infty \\ \mathscr{N}\to\infty}} \langle\sigma_{0,0}\sigma_{0,N}\rangle_{\mathscr{M},\mathscr{N}} = \langle\sigma_{0,0}\sigma_{0,N}\rangle. \tag{1.3}$$

The relation (1.2) has previously been discussed; see (II.5.43). For (1.2) to hold, it is necessary that not only the limit on the right-hand side exists, but also the more general limit

$$\lim_{M^2+N^2\to\infty} \langle\sigma_{0,0}\sigma_{M,N}\rangle \tag{1.4}$$

should exist and be independent of the ratio M/N. The existence of the limit in (1.4) will be verified in Chapter XII, where we compute the asymptotic behavior of $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ for large $M^2 + N^2$.

It must be strongly emphasized that the existence of the limit (1.4) is closely connected with the fact that we are considering Onsager's lattice. For most lattices which do not possess the translational symmetry of Onsager's lattice, the limits (1.2) and (1.4) do not exist. Therefore, in general (1.2) cannot be taken as a definition of the spontaneous magnetization. This point will be discussed in greater detail in Chapter XV.

The study of the general correlation function $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ is complicated. However, there are two special cases where this correlation function possesses the simplifying feature that it may be written as a Toeplitz determinant. [A Toeplitz determinant is the determinant of a matrix whose elements $a_{m,n}$ are functions of $m - n$ only. See (2.28).] These two cases are

(1) $M = 0$, N arbitrary (or, by symmetry, $N = 0$ and M arbitrary) and
(2) $M = N$.

The Toeplitz determinant for $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ will be derived in Sec. 2 by a straightforward procedure similar to that of Chapter VII, Sec. 2. The determinant for $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ is not simply derivable in this straightforward manner, and is computed in Sec. 3 by introducing a triangular Ising-model lattice. However, in compensation for the increased complexity of the derivation, the result will be simpler than the corresponding result for $\langle\sigma_{0,0}\sigma_{0,N}\rangle$. The effect of this simplification will be seen in detail in Sec. 4 of Chapter XI, where we study the behavior of these correlation functions for $T = T_c$.

The final section of this chapter is devoted to the study of the near-neighbor correlation functions $\langle\sigma_{0,0}\sigma_{0,1}\rangle$ and $\langle\sigma_{0,0}\sigma_{1,1}\rangle$.

1. The spontaneous M was originally obtained by Yang without using (1.2); see C. N. Yang, *Phys. Rev.* **85**, 808 (1952).

2. $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ IN TERMS OF AN $N \times N$ TOEPLITZ DETERMINANT

A precise discussion of any bulk quantity requires a specification of the boundary conditions satisfied by the lattice. However, if the problem under consideration is to be physically interesting, the dependence of any bulk quantity on the type of boundary condition imposed should vanish as the size of the lattice becomes infinite. In this section we shall be very specific about the boundary condition: cylindrical in the horizontal direction and free in the vertical direction. Let the rows be numbered $-\mathcal{M}' \leq j \leq \mathcal{M}$ and the columns $-\mathcal{N} + 1 \leq k \leq \mathcal{N}$; then the columns $-\mathcal{N} + 1$ and $\mathcal{N}$ interact with each other but the rows $-\mathcal{M}'$ and $\mathcal{M}$ do not. The interaction energy for this lattice is

$$\mathscr{E} = -E_1 \sum_{j=-\mathcal{M}'}^{\mathcal{M}} \sum_{k=-\mathcal{N}+1}^{\mathcal{N}} \sigma_{j,k}\sigma_{j,k+1} - E_2 \sum_{j=-\mathcal{M}'}^{\mathcal{M}-1} \sum_{k=-\mathcal{N}+1}^{\mathcal{N}} \sigma_{j,k}\sigma_{j+1,k}. \tag{2.1}$$

Let $\langle\sigma_{0,0}\sigma_{0,N}\rangle_{\mathcal{M},\mathcal{M}',\mathcal{N}}$ be the spin-spin correlation function for such a lattice. We shall obtain the desired $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ as the limit, when $\mathcal{M} \to \infty$, $\mathcal{M}' \to \infty$, and $\mathcal{N} \to \infty$, of this $\langle\sigma_{0,0}\sigma_{0,N}\rangle_{\mathcal{M},\mathcal{M}',\mathcal{N}}$.

The insistence on dealing rigorously with the boundary conditions forces us to give a derivation of $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ which is slightly more involved algebraically than is needed merely to derive the final result. Once we have obtained this result, we will see that this same result may be obtained if we adopt a more cavalier attitude toward the boundary conditions. Since this independence of boundary conditions is expected, we will use the algebraically simpler approach in Sec. 3.

From the discussion in Sec. 2 of Chapter V and Sec. 2 of Chapter VI, we know that the partition function derived from (2.1) may be written as

$$Z = (\cosh \beta E_1)^{2\mathcal{N}(\mathcal{M}+\mathcal{M}'+1)}(\cosh \beta E_2)^{2\mathcal{N}(\mathcal{M}+\mathcal{M}')}\,\mathrm{Pf}\,A, \tag{2.2}$$

where

$$A(j,k;j,k) = \begin{array}{c c} & \begin{array}{cccc} R & L & U & D \end{array} \\ \begin{array}{c} R \\ L \\ U \\ D \end{array} & \begin{bmatrix} 0 & 1 & -1 & -1 \\ -1 & 0 & 1 & -1 \\ 1 & -1 & 0 & 1 \\ 1 & 1 & -1 & 0 \end{bmatrix} \end{array} \tag{2.3a}$$

for $-\mathcal{M}' \leq j \leq \mathcal{M}$ and $-\mathcal{N} + 1 \leq k \leq \mathcal{N}$,

$$A(j,k;j,k+1) = -A^T(j,k+1;j,k) = \begin{bmatrix} 0 & z_1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{2.3b}$$

for $-\mathcal{M}' \leq j \leq \mathcal{M}$ and $-\mathcal{N} + 1 \leq k \leq \mathcal{N} - 1$,

$$A(j, \mathcal{N}; j, -\mathcal{N} + 1) = -A^T(j, -\mathcal{N} + 1; j, \mathcal{N}) = -A(j, 0; j, 1) \tag{2.3c}$$

for $-\mathcal{M}' \leq j \leq \mathcal{M}$, and

$$A(j, k; j + 1, k) = -A^T(j + 1, k; j, k) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & z_2 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{2.3d}$$

for $-\mathcal{M}' \leq j \leq \mathcal{M} - 1$ and $-\mathcal{N} + 1 \leq k \leq \mathcal{N}$. Furthermore,

$$\begin{aligned}\langle \sigma_{0,0}\sigma_{0,N} \rangle_{\mathcal{M},\mathcal{M}',\mathcal{N}} &= Z^{-1} \sum_{\sigma = \pm 1} \sigma_{0,0}\sigma_{0,N} e^{-\beta \mathscr{E}} \\ &= Z^{-1}(\cosh \beta E_1)^{2\mathcal{N}(\mathcal{M}+\mathcal{M}'+1)}(\cosh \beta E_2)^{2\mathcal{N}(\mathcal{M}+\mathcal{M}')} \\ &\quad \times \sum_{\sigma = \pm 1} \sigma_{0,0}\sigma_{0,N} \left[\prod_{j=-\mathcal{M}'}^{\mathcal{M}} \prod_{k=-\mathcal{N}+1}^{\mathcal{N}} (1 + z_1 \sigma_{j,k}\sigma_{j,k+1}) \right] \\ &\quad \times \left[\prod_{j=-\mathcal{M}'}^{\mathcal{M}-1} \prod_{k=-\mathcal{N}+1}^{\mathcal{N}} (1 + z_2 \sigma_{j,k}\sigma_{j+1,k}) \right].\end{aligned} \tag{2.4}$$

This may be rewritten using

$$\sigma_{0,0}\sigma_{0,N} = (\sigma_{0,0}\sigma_{0,1})(\sigma_{0,1}\sigma_{0,2})\cdots(\sigma_{0,N-1}\sigma_{0,N}) \tag{2.5}$$

and

$$\sigma_{0,l}\sigma_{0,l+1}(1 + z_1\, \sigma_{0,l}\sigma_{0,l+1}) = z_1(1 + z_1^{-1}\sigma_{0,l}\sigma_{0,l+1}) \tag{2.6}$$

as

$$\begin{aligned}&\langle \sigma_{0,0}\sigma_{0,N} \rangle_{\mathcal{M},\mathcal{M}',\mathcal{N}} \\ &= Z^{-1}(\cosh \beta E_1)^{2\mathcal{N}(\mathcal{M}+\mathcal{M}'+1)}(\cosh \beta E_2)^{2\mathcal{N}(\mathcal{M}+\mathcal{M}')} z_1^N \\ &\times \sum_{\sigma = \pm 1} \left[\prod_{k=0}^{N-1} (1 + z_1^{-1}\sigma_{0,k}\sigma_{0,k+1}) \right] \left[\prod_{j=-\mathcal{M}'}^{\mathcal{M}} \prod_{k=-\mathcal{N}+1}^{\mathcal{N}}{}' (1 + z_1 \sigma_{j,k}\sigma_{j,k+1}) \right] \\ &\times \left[\prod_{j=-\mathcal{M}'}^{\mathcal{M}-1} \prod_{k=-\mathcal{N}+1}^{\mathcal{N}} (1 + z_2 \sigma_{j,k}\sigma_{j+1,k}) \right],\end{aligned} \tag{2.7}$$

where $\prod_{k=-\mathcal{N}+1}^{\prime\mathcal{N}}$ means that the terms with $j = 0$ and $0 \leq k \leq N - 1$ are omitted. This expression is of the form of a partition function for some Ising counting lattice with the bonds z_1 on the straight line connecting sites $(0, 0)$ and $(0, N)$ replaced by z_1^{-1} (Fig. 8.1). Accordingly,

$$\langle \sigma_{0,0}\sigma_{0,N} \rangle_{\mathcal{M},\mathcal{M}',\mathcal{N}} = z_1^N \operatorname{Pf} A'/\operatorname{Pf} A, \tag{2.8}$$

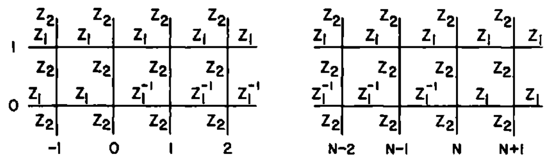


Fig. 8.1. Ising counting lattice with the bonds z_1 on the straight-line path between sites (0, 0) and (0, N) replaced by $1/z_1$.

where

$$\delta = A' - A \tag{2.9}$$

is given by

$$\delta(0,k;0,k+1) = -\delta^T(0,k+1;0,k)$$
$$= \begin{array}{c} \\ R \\ L \\ U \\ D \end{array} \begin{array}{c} \begin{array}{cccc} R & L & U & D \end{array} \\ \begin{bmatrix} 0 & z_1^{-1} - z_1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \end{array} \tag{2.10}$$

if $0 \le k \le N - 1$ and zero otherwise. Thus, if we define y as that $2N \times 2N$ submatrix of δ in the subspace where δ does not vanish identically and if we define Q as the $2N \times 2N$ submatrix of A^{-1} in this same subspace, we find

$$\begin{aligned} \langle\sigma_{0,0}\sigma_{0,N}\rangle^2_{\mathcal{M},\mathcal{M}',\mathcal{N}} &= z_1^{2N} \det(A + \delta)/\det A \\ &= z_1^{2N} \det(1 + A^{-1}\delta) \\ &= z_1^{2N} \det y \det(y^{-1} + Q), \end{aligned} \tag{2.11}$$

which is similar to (VII.2.11). Explicitly from (2.10)

$$y = \begin{array}{cc|cccc} & & 00 & 01 & \cdots & 0N-1 \\ & & R & R & & R \\ \hline 00 & R & 0 & 0 & \cdots & 0 \\ 01 & R & 0 & 0 & \cdots & 0 \\ \vdots & & \vdots & \vdots & \cdots & \vdots \\ 0N-1 & R & 0 & 0 & \cdots & 0 \\ 01 & L & -(z_1^{-1} - z_1) & 0 & \cdots & 0 \\ 02 & L & 0 & -(z_1^{-1} - z_1) & \cdots & 0 \\ \vdots & & \vdots & \vdots & \cdots & \vdots \\ 0N & L & 0 & 0 & \cdots & -(z_1^{-1} - z_1) \end{array}$$

$$
\begin{array}{cccc}
01 & 02 & \cdots & 0N \\
L & L & & L \\
z_1^{-1} - z_1 & 0 & \cdots & 0 \\
0 & z_1^{-1} - z_1 & \cdots & 0 \\
\vdots & \vdots & \cdots & \vdots \\
0 & 0 & \cdots & z_1^{-1} - z_1 \\
0 & 0 & \cdots & 0 \\
0 & 0 & \cdots & 0 \\
\vdots & \vdots & \cdots & \vdots \\
0 & 0 & \cdots & 0
\end{array}
\Bigg], \tag{2.12}
$$

so that

$$
\det y = (z_1^{-1} - z_1)^{2N}. \tag{2.13}
$$

Substitution into (2.11) then yields

$\langle \sigma_{0,0}\sigma_{0,N} \rangle^2_{\mathscr{M},\mathscr{M}',\mathscr{N}}$

$$
= (1 - z_1^2)^{2N} \det \left[
\begin{array}{ccc}
0 & \cdots & A^{-1}(0,0;0,N-1)_{RR} \\
A^{-1}(0,1;0,0)_{RR} & \cdots & A^{-1}(0,1;0,N-1)_{RR} \\
\vdots & \vdots & \vdots \\
A^{-1}(0,N-1;0,0)_{RR} & \cdots & 0 \\
A^{-1}(0,1;0,0)_{LR} + (z_1^{-1} - z_1)^{-1} & \cdots & A^{-1}(0,1;0,N-1)_{LR} \\
A^{-1}(0,2;0,0)_{LR} & \cdots & A^{-1}(0,2;0,N-1)_{LR} \\
\vdots & \vdots & \vdots \\
A^{-1}(0,N;0,0)_{LR} & \cdots & A^{-1}(0,N;0,N-1)_{LR} + (z_1^{-1} - z_1)^{-1}
\end{array}
\right.
$$

$$
\left.
\begin{array}{ccc}
A^{-1}(0,0;0,1)_{RL} - (z_1^{-1} - z_1)^{-1} & \cdots & A^{-1}(0,0;0,N)_{RL} \\
A^{-1}(0,1;0,1)_{RL} & \cdots & A^{-1}(0,1;0,N)_{RL} \\
\vdots & \vdots & \vdots \\
A^{-1}(0,N-1;0,1)_{RL} & \cdots & A^{-1}(0,N-1;0,N)_{RL} - (z_1^{-1} - z_1)^{-1} \\
0 & \cdots & A^{-1}(0,1;0,N)_{LL} \\
A^{-1}(0,2;0,1)_{LL} & \cdots & A^{-1}(0,2;0,N)_{LL} \\
\vdots & \vdots & \vdots \\
A^{-1}(0,N;0,1)_{LL} & \cdots & 0
\end{array}
\right]. \tag{2.14}
$$

To make this expression for $\langle\sigma_{0,0}\sigma_{0,N}\rangle_{\mathscr{M},\mathscr{M}',\mathscr{N}}$ explicit we must compute the required inverse matrix elements. Were A a matrix that was cyclic or nearly cyclic in both those indices referring to the rows of the lattice and those indices referring to the columns of the lattice, it would be a simple matter to apply the formulas developed in Sec. 3 of Chapter VII to compute its inverse. In fact, A fails to be (nearly) cyclic in the indices referring to the rows of the lattice. Therefore, to obtain a rigorously correct answer we will obtain the required matrix elements of A^{-1} by an extension of the calculation of Chapter VII. It is easily verified, however, that our final results are identical with those we would obtain if we modified A to be (nearly) cyclic in both its indices. The matrix A is nearly cyclic in the horizontal direction. Therefore, by (VII.3.9),

$$A^{-1}(j,k;j',k') = (2\mathscr{N})^{-1}\sum_{\theta} e^{i\theta(k-k')}[B^{-1}(\theta)]_{j,j'}, \tag{2.15}$$

where the sum over θ is over $\theta = \pi(2n-1)/2\mathscr{N}$ with $n = 1, 2, \ldots, 2\mathscr{N}$ and the $4[\mathscr{M}+\mathscr{M}'+1] \times 4[\mathscr{M}+\mathscr{M}'+1]$ matrix $B(\theta)$ is explicitly given by

$$B_{j,j}(\theta) = \begin{array}{c c} & \begin{array}{cccc} R & L & U & D \end{array} \\ \begin{array}{c} R \\ L \\ U \\ D \end{array} & \begin{bmatrix} 0 & 1+z_1e^{i\theta} & -1 & -1 \\ -1-z_1e^{-i\theta} & 0 & 1 & -1 \\ 1 & -1 & 0 & 1 \\ 1 & 1 & -1 & 0 \end{bmatrix} \end{array} \tag{2.16a}$$

for $-\mathscr{M}' \le j \le \mathscr{M}$,

$$B_{j,j+1}(\theta) = -B^T_{j+1,j}(\theta) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & z_2 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{2.16b}$$

for $-\mathscr{M}' \le j \le \mathscr{M}-1$, and all other matrix elements are zero. In Sec. 3 of Chapter VII we found that if all the R, L rows (columns) of $B(\theta)$ are rearranged to precede all the U, D rows (columns) and the resulting matrix is written

$$\begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix},$$

then

$$\begin{aligned}\begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}^{-1} &= \begin{bmatrix} b'_{11} & b'_{12} \\ 0 & b'_{22} \end{bmatrix}^{-1}\begin{bmatrix} 1 & 0 \\ t_{21} & 1 \end{bmatrix} \\ &= \begin{bmatrix} b'^{-1}_{11} & -b'^{-1}_{11}b'_{12}b'^{-1}_{22} \\ 0 & b'^{-1}_{22} \end{bmatrix}\begin{bmatrix} 1 & 0 \\ t_{21} & 1 \end{bmatrix},\end{aligned} \tag{2.17}$$

where t_{21} and the matrices $b_{ss'}$ and $b'_{ss'}$ ($s, s' = 1$ or 2) are of dimension $2(\mathscr{M} + \mathscr{M}' + 1)$. The only nonzero elements of the matrices t_{21} and $b'_{ss'}$ are

$$[t_{21}(\theta)]_{j,j} = \begin{array}{c|cc} & R & L \\ \hline U & (1 + z_1e^{i\theta})^{-1} & (1 + z_1e^{-i\theta})^{-1} \\ D & -(1 + z_1e^{i\theta})^{-1} & (1 + z_1e^{-i\theta})^{-1} \end{array} \tag{2.18}$$

for $-\mathscr{M}' \le j \le \mathscr{M}$,

$$[b'_{11}(\theta)]_{j,j} = \begin{array}{c|cc} & R & L \\ \hline R & 0 & 1 + z_1e^{i\theta} \\ L & -1 - z_1e^{-i\theta} & 0 \end{array} \tag{2.19}$$

for $-\mathscr{M}' \le j \le \mathscr{M}$,

$$[b'_{12}]_{j,j} = \begin{array}{c|cc} & U & D \\ \hline R & -1 & -1 \\ L & 1 & -1 \end{array} \tag{2.20}$$

for $-\mathscr{M}' \le j \le \mathscr{M}$,

$$[b'_{22}(\theta)]_{j,j} = \begin{array}{c|cc} & U & D \\ \hline U & \mathfrak{a} & -\mathfrak{b} \\ D & \mathfrak{b} & -\mathfrak{a} \end{array} \tag{2.21}$$

for $-\mathscr{M}' \le j \le \mathscr{M}$ [see (VI.3.7)], and

$$[b'_{22}(\theta)]_{j,j+1} = -[b'^{T}_{22}(\theta)]_{j+1,j} = \begin{array}{c|cc} & U & D \\ \hline U & 0 & z_2 \\ D & 0 & 0 \end{array} \tag{2.22}$$

for $-\mathscr{M}' \le j \le \mathscr{M} - 1$.

The only matrix elements of $[B^{-1}(\theta)]_{jl,j'l'}$ needed for the purpose of evaluating (2.14) are those where l and $l' = R$ or L. In this case (2.17) yields

$$[B^{-1}(\theta)]_{jl,j'l'} = \{b'^{-1}_{11}[1 - b'_{12}b'^{-1}_{22}t_{21}]\}_{jl,j'l'}. \tag{2.23}$$

To use this formula we need to know the elements of b'^{-1}_{11} and b'^{-1}_{22}. The elements of b'^{-1}_{22} may be readily obtained from those computed in Sec. 3 of Chapter VII if we replace j and j' of Chapter VII by $j + \mathscr{M}' + 1$ and $j' + \mathscr{M}' + 1$ and set z equal to zero. Therefore in the limit where $\mathscr{M} \to \infty$, $\mathscr{M}' \to \infty$ and j and j' are fixed,

$$\begin{aligned} [b'^{-1}_{22}]_{jU,j'U} &= -[b'^{-1}_{22}]^{*}_{j'U,jU} \\ &= -[b'^{-1}_{22}]_{jD,j'D} \\ &= \alpha^{j'-j}z_1z_2^{-1}(1 - z_1^2)^{-1}(e^{i\theta} - e^{-i\theta})(\alpha^{-1} - \alpha)^{-1} \end{aligned} \tag{2.24a}$$

for $j \geq j'$,

$$[b_{22}'^{-1}]_{jU,j'D} = -[b_{22}'^{-1}]^*_{j'D,jU}$$
$$= \alpha^{j'-j}z_2^{-1}(1-z_1^2)^{-1}(\alpha^{-1}-\alpha)^{-1}(-1+z_1^2+\alpha^{-1}z_2|1+z_1e^{i\theta}|^2) \quad (2.24b)$$

for $j \geq j'$, and

$$[b_{22}'^{-1}]_{jD,j'U} = -[b_{22}'^{-1}]^*_{j'U,jD}$$
$$= \alpha^{j'-j}z_2^{-1}(1-z_1^2)^{-1}(\alpha^{-1}-\alpha)^{-1}(1-z_1^2-\alpha z_2|1+z_1e^{i\theta}|^2) \quad (2.24c)$$

for $j > j'$. Furthermore, it follows trivially from (2.19) that

$$[b_{11}'^{-1}]_{j,j'} = \begin{array}{c c} & \begin{array}{cc} R & L \end{array} \\ \begin{array}{c} R \\ L \end{array} & \begin{bmatrix} 0 & -(1+z_1e^{-i\theta})^{-1} \\ (1+z_1e^{i\theta})^{-1} & 0 \end{bmatrix} \end{array} \delta_{j,j'}. \quad (2.25)$$

Therefore we combine (2.23) with (2.24) and (2.25) to find that in the thermodynamic limit

$$\begin{aligned}
&[B^{-1}(\theta)]_{jR,j'R} \\
&= |1+z_1e^{i\theta}|^{-2}\{[b_{22}'^{-1}(\theta)]_{UU} - [b_{22}'^{-1}(\theta)]_{DU} - [b_{22}'^{-1}(\theta)]_{UD} + [b_{22}'^{-1}(\theta)]_{DD}\}_{j,j'} \\
&= -|1+z_1e^{i\theta}|^{-2}\{[(b_{22}'^{-1}\theta)]_{DU} + [b_{22}'^{-1}(\theta)]_{UD}\}_{j,j'} \\
&= \begin{cases} -\alpha^{-|j'-j|}(1-z_1^2)^{-1} & \text{if } j \neq j' \\ 0 & j = j' \end{cases} \\
&= -[B^{-1}(\theta)]_{jL,j'L},
\end{aligned} \quad (2.26a)$$

and, using (V.3.3.),

$$\begin{aligned}
&[B^{-1}(\theta)]_{jR,j'L} \\
&= -[B^{-1}(\theta)]^*_{j'L,jR} \\
&= -(1+z_1e^{-i\theta})^{-1}\{\delta_{j,j'} - (1+z_1e^{-i\theta})^{-1}([b_{22}'^{-1}(\theta)]_{UU} - [b_{22}'^{-1}(\theta)]_{DD} \\
&\qquad - [b_{22}'^{-1}(\theta)]_{DU} + [b_{22}'^{-1}(\theta)]_{UD})_{j,j'}\} \\
&= z_1(1-z_1^2)^{-1}e^{i\theta}\delta_{j,j'} - \alpha^{-|j'-j|}(1-z_1^2)^{-1}e^{i\theta}\left[\frac{(1-\alpha_1e^{i\theta})(1-\alpha_2e^{-i\theta})}{(1-\alpha_1e^{-i\theta})(1-\alpha_2e^{i\theta})}\right]^{1/2}.
\end{aligned} \quad (2.26b)$$

Finally, we substitute this expression into (2.15) for the case $j = j' = 0$ and $\mathcal{N} \to \infty$ to obtain the needed elements of A^{-1}:

$$A^{-1}(0,k;0,k')_{RR} = A^{-1}(0,k;0,k')_{LL} = 0 \quad (2.27a)$$

and

$$\begin{aligned}
A^{-1}(0,k;0,k')_{RL} &= A^{-1}(0,k;0,k')_{LR} \\
&= z_1(1-z_1^2)^{-1}\delta_{k-k'+1,0} - (1-z_1^2)^{-1}(2\pi)^{-1} \\
&\quad \times \int_{-\pi}^{\pi} d\theta e^{i(k-k'+1)\theta}\left[\frac{(1-\alpha_1e^{i\theta})(1-\alpha_2e^{-i\theta})}{(1-\alpha_1e^{-i\theta})(1-\alpha_2e^{i\theta})}\right]^{1/2}.
\end{aligned} \quad (2.27b)$$

The vanishing of the RR and LL elements as given by (2.27a) leads to important simplifications for the determinantal expression (2.14). More explicitly, the $2N \times 2N$ determinant for S_N^2 reduces to an $N \times N$ determinant for S_N. Therefore, with an appropriate choice of sign to make the final expression for S_N positive, as given by Montroll, Potts, and Ward,

$$\pm S_N = \begin{vmatrix} a_0 & a_{-1} & a_{-2} & \cdots & a_{-N+1} \\ a_1 & a_0 & a_{-1} & \cdots & a_{-N+2} \\ a_2 & a_1 & a_0 & \cdots & a_{-N+3} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{N-1} & a_{N-2} & a_{N-3} & \cdots & a_0 \end{vmatrix}, \tag{2.28}$$

where

$$a_n = \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-in\theta} \phi(\theta), \tag{2.29}$$

with

$$\phi(\theta) = \left[\frac{(1 - \alpha_1 e^{i\theta})(1 - \alpha_2 e^{-i\theta})}{(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{i\theta})} \right]^{1/2}. \tag{2.30}$$

In (2.30) the square root is defined so that $\phi(\pi) > 0$.

A determinant of the form (2.28) is called a Toeplitz determinant. Toeplitz determinants are more general than cyclic determinants, which, besides the form (2.28), have the additional restriction that $a_k = a_{N+k}$. The behavior of Toeplitz determinants for large N is much more difficult to determine than the corresponding behavior of cyclic determinants. The next three chapters are concerned with the study of this large-N behavior of Toeplitz determinants.

3. $\langle \sigma_{0,0}\sigma_{N,N} \rangle$ IN TERMS OF AN $N \times N$ TOEPLITZ DETERMINANT

The method of computing spin-correlation functions as determinants presented in the previous section can be used to produce an expression for any spin-correlation function $\langle \sigma_{0,0}\sigma_{M,N} \rangle$. However, the expressions so produced are not at all unique. Even the nearest-neighbor correlation function $\langle \sigma_{0,0}\sigma_{0,1} \rangle$, which is found in (2.28) to be expressible as a single integral, has many alternative forms. For example, if, instead of connecting the sites (0, 0) and (0, 1) by a single bond, we connect them by the path with three bonds running from (0, 0) to (1, 0), (1, 1), and finally to (0, 1), we can write $\sigma_{0,0}\sigma_{0,1} = (\sigma_{0,0}\sigma_{1,0})(\sigma_{1,0}\sigma_{1,1})(\sigma_{1,1}\sigma_{0,1})$. This representation of $\sigma_{0,0}\sigma_{0,1}$ is much more complicated than the single integral we previously derived, and yet the two expressions obviously must be equal.

Because of this great arbitrariness in the manner in which the sites are connected, it is sometimes not obvious whether or not a given correlation function is expressed in the simplest possible form. Indeed, it is sometimes possible to simplify a result by seemingly complicating the problem. For example, one could compute the boundary spin-correlation function $\mathfrak{S}_{1,1}(N)$ at $\mathfrak{H} = 0$ by connecting the sites (0, 0) to (0, N) by a straight line. This would lead to a $2N \times 2N$ determinant. However, as we have seen in Chapter VII, if we complicate the problem by introducing the magnetic field $\mathfrak{H}$, we immediately obtain $\mathfrak{S}_{1,1}(N, \mathfrak{H})$ as a 4×4 determinant. The $\mathfrak{H} = 0$ result was easily obtained by letting $\mathfrak{H} \to 0$. The labor saved in following this latter approach is enormous.[2]

A similar situation arises in the case of the correlation $\langle\sigma_{0,0}\sigma_{N,N}\rangle$. A straightforward application of the previous procedure is to join the sites (0, 0) and (N, N) through the staircase arrangement of bonds (0, 0) to (0, 1), (0, 1) to (1, 1), . . . , ($N - 1$, N) to (N, N). This leads to a $4N \times 4N$ determinant. However, we may adopt a different point of view. Instead of considering a square lattice we study the triangular lattice[3] shown in Fig. 8.2. This lattice has bonds of strength E_3 connecting the sites (j, k)

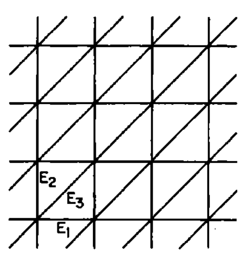


Fig. 8.2. Triangular Ising lattice.

to the sites ($j + 1$, $k + 1$). On this lattice we will compute $\langle\sigma_{0,0}\sigma_{N,N}\rangle_\Delta$ by joining (0, 0) with (N, N) by a straight line. We then will recover the result for Onsager's lattice by taking the limit $E_3 \to 0$. This achieves the significant simplification of obtaining $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ as an $N \times N$ Toeplitz determinant which is closely related to the determinant (2.28). In fact, this new determinant is simpler than (2.28) because its matrix elements are computed from formulas like (2.29) and (2.30) with $\alpha_1 = 0$.

2. Both methods of computation have actually been carried out but the analysis of the $2N \times 2N$ determinant is so tedious that it will forever remain unpublished.

3. Our treatment of the triangular lattice and its relation to $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ follows that of J. Stephenson, *J. Math. Phys.* **5**, 1009 (1964).

The interaction energy for the triangular lattice is

$$\mathscr{E}_\Delta = -E_1 \sum_{j=-\mathscr{M}'}^{\mathscr{M}} \sum_{k=-\mathscr{N}+1}^{\mathscr{N}} \sigma_{j,k}\sigma_{j,k+1} - E_2 \sum_{j=-\mathscr{M}'}^{\mathscr{M}-1} \sum_{k=-\mathscr{N}+1}^{\mathscr{N}} \sigma_{j,k}\sigma_{j+1,k}$$
$$-E_3 \sum_{j=-\mathscr{M}'}^{\mathscr{M}-1} \sum_{k=-\mathscr{N}+1}^{\mathscr{N}} \sigma_{j,k}\sigma_{j+1,k+1}. \tag{3.1}$$

To apply our previous method of computing spin-correlation functions to this problem we must show that we can compute the partition function of this lattice as the Pfaffian of an appropriate matrix. Since this construction is very similar to that of Chapter V, we shall be brief.

As in (V.2.8), Z_Δ may be written

$$Z_\Delta = (2\cosh\beta E_1)^{2\mathscr{N}(\mathscr{M}+\mathscr{M}'+1)}(\cosh\beta E_2)^{2\mathscr{N}(\mathscr{M}+\mathscr{M}')}$$
$$\times (\cosh\beta E_3)^{2\mathscr{N}(\mathscr{M}+\mathscr{M}')} \sum_{p,q,r} N_{pqr} z_1^p z_2^q z_3^r, \tag{3.2}$$

where $z_3 = \tanh\beta E_3$ and N_{pqr} are the number of figures that can be drawn on the lattice of Fig. 8.2 with the properties that: (1) each bond between nearest neighbors is used at most once, (2) any given lattice site must have only an even number of bonds of the figure with that site as one end, and (3) the figure contains p horizontal bonds, q vertical bonds, and r diagonal bonds. An example of an allowed figure is given in Fig. 8.3.

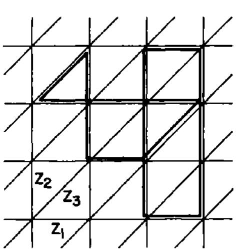


Fig. 8.3. The triangular Ising counting lattice with bond weights z_1, z_2, and z_3. On this lattice is shown an example of a closed figure that enters the sum (3.2).

The sum in (3.2) is the generating function for closed polygons on the lattice of Fig. 8.3. Since this lattice is planar (with cylindrical boundary conditions), we may reduce this problem to a dimer counting problem. This relation was simply made for the square lattice in Sec. 2 by drawing the cluster of dimer sites that corresponds to one Ising vertex and explicitly verifying in Fig. 5.3 that the eight possible arrangements of bonds at the Ising vertex are in one-to-one correspondence with the arrangement of dimers on the dimer lattice. This explicit verification can be done in the present case but, since there are now 32 different possible configurations of bonds at an Ising vertex, much labor is involved. Therefore it pays to be a bit more systematic.[4]

We proceed in two steps. First, we replace each vertex of Fig. 8.4(*a*) by the expanded site of Fig. 8.4(*b*), which has four vertices and three new

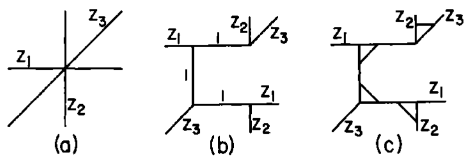


Fig. 8.4. (*a*) A vertex in the triangular Ising counting lattice; (*b*) the corresponding expanded vertex; (*c*) the corresponding cluster of vertices in the dimer lattice. All unlabeled bonds have weight 1.

internal bonds. The weight associated with the new bonds is 1, so the generating function for polygons on this expanded lattice is the same as on the original lattice. Now each vertex has three and only three lattice bonds attached to it. We next replace each of the three-bond vertices of Fig. 8.4(*b*) by a Δ-type site with three vertices and three new internal bonds as shown in Fig. 8.4(*c*). By Fig. 8.5, the polygons on the counting lattice of Fig. 8.3 are in one-to-one correspondence with the closest-packed dimer configurations of the lattice in Fig. 8.6. An example of such a correspondence is shown in Fig. 8.7. Thus we have reduced the computation of the sum in (3.2) to the computation of the generating function for closest-packed dimer configurations on the lattice of Fig. 8.6.

The last sentence requires some clarification because the one-to-one correspondence is between a polygon of weight $z_1^p z_2^q z_3^r$ and a closest-packed dimer configuration of weight

$$z_1^{2\mathcal{N}(\mathcal{M}+\mathcal{M}'+1)-p}\, z_2^{2\mathcal{N}(\mathcal{M}+\mathcal{M}')-q}\, z_3^{2\mathcal{N}(\mathcal{M}+\mathcal{M}')-r}.$$

Therefore the sum in (3.2) is really equal to

$$z_1^{2\mathcal{N}(\mathcal{M}+\mathcal{M}'+1)}\, z_2^{2\mathcal{N}(\mathcal{M}+\mathcal{M}')}\, z_3^{2\mathcal{N}(\mathcal{M}+\mathcal{M}')}$$

times the generating function for closest-packed dimer configurations on the lattice of Fig. 8.6 with each z_i replaced by z_i^{-1}. However, since we are considering cyclic boundary conditions in the horizontal direction on the original Ising counting lattice, the number of bonds at every lattice site is

4. We follow here the general prescription of M. E. Fisher, *J. Math. Phys.* **7**, 1776 (1966).

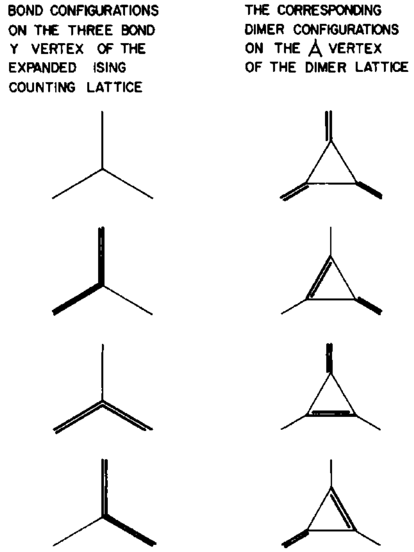


Fig. 8.5. The 1–1 correspondence between figures on an Ising vertex in the expanded lattice and dimer configurations on the cluster of sites in the associated dimer lattice.

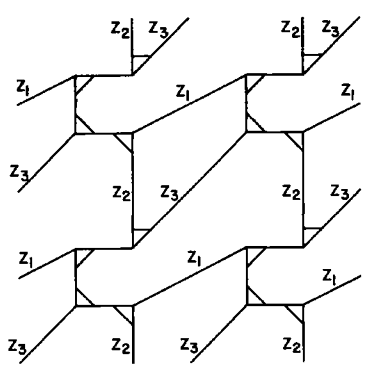


Fig. 8.6. Planar dimer lattice corresponding to the triangular Ising lattice. All unlabeled bonds have weight 1.

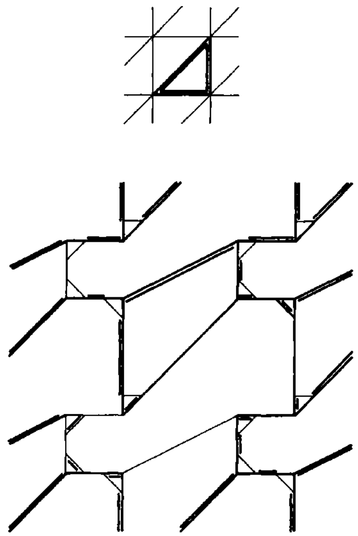


Fig. 8.7. A simple example of the 1–1 correspondence between closed polygons on the counting lattice and closest-packed dimer configurations on the associated dimer lattice.

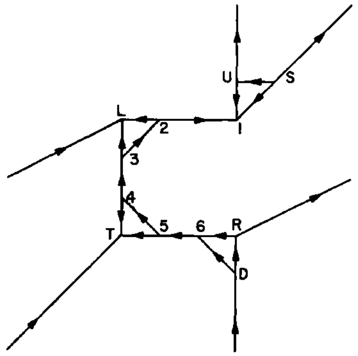


Fig. 8.8. Oriented planar dimer lattice corresponding to the triangular Ising lattice. With this assignment of arrows the orientation parity of every elementary polygon is clockwise odd.

even (including those sites on the boundary) and thus we have the identity

$$N_{pqr} = N_{[2\mathcal{N}(\mathcal{M}+\mathcal{M}'+1)-p][2\mathcal{N}(\mathcal{M}+\mathcal{M}')-q][2\mathcal{N}(\mathcal{M}+\mathcal{M}')-r]}. \tag{3.3}$$

Therefore the last statement of the preceding paragraph is correct.

We may compute the required generating function by the methods of Chapter IV if we can draw arrows on the lattice of Fig. 8.6 in such a way that the orientation parity of every elementary polygon is clockwise odd. It may easily be verified that one such set of arrows is that of Fig. 8.8. The matrix which corresponds to this set of arrows is

$$\bar{A}_\Delta(j,k;j,k) = \begin{array}{c} \\ U \\ S \\ R \\ D \\ T \\ L \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{array} \begin{array}{c} \begin{array}{cccccccccccc} U & S & R & D & T & L & 1 & 2 & 3 & 4 & 5 & 6 \end{array} \\ \begin{bmatrix} & 1 & & & & & -1 & & & & & \\ -1 & & & & & & -1 & & & & & \\ & & & 1 & & & & & & & & -1 \\ & & -1 & & & & & & & & & -1 \\ & & & & & & & & & 1 & 1 & \\ & & & & & & & 1 & 1 & & & \\ 1 & 1 & & & & & & 1 & & & & \\ & & & & & -1 & -1 & & 1 & & & \\ & & & & & -1 & & -1 & & 1 & & \\ & & & & -1 & & & & -1 & & 1 & \\ & & & & -1 & & & & & -1 & & 1 \\ & & 1 & 1 & & & & & & & -1 & \end{bmatrix} \end{array} \tag{3.4a}$$

for $-\mathcal{M}' \le j \le \mathcal{M}$, $-\mathcal{N}+1 \le k \le \mathcal{N}$,

$$\bar{A}_\Delta(j,k;j,k+1)_{RL} = -\bar{A}_\Delta(j,k+1;j,k)_{LR} = z_1 \tag{3.4b}$$

for $-\mathcal{M}' \le j \le \mathcal{M}$, $-\mathcal{N}+1 \le k \le \mathcal{N}-1$,

$$\bar{A}_\Delta(j,\mathcal{N};j,-\mathcal{N}+1)_{RL} = -\bar{A}_\Delta(j,-\mathcal{N}+1;j,\mathcal{N})_{LR} = -z_1 \tag{3.4c}$$

for $-\mathcal{M}' \le j \le \mathcal{M}$,

$$\bar{A}_\Delta(j,k;j+1,k)_{UD} = -\bar{A}_\Delta(j+1,k;j,k)_{DU} = z_2 \tag{3.4d}$$

for $-\mathcal{M}' \le j \le \mathcal{M}-1$, $-\mathcal{N}+1 \le k \le \mathcal{N}$,

$$\bar{A}_\Delta(j,k;j+1,k+1)_{ST} = -\bar{A}_\Delta(j+1,k+1;j,k)_{TS} = z_3 \tag{3.4e}$$

for $-\mathcal{M}' \le j \le \mathcal{M}-1$, $-\mathcal{N}+1 \le k \le \mathcal{N}-1$,

$$\bar{A}_\Delta(j,\mathcal{N};j+1,-\mathcal{N}+1)_{ST} = -\bar{A}_\Delta(j+1,-\mathcal{N}+1;j,\mathcal{N})_{TS} = -z_3 \tag{3.4f}$$

for $-\mathcal{M}' \le j \le \mathcal{M}-1$, and all the other matrix elements are zero. Therefore

$$\begin{aligned} Z_\Delta &= (2\cosh\beta E_1)^{2\mathcal{N}(\mathcal{M}+\mathcal{M}'+1)}(\cosh\beta E_2\cosh\beta E_3)^{2\mathcal{N}(\mathcal{M}+\mathcal{M}')}\,\mathrm{Pf}\,\bar{A}_\Delta \\ &= (2\cosh\beta E_1)^{2\mathcal{N}(\mathcal{M}+\mathcal{M}'+1)}(\cosh\beta E_2\cosh\beta E_3)^{2\mathcal{N}(\mathcal{M}+\mathcal{M}')}(\det\bar{A}_\Delta)^{1/2}. \end{aligned} \tag{3.5}$$

But, analogously to what we have seen in Sec. 2 of Chapter V, we may perform a set of row and column operations on det $\bar{A}_\Delta$ that will reduce the computing of the determinant to that of a smaller determinant which does not contain the indices $1-6$. One such set of row and column operations is as follows, in the indicated order:

row 1	is	added to	row 3
row 3	is	added to	row 5
row 6	is	added to	row 4
row 4	is	added to	row 2
row 1	is	subtracted from	row L
row 2	is	subtracted from	rows U and S
row 3	is	subtracted from	row T
row 4	is	added to	row L
row 5	is	added to	rows R and D
row 6	is	added to	row T.

Then

$$\det \bar{A}_\Delta = \det A_\Delta, \tag{3.6}$$

where A_Δ is the $6(2\mathcal{N})(\mathcal{M}+\mathcal{M}'+1)\times 6(2\mathcal{N})(\mathcal{M}+\mathcal{M}'+1)$ matrix whose nonvanishing elements are given by (3.4b–f) together with

$$A_\Delta(j,k;j,k) = \begin{array}{c c} & \begin{array}{cccccc} U & S & R & D & T & L \end{array} \\ \begin{array}{c} U \\ S \\ R \\ D \\ T \\ L \end{array} & \begin{bmatrix} 0 & 1 & -1 & -1 & 1 & 1 \\ -1 & 0 & -1 & -1 & 1 & 1 \\ 1 & 1 & 0 & 1 & -1 & -1 \\ 1 & 1 & -1 & 0 & -1 & -1 \\ -1 & -1 & 1 & 1 & 0 & 1 \\ -1 & -1 & 1 & 1 & -1 & 0 \end{bmatrix} \end{array}. \tag{3.7}$$

This new matrix may be considered as derived from the oriented counting lattice of Fig. 8.9.

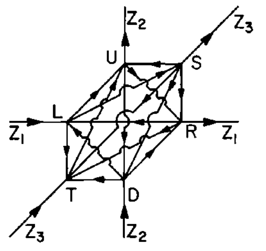


Fig. 8.9. An oriented six-site cluster which can replace an Ising-model vertex in the triangular lattice to construct directly the oriented counting lattice related to the matrix A_Δ of (3.7).

We could now continue and explicitly compute the partition function for the triangular lattice. However, since our only interest here is $\langle \sigma_{0,0}\sigma_{N,N}\rangle_\Delta$ in the limit $E_3 \to 0$, we will pass immediately to a discussion of correlation functions. Indeed, now that we possess a suitable counting matrix A_Δ, the discussion of the previous section may be taken over word for word. In particular, we join the site (0, 0) to (N, N) on the weighted Ising lattice by a straight line and replace all the z_3 on the line by z_3^{-1}. Then, in a notation analogous to that of Sec. 2, the matrix y_Δ is

$$y_\Delta = \begin{array}{ll} & \begin{array}{cccccccc} 00 & 11 & \cdots & N-1\;N-1 & 11 & 22 & \cdots & NN \\ S & S & & S & T & T & & T \end{array} \\ \begin{array}{r} 00\;S \\ 11\;S \\ \vdots\;\; \\ N-1\;N-1\;S \\ 11\;T \\ 22\;T \\ \vdots\;\; \\ NN\;T \end{array} & \left[\begin{array}{cccccccc} 0 & 0 & \cdots & 0 & z_3^{-1}-z_3 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 & 0 & z_3^{-1}-z_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & z_3^{-1}-z_3 \\ -(z_3^{-1}-z_3) & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 0 & -(z_3^{-1}-z_3) & \cdots & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & -(z_3^{-1}-z_3) & 0 & 0 & \cdots & 0 \end{array}\right] \end{array}, \tag{3.8}$$

and

$$\langle \sigma_{0,0}\sigma_{N,N}\rangle_\Delta^2 = z_3^{2N} \det y_\Delta \det (y_\Delta^{-1} + Q_\Delta), \tag{3.9}$$

where Q_Δ is the $2N \times 2N$ submatrix of A_Δ^{-1} in the subspace where y_Δ is defined.

We may now let $E_3 \to 0$ to obtain

$$\langle\sigma_{0,0}\sigma_{N,N}\rangle^2$$

$$= \det \left[\begin{array}{ccc|ccc}
A_0^{-1}(0,0;0,0)_{SS} & \cdots & A_0^{-1}(0,0;N-1,N-1)_{SS} & A_0^{-1}(0,0;1,1)_{ST} & \cdots & A_0^{-1}(0,0;N,N)_{ST} \\
A_0^{-1}(1,1;0,0)_{SS} & \cdots & A_0^{-1}(1,1;N-1,N-1)_{SS} & A_0^{-1}(1,1;1,1)_{ST} & \cdots & A_0^{-1}(1,1;N,N)_{ST} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
A_0^{-1}(N-1,N-1;0,0)_{SS} & \cdots & A_0^{-1}(N-1,N-1;N-1,N-1)_{SS} & A_0^{-1}(N-1,N-1;1,1)_{ST} & \cdots & A_0^{-1}(N-1,N-1;N,N)_{ST} \\
A_0^{-1}(1,1;0,0)_{TS} & \cdots & A_0^{-1}(1,1;N-1,N-1)_{TS} & A_0^{-1}(1,1;1,1)_{TT} & \cdots & A_0^{-1}(1,1;N,N)_{TT} \\
A_0^{-1}(2,2;0,0)_{TS} & \cdots & A_0^{-1}(2,2;N-1,N-1)_{TS} & A_0^{-1}(2,2;1,1)_{TT} & \cdots & A_0^{-1}(2,2;N,N)_{TT} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
A_0^{-1}(N,N;0,0)_{TS} & \cdots & A_0^{-1}(N,N;N-1,N-1)_{TS} & A_0^{-1}(N,N;1,1)_{TT} & \cdots & A_0^{-1}(N,N;N,N)_{TT}
\end{array}\right], \tag{3.10}$$

where

$$A_0^{-1}(j',k';j,k) = \lim_{E_3\to 0} A_\Delta^{-1}(j',k';j,k). \tag{3.11}$$

Finally, to obtain an explicit expression for $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ from this, we need to find formulas for the indicated inverse matrix elements of A_0. This could be done in a fashion analogous to that carried out in the previous section. However, it is simpler to notice that in the limit $\mathscr{M}$, $\mathscr{M}'$, and $\mathscr{N} \to \infty$ the matrix elements of A^{-1} of the previous section are precisely those which would be obtained if A were a cyclic (or nearly cyclic) matrix in both the index j which refers to the rows and the index k which refers to the columns of the Ising lattice. Therefore, the inverse matrix elements of A_0, as $\mathscr{M}$, $\mathscr{M}'$, and $\mathscr{N}$ all approach infinity, are exactly the same as those of the corresponding cyclic matrix. But we have seen in Sec. 3 of Chapter VII how to invert a cyclic matrix. Therefore, without further ado, we may write

$$A_\Delta^{-1}(j';k';j,k) = \frac{1}{2\pi}\int_0^{2\pi} d\phi_1 \frac{1}{2\pi}\int_0^{2\pi} d\phi_2 e^{i\phi_1(k'-k)+i\phi_2(j'-j)} A_\Delta^{-1}(\phi_1,\phi_2), \tag{3.12}$$

where $A_\Delta(\phi_1, \phi_2)$ is the 6×6 matrix

$$
\begin{aligned}
A_\Delta(\phi_1, \phi_2) &= A_\Delta(0,0;0,0) + A_\Delta(0,0;0,1)e^{i\phi_1} \\
&\quad + A_\Delta(0,0;0,-1)e^{-i\phi_1} + A_\Delta(0,0;1,0)e^{i\phi_2} \\
&\quad + A_\Delta(0,0;-1,0)e^{-i\phi_2} + A_\Delta(0,0;1,1)e^{i(\phi_1+\phi_2)} \\
&\quad + A_\Delta(0,0;-1,-1)e^{-i(\phi_1+\phi_2)}
\end{aligned}
$$

$$
= \begin{array}{c} \\ U \\ S \\ R \\ D \\ T \\ L \end{array}
\begin{array}{c}
\begin{array}{cccccc} U & S & R & D & T & L \end{array} \\
\left[\begin{array}{cccccc}
0 & 1 & -1 & -1 + z_2 e^{i\phi_2} & 1 & 1 \\
-1 & 0 & -1 & -1 & 1 + z_3 e^{i(\phi_1+\phi_2)} & 1 \\
1 & 1 & 0 & 1 & -1 & -1 + z_1 e^{i\phi_1} \\
1 - z_2 e^{-i\phi_2} & 1 & -1 & 0 & -1 & -1 \\
-1 & -1 - z_3 e^{-i(\phi_1+\phi_2)} & 1 & 1 & 0 & 1 \\
-1 & -1 & 1 - z_1 e^{-i\phi_1} & 1 & -1 & 0
\end{array}\right]
\end{array}. \quad (3.13)
$$

We are only interested in the case $E_3 \to 0$. Therefore, we make this specialization and find

$$
\begin{aligned}
&A_0^{-1}(\phi_1, \phi_2)_{TT} \\
&\quad = -A_0^{-1}(\phi_1, \phi_2)_{SS} \\
&\quad = \frac{z_2(1 - z_1^2)(e^{i\phi_2} - e^{-i\phi_2}) - z_1(1 - z_2^2)(e^{i\phi_1} - e^{-i\phi_1})}{(1 + z_1^2)(1 + z_2^2) - z_1(1 - z_2^2)(e^{i\phi_1} + e^{-i\phi_1}) - z_2(1 - z_1^2)(e^{i\phi_2} + e^{-i\phi_2})} \quad (3.14a)
\end{aligned}
$$

and

$$
\begin{aligned}
&A_0^{-1}(\phi_1, \phi_2)_{TS} \\
&\quad = A_0^{-1}(\phi_1, \phi_2)_{ST}^{*} \\
&\quad = \frac{4z_1 z_2 e^{-i(\phi_1+\phi_2)} - (1 - z_1^2)(1 - z_2^2)}{(1 + z_1^2)(1 + z_2^2) - z_1(1 - z_2^2)(e^{i\phi_1} + e^{-i\phi_1}) - z_2(1 - z_1^2)(e^{i\phi_2} + e^{-i\phi_2})}. \quad (3.14b)
\end{aligned}
$$

To obtain the desired expression for $\langle \sigma_{0,0}\sigma_{N,N} \rangle$ it remains to use (3.12) and (3.14) to write the inverse matrix elements in (3.10) as single integrals.

Consider first

$$
\begin{aligned}
A_0^{-1}&(k', k'; k, k)_{TT} \\
&= -A_0^{-1}(k', k'; k, k)_{SS} \\
&= \frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi_1 \frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi_2 e^{i(k'-k)(\phi_1+\phi_2)} \\
&\times \frac{z_2(1-z_1^2)(e^{i\phi_2}-e^{-i\phi_2}) - z_1(1-z_2^2)(e^{i\phi_1}-e^{-i\phi_1})}{(1+z_1^2)(1+z_2^2) - z_1(1-z_2^2)(e^{i\phi_1}+e^{-i\phi_1}) - z_2(1-z_1^2)(e^{i\phi_2}+e^{-i\phi_2})}. \qquad (3.15)
\end{aligned}
$$

We wish to show that this vanishes. This will be the case if we can demonstrate that

$$
\begin{aligned}
I = &\frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi_1 \frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi_2 \\
&\times \frac{e^{i(k'-k)(\phi_1+\phi_2)} z_2(1-z_1^2)(e^{i\phi_2}-e^{-i\phi_2})}{(1+z_1^2)(1+z_2^2) - z_1(1-z_2^2)(e^{i\phi_1}+e^{-i\phi_1}) - z_2(1-z_1^2)(e^{i\phi_2}+e^{-i\phi_2})} \qquad (3.16)
\end{aligned}
$$

is a symmetric function of z_1 and z_2. To show this, we transform to the variables

$$
\begin{aligned}
\phi_1 + \phi_2 &= \theta, \\
\phi_2 &= -\omega.
\end{aligned} \qquad (3.17)
$$

In terms of these variables, the denominator of (3.16) becomes

$$A + Be^{i\omega} + B^* e^{-i\omega}, \qquad (3.18a)$$

where

$$A = (1 + z_1^2)(1 + z_2^2) \quad \text{and} \quad B = -[z_2(1 - z_1^2) + z_1(1 - z_2^2)e^{i\theta}]. \qquad (3.18b)$$

Thus

$$I = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta \frac{1}{2\pi}\int_{-\pi}^{\pi} d\omega \frac{e^{i(k'-k)\theta} z_2(1 - z_1^2)(e^{-i\omega} - e^{i\omega})}{A + Be^{i\omega} + B^* e^{-i\omega}}. \qquad (3.19)$$

The ω integral may be evaluated as a contour integral. Specifically, the denominator vanishes when

$$e^{i\omega} = \alpha_0 \text{ or } \alpha_0^{-1*}, \qquad (3.20)$$

where

$$\alpha_0 = \frac{(1 + z_1^2)(1 + z_2^2) + |4z_1z_2 - (1 - z_1^2)(1 - z_2^2)e^{i\theta}|}{2[z_2(1 - z_1^2) + z_1(1 - z_2^2)e^{i\theta}]} \qquad (3.21a)$$

and

$$\alpha_0^{-1*} = \frac{(1 + z_1^2)(1 + z_2^2) - |4z_1z_2 - (1 - z_1^2)(1 - z_2^2)e^{i\theta}|}{2[z_2(1 - z_1^2) + z_1(1 - z_2^2)e^{i\theta}]}. \qquad (3.21b)$$

Furthermore, it is easily verified that for $0 \le \theta \le 2\pi$

$$|\alpha_0| \ge 1 \tag{3.22}$$

and that $|\alpha_0| = 1$ only if $e^{i\theta} = +1$ and

$$4z_1z_2 = (1 - z_1^2)(1 - z_2^2). \tag{3.23}$$

This condition is, of course, fulfilled only if $T = T_c$. Therefore, if for the moment we consider $T \neq T_c$, we evaluate (3.19) and find

$$\begin{aligned} I = \frac{1}{4\pi}\int_{-\pi}^{\pi} & d\theta e^{i(k'-k)\theta} z_2(1 - z_1^2)z_1(1 - z_2^2)(e^{i\theta} - e^{-i\theta}) \\ & \times [1 - (1 + z_1^2)(1 + z_2^2)|4z_1z_2 - (1 - z_1^2)(1 - z_2^2)e^{i\theta}|^{-1}] \\ & \times [z_2^2(1 - z_1^2)^2 + z_1^2(1 - z_2^2)^2 + z_1z_2(1 - z_1^2)(1 - z_2^2)(e^{i\theta} - e^{-i\theta})]^{-1}. \end{aligned} \tag{3.24}$$

This is symmetric in z_1 and z_2 so, at least for $T \neq T_c$,

$$A_0^{-1}(k', k'; k, k)_{TT} = -A_0^{-1}(k', k'; k, k)_{SS} = 0 \tag{3.25}$$

and by continuity the restriction $T \neq T_c$ is removed.

The remaining matrix elements in (3.10) are

$$\begin{aligned} & A_0^{-1}(k', k'; k, k)_{TS} \\ & = -A_0^{-1}(k, k; k', k')_{ST} \\ & = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi_1 \frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi_2 e^{i(k'-k)(\phi_1+\phi_2)} \\ & \times \frac{4z_1z_2e^{-i(\phi_1+\phi_2)} - (1 - z_1^2)(1 - z_2^2)}{(1 + z_1^2)(1 + z_2^2) - z_1(1 - z_2^2)(e^{i\phi_1} + e^{-i\phi_1}) - z_2(1 - z_1^2)(e^{i\phi_2} + e^{-i\phi_2})}. \end{aligned} \tag{3.26}$$

By the change of variable (3.17), we may again use (3.20) to perform the integration over the variable ω to find

$$\begin{aligned} & A_0^{-1}(k', k'; k, k)_{TS} \\ & = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta e^{i(k'-k)\theta} \\ & \times \frac{(1 - z_1^2)(1 - z_2^2) - 4z_1z_2e^{-i\theta}}{\{[4z_1z_2 - (1 - z_1^2)(1 - z_2^2)e^{i\theta}][4z_1z_2 - (1 - z_1^2)(1 - z_2^2)e^{-i\theta}]\}^{1/2}}, \end{aligned} \tag{3.27}$$

where the square root is defined to be nonnegative when $\theta = \pi$. Therefore

$$\begin{aligned} & A_0^{-1}(k', k'; k, k)_{TS} \\ & = -A_0^{-1}(k, k; k', k')_{ST} \\ & = -\frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta e^{i(k'-k-1)\theta}\left[\frac{4z_1z_2 - (1 - z_1^2)(1 - z_2^2)e^{i\theta}}{4z_1z_2 - (1 - z_1^2)(1 - z_2^2)e^{-i\theta}}\right]^{1/2}. \end{aligned} \tag{3.28}$$

Finally, we substitute (3.25) and (3.28) into (3.10) and note that

$$2z_k(1 - z_k^2)^{-1} = \sinh 2\beta E_k, \qquad k = 1, 2,$$

to obtain the desired result:

$$\langle\sigma_{0,0}\sigma_{N,N}\rangle = \begin{vmatrix} \tilde{a}_0 & \tilde{a}_{-1} & \cdots & \tilde{a}_{-N+1} \\ \tilde{a}_1 & \tilde{a}_0 & \cdots & \tilde{a}_{-N+2} \\ \vdots & \vdots & \vdots & \vdots \\ \tilde{a}_{N-1} & \tilde{a}_{N-2} & \cdots & \tilde{a}_0 \end{vmatrix}, \tag{3.29}$$

where

$$\tilde{a}_n = \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{-in\theta}\tilde{\phi}(\theta), \tag{3.30}$$

with

$$\tilde{\phi}(\theta) = \left[\frac{\sinh 2\beta E_1 \sinh 2\beta E_2 - e^{-i\theta}}{\sinh 2\beta E_1 \sinh 2\beta E_2 - e^{i\theta}}\right]^{1/2}. \tag{3.31}$$

The function $\tilde{\phi}(\theta)$ should be compared with the function $\phi(\theta)$ of (2.30); $\tilde{\phi}(\theta)$ is clearly obtained from $\phi(\theta)$ by the replacements $\alpha_1 \to 0$ and $\alpha_2 \to (\sinh 2\beta E_1 \sinh 2\beta E_2)^{-1}$. The fact that $\tilde{\phi}(\theta)$ corresponds to $\phi(\theta)$ with $\alpha_1 = 0$ makes $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ a somewhat simpler object to study than $\langle\sigma_{0,0}\sigma_{0,N}\rangle$. The nature of the simplification will become apparent in Chapter XI.

4. THE NEAR-NEIGHBOR CORRELATION FUNCTIONS $\langle\sigma_{0,0}\sigma_{0,1}\rangle$ AND $\langle\sigma_{0,0}\sigma_{1,1}\rangle$

Our primary interest in spin-spin correlation functions is in their behavior when the separation between the spins is large. However, before we embark on the study of this asymptotic behavior it is useful to discuss briefly the correlation functions of two spins close to each other.

Consider first the nearest-neighbor correlation function $\langle\sigma_{0,0}\sigma_{0,1}\rangle$. From (2.28) we find that it is

$$\langle\sigma_{0,0}\sigma_{0,1}\rangle = \frac{1}{2\pi}\int_0^{2\pi} d\theta \left[\frac{(1 - \alpha_1 e^{i\theta})(1 - \alpha_2 e^{-i\theta})}{(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{i\theta})}\right]^{1/2}. \tag{4.1}$$

The correlation function $\langle\sigma_{0,0}\sigma_{1,0}\rangle$ is obtained from (4.1) by the replacement $E_2 \leftrightarrow E_1$. Therefore, comparing (4.1) with (V.3.64) we find that, as expected from (II.5.32),

$$u = -E_1\langle\sigma_{0,0}\sigma_{0,1}\rangle - E_2\langle\sigma_{0,0}\sigma_{1,0}\rangle. \tag{4.2}$$

The most interesting features of $\langle\sigma_{0,0}\sigma_{0,1}\rangle$ and $\langle\sigma_{0,0}\sigma_{1,1}\rangle$ are to be found near T_c. In particular, both of these correlation functions are continuous at T_c and their first derivative with respect to T diverges logarithmically as $T \to T_c$. Indeed, these not only are properties of $\langle\sigma_{0,0}\sigma_{0,1}\rangle$ and $\langle\sigma_{0,0}\sigma_{1,1}\rangle$ but can also be seen to be the case for $\langle\sigma_{0,0}\sigma_{0,N}\rangle$, $\langle\sigma_{0,0}\sigma_{N,N}\rangle$, and even for $\langle\sigma_{0,0}\sigma_{M,N}\rangle$. To make these properties manifest it is sufficient to expand the correlation functions for $T \sim T_c$. This can be done directly in terms of the integrals (2.29) and (3.30). However, since we are confining our interest to $\langle\sigma_{0,0}\sigma_{0,1}\rangle$ and $\langle\sigma_{0,0}\sigma_{1,1}\rangle$, we will study the $T \sim T_c$ behavior by first writing $\langle\sigma_{0,0}\sigma_{0,1}\rangle$ and $\langle\sigma_{0,0}\sigma_{1,1}\rangle$ in terms of complete elliptic integrals and then using the expansion developed in Chapter V. This has the advantage that we can use tables of complete elliptic integrals to obtain rapidly numerical values for the correlations.

The reduction of $\langle\sigma_{0,0}\sigma_{0,1}\rangle$ to complete elliptic integrals has, in effect, already been carried out in Chapter V, where u was written in terms of Π_1 and $\mathbf{K}$. Therefore, we find from (V.3.82) that for $T > T_c$

$$\langle\sigma_{0,0}\sigma_{0,1}\rangle = (2/\pi)\coth 2\beta E_1 \cosh 2\beta E_1 \cosh 2\beta E_2 \times [\Pi_1(\sinh^2 2\beta E_1, k_>) - \operatorname{sech}^2 2\beta E_1\, \mathbf{K}(k_>)] \tag{4.3a}$$

and from (V.3.103) that for $T < T_c$

$$\langle\sigma_{0,0}\sigma_{0,1}\rangle = (2/\pi)\coth^2 2\beta E_1 \coth 2\beta E_2 \times [\Pi_1(\operatorname{csch}^2 2\beta E_1, k_<) - \operatorname{sech}^2 2\beta E_1\, \mathbf{K}(k_<)], \tag{4.3b}$$

where we recall from (V.3.71) that

$$k_> = \sinh 2\beta E_1 \sinh 2\beta E_2 = k_<^{-1}. \tag{4.4}$$

When $E_1 = E_2$ we use (V.3.84) to show that if $T > T_c$

$$\langle\sigma_{0,0}\sigma_{0,1}\rangle = \coth 2\beta E[\tfrac{1}{2} + \pi^{-1}\cosh^2 2\beta E(2\tanh^2 2\beta E - 1)\mathbf{K}(k_>)] \tag{4.5a}$$

and if $T < T_c$

$$\langle\sigma_{0,0}\sigma_{0,1}\rangle = \coth 2\beta E[\tfrac{1}{2} + \pi^{-1}(2 - \coth^2 2\beta E)\mathbf{K}(k_<)]. \tag{4.5b}$$

The correlation function $\langle\sigma_{0,0}\sigma_{1,1}\rangle$ is found from (3.29) to be

$$\langle\sigma_{0,0}\sigma_{1,1}\rangle = \frac{1}{2\pi}\int_0^{2\pi} d\theta \left(\frac{\sinh 2\beta E_1 \sinh 2\beta E_2 - e^{-i\theta}}{\sinh 2\beta E_1 \sinh 2\beta E_2 - e^{i\theta}}\right)^{1/2}. \tag{4.6}$$

When $T < T_c$ we reduce this to a complete elliptic integral by first using the substitution $\zeta = e^{-i\theta}$ and deforming the contour of integration from the unit circle $|\zeta| = 1$ to the real axis to rewrite (4.6) as

$$\langle\sigma_{0,0}\sigma_{1,1}\rangle = \frac{1}{\pi}\int_0^{k_<} \frac{d\zeta}{\zeta}\left(\frac{1 - k_<\zeta}{\zeta^{-1}k_< - 1}\right)^{1/2}. \tag{4.7}$$

Then if we further let

$$\zeta = k_< \sin^2\phi, \tag{4.8}$$

we obtain

$$\langle\sigma_{0,0}\sigma_{1,1}\rangle = (2/\pi)\mathbf{E}(k_<). \tag{4.9a}$$

Similarly, when $T > T_c$ we find

$$\langle\sigma_{0,0}\sigma_{1,1}\rangle = (2/\pi k_>)[\mathbf{E}(k_>) + (k_>^2 - 1)\mathbf{K}(k_>)]. \tag{4.9b}$$

The values of $\langle\sigma_{0,0}\sigma_{0,1}\rangle$ and $\langle\sigma_{0,0}\sigma_{1,1}\rangle$ at T_c may now be found from the expansions of complete elliptic integrals given by (V.3.46), (V.3.53), and (V.3.116). We obtain

$$\langle\sigma_{0,0}\sigma_{0,1}\rangle = (2/\pi)\coth 2\beta_c E_1 \operatorname{gd} 2\beta_c E_1 \tag{4.10a}$$

and

$$\langle\sigma_{0,0}\sigma_{1,1}\rangle = (2/\pi) \sim 0.5366198. \tag{4.10b}$$

In the isotropic case when $E_1 = E_2$ we have

$$\operatorname{gd} 2\beta_c E_1 = \pi/4 \tag{4.11}$$

and thus (4.10*a*) reduces to

$$\langle\sigma_{0,0}\sigma_{0,1}\rangle = 1/\sqrt{2} \sim 0.7071067. \tag{4.12}$$

The logarithmic divergence in the derivative of these correlation functions with respect to T is also easily obtained. In particular, from (V.3.119) we find that near T_c

$$\begin{aligned}(d/dT)&\langle\sigma_{0,0}\sigma_{0,1}\rangle\\ &\sim (2/\pi k T_c^2)\{(E_1 \sinh^2 2\beta_c E_2 + E_2)\\ &\qquad\times [\ln|1 - T/T_c| + \ln \tfrac{1}{4}\beta_c(E_1\coth 2\beta_c E_1 + E_2 \coth 2\beta_c E_2)]\\ &\qquad + 2E_1 \sinh^2 2\beta_c E_2 \operatorname{gd} 2\beta_c E_1 + 2E_2\}.\end{aligned} \tag{4.13a}$$

In the isotropic case we may use (4.11) to show that (4.13*a*) reduces to

$$\begin{aligned}(d/dT)\langle\sigma_{0,0}\sigma_{0,1}\rangle &\sim (4/\pi k T_c^2)E\\ &\qquad\times [\ln|1 - T/T_c| + \ln(E/kT_c\sqrt{2}) + \tfrac{1}{4}\pi + 1].\end{aligned} \tag{4.14a}$$

To study $\langle\sigma_{0,0}\sigma_{1,1}\rangle$ we first differentiate $\mathbf{E}(k)$ to find

$$\frac{d\mathbf{E}(k)}{dk} = k\int_0^{\pi/2} d\phi\, \frac{\sin^2\phi}{(1 - k^2\sin^2\phi)^{1/2}} = \frac{1}{k}[\mathbf{K}(k) - \mathbf{E}(k)]. \tag{4.15}$$

Then we use (V.3.42), (V.3.46), and (V.3.53) to show that near T_c

$$\begin{aligned}(d/dT)&\langle\sigma_{0,0}\sigma_{1,1}\rangle\\ &\sim (2/\pi k T_c^2)[E_1\coth 2\beta_c E_1 + E_2\coth 2\beta_c E_2]\\ &\qquad\times [\ln|1 - T/T_c| + \ln\tfrac{1}{4}\beta_c(E_1\coth 2\beta_c E_1 + E_2\coth 2\beta_c E_2)],\end{aligned} \tag{4.13b}$$

which, when $E_1 = E_2 = E$, reduces to

$$(d/dT)\langle\sigma_{0,0}\sigma_{1,1}\rangle \sim (4\sqrt{2}/\pi^2 kT_c^2)E[\ln|1 - T/T_c| + \ln(E/kT_c\sqrt{2})]. \tag{4.14b}$$

To complete our discussion of near-neighbor correlations we use (4.3) and (4.9) to plot $\langle\sigma_{0,0}\sigma_{0,1}\rangle$ and $\langle\sigma_{0,0}\sigma_{1,1}\rangle$ in Fig. 8.10. There we see that,

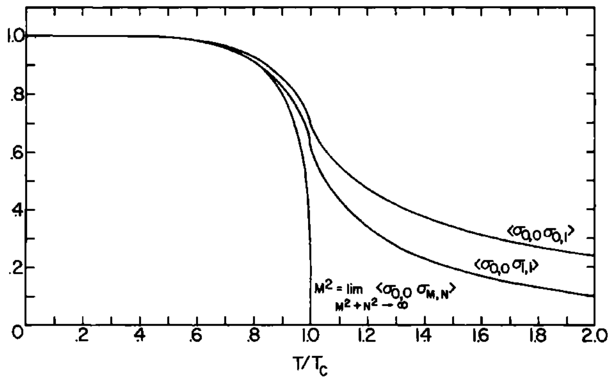


Fig. 8.10. Plot of the near-neighbor correlation functions $\langle\sigma_{0,0}\sigma_{0,1}\rangle$ and $\langle\sigma_{0,0}\sigma_{1,1}\rangle$ in the isotopic case $E_1 = E_2$. For comparison, $M^2 = \lim_{M^2+N^2\to\infty}\langle\sigma_{0,0}\sigma_{M,N}\rangle$ is also shown.

as expected,

$$\langle\sigma_{0,0}\sigma_{0,1}\rangle \geq \langle\sigma_{0,0}\sigma_{1,1}\rangle. \tag{4.16}$$

For comparison we also plot in Fig. 8.10 the limiting value $M^2 = \lim_{N\to\infty}\langle\sigma_{0,0}\sigma_{0,N}\rangle$ which will be computed in Chapter X. Both $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ and $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ approach M^2 as $N \to \infty$. Now M^2 vanishes at T_c. However, just because M^2 vanishes at the same temperature where $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ (and $\langle\sigma_{0,0}\sigma_{N,N}\rangle$) behave as

$$A(N) + B(N)(T - T_c)\ln|T - T_c| + \cdots, \tag{4.17}$$

it may not be concluded that $M^2 \sim (T - T_c)\ln|T - T_c|$ as $T \to T_c^-$. In fact, we find in Chapter X that M^2 vanishes as $(T_c - T)^{1/4}$ as $T \to T_c^-$. Therefore, when N is large, even though an expansion of the form (4.17) exists when T is sufficiently close to T_c, this range of T in which (4.17) is a useful expansion vanishes as $N \to \infty$. However, though we will be able to make some precise remarks in the last section of Chapter XII, complete details of the behavior of $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ when $M^2 + N^2$ is large and T is very close to T_c do not exist.

CHAPTER IX
Wiener-Hopf Sum Equations

1. INTRODUCTION

The infinite set of simultaneous linear equations

$$\sum_{m=0}^{\infty} c_{n-m} x_m = y_n, \qquad 0 \le n, \tag{1.1}$$

where c_n and y_n are known and x_n are unknown, is referred to as a Wiener-Hopf sum equation.[1] These sum equations are distinguished from the most general sum equation in two respects: (1) the set of numbers c_{n-m} depends on $n - m$ only instead of on n and m separately, and (2) the summation runs from 0 to ∞. For all applications in this book y_n will satisfy

$$\sum_{n=0}^{\infty} |y_n| < \infty \tag{1.2}$$

and we will be interested in solutions x_n which also satisfy

$$\sum_{n=0}^{\infty} |x_n| < \infty. \tag{1.3}$$

In order to solve (1.1) it is necessary to impose some restrictions on the numbers c_n. For the purposes of this book we will restrict ourselves to sequences c_n satisfying

$$\sum_{n=-\infty}^{\infty} |c_n| < \infty. \tag{1.4}$$

1. A good discussion of the equation of Wiener and Hopf is to be found in M. G. Krein, *Am. Math. Soc. Transl.* **22**, 163 (1962).

The solution of (1.1) is by no means obvious. Therefore, to provide some orientation, it is useful to consider the much simpler equations obtained from (1.1) and (1.2) by extending the lower limit of summation from 0 to $-\infty$; namely

$$\sum_{m=-\infty}^{\infty} c_{n-m}x_m = y_n, \qquad -\infty < n < \infty, \tag{1.5}$$

and

$$\sum_{n=-\infty}^{\infty} |y_n| < \infty. \tag{1.6}$$

We seek solutions which obey the restriction similar to (1.3),

$$\sum_{n=-\infty}^{\infty} |x_n| < \infty. \tag{1.7}$$

These solutions may be found if we define the Fourier series

$$X(e^{i\theta}) = \sum_{n=-\infty}^{\infty} x_n e^{in\theta}, \tag{1.8}$$

$$Y(e^{i\theta}) = \sum_{n=-\infty}^{\infty} y_n e^{in\theta}, \tag{1.9}$$

$$C(e^{i\theta}) = \sum_{n=-\infty}^{\infty} c_n e^{in\theta}. \tag{1.10}$$

Because of the conditions (1.4), (1.6), and (1.7), these Fourier series are all uniformly convergent for $0 \le \theta \le 2\pi$, so that $X(e^{i\theta})$, $Y(e^{i\theta})$, and $C(e^{i\theta})$ are all continuous (though not necessarily analytic) on the interval $0 \le \theta \le 2\pi$. Furthermore, because the series are uniformly convergent, they may be integrated term by term so that x_n is easily obtained from $X(e^{i\theta})$ as

$$\begin{aligned}\frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta e^{-in\theta}X(e^{i\theta}) &= \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta e^{-in\theta}\sum_{m=-\infty}^{\infty} x_m e^{im\theta}\\ &= \frac{1}{2\pi}\sum_{m=-\infty}^{\infty} x_m \int_{-\pi}^{\pi} d\theta e^{-i(n-m)\theta} = x_n.\end{aligned} \tag{1.11}$$

We may now solve (1.5) if we multiply both sides by $e^{in\theta}$ and sum over n. Therefore, for $0 \le \theta \le 2\pi$,

$$\begin{aligned}Y(e^{i\theta}) &= \sum_{n=-\infty}^{\infty} e^{in\theta}\sum_{m=-\infty}^{\infty} c_{n-m}x_m\\ &= \sum_{n=-\infty}^{\infty} e^{in\theta}\sum_{m=-\infty}^{\infty} c_{n-m}e^{-im\theta}x_m e^{im\theta}\\ &= \sum_{m=-\infty}^{\infty} x_m e^{im\theta}\sum_{n=-\infty}^{\infty} c_{n-m}e^{i\theta(n-m)}\\ &= C(e^{i\theta})X(e^{i\theta}),\end{aligned} \tag{1.12}$$

where we have been allowed to interchange the order of summation over m and n because of the uniform convergence of the series for $C(e^{i\theta})$ and $X(e^{i\theta})$ for real θ. From this we have only to divide both sides by $C(e^{i\theta})$ and apply the inversion formula (1.11) to obtain the formal solution

$$x_n = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{d\theta\, Y(e^{i\theta})}{C(e^{i\theta})}. \tag{1.13}$$

This formal solution is not necessarily a solution satisfying (1.7) for all possible $C(e^{i\theta})$. In particular, (1.7) guarantees that $X(e^{i\theta})$ must be continuous for $0 \le \theta \le 2\pi$. Therefore it is necessary to require that

$$C(e^{i\theta}) \neq 0 \qquad \text{for } 0 \le \theta \le 2\pi \tag{1.14}$$

if x_n is to satisfy (1.5) and (1.7) for an arbitrary sequence y_n satisfying (1.6).

It is also true that (1.14) is sufficient for $Y(e^{i\theta})/C(e^{i\theta})$ to be represented as a Fourier series whose coefficients are absolutely summable. The necessary theorems are somewhat technical and they will be dealt with in the next section. These theorems are also needed to prove that the formal solution which we will obtain for the Wiener-Hopf sum equation (1.1) is in fact a solution which satisfies (1.3).

The foregoing discussion of (1.5) suggests that the dependence of c_{n-m} in (1.1) on $n - m$ alone may be usefully exploited if we perform a Fourier transformation. Since (1.1) holds only for $n \ge 0$, we define

$$y_n = 0 \qquad \text{if } n < 0, \tag{1.15}$$

$$v_n = \sum_{m=0}^{\infty} c_{n-m}x_m \qquad \text{if } n < 0, \tag{1.16a}$$

and

$$v_n = 0 \qquad \text{if } n \ge 0. \tag{1.16b}$$

Then we may write

$$\sum_{m=-\infty}^{\infty} c_{n-m}x_m = y_n + v_n \qquad \text{for } -\infty < n < \infty. \tag{1.17}$$

We note that

$$\sum_{n=-\infty}^{\infty} |v_n| = \sum_{n=-\infty}^{\infty} \left| \sum_{m=0}^{\infty} c_{n-m}x_m \right| < \sum_{n=-\infty}^{\infty} |c_n| \sum_{m=0}^{\infty} |x_m| < \infty, \tag{1.18}$$

where the interchange of the order of summation over m and n is justified because the final expression is finite.

Let $e^{i\theta} = \xi$, define $C(\xi)$ for $|\xi| = 1$ by (1.10), and

$$X(\xi) = \sum_{n=0}^{\infty} x_n\xi^n, \tag{1.19}$$

$$Y(\xi) = \sum_{n=0}^{\infty} y_n\xi^n, \tag{1.20}$$

and

$$V(\xi) = \sum_{n=-\infty}^{-1} v_n \xi^n. \tag{1.21}$$

By (1.3), (1.2), and (1.18), these three functions of ξ are continuous when $|\xi| = 1$. With these definitions, we multiply (1.17) by ξ^n and sum over all n to find that, for $|\xi| = 1$,

$$C(\xi)X(\xi) = Y(\xi) + V(\xi). \tag{1.22}$$

This equation is dramatically different from (1.12). Equation (1.12) contains only one unknown function and hence, if (1.14) is satisfied, is easily solved. Equation (1.22) contains two unknown functions and hence it is by no means clear that it can be solved at all.

The purpose of this chapter is to explain in detail how this apparent difficulty of having one equation for two unknowns may be overcome by exploiting the analyticity properties of the four functions in (1.22). More specifically, in Sections 3–6, we will find all solutions of (1.1) satisfying (1.3) when y_n satisfies (1.2), c_n satisfies (1.4), and $C(\xi) \neq 0$ for $|\xi| = 1$. However, in order to make the work of these sections mathematically rigorous, it is necessary to introduce a few theorems of a rather technical nature. These theorems are set forth in Sec. 2 and may be omitted if one is not overly concerned with technical details.

2. MATHEMATICAL TECHNICALITIES

The space of all sequences x_n satisfying $\sum_{n=-\infty}^{\infty} |x_n| < \infty$ will be denoted by l. The space of all functions

$$X(e^{i\theta}) = \sum_{n=-\infty}^{\infty} x_n e^{in\theta} \tag{2.1}$$

derivable from the sequences of l for real θ will be denoted by l^*. With these definitions we may formulate several theorems needed later in this chapter.

Theorem 1. If $f_n \in l$ and $g_n \in l$ then $h_n = \sum_{m=-\infty}^{\infty} f_{n-m} g_m \in l$.

This is easily proved since

$$\sum_{n=-\infty}^{\infty} |h_n| < \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} |f_{n-m}|\,|g_m| = \sum_{m=-\infty}^{\infty} |g_m| \sum_{n=-\infty}^{\infty} |f_n| < \infty, \tag{2.2}$$

where we have been allowed to interchange the order of summation because the resulting expression is finite.

We may now multiply

$$h_n = \sum_{m=-\infty}^{\infty} f_{n-m} g_m \tag{2.3}$$

by $e^{in\theta}$ and sum over n from $-\infty$ to $+\infty$. Then, because of the absolute convergence for real θ of all series involved,

$$
\begin{aligned}
H(e^{i\theta}) &= \sum_{n=-\infty}^{\infty} h_n e^{in\theta} = \sum_{n=-\infty}^{\infty} e^{in\theta} \sum_{m=-\infty}^{\infty} f_{n-m} g_m \\
&= \sum_{m=-\infty}^{\infty} e^{im\theta} g_m \sum_{n=-\infty}^{\infty} e^{i(n-m)\theta} f_{n-m} = F(e^{i\theta})G(e^{i\theta}).
\end{aligned}
\tag{2.4}
$$

Therefore we have proved

Theorem 2. If $F \in l^*$ and $G \in l^*$ then $FG \in l^*$.

To illustrate the uses to which Theorem 2 will be put, consider the expression $Y(e^{i\theta})/C(e^{i\theta})$ encountered in the previous section. We saw there that to demonstrate the validity of our formal solution of (1.5) we had to prove that $Y(e^{i\theta})/C(e^{i\theta}) \in l^*$. Theorem 2 now guarantees that $Y(e^{i\theta})/C(e^{i\theta}) \in l^*$ if $Y(e^{i\theta}) \in l^*$ and $C(e^{i\theta})^{-1} \in l^*$. But, by (1.2), $Y(e^{i\theta}) \in l^*$. Therefore we will have proved that (1.13) is a rigorous solution to (1.5) which satisfies (1.3) if we can prove that the conditions $C(e^{i\theta}) \in l^*$ and $C(e^{i\theta}) \neq 0$ for real θ are sufficient to guarantee that $C(e^{i\theta})^{-1} \in l^*$. This result follows as a special case of a much more general theorem of Wiener and Lévy.

Wiener-Lévy Theorem. Let $\Phi(z)$ be a function analytic in a region R and let $F(e^{i\theta}) \in l^*$ be such that the curve $z = F(e^{i\theta})$, $0 \leq \theta \leq 2\pi$, lies entirely inside the region R. Then $\Phi(F(e^{i\theta})) \in l^*$.

This theorem is intuitively obvious. However, as is often the case with obvious theorems, its proof is highly nontrivial.[2]

For the purposes of this book we need, in particular, the two following special cases of the Wiener-Lévy theorem:

(1) If $F(e^{i\theta}) \in l^*$ and if $F(e^{i\theta}) \neq 0$ for real θ, then $F(e^{i\theta})^{-1} \in l^*$; this is the theorem needed to justify solution (1.13) of (1.5);

(2) If $F(e^{i\theta}) \in l^*$ and if $\ln F(e^{i\theta})$ is continuous when $0 \leq \theta \leq 2\pi$ then $\ln F(e^{i\theta}) \in l^*$.

The final theorem we will need, to make the work of this chapter rigorous, is Pollard's generalization of Cauchy's theorem.

Pollard's Theorem. If a function $f(z)$ is analytic inside and continuous on a simple closed contour C, then

$$\oint_C f(z)\, dz = 0. \tag{2.5}$$

The generalization this theorem makes over the more familiar theorem of Cauchy is that in Cauchy's theorem $f(z)$ is required to be analytic and not merely continuous on C. The proof of this theorem is involved and will again be omitted.

2. We refer the reader to, for example, N. I. Achieser, *Theory of Approximation* (Ungar, New York, 1956), pp. 230 ff.

3. FACTORIZATION

The functions $X(\xi)$ and $Y(\xi)$ in (1.22) have the property that, for $|\xi| = 1$, they may be expanded into a Laurent series of the form

$$\sum_{n=0}^{\infty} a_n \xi^n, \tag{3.1}$$

with

$$\sum |a_n| < \infty. \tag{3.2}$$

When (3.2) is satisfied, the series (3.1) defines a function, called a + function, which is analytic for $|\xi| < 1$ and continuous for $|\xi| \le 1$. Similarly, the $V(\xi)$ in (1.22) has the property that for $|\xi| = 1$ it may be expanded into a Laurent series

$$\sum_{n=-\infty}^{-1} a_n \xi^n, \tag{3.3}$$

where (3.2) is again satisfied. Because of (3.2), (3.3) defines a function, called a $-$ function, which is analytic for $|\xi| > 1$ and continuous for $|\xi| \ge 1$, and approaches zero as $\xi \to \infty$.

We may exploit these analyticity properties of X, Y, and V if we can factorize $C(\xi)$ for $|\xi| = 1$ as

$$C(\xi) = P(\xi)^{-1} Q(\xi^{-1})^{-1}, \tag{3.4}$$

where both $P(\xi)$ and $Q(\xi)$ are + functions which are nonzero for $|\xi| \le 1$. Such a factorization is called canonical. Clearly $P(\xi)$ and $Q(\xi^{-1})$ are not unique since we may multiply $P(\xi)$ by a constant c if we also divide $Q(\xi^{-1})$ by c. For definiteness we will eliminate this trivial ambiguity by requiring that $Q(0) = 1$. Then we may write

$$P(\xi) = e^{G_+(\xi)} \tag{3.5a}$$

and

$$Q(\xi^{-1}) = e^{G_-(\xi)}, \tag{3.5b}$$

where $G_+(\xi)$ $[G_-(\xi)]$ is a + $[-]$ function.

How can the functions $G_+(\xi)$ and $G_-(\xi)$ be found? Since $C(\xi)$ is always assumed to be nonzero on the unit circle $|\xi| = 1$, the logarithm of $C(e^{i\theta})$ can always be defined in such a way that it is continuous for $0 < \theta < 2\pi$. The Wiener-Lévy theorem, discussed in Sec. 2, implies that $\ln C(\xi)$ has a Laurent-series expansion whose coefficients are absolutely summable if, in addition to the non-vanishing of $C(\xi)$ on the unit circle, $\ln C(\xi)$ is continuous on the unit circle. This condition is satisfied if and only if

$$\ln C(e^{2\pi i}) = \ln C(e^{0i}).$$

More generally, define the index of $C(\xi)$ by

$$\nu = \text{Ind } C(\xi) = (1/2\pi i)[\ln C(e^{2\pi i}) - \ln C(e^{0i})]. \tag{3.6}$$

Since $C(\xi)$ is continuous and nonzero on the unit circle, ν is well defined and is in fact an integer. Ind $C(\xi)$ is the number of times $C(\xi)$ goes around the point $C(\xi) = 0$ in the counterclockwise direction when ξ goes once around $\xi = 0$ in the counterclockwise direction with $|\xi| = 1$. For example, if

$$C(\xi) = \xi^n, \tag{3.7}$$

then

$$\text{Ind } C(\xi) = n. \tag{3.8}$$

From any function of the form

$$F(\xi) = \sum_{n=-\infty}^{\infty} d_n \xi^n \qquad \text{for } |\xi| = 1, \tag{3.9a}$$

with

$$\sum_{n=-\infty}^{\infty} |d_n| < \infty, \tag{3.9b}$$

we may define a + function $[F(\xi)]_+$ by

$$[F(\xi)]_+ = \sum_{n=0}^{\infty} d_n \xi^n \qquad \text{for } |\xi| \le 1, \tag{3.10a}$$

and a $-$ function $[F(\xi)]_-$ by

$$[F(\xi)]_- = \sum_{n=-\infty}^{-1} d_n \xi^n \qquad \text{for } |\xi| \ge 1. \tag{3.10b}$$

Clearly, when $|\xi| = 1$,

$$F(\xi) = [F(\xi)]_+ + [F(\xi)]_-. \tag{3.11}$$

As stated above, if $C(\xi) \neq 0$ for $|\xi| = 1$ and Ind $C(\xi) = 0$, then the Wiener-Lévy theorem guarantees that $\ln C(\xi)$ is of the form (3.9). Thus (3.10) may be used to define

$$G_+(\xi) = -[\ln C(\xi)]_+ \tag{3.12a}$$

and

$$G_-(\xi) = -[\ln C(\xi)]_-, \tag{3.12b}$$

and it follows from (3.11) that, as desired,

$$C(\xi) = e^{-G_+(\xi)} e^{-G_-(\xi)} \tag{3.13}$$

for $|\xi| = 1$.

In practice, for the applications of this book, $G_+(\xi)$ and $G_-(\xi)$ will be determined by inspection. However, for other purposes we will need general formulas for $[F(\xi)]_+$ and $[F(\xi)]_-$ in terms of $F(\xi)$ itself. Let ξ satisfy $|\xi| > 1$. Then, by Pollard's theorem,

$$[F(\xi)]_- = -\frac{1}{2\pi i}\oint_{|\xi'|=1} d\xi' \frac{[F(\xi')]_-}{\xi' - \xi} \tag{3.14}$$

and

$$0 = \frac{1}{2\pi i}\oint_{|\xi'|=1} d\xi' \frac{[F(\xi')]_+}{\xi' - \xi}, \tag{3.15}$$

where the contour of integration is counterclockwise along the unit circle. By (3.14), (3.15), and (3.11),

$$\begin{aligned}[F(\xi)]_- &= -\frac{1}{2\pi i}\oint_{|\xi'|=1} d\xi' \frac{[F(\xi')]_+ + [F(\xi')]_-}{\xi' - \xi} \\ &= -\frac{1}{2\pi i}\oint_{|\xi'|=1} d\xi' \frac{F(\xi')}{\xi' - \xi}.\end{aligned} \tag{3.16a}$$

In particular, by (3.12*b*),

$$G_-(\xi) = \frac{1}{2\pi i}\oint_{|\xi'|=1} d\xi' \frac{\ln C(\xi')}{\xi' - \xi}. \tag{3.17a}$$

Similarly, for $|\xi| < 1$,

$$[F(\xi)]_+ = \frac{1}{2\pi i}\oint_{|\xi'|=1} d\xi' \frac{F(\xi')}{\xi' - \xi}, \tag{3.16b}$$

and, in particular,

$$G_+(\xi) = -\frac{1}{2\pi i}\oint_{|\xi'|=1} d\xi' \frac{\ln C(\xi')}{\xi' - \xi}. \tag{3.17b}$$

If Ind $C(\xi) = \nu \neq 0$ we cannot find a canonical factorization of the form (3.4) for $C(\xi)$. However, $\xi^{-\nu}C(\xi)$ will possess such a factorization. Thus we can study the more general case by first multiplying (1.22) by $\xi^{-\nu}$. However, we shall see that the nature of the solution is quite different, depending on whether $\nu < 0$, $\nu = 0$, or $\nu > 0$. Therefore, we shall consider each of these three cases separately.

4. Ind $C(\xi) = 0$

When Ind $C(\xi) = 0$ we use the canonical factorization (3.13) to obtain from (1.22)

$$e^{-G_+(\xi)}X(\xi) = e^{G_-(\xi)}Y(\xi) + e^{G_-(\xi)}V(\xi) \tag{4.1}$$

for $|\xi| = 1$. The function $e^{-G_+(\xi)}X(\xi)$, being the product of two + functions, is a + function. Similarly, $e^{G_-(\xi)}V(\xi)$ is a − function. The remaining function $e^{G_-(\xi)}Y(\xi)$ is known but is neither a + nor a − function. However, by Theorem 2 of Sec. 2, it is of the form (3.9), and thus by (3.10) and (3.11) may be decomposed into the sum of a + function and a − function. Therefore, for $|\xi| = 1$,

$$e^{-G_+(\xi)}X(\xi) - [e^{G_-(\xi)}Y(\xi)]_+ = e^{G_-(\xi)}V(\xi) + [e^{G_-(\xi)}Y(\xi)]_-. \tag{4.2}$$

The left-hand side of this equation defines a function analytic for $|\xi| < 1$ and continuous for $|\xi| \leq 1$, and the right-hand side defines a function analytic for $|\xi| > 1$ and continuous for $|\xi| \geq 1$. Since these two functions are equal on the circle $|\xi| = 1$,

$$e^{-G_+(\xi)}X(\xi) - [e^{G_-(\xi)}Y(\xi)]_+ = E(\xi) \tag{4.3a}$$

for $|\xi| \leq 1$ and

$$e^{G_-(\xi)}V(\xi) + [e^{G_-(\xi)}Y(\xi)]_- = E(\xi) \tag{4.3b}$$

for $|\xi| \geq 1$ define together a function $E(\xi)$ which is (1) continuous for all ξ and (2) analytic for all ξ except possibly on the circle $|\xi| = 1$. However, it may be seen that a function $E(\xi)$ with these two properties is entire (that is, is analytic in the entire ξ-plane).

To see this we use the following well-known theorem from the theory of complex variables:

If in an open set R in the x, y-plane, $h(x, y)$ has continuous first derivatives and satisfies

$$\frac{\partial h}{\partial x} = -i\frac{\partial h}{\partial y}, \tag{4.4}$$

then $h(x, y)$ is an analytic function of $x + iy$ in R.

We use this theorem to prove that $E(\xi)$ is entire by examining the function

$$h(x, y) = \int_\Gamma E(\xi')\, d\xi', \tag{4.5}$$

where the contour Γ runs from 0 to $\xi = x + iy$ as shown in Fig. 9.1(a). If $|\xi| < 1$ we use Cauchy's theorem and the fact that $E(\xi)$ is given to be analytic for $|\xi| < 1$ to conclude that

$$h(\xi) = \int_\daleth E(\xi')\, d\xi', \tag{4.6}$$

where $\daleth$ is the contour shown in Fig. 9.1(b). Equation (4.6) is also true if $|\xi| > 1$. To see this, consider the closed contour c shown in Fig. 9.2(a) made up of Γ traversed from 0 to ξ and $\daleth$ traversed from ξ to 0.

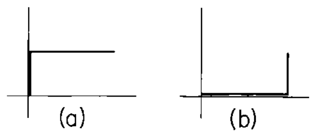


Fig. 9.1. (*a*) The contour Γ; (*b*) the contour ⅃.

This integral may be rewritten as

$$\oint_c d\xi' E(\xi') = \oint_{c_+} d\xi' E(\xi') + \oint_{c_-} d\xi' E(\xi'), \tag{4.7}$$

where c_+ and c_- are shown in Fig. 9.2(*b*). (The contours c_+ and c_- have

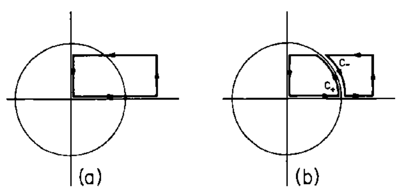


Fig. 9.2. (*a*) The contour c and its relation to the unit circle; (*b*) the contours c_+ and c_-.

part of the unit circle in common.) But $E(\xi)$ is analytic in the region enclosed by c_+ and c_- and is moreover continuous on c_+ and c_-. Hence, by Pollard's Theorem, both integrals on the right-hand side of (4.7) vanish and therefore (4.6) holds without restriction on ξ. We now differentiate (4.5) with respect to x, to find

$$\frac{\partial h(x, y)}{\partial x} = E(x + iy), \tag{4.8a}$$

and differentiate (4.6) with respect to y, to find

$$\frac{\partial h(x, y)}{\partial y} = iE(x + iy). \tag{4.8b}$$

Thus (4.4) is satisfied and, since $E(\xi)$ is a continuous function of ξ, we conclude from the above-stated theorem that $h(x, y)$ is an entire function of ξ. Hence, it follows that $E(\xi)$ itself is entire and that both equations in (4.3) may be analytically continued to all ξ.

We can easily determine $E(\xi)$. Since $E(\xi)$ is entire, the Taylor series

$$E(\xi) = \sum_{n=0}^{\infty} e_n \xi^n \tag{4.9}$$

must be convergent for all ξ and in particular for $|\xi| \geq 1$. Since the left-hand side of (4.3b) is a $-$ function, a comparison with (4.9) shows that

$$e_n = 0 \tag{4.10}$$

for all n. Accordingly,

$$E(\xi) = 0. \tag{4.11}$$

It follows from (4.11) and (4.3a) that, for $|\xi| < 1$,

$$X(\xi) = e^{G_+(\xi)}[e^{G_-(\xi)}Y(\xi)]_+. \tag{4.12}$$

The right-hand side of this expression is the product of two + functions and hence, by Theorem 2 of Sec. 2, a + function itself. Thus we may invert the Fourier series by means of (1.11) to obtain the desired unique solution,

$$x_n = \frac{1}{2\pi i} \oint_{|\xi|=1} d\xi \xi^{-n-1} e^{G_+(\xi)}[e^{G_-(\xi)}Y(\xi)]_+. \tag{4.13}$$

5. Ind $C(\xi) < 0$

This case differs from the preceding one in that the general solution of (1.1) now contains $-\text{Ind } C(\xi)$ arbitrary constants and hence is not unique.

We cannot make a canonical factorization of $C(\xi)$ itself if Ind $C(\xi) = \nu \neq 0$, but we can find a canonical factorization for

$$\xi^{-\nu}C(\xi) = Q(\xi^{-1})^{-1}P(\xi)^{-1} = e^{-G_-(\xi)}e^{-G_+(\xi)} \tag{5.1}$$

where $P(\xi)$ and $Q(\xi)$ are + functions without any zeros in $|\xi| \leq 1$, and, instead of (3.12),

$$G_+(\xi) = -[\ln(\xi^{-\nu}C(\xi))]_+ \tag{5.2a}$$

and

$$G_-(\xi) = -[\ln(\xi^{-\nu}C(\xi))]_-. \tag{5.2b}$$

Therefore we find from (1.22) that, for $|\xi| = 1$,

$$e^{-G_+(\xi)}X(\xi) = \xi^{-\nu}e^{G_-(\xi)}Y(\xi) + \xi^{-\nu}e^{G_-(\xi)}V(\xi), \tag{5.3}$$

and we may split $\xi^{-\nu}e^{G_-(\xi)}Y(\xi)$ into its + and $-$ parts to obtain, again for $|\xi| = 1$,

$$e^{-G_+(\xi)}X(\xi) - [\xi^{-\nu}e^{G_-(\xi)}Y(\xi)]_+ = \xi^{-\nu}e^{G_-(\xi)}V(\xi) + [\xi^{-\nu}e^{G_-(\xi)}Y(\xi)]_-. \tag{5.4}$$

The left-hand side of this equation is a + function and thus is analytic for $|\xi| < 1$ and continuous for $|\xi| \leq 1$. The right-hand side is not a $-$ function because a $-$ function multiplied by $\xi^{-\nu}$ is not necessarily a $-$ function. Nevertheless, the right-hand side is still analytic for $|\xi| > 1$ and continuous for $|\xi| \geq 1$. Therefore, as before, there is an entire function $E(\xi)$ such that, for $|\xi| \leq 1$

$$e^{-G_+(\xi)}X(\xi) - [\xi^{-\nu}e^{G_-(\xi)}Y(\xi)]_+ = E(\xi) \tag{5.5a}$$

and for $|\xi| \geq 1$

$$\xi^{-\nu}e^{G_-(\xi)}V(\xi) + [\xi^{-\nu}e^{G_-(\xi)}Y(\xi)]_- = E(\xi). \tag{5.5b}$$

To determine this entire function $E(\xi)$, we first note that the left-hand side of (5.5*b*), being a product of $\xi^{-\nu}$ with a $-$ function, is of the form

$$\sum_{n=-\infty}^{|\nu|-1} a_n\xi^n. \tag{5.6}$$

A comparison of (5.6) with (4.9), the Taylor-series expansion of $E(\xi)$, shows that $E(\xi)$ is a polynomial,

$$E(\xi) = \sum_{n=0}^{|\nu|-1} a_n\xi^n, \tag{5.7}$$

and we have no further way of determining a_n. We thus may substitute (5.7) in (5.5*a*) to find

$$X(\xi) = e^{G_+(\xi)}\{[\xi^{-\nu}e^{G_-(\xi)}Y(\xi)]_+ + E(\xi)\} \tag{5.8}$$

and use (1.11) to obtain the final result

$$x_n = \frac{1}{2\pi i}\int_{|\xi|=1} d\xi\xi^{-1-n}e^{G_+(\xi)}\left\{[\xi^{-\nu}e^{G_-(\xi)}Y(\xi)]_+ + \sum_{m=0}^{|\nu|-1} a_m\xi^m\right\}, \tag{5.9}$$

a result that contains $-\nu$ undetermined constants.

6. Ind $C(\xi) > 0$

This final case to be considered differs from the two previous cases in that a solution is possible only if certain extra relations hold between $Y(\xi)$ and $C(\xi)$.

As in the previous case, a canonical factorization of $C(\xi)$ does not exist and we consider $\xi^{-\nu}C(\xi)$, which possesses the canonical factorization (5.1). Then from (1.22) we obtain for $|\xi| = 1$

$$\xi^{\nu}e^{-G_+(\xi)}X(\xi) - [e^{G_-(\xi)}Y(\xi)]_+ = e^{G_-(\xi)}V(\xi) + [e^{G_-(\xi)}Y(\xi)]_-. \tag{6.1}$$

The right-hand side of this equation is a $-$ function and the left-hand side is a $+$ function, so we argue, as in Sec. 4, that each side is separately equal to the entire function $E(\xi)$, which is zero. Therefore

$$\xi^{\nu}e^{-G_+(\xi)}X(\xi) = [e^{G_-(\xi)}Y(\xi)]_+, \tag{6.2}$$

and, since $e^{-G_+(\xi)}$ does not vanish for $|\xi| < 1$, we have

$$X(\xi) = \xi^{-\nu} e^{G_+(\xi)} [e^{G_-(\xi)} Y(\xi)]_+. \tag{6.3}$$

The right-hand side of (6.3) is, however, not necessarily a + function. In general the Laurent expansion of (6.3) begins with $\xi^{-\nu}$. To insure that $X(\xi)$ is a + function we must demand that the Laurent expansion of the right-hand side of (6.3) begins with ξ^0. Therefore, only if the conditions

$$\oint_{|\xi|=1} d\xi \xi^{-n-1} e^{G_+(\xi)} [e^{G_-(\xi)} Y(\xi)]_+ = 0, \tag{6.4}$$

for $n = 0, 1, \ldots, \nu - 1$, are satisfied, will $X(\xi)$ as defined by (6.4) be a + function, and we obtain the final result

$$x_n = \frac{1}{2\pi i} \oint_{|\xi|=1} d\xi \xi^{-n-1-\nu} e^{G_+(\xi)} [e^{G_-(\xi)} Y(\xi)]_+. \tag{6.5}$$

CHAPTER X
Spontaneous Magnetization

1. INTRODUCTION

The ultimate goal of this chapter is to compute the spontaneous magnetization of Onsager's lattice when $T < T_c$, $E_1 > 0$, and $E_2 > 0$ from the formulas

$$M^2 = \lim_{N\to\infty} \langle \sigma_{0,0}\sigma_{0,N} \rangle \tag{1.1a}$$

and

$$M^2 = \lim_{N\to\infty} \langle \sigma_{0,0}\sigma_{N,N} \rangle, \tag{1.1b}$$

and to show that they are the same. This will be carried out in Sec. 4, where we also discuss some of the physical questions connected with this result.

The limits on the right-hand side of (1.1) may be evaluated when $T < T_c$ as a special case of the following theorem on the $N \to \infty$ limit of the $N \times N$ Toeplitz determinant

$$D_N = \begin{vmatrix} c_0 & c_{-1} & \cdots & c_{-N+1} \\ c_1 & c_0 & \cdots & c_{-N+2} \\ \vdots & \vdots & \vdots & \vdots \\ c_{N-1} & c_{N-2} & \cdots & c_0 \end{vmatrix}, \tag{1.2}$$

where

$$c_n = \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{-in\theta} C(e^{i\theta}). \tag{1.3}$$

"*Szegö's Theorem.*" If Ind $C(\xi) = 0$ [see (IX.3.6)], then, under suitable additional conditions,

$$\lim_{N\to\infty} D_N/\mu^N = \exp\left(\sum_{n=1}^{\infty} ng_{-n}g_n\right), \tag{1.4}$$

where

$$\mu = \exp\left[\frac{1}{2\pi}\int_0^{2\pi} d\theta \ln C(e^{i\theta})\right] \tag{1.5}$$

and

$$g_n = \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{-in\theta} \ln C(e^{i\theta}). \tag{1.6}$$

As we have stated it, this version of Szegö's theorem is not really a theorem at all, because the additional conditions[1] on $C(e^{i\theta})$ have not been given. For the purpose of evaluating M^2 from (1.1) it is sufficient to prove Szegö's theorem under the additional hypothesis that, as $|n| \to \infty$,

$$c_n = O(K^{-|n|}), \tag{1.7}$$

where $K > 1$. However, (1.7) is much stronger than is necessary. Therefore, since Szegö's theorem is of independent interest, we will prove in Sec. 3 that (1.4) holds under conditions on c_n much weaker than (1.7).

To say that Szegö's theorem is unfamiliar to many physicists is most assuredly an understatement. Moreover, the full-blown proof is filled with innumerable details and lemmas which often obscure the basic point. Were we mathematicians this would pose no problem, since we could simply give some references[2-5] and let the reader fend for himself. However, since we are physicists, we will proceed differently. Instead of going directly to the precise statement and rigorous proof of Szegö's theorem, which is given in Sec. 3, we will give in Sec. 2 a heuristic derivation in which we freely interchange the orders of limiting procedures and are not attentive to questions of technical detail. In this fashion we hope not only to prove that Szegö's theorem is true but also to give the reader a feeling of why it is true. The rigorous proof given in

1. We remark that the condition Ind $C(\xi) = 0$ is clearly needed, for otherwise the values of μ and g_n depend on where we put the discontinuity of ln $C(e^{i\theta})$. Alternatively, we may take the view that, when Ind $C(\xi) \neq 0$, the sum on the right-hand side of (1.4) diverges and we get the uninteresting result $\lim_{N\to\infty} D_N/\mu^N = 0$.

2. G. Szegö, *Commun. Seminair. Math. Univ. Lund,* suppl. dédié à Marcel Riesz, 228 (1952).

3. U. Grenander and G. Szegö, *Toeplitz Forms and Their Applications* (University of California Press, Berkeley and Los Angeles, 1958).

4. I. I. Hirschman, Jr., *J. Anal. Math.* **14,** 225 (1965).

5. A. Devinatz, *Illinois J. Math.* **11,** 160 (1967).

Sec. 3 is included because we are writing as honest a book as possible and do not want to swindle the careful reader. However, we strongly advise all readers, both interested and dedicated, to omit Sec. 3 and to be content with the warm, reassuring feeling that all the technical questions left unanswered in Sec. 2 cause no trouble in the end.

2. DISCOVERING SZEGÖ'S THEOREM

(*A*) Behavior of D_N/D_{N+1} for large N

It is difficult to study D_N directly because determinants are very complicated objects. However, it is possible to study D_N through the connection that Toeplitz determinants have with Wiener-Hopf sum equations. To see this connection define the quantities $x_n^{(N)}$, $0 \leq n \leq N$, as the solution of the system of linear equations

$$\sum_{m=0}^{N} c_{n-m} x_m^{(N)} = \delta_{n,0}. \tag{2.1}$$

These equations uniquely define $x_n^{(N)}$ if

$$D_{N+1} \neq 0. \tag{2.2}$$

If (2.2) is satisfied, then Cramer's rule gives that

$$\mu_N = D_{N+1}/D_N = [x_0^{(N)}]^{-1}. \tag{2.3}$$

We are primarily interested in the behavior of μ_N when N is large. Knowledge of this behavior, although not enough to determine the behavior of D_N for large N, is sufficient to demonstrate that $\lim_{N\to\infty} D_N/\mu_N^N$ exists. In particular, it is clear that, if $\lim_{N\to\infty} x_0^{(N)} \neq 1$, then D_N must tend to zero or infinity as $N \to \infty$.

It is natural to expect that, for at least some class of functions $C(e^{i\theta})$, $\lim_{N\to\infty} x_0^{(N)}$ exists and, moreover, that the limiting value

$$x_0^{(\infty)} = \lim_{N\to\infty} x_0^{(N)} \tag{2.4}$$

can be found by solving the Wiener-Hopf sum equation, for $n \geq 0$,

$$\sum_{m=0}^{\infty} c_{n-m} x_m^{(\infty)} = \delta_{n,0}. \tag{2.5}$$

From the general theory of the Chapter IX we know that if

$$C(e^{i\theta}) \neq 0 \qquad \text{for } \theta \text{ real}, \tag{2.6a}$$

$$\operatorname{Ind} C(e^{i\theta}) = 0, \tag{2.6b}$$

and

$$\sum_{n=-\infty}^{\infty} |c_n| < \infty, \tag{2.6c}$$

then (2.5) has a unique solution satisfying

$$\sum_{n=0}^{\infty} |x_n^{(\infty)}| < \infty. \tag{2.7}$$

More specifically, we have seen that, when $C(e^{i\theta})$ satisfies (2.6), $C(\xi)$ has the unique factorization (IX.3.4) (up to a multiplicative constant), where $P(\xi)$ and $Q(\xi)$ are both analytic for $|\xi| < 1$ and continuous and nonzero for $|\xi| \leq 1$. Furthermore, the function $Y(\xi)$ defined by (IX.1.9) is, in this application, simply

$$Y(\xi) = \sum_{n=0}^{\infty} \xi^n \delta_{n,0} = 1. \tag{2.8}$$

Therefore from (IX.4.13) we immediately find

$$x_n^{(\infty)} = \frac{1}{2\pi i} \oint_{|\xi|=1} d\xi \, \frac{1}{\xi^{n+1}} P(\xi)[Q(\xi^{-1})]_+. \tag{2.9}$$

But, by (IX.3.16),

$$[Q(\xi^{-1})]_+ = Q(0), \tag{2.10}$$

so that

$$x_n^{(\infty)} = \frac{1}{2\pi i} Q(0) \oint_{|\xi|=1} d\xi \, \frac{1}{\xi^{n+1}} P(\xi). \tag{2.11}$$

Since $P(\xi)$ is analytic for $|\xi| < 1$, we find that

$$x_0^{(\infty)} = Q(0)P(0). \tag{2.12}$$

The right-hand side of this expression is easily computed directly in terms of $C(e^{i\theta})$ using the work of Sec. IX.3. From (IX.3.5), if we use the canonical factorization,

$$P(0) = e^{G_+(0)} \tag{2.13}$$

and

$$Q(0) = e^{G_-(\infty)} = 1, \tag{2.14}$$

because $G_-(\xi)$ is a $-$ function and thus vanishes as $\xi \to \infty$. Furthermore, from (IX.3.17b),

$$G_+(0) = -\frac{1}{2\pi} \int_0^{2\pi} d\theta \ln C(e^{i\theta}). \tag{2.15}$$

Thus we have the explicit expression

$$\lim_{N\to\infty} D_N/D_{N+1} = \mu^{-1}, \tag{2.16}$$

where μ is defined by (1.5).

The next fact we would like to establish about D_N is that

$$\lim_{N\to\infty} \frac{D_N}{\mu^N} = \text{const} \neq 0. \tag{2.17}$$

In particular, to obtain (2.17) we assume there is some N_0 such that

$$D_N \neq 0 \qquad \text{for all } N \geq N_0. \tag{2.18}$$

Then

$$\begin{aligned}\lim_{N\to\infty} \frac{D_N}{\mu^N} &= \lim_{N\to\infty} \frac{\mu_{N-1}}{\mu}.\frac{\mu_{N-2}}{\mu}\cdots\frac{\mu_{N_0}}{\mu}\frac{D_{N_0}}{\mu^{N_0}} \\ &= \lim_{N\to\infty} \frac{D_{N_0}}{\mu^{N_0}} \prod_{n=N_0}^{N-1} \frac{\mu_n}{\mu},\end{aligned} \tag{2.19}$$

and the limit of the product in (2.19) exists and is not zero if

$$\sum_{N=N_0}^{\infty} \left| 1 - \frac{\mu}{\mu_N} \right| < \infty. \tag{2.20}$$

Under suitable restrictions on $C(e^{i\theta})$ we will prove in Sec. 3(C) that this series does in fact converge.

The existence of an N_0 such that (2.18) is satisfied will be proved for a suitable class of functions $C(e^{i\theta})$ as corollary 1 in the next section. It should be remarked at this point, however, that the existence of such an N_0 is intimately connected with restrictions (2.6) and in particular (2.6b). For example, consider the simple case $C(e^{i\theta}) = e^{i\theta}$ for which (2.6a) and (2.6c) hold but (2.6b) is violated. The $N \times N$ Toeplitz determinant associated with this function is zero for every N because all the elements in the first row are zero.

(B) Szegö's Theorem

We must now determine the value of $\lim_{N\to\infty} D_N/\mu^N$. Again we shall not do this directly, but instead shall study the dependence of this limiting value on the function $C(\xi)$. For this purpose, consider a second $N \times N$ Toeplitz determinant

$$\bar{D}_N = \begin{vmatrix} \bar{c}_0 & \bar{c}_{-1} & \cdots & \bar{c}_{-N+1} \\ \bar{c}_1 & \bar{c}_0 & \cdots & \bar{c}_{-N+2} \\ \vdots & \vdots & \vdots & \vdots \\ \bar{c}_{N-1} & \bar{c}_{N-2} & \cdots & \bar{c}_0 \end{vmatrix}, \tag{2.21}$$

where

$$\bar{c}_n = \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{-in\theta}\bar{C}(e^{i\theta}). \tag{2.22}$$

We shall choose $\bar{C}(e^{i\theta})$ so that it satisfies not only (2.6) but also

$$\int_0^{2\pi} d\theta \ln \bar{C}(e^{i\theta}) = \int_0^{2\pi} d\theta \ln C(e^{i\theta}), \tag{2.23}$$

and study the ratio $\bar{D}_N/D_N$ for large N. This ratio may be studied by an extension of the previous Wiener-Hopf procedure. If $\bar{D}_N$ is sufficiently simple that it may be explicitly evaluated, the behavior of D_N for large N is thus found.

To begin with we ask the question how D_N and $\bar{D}_N$ are related for large N if

$$\bar{C}(e^{i\theta}) = C(e^{i\theta})(1 - \alpha e^{-i\theta}), \tag{2.24}$$

where $|\alpha| < 1$.

By (1.3), (2.22), and (2.23),

$$\bar{c}_n = c_n - \alpha c_{n+1}, \tag{2.25}$$

so that by (2.21)

$$\bar{D}_N = \begin{vmatrix} c_0-\alpha c_1 & c_{-1}-\alpha c_0 & c_{-2}-\alpha c_{-1} & \cdots & c_{-N+1}-\alpha c_{-N+2} \\ c_1-\alpha c_2 & c_0-\alpha c_1 & c_{-1}-\alpha c_0 & \cdots & c_{-N+2}-\alpha c_{-N+3} \\ c_2-\alpha c_3 & c_1-\alpha c_2 & c_0-\alpha c_1 & \cdots & c_{-N+3}-\alpha c_{-N+4} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ c_{N-1}-\alpha c_N & c_{N-2}-\alpha c_{N-1} & c_{N-3}-\alpha c_{N-2} & \cdots & c_0-\alpha c_1 \end{vmatrix}. \tag{2.26}$$

Accordingly, $\bar{D}_N$ can be expressed as an $(N + 1) \times (N + 1)$ determinant in the form

$$\bar{D}_N = \begin{vmatrix} 1 & \alpha & \alpha^2 & \alpha^3 & \cdots & \alpha^N \\ c_1 & c_0 & c_{-1} & c_{-2} & \cdots & c_{-N+1} \\ c_2 & c_1 & c_0 & c_{-1} & \cdots & c_{-N+2} \\ c_3 & c_2 & c_1 & c_0 & \cdots & c_{-N+3} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ c_N & c_{N-1} & c_{N-2} & c_{N-3} & \cdots & c_0 \end{vmatrix}. \tag{2.27}$$

Define the $N + 1$ quantities $\bar{x}_j^{(N)}$, $0 \le j \le N$, as the solutions of the $N + 1$ simultaneous linear equations

$$\sum_{m=0}^{N} \alpha^m \bar{x}_m^{(N)} = 1 \tag{2.28}$$

and

$$\sum_{m=0}^{N} c_{n-m}\bar{x}_m^{(N)} = 0, \qquad \text{for } 1 \le n \le N. \tag{2.29}$$

Then we use Cramer's rule to find

$$\bar{x}_0^{(N)} = D_N/\bar{D}_N. \tag{2.30}$$

As $N \to \infty$, we assume as before that

$$\bar{x}_0^{(N)} \to \bar{x}_0^{(\infty)}, \tag{2.31}$$

where $\bar{x}_j^{(\infty)}$, $0 \le j$, satisfy

$$\sum_{m=0}^{\infty} \alpha^m \bar{x}_m^{(\infty)} = 1 \tag{2.32}$$

and

$$\sum_{m=0}^{\infty} c_{n-m}\bar{x}_m^{(\infty)} = 0, \qquad \text{for } 1 \le n. \tag{2.33}$$

The precise sense in which (2.31) holds will be discussed in Sec. 3(D).

To solve (2.32) and (2.33), define y_0 by

$$\sum_{m=0}^{\infty} c_{-m}\bar{x}_m^{(\infty)} = y_0. \tag{2.34}$$

Then (2.34) and (2.33) together form a Wiener-Hopf sum equation. Since $C(e^{i\theta})$ satisfies (2.6), it follows from (IX.4.13) that (2.33) and (2.34) have the unique solution

$$\bar{X}^{(\infty)}(\xi) = P(\xi)[Q(\xi^{-1})y_0]_+ = y_0 Q(0)P(\xi), \tag{2.35}$$

where we recall that

$$\bar{X}^{(\infty)}(\xi) = \sum_{n=0}^{\infty} \bar{x}_n^{(\infty)}\xi^n.$$

In order to determine y_0 we note that (2.32) is just

$$\bar{X}^{(\infty)}(\alpha) = 1. \tag{2.36}$$

Accordingly,

$$y_0 Q(0)P(\alpha) = 1, \tag{2.37}$$

and thus

$$\bar{X}^{(\infty)}(\xi) = \frac{P(0)}{P(\alpha)}. \tag{2.38}$$

It then follows from (2.30) and (2.31) that

$$\lim_{N\to\infty} \frac{D_N}{\bar{D}_N} = \frac{P(0)}{P(\alpha)}. \tag{2.39}$$

We now rewrite (2.39) by explicitly computing $P(\xi)$ in terms of $C(e^{i\theta})$ and $\bar{C}(e^{i\theta})$. To do this, recall (1.6) and define similarly

$$\bar{g}_n = \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{-in\theta} \ln \bar{C}(e^{i\theta}). \tag{2.40}$$

Then by (2.24)

$$\bar{g}_n = g_n \qquad \text{for } n \ge 0$$

and

$$\bar{g}_n = g_n + \alpha^{-n}/n \qquad \text{for } n < 0. \tag{2.41}$$

On the other hand, from (IX.3.5*a*) and (IX.3.17*b*),

$$P(\xi) = P(0) \exp\left(-\sum_{l=1}^{\infty} g_l \xi^l\right). \tag{2.42}$$

The substitution of (2.41) and (2.42) in (2.39) gives the desired result

$$\lim_{N\to\infty} \frac{D_N}{\bar{D}_N} = \exp \sum_{l=1}^{\infty} g_l \alpha^l = \exp \sum_{l=1}^{\infty} l(g_{-l} g_l - \bar{g}_{-l} \bar{g}_l). \tag{2.43}$$

We next consider exactly the same problem except that instead of (2.24) we have

$$\bar{C}(e^{i\theta}) = C(e^{i\theta})(1 - \alpha e^{i\theta}). \tag{2.44}$$

In this case we can apply (2.43) to the complex conjugate functions to obtain

$$\lim_{N\to\infty} \frac{D_N^*}{\bar{D}_N^*} = \exp \sum_{l=1}^{\infty} l(g_{-l}^* g_l^* - \bar{g}_{-l}^* \bar{g}_l^*). \tag{2.45}$$

Therefore (2.43) holds for this case as well.

If we use (2.43) a finite number of times, we obtain the following result. Let D_N and $\bar{D}_N^{(n_1, n_2)}$ be two $N \times N$ Toeplitz determinants whose elements are the Fourier coefficients of $C(e^{i\theta})$ and $\bar{C}(e^{i\theta})$ respectively, let $C(e^{i\theta})$ obey (2.6), and let

$$\bar{C}(e^{i\theta}) = C(e^{i\theta}) \prod_{n=1}^{n_1} (1 - \alpha^{(n)} e^{-i\theta}) \prod_{n=1}^{n_2} (1 - \bar{\alpha}^{(n)} e^{i\theta}) \tag{2.46}$$

with all the α's and $\bar{\alpha}$'s less than 1 in magnitude. Then

$$\lim_{N\to\infty} \frac{D_N}{\bar{D}_N^{(n_1,n_2)}} = \exp \sum_{l=1}^{\infty} l(g_{-l} g_l - \bar{g}_{-l}^{(n_1,n_2)} \bar{g}_l^{(n_1,n_2)}). \tag{2.47}$$

Our principal interest lies, however, not in the determinants D_N and $\bar{D}_N^{(n_1,n_2)}$ which are related by (2.46), but rather in the limiting case where

$$\bar{C}(e^{i\theta}) = C(e^{i\theta}) \lim_{n\to\infty} \prod_{j=-n}^{n} (1 - \alpha^{(j)} e^{-i\theta})(1 - \bar{\alpha}^{(j)} e^{i\theta}) \tag{2.48}$$

with all $|\alpha^{(j)}| < 1$ and $|\bar{\alpha}^{(j)}| < 1$. If we call $\bar{D}_N^{(n)}$ the Toeplitz determinant formed from

$$\bar{C}^{(n)}(e^{i\theta}) = C(e^{i\theta}) \prod_{j=-n}^{n} (1 - \alpha^{(j)} e^{-i\theta})(1 - \bar{\alpha}^{(j)} e^{i\theta}), \tag{2.49}$$

then, if we write

$$\lim_{N\to\infty} \frac{D_N}{\bar{D}_N} = \lim_{N\to\infty} \lim_{n\to\infty} \frac{D_N}{\bar{D}_N^{(n)}} \tag{2.50}$$

and interchange the two limiting processes, we may apply (2.47) to obtain

$$\lim_{N\to\infty} \frac{D_N}{\bar{D}_N} = \lim_{n\to\infty} \lim_{N\to\infty} \frac{D_N}{\bar{D}_N^{(n)}} = \lim_{n\to\infty} \exp \sum_{l=1}^{\infty} l(g_{-l}g_l - \bar{g}_{-l}^{(n)}\bar{g}_l^{(n)}). \tag{2.51}$$

If we further assume that

$$\bar{g}_l = \lim_{n\to\infty} \bar{g}_l^{(n)} \tag{2.52}$$

exists and that summation and limit may be interchanged in (2.51), we arrive at the result that when (2.48) holds,

$$\lim_{N\to\infty} \frac{D_N}{\bar{D}_N} = \exp \sum_{l=1}^{\infty} l(g_{-l}g_l - \bar{g}_{-l}\bar{g}_l). \tag{2.53}$$

To get from (2.53) to Szegö's theorem (1.4), we choose $\bar{C}(e^{i\theta})$ to be a constant. Owing to the restriction (2.23), we must take

$$\bar{C}(e^{i\theta}) = \mu. \tag{2.54}$$

With this choice, $\bar{D}_N = \mu^N$, $\bar{g}_l = 0$ for all $l \neq 0$, and (2.53) reduces to (1.4).

To obtain (1.4), we have interchanged several limiting operations. The validity of these interchanges will be studied in the next section.

3. A RIGOROUS PROOF OF SZEGÖ'S THEOREM

(*A*) Historical Introduction

The demonstration of (1.4) in the previous section leads us to suspect that under quite general conditions

$$\ln D_N = N \frac{1}{2\pi} \int_0^{2\pi} d\theta \ln C(e^{i\theta}) + \sum_{n=1}^{\infty} n g_{-n} g_n + o(1) \tag{3.1}$$

as $N \to \infty$. The validity of this expression was first studied by Szegö in 1952. He proved that (3.1) holds if $\phi(\theta) = C(e^{i\theta})$ is real, positive, continuous, and periodic with period 2π, and if $\phi'(\theta)$ exists and satisfies the Lipschitz condition of order ϵ,

$$|\phi'(\theta_1) - \phi'(\theta_2)| \leq K|\theta_1 - \theta_2|^{\epsilon}, \tag{3.2}$$

with $K > 0$ and $\epsilon > 0$. Because of this pioneering work of Szegö, generalizations of this theorem which prove that (3.1) holds under other (less restrictive) hypotheses on $C(e^{i\theta})$ are also referred to as Szegö's theorem.

Szegö's original theorem is not good enough for our purposes because the function $\phi(\theta)$ of (VIII.2.30) is not real except for $\theta = 0$ and π. Various generalizations of Szegö's work to the case of complex $C(e^{i\theta})$ and to the case of functions which do not necessarily satisfy the Lipschitz condition (3.2) have appeared in the mathematical literature. We will not prove the most general of these theorems. On the other hand we wish to avoid giving the reader the false impression that all the conditions which we will impose on $C(e^{i\theta})$ to secure the validity of (3.1) are actually necessary. In fact, necessary and sufficient conditions for the validity of (3.1) are not known. Therefore we mention the following results which are the best that presently exist.

(A) Hirschman[4] proved in 1965 that (3.1) holds when $C(e^{i\theta})$ satisfies the following requirements:

(1′) $\sum_{n=-\infty}^{\infty} |c_n| < \infty$,
(2′) $\sum_{n=-\infty}^{\infty} n|c_n|^2 < \infty$,
(3′) $C(\xi) \neq 0$ for $|\xi| = 1$,

and

(4′) Ind $C(\xi) = 0$.

(B) Devinatz[5] proved in 1967 that (3.1) holds for a slightly wider class of functions. He requires that

(1″) $C(\xi)$ is continuous and nonzero for $|\xi| = 1$,
(2″) $\sum_{n=-\infty}^{\infty} n|c_n|^2 < \infty$,
(3″) Ind $C(\xi) = 0$,
(4″) The function $\sum_{n=-\infty}^{\infty} (\operatorname{sgn} n) c_n e^{in\theta}$ is continuous.

For the purposes of this book there is nothing to be gained by including the extra details needed to prove either Hirschman's or Devinatz's form of Szegö's theorem and we will content ourselves with the following slightly less general version:

Szegö's Theorem. Let $C(e^{i\theta}) = \phi(\theta)$ be such that: (1) $\ln \phi(\theta)$ is continuous and periodic for $0 \leq \theta \leq 2\pi$, and (2) $\phi'(\theta)$ exists and satisfies the Lipschitz condition of order ϵ,

$$|\phi'(\theta_1) - \phi'(\theta_2)| \leq K|\theta_1 - \theta_2|^{\epsilon}, \tag{3.3}$$

where $0 < \epsilon$. Then (1.4) holds.

Our proof will consist of separate demonstrations of the several assumptions made in the previous section.

(B) Proof that $D_N \neq 0$ and that $\lim_{N\to\infty} \mu_N = \mu$

The first assumptions of the previous section which we will prove are (i) that there exists an N_0 such that, for all finite N satisfying $N \geq N_0$, $D_N \neq 0$ [see (2.18)] and (ii) that as $N \to \infty$, $x_0^{(N)} \to x_0^{(\infty)}$ [see (2.4)].

In the case of interest in the previous section $x_0^{(N)}$, $0 \leq n \leq N$, and $x_n^{(\infty)}$, $0 \leq n$, are defined as the solutions of

$$\sum_{m=0}^{N} c_{n-m} x_m^{(N)} = y_n, \qquad 0 \leq n \leq N, \tag{3.4a}$$

and

$$\sum_{m=0}^{\infty} c_{n-m} x_m^{(\infty)} = y_n, \qquad 0 \leq n, \tag{3.4b}$$

with

$$\sum_{m=0}^{\infty} |x_m^{(\infty)}| < \infty \tag{3.5}$$

and

$$y_n = \delta_{n,0}. \tag{3.6}$$

However, for the moment it is convenient to let y_n be arbitrary, subject only to the condition

$$\sum_{n=0}^{\infty} |y_n| < \infty. \tag{3.7}$$

We then will have proved assumption (i) if we can show that if y_n satisfies (3.7) and $C(e^{i\theta})$ satisfies conditions (1) and (2) then (3.4*a*) has a unique solution if N is sufficiently large.

To study the uniqueness of the solution of (3.4*a*) we first prove that the Wiener-Hopf sum equation (3.4*b*) has a unique solution. By the result of Sec. 4 of Chapter IX this uniqueness will follow if we can show that (IX.1.4) is satisfied, that is, that

$$\sum_{n=-\infty}^{\infty} |c_n| < \infty. \tag{3.8}$$

To establish this from assumptions (1) and (2) we first prove the following lemma:

Lemma 1. If $f(\theta)$ satisfies the Lipschitz condition

$$|f(\theta_1) - f(\theta_2)| \leq K|\theta_1 - \theta_2|^{\epsilon}, \tag{3.9}$$

then f_n, the Fourier components of $f(\theta)$, satisfy

$$f_n = O(|n|^{-\epsilon}) \quad \text{as} \quad |n| \to \infty. \tag{3.10}$$

Proof. By definition,

$$f_n = \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-in\theta} f(\theta). \tag{3.11}$$

But if we replace θ by $\theta + \pi/n$ we also have

$$f_n = -\frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-in\theta} f\left(\theta + \frac{\pi}{n}\right). \tag{3.12}$$

Adding these two expressions and dividing by 2 gives

$$f_n = \frac{1}{4\pi} \int_0^{2\pi} d\theta e^{-in\theta} \left[f(\theta) - f\left(\theta + \frac{\pi}{n}\right)\right]. \tag{3.13}$$

Therefore, since $f(\theta)$ obeys (3.9),

$$|f_n| \le \frac{1}{4\pi}\int_0^{2\pi} d\theta \left| f(\theta) - f\left(\theta + \frac{\pi}{n}\right)\right| \le \frac{K}{4\pi}\left|\frac{\pi}{n}\right|^{\epsilon}\int_0^{2\pi} d\theta, \tag{3.14}$$

which proves the lemma.

Lemma 1 and condition (2) guarantee that the Fourier coefficients of $\phi'(\theta)$ are of order $O(|n|^{-\epsilon})$ as $|n| \to \infty$. Therefore the Fourier coefficients of $\phi(\theta)$ are of order $O(|n|^{-1-\epsilon})$ as $|n| \to \infty$ and hence (3.8) is satisfied.

We now may prove a theorem from which the assumptions (i) and (ii) will follow as simple corollaries.

Theorem 1. If y_n are given, if $C(e^{i\theta})$ satisfies conditions (1) and (2), and if $x_n^{(N)}$ satisfies (3.4a), then there is some $K > 0$ and some $N_0 > 0$, both of which may depend on r in such a way that for all $N \ge N_0$

$$\sum_{n=0}^{N} |x_n^{(N)}|^r \le K \sum_{n=0}^{N} |y_n|^r, \quad \text{for any} \quad r \ge 1. \tag{3.15}$$

Proof. For convenience we introduce the following notation. Let f_n be the Fourier coefficients of the function $f(e^{i\theta})$. Then we define

$$\|f\|_r = \left(\sum_{n=-\infty}^{\infty} |f_n|^r\right)^{1/r}. \tag{3.16}$$

This expression will be called an r norm. It has the following two useful properties, which we will often use

(1) Minkowski's inequality,

$$\|f + g\|_r \le \|f\|_r + \|g\|_r. \tag{3.17}$$

The proof of this inequality is well known and will be omitted. The existence of this triangle inequality and the fact that $\|f\|_r = 0$ if and only if $f(e^{i\theta})$ is zero except on a set of measure zero are the reasons that the object defined by (3.16) is entitled to be called a norm.

$$\text{(2) If} \quad \|g\|_1 < \infty, \quad \text{then} \quad \|fg\|_r \le \|f\|_r \|g\|_1. \tag{3.18}$$

This inequality is not so well known as that of Minkowski. However, it follows at once from the well-known Hölder's inequality, which states that if r and s are positive and satisfy

$$\frac{1}{r} + \frac{1}{s} = 1, \tag{3.19}$$

and if $a(e^{i\theta})$ and $b(e^{i\theta})$ are such that

$$\|a\|_r < \infty \quad \text{and} \quad \|b\|_s < \infty, \tag{3.20}$$

then

$$\sum_{k=-\infty}^{\infty} |a_k b_k| \le \left(\sum_{k=-\infty}^{\infty} |a_k|^r\right)^{1/r} \left(\sum_{k=-\infty}^{\infty} |b_k|^s\right)^{1/s}$$
$$= \|a\|_r \|b\|_s. \tag{3.21}$$

Using Hölder's inequality we see that

$$\left|\sum_{l=-\infty}^{\infty} f_l g_{k-l}\right|^r \le \left(\sum_{l=-\infty}^{\infty} |f_l|\,|g_{k-l}|\right)^r$$
$$= \left(\sum_{l=-\infty}^{\infty} |f_l|\,|g_{k-l}|^{1/r}|g_{k-l}|^{1/s}\right)^r$$
$$\le \left(\sum_{l=-\infty}^{\infty} |f_l|^r|g_{k-l}|\right)\left(\sum_{l=-\infty}^{\infty} |g_{k-l}|\right)^{r/s}$$
$$= \left(\sum_{l=-\infty}^{\infty} |f_l|^r|g_{k-l}|\right)\left(\sum_{l=-\infty}^{\infty} |g_l|\right)^{r/s}, \tag{3.22}$$

from which it follows that

$$\|fg\|_r^r = \sum_{k=-\infty}^{\infty}\left|\sum_{l=-\infty}^{\infty} f_l g_{k-l}\right|^r$$
$$\le \left(\sum_{l=-\infty}^{\infty} |g_l|\right)^{r/s} \sum_{k=-\infty}^{\infty}\sum_{l=-\infty}^{\infty} |f_l|^r|g_{k-l}|. \tag{3.23}$$

Therefore, if we invert the order of summation and use (3.19) we obtain

$$\|fg\|_r^r \le \left(\sum_{l=-\infty}^{\infty} |g_l|\right)^r \sum_{k=-\infty}^{\infty} |f_l|^r, \tag{3.24}$$

and hence (3.18) follows.

In addition to these two properties of the r norm we also note the two obvious inequalities

$$\|[f]_+\|_r \le \|f\|_r \tag{3.25a}$$

and

$$\|[f]_-\|_r \le \|f\|_r. \tag{3.25b}$$

We may now prove Theorem 1 by an extension of the Wiener-Hopf technique of the previous section. Define

$$x_n^{(N)} = 0 \qquad \text{if } n < 0 \quad \text{or} \quad n > N, \tag{3.26}$$

$$y_n^{(N)} = \begin{cases} y_n & \text{if } 0 \le n \le N \\ 0 & \text{if } n < 0 \quad \text{or} \quad n > N; \end{cases} \tag{3.27}$$

$$u_n = \begin{cases} \displaystyle\sum_{m=0}^{N} c_{N+n-m} x_m^{(N)} & \text{if } n > 0, \\ 0 & \text{if } n \le 0; \end{cases} \tag{3.28}$$

and

$$v_n = \begin{cases} \sum_{m=0}^{N} c_{-n-m} x_m^{(N)} & \text{if } n > 0, \\ 0 & \text{if } n \le 0. \end{cases} \tag{3.29}$$

We further define

$$X^{(N)}(\xi) = \sum_{n=0}^{N} x_n^{(N)} \xi^n, \tag{3.30}$$

$$Y^{(N)}(\xi) = \sum_{n=0}^{N} y_n \xi^n, \tag{3.31}$$

$$U(\xi) = \sum_{n=1}^{\infty} u_n \xi^n, \tag{3.32}$$

and

$$V(\xi) = \sum_{n=1}^{\infty} v_n \xi^n. \tag{3.33}$$

Then we may Fourier transform (3.4a) and obtain for $|\xi| = 1$

$$C(\xi)X^{(N)}(\xi) = Y^{(N)}(\xi) + U(\xi)\xi^N + V(\xi^{-1}). \tag{3.34}$$

By condition (1), $C(\xi) \neq 0$ for $|\xi| = 1$. Thus we may divide (3.34) by $C(\xi)$, take the r norm, and use (3.17) and (3.18) to obtain

$$\begin{aligned} \|X^{(N)}(\xi)\|_r &= \|[C(\xi)]^{-1}[Y^{(N)}(\xi) + U(\xi)\xi^N + V(\xi^{-1})]\|_r \\ &\le \|[C(\xi)]^{-1}\|_1\{\|Y^{(N)}(\xi)\|_r + \|U(\xi)\xi^N\|_r + \|V(\xi^{-1})\|_r\}. \end{aligned} \tag{3.35}$$

From Lemma 1 we saw that

$$\|C(\xi)\|_1 < \infty, \tag{3.36}$$

so that it follows from conditions (1) and (2) on $C(e^{i\theta})$ and the Wiener-Lévy theorem that

$$\|[C(\xi)]^{-1}\|_1 < \infty. \tag{3.37}$$

Therefore we will have proved Theorem 1 if we can prove that for all sufficiently large N

$$\|U(\xi)\|_r \le \text{const } \|Y^{(N)}(\xi)\|_r \tag{3.38a}$$

and

$$\|V(\xi^{-1})\|_r \le \text{const } \|Y^{(N)}(\xi)\|_r. \tag{3.38b}$$

We obtain the required bounds (3.38) by applying a Wiener-Hopf argument to (3.34). Because $C(e^{i\theta})$ satisfies conditions (1) and (2) it may be factored [see (IX.3.4)] for $|\xi| = 1$ as

$$[C(\xi)]^{-1} = P(\xi)Q(\xi^{-1}), \tag{3.39}$$

where $P(\xi)$ and $Q(\xi)$ are both analytic for $|\xi| < 1$, are continuous and nonzero for $|\xi| \leq 1$, and satisfy

$$\|Q(\xi)\|_1 < \infty \quad \text{and} \quad \|P(\xi)\|_1 < \infty. \tag{3.40}$$

Thus (3.34) may be rewritten when $|\xi| = 1$ to give

$$\begin{aligned}&[P(\xi)]^{-1}X^{(N)}(\xi) - [Q(\xi^{-1})Y^{(N)}(\xi)]_+ - [Q(\xi^{-1})U(\xi)\xi^N]_+ \\ &\qquad = Q(\xi^{-1})V(\xi^{-1}) + [Q(\xi^{-1})Y^{(N)}(\xi)]_- + [Q(\xi^{-1})U(\xi)\xi^N]_-.\end{aligned} \tag{3.41}$$

We apply the Wiener-Hopf argument of Sec. 4 of Chapter IX to this equation by noticing that the left-hand side is analytic inside the unit circle, whereas the right-hand side is analytic outside the unit circle and approaches zero as $\xi \to \infty$. Therefore

$$X^{(N)}(\xi) = P(\xi)\{[Q(\xi^{-1})Y^{(N)}(\xi)]_+ + [Q(\xi^{-1})U(\xi)\xi^N]_+\} \tag{3.42a}$$

and

$$V(\xi^{-1}) = -[Q(\xi^{-1})]^{-1}\{[Q(\xi^{-1})Y^{(N)}(\xi)]_- + [Q(\xi^{-1})U(\xi)\xi^N]_-\}. \tag{3.43a}$$

Not only is $X^{(N)}(\xi)$ a + function but so also is $\xi^N X^{(N)}(\xi^{-1})$. Therefore, we may replace ξ by ξ^{-1} in (3.34), multiply by ξ^N, and apply an argument similar to the foregoing to find

$$\xi^N X^{(N)}(\xi^{-1}) = Q(\xi)\{[P(\xi^{-1})Y^{(N)}(\xi^{-1})\xi^N]_+ + [P(\xi^{-1})V(\xi)\xi^N]_+\} \tag{3.42b}$$

and

$$U(\xi^{-1}) = -[P(\xi^{-1})]^{-1}\{[P(\xi^{-1})Y^{(N)}(\xi^{-1})\xi^N]_- + [P(\xi^{-1})V(\xi)\xi^N]_-\}. \tag{3.43b}$$

To proceed further we take the r norm of (3.43) and find

$$\|V(\xi^{-1})\|_r \leq K_1\|Y^{(N)}(\xi)\|_r + K_2\|[Q(\xi^{-1})U(\xi)\xi^N]_-\|_r \tag{3.44a}$$

and

$$\|U(\xi^{-1})\|_r \leq K_3\|Y^{(N)}(\xi)\|_r + K_4\|[P(\xi^{-1})V(\xi)\xi^N]_-\|_r. \tag{3.44b}$$

Define $S_N(f)$, the Nth partial sum of the Fourier series of the function f, by

$$S_N(f) = \sum_{n=-N}^{N} f_n e^{in\theta}. \tag{3.45}$$

From (3.40) we conclude that the Fourier series for $P(e^{i\theta})$ is absolutely and uniformly convergent. Therefore, given an $\bar{\epsilon}$ [unrelated to the ϵ of condition (2)], there exists an N_0 such that, for all $N \geq N_0$,

$$\|P(e^{i\theta}) - S_N[P(e^{i\theta})]\|_1 < \bar{\epsilon} \tag{3.46a}$$

and

$$\|Q(e^{i\theta}) - S_N[Q(e^{i\theta})]\|_1 \leq \bar{\epsilon}. \tag{3.46b}$$

Then, since

$$[S_N(P(\xi^{-1}))V(\xi)\xi^N]_- = 0 \tag{3.47a}$$

and

$$[S_N(Q(\xi^{-1}))U(\xi)\xi^N]_- = 0, \tag{3.47b}$$

we may use (3.18) and (3.46) to rewrite (3.44) when $N \geq N_0$ as

$$\|V(\xi)\|_r \leq K_1\|Y^{(N)}(\xi)\|_r + K_2\bar{\epsilon}\|U(\xi)\|_r \tag{3.48a}$$

and

$$\|U(\xi)\|_r \leq K_3\|Y^{(N)}(\xi)\|_r + K_4\bar{\epsilon}\|V(\xi)\|_r. \tag{3.48b}$$

But since K_1, K_2, K_3, and K_4 are positive numbers independent of $\bar{\epsilon}$, $\bar{\epsilon}$ may be chosen so small that

$$1 - K_2K_4\bar{\epsilon}^2 > 0. \tag{3.49}$$

Therefore we may solve the simultaneous inequalities (3.48) to obtain the desired inequalities (3.38), which completes the proof of the theorem.

The proof of assumption (i) now follows as a simple corollary of Theorem 1.

Corollary 1. If $C(e^{i\theta})$ satisfies conditions (1) and (2), then there exists an N_0 such that, for every finite N satisfying $N \geq N_0$, $D_N \neq 0$.

Proof: If $D_{N+1} = 0$ there exists a solution $x_n^{(N)}$ to the set of equations (3.4*a*) with $y_n = 0$ for $0 \leq n \leq N$ such that

$$0 < \sum_{n=0}^{N} |x_n^{(N)}|^r \leq K \sum_{n=0}^{N} |y_n|^r = 0, \tag{3.50}$$

which is a contradiction. Hence the corollary follows.

Corollary 1 guarantees that the ratios $D_{N+1}/D_N = \mu_N$ exist for all sufficiently large N. Therefore we may proceed to prove that $\lim_{N\to\infty} \mu_N = \mu$. We first prove

Theorem 2. If $x_n^{(N)}$, $0 \leq n \leq N$, satisfies (3.4*a*), $x_n^{(\infty)}$, $0 \leq n$, satisfies (3.4*b*), and $C(e^{i\theta})$ satisfies conditions (1) and (2), then for all $r \geq 1$

$$\sum_{n=0}^{N} |x_n^{(\infty)} - x_n^{(N)}|^r \leq \text{const} \sum_{n=N+1}^{\infty} |x_n^{(\infty)}|^r. \tag{3.51}$$

Proof: We combine (3.4*a*) and (3.4*b*) as

$$\sum_{m=0}^{N} c_{n-m}(x_m^{(N)} - x_m^{(\infty)}) = \sum_{m=N+1}^{\infty} c_{n-m}x_m^{(\infty)} \qquad \text{for } 0 \leq n \leq N. \tag{3.52}$$

But this is again an equation of the form (3.4*a*) with $x_m^{(N)}$ replaced by

$x_m^{(N)} - x_m^{(\infty)}$ and y_n by $\sum_{m=N+1}^{\infty} c_{n-m}x_m^{(\infty)}$. Therefore we may apply Theorem 1 to (3.52) to find

$$\begin{aligned}\left(\sum_{n=0}^{N} |x_n^{(N)} - x_n^{(\infty)}|^r\right)^{1/r} &\leq K\left(\sum_{n=0}^{N} \left|\sum_{m=N+1}^{\infty} c_{n-m}x_m^{(\infty)}\right|^r\right)^{1/r} \\ &\leq K\left(\sum_{n=-\infty}^{\infty} \left|\sum_{m=N+1}^{\infty} c_{n-m}x_m^{(\infty)}\right|^r\right)^{1/r} \\ &= K\|C(\xi)\{X^{(\infty)}(\xi) - S_N[X^{(\infty)}(\xi)]\}\|_r \\ &\leq K\|C(\xi)\|_1\|X^{(\infty)}(\xi) - S_N[X^{(\infty)}(\xi)]\|_r \\ &= K\|C(\xi)\|_1\left(\sum_{n=N+1}^{\infty} |x_n^{(\infty)}|^r\right)^{1/r},\end{aligned} \tag{3.53}$$

which establishes the theorem.

The proof of assumption (ii) now follows as a simple consequence of this theorem if we consider the special case $y_n = \delta_{n,0}$. Then we instantly find from Theorem 2 that for any $r \geq 1$

$$|1 - x_0^{(N)}/x_0^{(\infty)}| \leq \text{const}\left(\sum_{n=N+1}^{\infty} |x_n^{(\infty)}|^r\right)^{1/r}. \tag{3.54}$$

But from (2.3) we recall that $x_0^{(N)} = \mu_N^{-1}$ and from (2.12), (2.15), and (1.5) that $x_0^{(\infty)} = \mu^{-1}$. Furthermore, Sec. 4 of Chapter IX guarantees that $\sum_{n=0}^{\infty} |x_n^{(\infty)}| < \infty$, so the right-hand side of (3.54) vanishes as $N \to \infty$. Thus we have established that

$$\lim_{N\to\infty} \mu_N = \mu. \tag{3.55}$$

(*C*) Proof that $\sum_{N=N_0}^{\infty} |1 - \mu/\mu_N| < \infty$

The next assumption of the previous section which must be proved is (2.20), namely, that if $C(e^{i\theta})$ satisfies conditions (1) and (2) and N_0 is such that $D_N \neq 0$ for $N \geq N_0$ then

$$\sum_{N=N_0}^{\infty} \left|1 - \frac{\mu}{\mu_N}\right| < \infty. \tag{3.56}$$

As seen in (2.19), this statement guarantees the existence of $\lim_{N\to\infty} D_N/\mu^N$. Furthermore, from (3.56) we immediately obtain the weaker statement that, as $N \to \infty$,

$$\mu_N = \mu + o(N^{-1}). \tag{3.57}$$

Therefore,

$$\ln(\mu/\mu_N) = o(N^{-1}) \tag{3.58}$$

and hence we may use

$$(\mu/\mu_N)^N = e^{N\ln(\mu/\mu_N)} \tag{3.59}$$

to conclude that

$$\lim_{N\to\infty} (\mu/\mu_N)^N = 1. \tag{3.60}$$

Thus, combining (2.17) and (3.60), we have

$$\lim_{N\to\infty} \frac{D_N}{\mu^N} = \lim_{N\to\infty} \frac{D_N}{\mu_N^N} = \text{const.} \tag{3.61}$$

This fact will be needed in subsection (D).

We establish (3.56) by using the bound on $|1 - \mu/\mu_N|$ given by (3.54) in conjunction with the expression (2.11) for $x_n^{(\infty)}$ and the Lipschitz condition (3.3). To do this we establish the following theorem due to Privalov:

Theorem 3 (Privalov's). If $f(x)$ satisfies a Lipschitz condition of order ϵ, where $0 < \epsilon < 1$, that is, if

$$|f(x + h) - f(x)| \leq K|h|^\epsilon, \qquad -\pi \leq x \leq \pi, \tag{3.62}$$

then the function

$$\bar{f}(x) = -\frac{1}{\pi}\int_{-\pi}^{\pi} dt\, \frac{f(x + t) - f(x)}{2\tan t/2} \tag{3.63}$$

also satisfies a Lipschitz condition of the same order.

Proof.[6] We must show that there is some K' such that

$$|\bar{f}(x + h) - \bar{f}(x)| \leq K'|h|^\epsilon, \tag{3.64}$$

where $\bar{f}(x)$ is given by (3.63) and

$$\bar{f}(x + h) = -\frac{1}{\pi}\int_{-\pi}^{\pi} dt\, \frac{f(x + t) - f(x + h)}{2\tan (t - h)/2}. \tag{3.65}$$

Consider $h > 0$ (since the proof for $h < 0$ is identical). We first show that if in the integrals of (3.63) and (3.65) the integration is carried out over the interval $(-2h, 2h)$ then the integrals are of the order $O(h^\epsilon)$. This follows for (3.63) since

$$\left|\frac{f(x + t) - f(x)}{2\tan t/2}\right| \leq \frac{K|t|^\epsilon}{|t|} \leq K|t|^{\epsilon-1}, \tag{3.66}$$

so that

$$\left|\int_{-2h}^{2h} dt\, \frac{f(x + t) - f(x)}{2\tan t/2}\right| \leq 2K\int_0^{2h} dt t^{\epsilon-1} = O(h^\epsilon). \tag{3.67}$$

6. This proof is taken from N. K. Bary, *A Treatise on Trigonometric Series* (Macmillan, New York, 1964), vol. 2, pp. 99–103.

The same argument applies to (3.65) if we let $t - h = u$. Therefore

$$\bar{f}(x) = -\frac{1}{\pi}\left[\int_{-\pi}^{-2h} dt\,\frac{f(x+t) - f(x)}{2\tan t/2} + \int_{2h}^{\pi} dt\,\frac{f(x+t) - f(x)}{2\tan t/2}\right] + O(h^{\epsilon}) \quad (3.68a)$$

and

$$\bar{f}(x+h) = -\frac{1}{\pi}\left[\int_{-\pi}^{-2h} dt\,\frac{f(x+t) - f(x+h)}{2\tan(t-h)/2}\right.$$
$$\left. + \int_{2h}^{\pi} dt\,\frac{f(x+t) - f(x+h)}{2\tan(t-h)/2}\right] + O(h^{\epsilon}). \quad (3.68b)$$

Furthermore, we may write

$$\frac{f(x+t) - f(x)}{2\tan t/2} - \frac{f(x+t) - f(x+h)}{2\tan(t-h)/2}$$
$$= [f(x+t) - f(x)]\left[\frac{1}{2\tan t/2} - \frac{1}{2\tan(t-h)/2}\right]$$
$$+ [f(x+h) - f(x)]\,\frac{1}{2\tan(t-h)/2}. \quad (3.69)$$

Thus we find

$$\bar{f}(x+h) - \bar{f}(x) = I_1 + I_2 + O(h^{\epsilon}), \quad (3.70)$$

where

$$I_1 = -\frac{1}{\pi}\left(\int_{-\pi}^{-2h} + \int_{2h}^{\pi}\right) dt[f(x+t) - f(x)]\left[\frac{1}{2\tan t/2} - \frac{1}{2\tan(t-h)/2}\right] \quad (3.71a)$$

and

$$I_2 = -[f(x+h) - f(x)]\,\frac{1}{\pi}\left(\int_{-\pi}^{-2h} + \int_{2h}^{\pi}\right)\frac{dt}{2\tan(t-h)/2}. \quad (3.71b)$$

We estimate I_1 by noting that

$$\frac{1}{2\tan t/2} - \frac{1}{2\tan(t-h)/2} = -\frac{1}{2}\,\frac{\sin h/2}{\sin t/2\,\sin(t-h)/2} \quad (3.72)$$

and that for $|t| \geq 2h$ we have

$$|(t-h)/2| \geq |t|/4. \quad (3.73)$$

Therefore, recalling that $\epsilon < 1$,

$$\left|\int_{2h}^{\pi} dt[f(x+t) - f(x)]\left[\frac{1}{2\tan t/2} - \frac{1}{2\tan(t-h)/2}\right]\right| \leq 4K\int_{2h}^{\pi} dt\,|t|^{\epsilon}\,\frac{h}{t^2}$$
$$= O(h^{\epsilon}). \quad (3.74)$$

A similar estimate holds for the integral from $-\pi$ to $-2h$. Therefore

$$|I_1| = O(h^\epsilon). \tag{3.75}$$

Finally we estimate I_2 by remarking that

$$\begin{aligned}\left(\int_{-\pi}^{-2h} + \int_{2h}^{\pi}\right)\frac{dt}{2\tan(t-h)/2} &= \int_{2h}^{\pi} dt\left(\frac{1}{\tan(t-h)/2} - \frac{1}{\tan(t+h)/2}\right)\\ &= \int_{2h}^{\pi} dt\,\frac{\sin h}{\sin(t-h)/2\sin(t+h)/2}\\ &= O(h)\int_{2h}^{\pi}\frac{dt}{t^2}\\ &= O(1),\end{aligned} \tag{3.76}$$

where we have used relations similar to (3.72) and (3.73). Therefore, since $f(x)$ obeys (3.62), we obtain

$$|I_2| = O(h^\epsilon). \tag{3.77}$$

Combining (3.70), (3.77), and (3.75) completes the proof of the theorem, that is,

$$|\bar{f}(x+h) - \bar{f}(x)| \le K'|h|^\epsilon. \tag{3.78}$$

The following lemma is now a simple consequence of Privalov's theorem.

Lemma 2. If $\ln\phi(\theta)$ is continuous and periodic for $0 \le \theta \le 2\pi$, if $\phi'(\theta)$ exists and satisfies the Lipschitz condition (3.3), and if

$$\phi(\theta)^{-1} = P(e^{i\theta})Q(e^{-i\theta}), \tag{3.79}$$

where $P(e^{i\theta})$ and $Q(e^{i\theta})$ are + functions that are nonzero for $|e^{i\theta}| \le 1$, then as $n \to \infty$

$$p_n = O(n^{-1-\epsilon}) \quad\text{and}\quad q_n = O(n^{-1-\epsilon}), \tag{3.80}$$

where p_n and q_n are the Fourier coefficients of $P(e^{i\theta})$ and $Q(e^{i\theta})$.

Proof. We consider only p_n, since the proof for q_n is identical. From (IX.3.5) and (IX.3.17) we see that, for $|\xi| < 1$,

$$\ln P(\xi) = -\frac{1}{2\pi i}\oint_{|\xi'|=1} d\xi'\,\frac{\ln C(\xi')}{\xi' - \xi} \tag{3.81}$$

where, if $|\xi| = 1$, (3.81) holds in the sense of a limit as $\xi \to 1$ from inside the unit circle $|\xi| = 1$. Letting $\xi = e^{i\theta}$ for $-\pi \le \theta \le \pi$, we may rewrite (3.81) as

$$\ln P(e^{i\theta}) = -\ln\phi(\theta) - \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta'\,\frac{\ln\phi(\theta'+\theta) - \ln\phi(\theta)}{1 - e^{-i\theta'}}. \tag{3.82}$$

Therefore, if we note that

$$\frac{1}{1 - e^{-i\theta'}} - \frac{1}{2} = \frac{-i}{2 \tan \theta'/2}, \tag{3.83}$$

we obtain

$$\ln P(e^{i\theta}) = -\frac{1}{2}\left[\ln \phi(\theta) + \frac{1}{4\pi}\int_{-\pi}^{\pi} d\theta' \ln \phi(\theta') - \frac{i}{\pi}\int_{-\pi}^{\pi} d\theta' \times \frac{\ln \phi(\theta' + \theta) - \ln \phi(\theta)}{2 \tan \theta'/2}\right]. \tag{3.84}$$

The last integral is of the type considered in Privalov's theorem.

In order to apply the Lipschitz condition (3.3) to (3.84) we differentiate with respect to θ to find

$$\frac{1}{P(e^{i\theta})}\frac{\partial P(e^{i\theta})}{\partial \theta} = -\frac{1}{2}\left[\frac{\phi'(\theta)}{\phi(\theta)} - \frac{i}{\pi}\int_{-\pi}^{\pi} d\theta' \frac{\phi'(\theta' + \theta)/\phi(\theta' + \theta) - \phi'(\theta)/\phi(\theta)}{2 \tan \theta'/2}\right]. \tag{3.85}$$

To obtain (3.85) we have interchanged the order of differentiation and integration. However, since $\phi(\theta) \neq 0$ and $\phi'(\theta)$ satisfies (3.3), $\phi'(\theta)/\phi(\theta)$ also satisfies (3.3) with $\epsilon > 0$. Therefore, Privalov's theorem implies that the integral in (3.85) is a continuous function of θ. Furthermore, since $\phi'(\theta)/\phi(\theta)$ satisfies (3.3), the integrand in (3.85) is integrable with respect to θ for $-\pi \leq \theta \leq \pi$ and also the double integral with respect to θ and θ' exists. Therefore, (3.85) holds.

But Privalov's theorem does more than just guarantee that (3.85) is valid. It guarantees that the right-hand side of (3.85) satisfies a Lipschitz condition of order $0 < \epsilon < 1$.

However, the fact that $P(e^{i\theta})^{-1}(\partial P(e^{i\theta})/\partial\theta)$ satisfies a Lipschitz condition with $0 < \epsilon$ guarantees that $\partial P(e^{i\theta})/\partial\theta$ exists for $0 \leq \theta \leq 2\pi$. Therefore, $P(e^{i\theta})$ must obey a Lipschitz condition with $\epsilon = 1$, so we conclude that

$$\left|\frac{\partial P(e^{i\theta_1})}{\partial \theta_1} - \frac{\partial P(e^{i\theta_2})}{\partial \theta_2}\right| \leq K|\theta_1 - \theta_2|^{\epsilon}. \tag{3.86}$$

But

$$\frac{\partial P(e^{i\theta})}{\partial \theta} = i \sum_{n=1}^{\infty} n p_n e^{in\theta}, \tag{3.87}$$

so that we may use Lemma 1 to conclude that, as $n \to \infty$,

$$n p_n = O(n^{-\epsilon}). \tag{3.88}$$

Similarly,

$$n q_n = O(n^{-\epsilon}). \tag{3.89}$$

Therefore Lemma 2 is established.

It is now a simple matter to prove that conditions (1) and (2) guarantee that (3.56) holds where N_0 is the number whose existence is guaranteed by Corollary 1. From (3.54),

$$|\mu - \mu_N| \leq \text{const} \left(\sum_{n=N+1}^{\infty} |x_n^{(\infty)}|^r \right)^{1/r}. \tag{3.90}$$

But (2.11) and Lemma 2 show that

$$x_n^{(\infty)} = O(n^{-1-\epsilon}) \quad \text{as} \quad n \to \infty. \tag{3.91}$$

But

$$|\mu - \mu_N| \leq \text{const}\, N^{-1-\epsilon/2} \left(\sum_{n=N+1}^{\infty} |n^{1+\epsilon/2} x_n^{(\infty)}|^r \right)^{1/r}, \tag{3.92}$$

and, since $\epsilon > 0$, r may be chosen larger than $2/\epsilon$, so that

$$\sum_{n=N_0}^{\infty} |n^{1+\epsilon/2} x_n^{(\infty)}|^r < \infty. \tag{3.93}$$

Therefore we find that

$$|\mu - \mu_N| = O(N^{-1-\epsilon/2}) \tag{3.94}$$

and the convergence of $\sum_{N=N_0}^{\infty} |1 - \mu/\mu_N|$ follows.

(*D*) Proof that $\lim_{N\to\infty} D_N/\mu^N = \exp \sum_{n=1}^{\infty} n g_{-n} g_n$

We now turn to the proof of the fact that conditions (1) and (2) not only guarantee the existence of $\lim_{N\to\infty} D_N/\mu^N$ but are also sufficient to guarantee the more precise statement that

$$\lim_{N\to\infty} \frac{D_N}{\mu^N} = \sum_{n=1}^{\infty} n g_{-n} g_n. \tag{3.95}$$

To begin with, we remark that conditions (1) and (2) guarantee that the infinite series on the right-hand side of (3.95) converges. We do this by first proving

Lemma 3. If $\ln f(\theta)$ is continuous and periodic for $0 \leq \theta \leq 2\pi$ and if $f'(\theta)$ obeys the Lipschitz condition (3.3), then, as $|n| \to \infty$,

$$\frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-in\theta} \ln f(\theta) = O(|n|^{-1-\epsilon}). \tag{3.96}$$

Proof. Integrating by parts we have

$$\frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-in\theta} \ln f(\theta) = \frac{1}{2\pi i n} \int_0^{2\pi} d\theta e^{-in\theta} \frac{f'(\theta)}{f(\theta)}. \tag{3.97}$$

But $f'(\theta)$ satisfies the Lipschitz condition (3.3) and $f(\theta) \neq 0$, so $f'(\theta)/f(\theta)$

also satisfies (3.3). Hence we apply Lemma 1 to $f'(\theta)/f(\theta)$ and conclude that, as $|n| \to \infty$,

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta e^{-in\theta} \ln f(\theta) = n^{-1}O(|n|^{-\epsilon}) = O(|n|^{-1-\epsilon}), \tag{3.98}$$

which proves the lemma.

In the case of interest we note that, since by hypothesis the function $\phi(\theta)$ satisfies the Lipschitz condition (3.3), Lemma 3 guarantees that

$$g_n = O(|n|^{-1-\epsilon}) \quad \text{as} \quad |n| \to \infty. \tag{3.99}$$

Therefore the convergence of the series in (3.95) follows.

Now that we have proved that conditions (1) and (2) are sufficient to guarantee that both sides of (3.95) exist, we turn to the proof that these conditions are also sufficient to guarantee that the two sides of (3.95) are equal. To construct such a proof we first prove

Theorem 4. If $C(e^{i\theta})$ satisfies conditions (1) and (2), then for all sufficiently large N there exists a polynomial of the Nth degree,

$$B^{(N)}(e^{i\theta}) = \prod_{n=1}^{N} (1 - \bar{\alpha}_N^{(n)} e^{i\theta}), \tag{3.100}$$

where

$$|\bar{\alpha}_N^{(n)}| < 1, \qquad 1 \le n \le N, \tag{3.101}$$

such that

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta e^{-ik\theta} C(e^{i\theta}) B^{(N)}(e^{i\theta}) = \mu_N \, \delta_{k,0} \qquad \text{for } 0 \le k \le N. \tag{3.102}$$

Proof. Denote by $B_n^{(N)}$ the Fourier coefficients of $B^{(N)}(e^{i\theta})$. Then (3.102) may be rewritten as

$$\sum_{m=0}^{N} c_{k-m} B_m^{(N)} = \mu_N \, \delta_{k,0}. \tag{3.103}$$

This equation has a unique solution if $D_{N+1} \neq 0$ and, since $C(e^{i\theta})$ satisfies conditions (1) and (2), Corollary 1 guarantees that $D_{N+1} \neq 0$ for all sufficiently large N. Indeed, $\mu_N^{-1} B_m^{(N)}$ satisfies precisely the same set of equations (2.1) as does $x_m^{(N)}$. Therefore, at least for all sufficiently large N,

$$B_m^{(N)} = \mu_N x_m^{(N)}. \tag{3.104}$$

In particular, since from (2.3) $x_0^{(N)} = \mu_N^{-1}$,

$$B_0^{(N)} = 1. \tag{3.105}$$

Moreover, if we use (3.104) and (2.11) in (3.51) we see that, as $N \to \infty$,

$$\sum_{n=0}^{N} |B_n^{(N)} - \mu_N p_n| \le \text{const} \sum_{n=N+1}^{\infty} |p_n| \to 0. \tag{3.106}$$

Therefore $B^{(N)}(\xi)$ converges uniformly to $\mu_N P(\xi)$ when $|\xi| \leq 1$. But $P(\xi)$ has no zeroes for $|\xi| \leq 1$. Thus, for sufficiently large N, $B^{(N)}(\xi)$ has no zeroes for $|\xi| \leq 1$ and Theorem 4 follows.

In a manner identical to the proof of Theorem 4 we also establish that for sufficiently large N there exists a polynomial of the Nth degree,

$$\tilde{B}^{(N)}(e^{-i\theta}) = \prod_{n=1}^{N} (1 - \alpha_N^{(n)} e^{-i\theta}), \tag{3.107}$$

where

$$|\alpha_N^{(n)}| < 1, \qquad 1 \leq n \leq N,$$

such that

$$\frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-ik\theta} C(e^{i\theta}) \tilde{B}^{(N)}(e^{-i\theta}) = \mu_N \delta_{k,0} \qquad \text{for } -N \leq k \leq 0. \tag{3.108}$$

We now may consider the $(N + 1) \times (N + 1)$ Toeplitz determinant $\bar{D}_{N+1}^{(N)}$ formed from

$$\bar{C}^{(N)}(e^{i\theta}) = \frac{\mu_N}{B^{(N)}(e^{i\theta}) \tilde{B}^{(N)}(e^{-i\theta})}. \tag{3.109}$$

The significance of $\bar{C}^{(N)}(e^{i\theta})$ is twofold. First of all, as we will shortly see, $\bar{D}_{N+1}^{(N)}$ may be exactly computed in terms of $B^{(N)}$ and $\tilde{B}^{(N)}$. Secondly we have

Theorem 5. If $C(e^{i\theta})$ satisfies conditions (1) and (2), and if $-N \leq k \leq N$, then

$$\frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-ik\theta} \left[C(e^{i\theta}) - \frac{\mu_N}{B^{(N)}(e^{i\theta}) \tilde{B}^{(N)}(e^{-i\theta})} \right] = 0. \tag{3.110}$$

Proof. Denote the left-hand side of (3.110) by f_k and consider the $2(N + 1)$ equations

$$\sum_{k=-N}^{N} B_{l-k}^{(N)} f_k = y_l, \qquad 0 \leq l \leq N, \tag{3.111a}$$

and

$$\sum_{k=-N}^{N} \tilde{B}_{l-k}^{(N)} f_k = \tilde{y}_l, \qquad -N \leq l \leq 0. \tag{3.111b}$$

Since $\tilde{B}^{(N)}(e^{i\theta})$ and $B^{(N)}(e^{i\theta})$ are each polynomials in $e^{i\theta}$ of degree N, we may extend the range of summation from $-\infty$ to ∞. Thus we find

$$y_l = \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-il\theta} \left[B^{(N)}(e^{i\theta}) C(e^{i\theta}) - \frac{\mu_N}{\tilde{B}^{(N)}(e^{-i\theta})} \right] \qquad \text{for } 0 \leq l \leq N \tag{3.112a}$$

and

$$\tilde{y}_l = \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{-il\theta}\left[\tilde{B}^{(N)}(e^{-i\theta})C(e^{i\theta}) - \frac{\mu_N}{B^{(N)}(e^{i\theta})}\right] \qquad \text{for } -N \le l \le 0, \quad (3.112b)$$

and, if we use the equations (3.102) and (3.108), which define $B^{(N)}(e^{i\theta})$ and $\tilde{B}^{(N)}(e^{i\theta})$, we find

$$\sum_{k=-N}^{N} B_{l-k}^{(N)} f_k = y_l = 0 \qquad \text{for } 0 \le l \le N \quad (3.113a)$$

and

$$\sum_{k=-N}^{N} \tilde{B}_{l-k}^{(N)} f_k = \tilde{y}_l = 0 \qquad \text{if } -N \le l \le 0. \quad (3.113b)$$

Therefore, the scalar products of the vector $\{f_k^*\}$ with the $N + 1$ vectors, $0 \le l \le N$,

$$[B_l^{(N)}]_k = \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{ik\theta}[e^{-il\theta}B^{(N)}(e^{i\theta})] \quad (3.114a)$$

and the $N + 1$ vectors, $-N \le l \le 0$,

$$[\tilde{B}_l^{(N)}]_k = \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{-ik\theta}[e^{il\theta}\tilde{B}^{(N)}(e^{-i\theta})] \quad (3.114b)$$

vanish. This implies that f_k vanishes for $-N \le k \le N$ if we can prove that these $2(N + 1)$ vectors span the $2N + 1$-dimensional space spanned by $e^{ik\theta}$ with $-N \le k \le N$.

Clearly $2(N + 1)$ vectors in a space of $2N + 1$ dimensions cannot be linearly independent. Therefore there must exist at least one set of numbers h_l and $\tilde{h}_l$, $0 \le l \le N$, such that

$$0 = \sum_{l=0}^{N} h_l e^{-il\theta}B^{(N)}(e^{i\theta}) - \sum_{l=0}^{N} \tilde{h}_l e^{il\theta}\tilde{B}^{(N)}(e^{-i\theta}), \quad (3.115)$$

where at least one $h_l \neq 0$ or $\tilde{h}_l \neq 0$. To prove our theorem it suffices to prove that up to a multiplicative constant there is only one set of h_l and $\tilde{h}_l$ which satisfies (3.115). But (3.115) may be rewritten as

$$\frac{B^{(N)}(e^{i\theta})}{\tilde{B}^{(N)}(e^{-i\theta})} = \frac{\sum_{l=0}^{N} \tilde{h}_l e^{il\theta}}{\sum_{l=0}^{N} h_l e^{-il\theta}}, \quad (3.116)$$

and hence, since $B^{(N)}(0) = \tilde{B}^{(N)}(0) = 1$ and $B^{(N)}(e^{i\theta})$ and $\tilde{B}^{(N)}(e^{-i\theta})$ have no common factors, we conclude that h_l and $\tilde{h}_l$ are uniquely determined up to a common multiplicative constant from

$$B^{(N)}(e^{i\theta}) = \sum_{l=0}^{N} \tilde{h}_l e^{il\theta} \quad (3.117a)$$

and

$$\tilde{B}^{(N)}(e^{i\theta}) = \sum_{l=0}^{N} h_l e^{-il\theta}. \tag{3.117b}$$

Therefore Theorem 5 holds.

The importance of Theorem 5 is that it immediately implies that if $\bar{C}^{(N-1)}(e^{i\theta})$ is determined from (3.109) then we have the exact relation

$$\bar{D}_N^{(N-1)} = D_N, \tag{3.118}$$

where $\bar{D}_N^{(N-1)}$ is the $N \times N$ Toeplitz determinant formed from $\bar{C}^{(N-1)}(e^{i\theta})$. But on the other hand we may exactly evaluate $\bar{D}_N^{(N-1)}$ by combining the Wiener-Hopf computation of Sec. 2(*B*) with Theorem 2. Consider

$$\bar{\bar{C}}_{(1)}^{(N-1)}(e^{i\theta}) = (1 - \bar{\alpha}_{N-1}^{(1)} e^{i\theta})\bar{C}^{(N-1)}(e^{i\theta}). \tag{3.119}$$

Then if we let $\bar{\bar{D}}_{(1)N}^{(N-1)}$ be the $N \times N$ Toeplitz determinant formed from $\bar{\bar{C}}_{(1)}^{(N-1)}$ we know from (2.30) that

$$\bar{D}_N^{(N-1)}/\bar{\bar{D}}_{(1)N}^{(N-1)} = \bar{x}_0^{(N-1)}, \tag{3.120}$$

where

$$\sum_{m=0}^{N-1} \bar{c}_{n-m}^{(N-1)} \bar{x}_m^{(N-1)} = 0, \qquad 1 \le n \le N-1, \tag{3.121a}$$

and

$$\sum_{m=0}^{N-1} \bar{\alpha}_{N-1}^{(1)m} \bar{x}_m^{(N-1)} = 1. \tag{3.121b}$$

In Sec. 2 we assumed that $\lim_{N\to\infty} \bar{x}_n^{(N-1)} = \bar{x}_n^{(\infty)}$, where

$$\sum_{m=0}^{\infty} \bar{c}_{n-m}^{(N-1)} \bar{x}_m^{(\infty)} = y_0 \delta_{n,0}, \qquad 0 \le n \le N-1, \tag{3.122}$$

and y_0 is determined from the requirement

$$\sum_{m=0}^{\infty} \bar{\alpha}_{N-1}^{(1)m} \bar{x}_m^{(\infty)} = 1. \tag{3.123}$$

We now know from Theorem 2 that

$$\sum_{n=0}^{N-1} |\bar{x}_n^{(\infty)} - \bar{x}_n^{(N-1)}| \le \text{const} \sum_{n=N}^{\infty} |\bar{x}_n^{(\infty)}|. \tag{3.124}$$

and further we know from (2.35) that

$$\bar{X}^{(\infty)}(\xi) = y_0 Q(0) P(\xi). \tag{3.125}$$

But from the definition of $\bar{C}^{(N-1)}(e^{i\theta})$ in (3.109) we see that

$$P(e^{i\theta}) = \mu_N^{-1} B^{(N-1)}(e^{i\theta}), \tag{3.126}$$

where $B^{(N-1)}(e^{i\theta})$ is a polynomial of degree no higher than $N-1$. Therefore

$$\bar{x}_n^{(\infty)} = 0 \qquad \text{if } n \geq N, \tag{3.127}$$

and so we conclude from (3.124) that for this special case

$$\bar{x}_n^{(\infty)} = \bar{x}_n^{(N-1)}. \tag{3.128}$$

Thus the derivation of (2.43) given in the previous section may be carried out except that instead of $\lim_{N\to\infty} \bar{D}_N^{(N-1)}/\bar{\bar{D}}_{(1)N}^{(N-1)}$ the result holds exactly for $\bar{D}_N^{(N-1)}/\bar{\bar{D}}_{(1)N}^{(N-1)}$. Accordingly we find that

$$\frac{\bar{D}_N^{(N-1)}}{\bar{\bar{D}}_{(1)N}^{(N-1)}} = \exp\left[\sum_{l=1}^{\infty} l(\bar{g}_{-l}^{(N-1)}\bar{g}_l^{(N-1)} - \bar{\bar{g}}_{(1)-l}^{(N-1)}\bar{\bar{g}}_{(1)l}^{(N-1)})\right], \tag{3.129}$$

where

$$\bar{g}_l^{(N-1)} = \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{-il\theta} \ln \bar{C}^{(N-1)}(e^{i\theta}) \tag{3.130a}$$

and

$$\bar{\bar{g}}_{(1)l}^{(N-1)} = \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{-il\theta} \ln \bar{\bar{C}}_{(1)}^{(N-1)}(e^{i\theta}). \tag{3.130b}$$

Because $\bar{C}^{(N-1)}(e^{i\theta})$ and $\bar{\bar{C}}_{(1)}^{(N-1)}(e^{i\theta})$ are rational functions of $e^{i\theta}$ that do not vanish for $0 \leq \theta \leq 2\pi$, $\bar{g}_l^{(N-1)}$ and $\bar{\bar{g}}_{(1)l}^{(N-1)}$ vanish exponentially rapidly as $l \to \infty$. Therefore the series in (3.129) converges.

The foregoing argument not only allows us to compute $\bar{D}_N^{(N-1)}/\bar{\bar{D}}_{(1)N}^{(N-1)}$ exactly, it also allows us to consider

$$\bar{\bar{C}}_{(2)}^{(N-1)}(e^{i\theta}) = \bar{\bar{C}}_{(1)}^{(N-1)}(e^{i\theta})(1 - \bar{\alpha}_N^{(2)}e^{i\theta}) \tag{3.131}$$

and to compute exactly the ratio $\bar{D}_N^{(N-1)}/\bar{\bar{D}}_{(2)N}^{(N-1)}$. Indeed, this process may be continued until all factors in $\bar{C}^{(N-1)}(e^{i\theta})$ have been removed and we find

$$\frac{\bar{D}_N^{(N-1)}}{\mu_{N-1}^N} = \exp\sum_{l=1}^{\infty} l\bar{g}_{-l}^{(N-1)}\bar{g}_l^{(N-1)}, \tag{3.132}$$

which, if we recall (3.118), may be used to give

$$\frac{D_N}{\mu_{N-1}^N} = \exp\sum_{l=1}^{\infty} l\bar{g}_{-l}^{(N-1)}\bar{g}_l^{(N-1)}. \tag{3.133}$$

The quantities $\bar{g}_l^{(N-1)}$ are not known explicitly because $B^{(N-1)}(e^{i\theta})$ and $\tilde{B}^{(N-1)}(e^{i\theta})$ are only implicitly defined by (3.102) and (3.108). However, we are only interested in the $N \to \infty$ limit. Therefore, to establish Szegö's theorem, we need only prove

$$\lim_{N\to\infty}\sum_{l=1}^{\infty} l\bar{g}_{-l}^{(N)}\bar{g}_l^{(N)} = \sum_{l=1}^{\infty} lg_{-l}g_l. \tag{3.134}$$

From (3.106) we see that $\mu_N^{-1}B^{(N)}(e^{i\theta}) \to P(e^{i\theta})$ uniformly in θ as $N \to \infty$. Similarly, $\tilde{B}^{(N)}(e^{i\theta}) \to Q(e^{i\theta})$ uniformly in θ as $N \to \infty$. Furthermore, since $\partial Q/\partial\theta$ exists, we may use Parseval's theorem to write

$$\begin{aligned}\sum_{l=1}^{\infty} l\bar{g}_{-l}^{(N)}g_l^{(N)} &= \int_0^{2\pi} d\theta \ln [B^{(N)}(e^{i\theta})] \frac{d}{d\theta} \ln \tilde{B}^{(N)}(e^{-i\theta}) \\ &= \int_0^{2\pi} d\theta \ln [\mu_N^{-1}B^{(N)}(e^{i\theta})] \frac{d}{d\theta} \ln \tilde{B}^{(N)}(e^{-i\theta}) \end{aligned} \tag{3.135a}$$

and

$$\sum_{l=1}^{\infty} lg_{-l}g_l = \int_0^{2\pi} d\theta \ln P(e^{i\theta}) \frac{d}{d\theta} \ln Q(e^{-i\theta}). \tag{3.135b}$$

Therefore

$$\begin{aligned}&\sum_{l=1}^{\infty} l\bar{g}_{-l}^{(N)}\bar{g}_l^{(N)} - \sum_{l=1}^{\infty} lg_{-l}g_l \\ &\quad= \int_0^{2\pi} d\theta[\ln \mu_N^{-1}B^{(N)}(e^{i\theta}) - \ln P(e^{i\theta})] \frac{d}{d\theta} \ln \tilde{B}^{(N)}(e^{-i\theta}) \\ &\qquad+ \int_0^{2\pi} d\theta \ln P(e^{i\theta})\left[\frac{d}{d\theta} \ln \tilde{B}^{(N)}(e^{-i\theta}) - \ln Q(e^{-i\theta})\right].\end{aligned} \tag{3.136}$$

Because $\ln P(e^{i\theta})$ is differentiable, the second integral may be integrated by parts. Furthermore, because $\mu_N^{-1}B^{(N)}(e^{i\theta}) \to P(e^{i\theta})$ and $\tilde{B}^{(N)}(e^{i\theta}) \to Q(e^{i\theta})$ uniformly and because $P(e^{i\theta})$ and $Q(e^{i\theta})$ do not vanish for $0 \le \theta \le 2\pi$, we have that $\ln \mu_N^{-1}B^{(N)}(e^{i\theta}) \to \ln P(e^{i\theta})$ and $\ln \tilde{B}^{(N)}(e^{i\theta}) \to \ln Q(e^{i\theta})$ uniformly as $N \to \infty$. Therefore, given an arbitrary $\delta > 0$, there exists an N_1 such that for all $N > N_1$

$$\left|\sum_{l=1}^{\infty} l\bar{g}_{-l}^{(N)}\bar{g}_l^{(N)} - \sum_{l=1}^{\infty} lg_{-l}g_l\right| \le \delta\left[\int_0^{2\pi} \left|d \ln \tilde{B}^{(N)}(e^{i\theta})\right| + \int_0^{2\pi} \left|d \ln P(e^{i\theta})\right|\right], \tag{3.137}$$

and hence (3.134) follows.

Thus we have proved that when $C(e^{i\theta})$ obeys conditions (1) and (2)

$$\lim_{N\to\infty} \frac{D_N}{\mu_{N-1}^N} = \exp \sum_{l=1}^{\infty} lg_{-l}g_l. \tag{3.138}$$

This is not yet Szegö's theorem since it involves μ_{N-1} instead of μ. But we have already seen in (3.61) that $\lim_{N\to\infty} D_N/\mu^N = \lim_{N\to\infty} D_N/\mu_N^N$ and hence Szegö's theorem follows. That is to say that if $C(e^{i\theta})$ obeys conditions (1) and (2) then

$$\lim_{N\to\infty} \frac{D_N}{\mu^N} = \exp \sum_{l=1}^{\infty} lg_{-l}g_l. \tag{3.139}$$

We have now completed our proof of Szegö's theorem.

Before we leave the subject we wish to make a few remarks on the differences between the weaker version of Szegö's theorem derived here and the stronger theorems proved by Hirschman[4] and by Devinatz.[5]

We first remark that the condition of Hirschman and of Devinatz,

$$\sum_{n=-\infty}^{\infty} n|c_n|^2 < \infty, \tag{3.140}$$

is certainly weaker than our condition that $dC(e^{i\theta})/d\theta$ satisfy a Lipschitz condition of order ϵ where $\epsilon > 0$. Indeed, we proved from Lemma 1 that under conditions (1) and (2) as $n \to \infty$

$$c_n = O(|n|^{-1-\epsilon}). \tag{3.141}$$

This certainly guarantees that (3.140) holds. However, the function defined by

$$c_n = \begin{cases} n^{1/2} & \text{if } n = m^3 \text{ when } m = 1, 2, \ldots \\ 0 & \text{otherwise} \end{cases} \tag{3.142}$$

demonstrates that (3.140) may hold even if (3.141) is violated.

There are several places in our proof where the Lipschitz condition has been used, of which the most essential was in the derivation of the result

$$\mu_N = \mu + o(N^{-1}), \tag{3.143}$$

which was needed to pass from (3.138) to (3.139). How the use of the Lipschitz condition can be removed is thoroughly discussed in the original papers of Hirschman[4] and Devinatz.[5]

We terminate our remarks on Szegö's theorem at this point and return from this mathematical interlude to the calculation of the spontaneous magnetization.

4. EXPLICIT CALCULATION OF THE SPONTANEOUS MAGNETIZATION

The spontaneous magnetization is now simply obtained by applying Szegö's theorem (1.4) to the Toeplitz determinants (VIII.2.28) and (VIII.3.29). Consider first the more complicated correlation function $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ as given by (VIII.2.28). We may apply Szegö's theorem when $T < T_c$, $\alpha_2 < 1$, since it is easily verified that $\phi(\theta)$ defined by (VIII.2.30) satisfies conditions (1) and (2) of the previous section.

We first find

$$\ln \mu = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta \ln \left[\frac{(1 - \alpha_1 e^{i\theta})(1 - \alpha_2 e^{-i\theta})}{(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{i\theta})}\right]^{1/2} = 0 \tag{4.1}$$

since the integrand is an odd function of θ. Therefore

$$\mu = 1. \tag{4.2}$$

Secondly, we need

$$g_n = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta e^{-in\theta} \ln\left[\frac{(1-\alpha_1 e^{i\theta})(1-\alpha_2 e^{-i\theta})}{(1-\alpha_1 e^{-i\theta})(1-\alpha_2 e^{i\theta})}\right]^{1/2}. \tag{4.3}$$

Since $0 \leq \alpha_1 \leq \alpha_2 < 1$, we use the formula

$$\ln(1-\alpha_j e^{i\theta}) = -\sum_{l=1}^{\infty} l^{-1}(\alpha_j e^{i\theta})^l \tag{4.4}$$

to write (4.3) as

$$g_n = \frac{1}{4\pi}\int_{-\pi}^{\pi} d\theta e^{-in\theta}\left\{\sum_{l=1}^{\infty} l^{-1}[(\alpha_1 e^{-i\theta})^l + (\alpha_2 e^{i\theta})^l - (\alpha_1 e^{i\theta})^l - (\alpha_2 e^{-i\theta})^l]\right\}. \tag{4.5}$$

We may integrate term by term to obtain, for $n > 0$,

$$g_n = \frac{1}{2n}[\alpha_2^n - \alpha_1^n], \tag{4.6a}$$

$$g_{-n} = -\frac{1}{2n}[\alpha_2^n - \alpha_1^n]. \tag{4.6b}$$

So we find

$$\begin{aligned}\sum_{n=1}^{\infty} n g_{-n} g_n &= -\frac{1}{4}\sum_{n=1}^{\infty} n^{-1}[\alpha_2^n - \alpha_1^n]^2 \\ &= -\frac{1}{4}\sum_{n=1}^{\infty} n^{-1}[\alpha_2^{2n} + \alpha_1^{2n} - 2\alpha_1^n\alpha_2^n] \\ &= \frac{1}{4}\ln\left[\frac{(1-\alpha_2^2)(1-\alpha_1^2)}{(1-\alpha_1\alpha_2)^2}\right].\end{aligned} \tag{4.7}$$

Hence (1.4) yields

$$\lim_{N\to\infty}\langle\sigma_{0,0}\sigma_{0,N}\rangle = \left[\frac{(1-\alpha_2^2)(1-\alpha_1^2)}{(1-\alpha_1\alpha_2)^2}\right]^{1/4}. \tag{4.8}$$

Finally, we substitute (4.8) in (1.1a) and recall the definitions of α_1 and α_2 from (V.3.4) to obtain the desired result,

$$M = \left[\frac{(1-\alpha_2^2)(1-\alpha_1^2)}{(1-\alpha_1\alpha_2)^2}\right]^{1/8} = [1 - (\sinh 2\beta E_1 \sinh 2\beta E_2)^{-2}]^{1/8}. \tag{4.9}$$

As expected, M is invariant under the interchange of E_1 and E_2.

The last form in (4.9) is the one in which the spontaneous magnetization was first exhibited by Onsager in 1948.[7] The first derivation of this

7. L. Onsager, *Nuovo Cimento* **6** (Supplement), 261 (1949).

result (with the restriction $E_1 = E_2$) was given by Yang in 1952.[8] The straightforward generalization of Yang's procedure to the case $E_1 \neq E_2$ was first made by Chang.[9]

It is now trivial to verify that the necessary identity

$$\lim_{N\to\infty} \langle \sigma_{0,0}\sigma_{0,N} \rangle = \lim_{N\to\infty} \langle \sigma_{0,0}\sigma_{N,N} \rangle \tag{4.10}$$

in fact holds. We saw from (VIII.3.29) that, for any N, $\langle \sigma_{0,0}\sigma_{N,N} \rangle$ was obtained from $\langle \sigma_{0,0}\sigma_{0,N} \rangle$ by replacing α_1 by 0 and α_2 by

$$(\sinh 2\beta E_1 \sinh 2\beta E_2)^{-1}.$$

Substituting these values in (4.8) we find

$$\lim_{N\to\infty} \langle \sigma_{0,0}\sigma_{N,N} \rangle = [1 - (\sinh 2\beta E_1 \sinh 2\beta E_2)^{-2}]^{1/4}, \tag{4.11}$$

which verifies (4.10).

It seems only fair that after working so hard to obtain (4.9) we pause a bit and discuss what we have found.

When $T \to T_c^-$,

$$M \sim [4\beta_c(E_1 \coth 2\beta_c E_1 + E_2 \coth 2\beta_c E_2)(1 - T/T_c)]^{1/8}. \tag{4.12}$$

Thus, for any ratio $E_1/E_2 > 0$, the spontaneous magnetization vanishes as $T \to T_c^-$ as a one-eighth root. This is to be compared with the boundary magnetization $\mathfrak{M}_1$ given by (VI.5.20), which vanishes as a square root as $T \to T_c^-$. For further comparison we plot both M and $\mathfrak{M}_1$ together in Fig. 10.1. We see there that $M \geq \mathfrak{M}_1$. This inequality is quite natural,

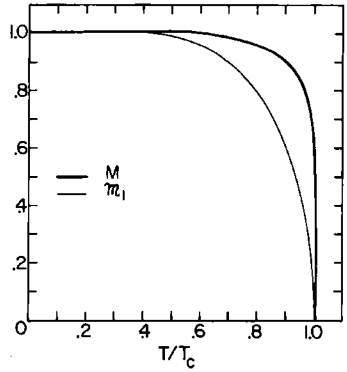


Fig. 10.1. Comparison of M with the boundary spontaneous magnetization $\mathfrak{M}_1$ for $E_1 = E_2$ as a function of temperature.

8. C. N. Yang, *Phys. Rev.* **85**, 808 (1952).
9. C. H. Chang, *Phys. Rev.* **88**, 1422 (1952).

since one expects that the more neighbors a spin has the greater the average value of that spin should be. Such an intuitive statement can be given a precise statement and a general proof. This is done in Appendix A.

In Chapter XIII, in the course of our discussion of the hysteresis type of phenomena exhibited by $\mathfrak{M}_1(\mathfrak{H})$, we derive an expression for the spontaneous magnetization $\mathfrak{M}_J$ in the Jth row of the half-plane Onsager lattice. From that expression we conjecture that for every finite value of J, as $T \to T_c$,

$$\mathfrak{M}_J \sim (1 - T/T_c)^{1/2}. \tag{4.13}$$

Furthermore, although no one has succeeded in providing a proof, it is physically obvious that for fixed T

$$\lim_{J\to\infty} \mathfrak{M}_J = M. \tag{4.14}$$

Hence (4.13) and (4.14) show that, although the quantity

$$\lim_{T\to T_c} \mathfrak{M}_J(T_c - T)^{-1/2} \tag{4.15}$$

exists for each J, it is unbounded as $J \to \infty$. This unboundedness means that as $T \to T_c$ the influence of the boundary "penetrates" further and further into the lattice. Such a "penetration" of the influence of the boundary into the bulk is intimately connected with the pole divergence in the boundary specific heat found in (VI.4.43).

Though $M(H)$ is not known as a function of H, it has been possible to evaluate M at one particular value of H other than $H = 0$, namely,[10,11]

$$H = i\tfrac{1}{2}\pi/\beta. \tag{4.16}$$

Note that the value of this magnetic field depends on temperature. Since this magnetic field is purely imaginary, the corresponding magnetization is not physically observable. This magnetization is more difficult to compute than M was because $M(i\frac{1}{2}\pi/\beta)$ is expressible not as the limit $N \to \infty$ of an $N \times N$ Toeplitz determinant, but as the limit $N \to \infty$ of an $N \times N$ block Toeplitz determinant, that is, a determinant of the Toeplitz form except that the matrix elements c_n are no longer numbers but are 2×2 matrices. Such an unpleasant situation would have occurred in the computation of this chapter were it not for the fortunate fact that $A^{-1}(0, k; 0, k')_{RR} = A^{-1}(0, k; 0, k')_{LL} = 0$. Since coupled Wiener-Hopf equations are in general not explicitly solvable, no analogue of Szegö's theorem exists for block Toeplitz determinants and at several points in the remainder of this book we will not be able to carry out some desired calculations precisely because block Toeplitz determinants are

10. T. D. Lee and C. N. Yang, *Phys. Rev.* **87**, 410 (1952).
11. B. M. McCoy and T. T. Wu, *Phys. Rev.* **155**, 438 (1967).

involved. However, for the case of evaluating $M(i\frac{1}{2}\pi/\beta)$ special circumstances obtain which enable us to evaluate such a limit and we find[10,11]

$$M(i\tfrac{1}{2}\pi/\beta) = [\tfrac{1}{4}(z_1^{-1} + z_1)(z_2^{-1} + z_2)(z_1^{-2} + z_1^2 + z_2^{-2} + z_2^2)^{-1/2}]^{1/4}. \tag{4.17}$$

Our final remark is the obvious and at the same time profound observation that T_c, which has here been shown to be the temperature at which M vanishes as T is increased from zero, is the same T_c as that found in Chapter V at which the specific heat becomes logarithmically infinite. It would seem inconceivable that these two temperatures could be different. Therefore, it would be most useful if a proof could be constructed which would establish the identity of these two temperatures without first having to compute explicitly both c and M. One would further expect that if such a proof exists for the Ising model it should be generalizable to a wide class of other more realistic magnetic systems. Unfortunately, no such proof has yet been found. Therefore, we have no fundamental understanding of how, or even if, the singularity in the specific heat is related to the vanishing of the spontaneous magnetization.

CHAPTER XI

Behavior of the Correlation Functions $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ and $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ for Large N

1. INTRODUCTION[1]

In the preceding chapters we derived the following facts about

$$S_N = \lim_{\substack{\mathscr{M}\to\infty \\ \mathscr{N}\to\infty}} \langle\sigma_{0,0}\sigma_{0,N}\rangle_{\mathscr{M},\mathscr{N}} \quad \text{and} \quad \langle\sigma_{0,0}\sigma_{N,N}\rangle = \lim_{\substack{\mathscr{M}\to\infty \\ \mathscr{N}\to\infty}} \langle\sigma_{0,0}\sigma_{N,N}\rangle_{\mathscr{M},\mathscr{N}}$$

in Onsager's lattice:

(1)

$$S_N = \begin{vmatrix} a_0 & a_{-1} & a_{-2} & \cdots & a_{-N+1} \\ a_1 & a_0 & a_{-1} & \cdots & a_{-N+2} \\ a_2 & a_1 & a_0 & \cdots & a_{-N+3} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{N-1} & a_{N-2} & a_{N-3} & \cdots & a_0 \end{vmatrix}, \tag{1.1}$$

where

$$a_n = (2\pi)^{-1}\int_0^{2\pi} d\theta e^{-in\theta}\phi(\theta), \tag{1.2}$$

with

$$\phi(\theta) = \left[\frac{(1-\alpha_1 e^{i\theta})(1-\alpha_2 e^{-i\theta})}{(1-\alpha_1 e^{-i\theta})(1-\alpha_2 e^{i\theta})}\right]^{1/2}, \tag{1.3}$$

$$\alpha_1 = z_1\left(\frac{1-z_2}{1+z_2}\right), \qquad \alpha_2 = z_1^{-1}\left(\frac{1-z_2}{1+z_2}\right). \tag{1.4}$$

1. This chapter is based partly on T. T. Wu, *Phys. Rev.* **149**, 380 (1966).

In (1.3) the square root is taken so that $\phi(\pi) > 0$ and we remind the reader that without loss of generality we have taken $E_1 > 0$ and $E_2 > 0$.

(2) $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ is obtained from S_N by making the replacements

$$\begin{aligned}\alpha_1 &\rightarrow 0,\\ \alpha_2 &\rightarrow [\sinh 2\beta E_1 \sinh 2\beta E_2]^{-1}.\end{aligned} \tag{1.5}$$

(3) When $T < T_c$,

$$\begin{aligned}M^2 = \lim_{N\to\infty} S_N = \lim_{N\to\infty} \langle\sigma_{0,0}\sigma_{N,N}\rangle &= \left[\frac{(1-\alpha_1^2)(1-\alpha_2^2)}{(1-\alpha_1\alpha_2)^2}\right]^{1/4}\\ &= \left[1 - \frac{1}{(\sinh 2\beta E_1 \sinh 2\beta E_2)^2}\right]^{1/4}.\end{aligned} \tag{1.6}$$

We continue the study of $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ and $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ in this chapter by considering their behavior when N is large and T is fixed. The leading term is, of course, M^2. In order of increasing complexity, we treat three cases: $T > T_c$, $T < T_c$, and $T = T_c$. In the first two cases, we will study first $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ and then obtain $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ by making the replacement indicated in (2) above. For the case $T = T_c$, however, the asymptotic expansion of $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ is much more difficult to obtain than that of $\langle\sigma_{0,0}\sigma_{N,N}\rangle$. Accordingly, the expansion at T_c of $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ will be studied by itself in Sec. 4. This expansion will then be combined with a generalization of Szegö's theorem in Sec. 5 to obtain the leading term of the expansion of $\langle\sigma_{0,0}\sigma_{0,N}\rangle$. The computation of higher-order terms in the expansion of $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ is more involved and is carried out in Secs. 6 and 7.

The three cases have the following qualitative differences:

(*a*) When $T > T_c$, we have $0 \leq \alpha_1 < 1 < \alpha_2$

and

$$\ln \phi(2\pi) - \ln \phi(0) = -2\pi i; \tag{1.7}$$

(*b*) When $T < T_c$, we have $0 \leq \alpha_1 \leq \alpha_2 < 1$ and

$$\ln \phi(2\pi) - \ln \phi(0) = 0; \tag{1.8}$$

and

(*c*) When $T = T_c$, we have $\alpha_1 < \alpha_2 = 1$ and

$$\phi(0) = -\phi(2\pi) = -i. \tag{1.9}$$

All three cases will be investigated by an extension of the Wiener-Hopf technique of Chapter IX, and these qualitative features determine the type of procedure to be used. A general discussion of the results obtained will be deferred until the next chapter, when we will have generalized some of this work to $\langle\sigma_{0,0}\sigma_{M,N}\rangle$.

2. SPIN CORRELATIONS ABOVE THE CRITICAL TEMPERATURE

We treat first the case $T > T_c$. From the theory of the Wiener-Hopf sum equation, it is convenient to work with a kernel whose index is zero, that is, a kernel with the property that its logarithm is continuous and periodic. Because of (1.7), we introduce

$$\phi_1(\theta) = \phi(\theta)e^{i\theta} \tag{2.1}$$

and

$$b_n = \frac{1}{2\pi}\int_0^{2\pi} \phi_1(\theta)e^{-in\theta}\, d\theta. \tag{2.2}$$

Therefore

$$b_n = a_{n-1}. \tag{2.3}$$

Let R_N be the $N \times N$ Toeplitz determinant formed from b_n, that is, R_N is given by the right-hand side of (1.1) with all the a's replaced by b's. Szegö's theorem can be immediately applied to R_N to give

$$\lim_{N\to\infty} (-1)^N R_N = \left[(1 - \alpha_1^2)\left(1 - \frac{1}{\alpha_2^2}\right)\left(1 - \frac{\alpha_1}{\alpha_2}\right)^2\right]^{1/4}. \tag{2.4}$$

For large N, the difference between R_N and this limiting value is exponentially small in N.

Consider the linear equations

$$\sum_{m=0}^{N} b_{n-m}x_m^{(N)} = \delta_{n,0} \tag{2.5}$$

for $0 \le n \le N$. Because of (2.3), we may use Cramer's rule to see that S_N is given by

$$S_N = (-1)^N R_{N+1}x_N^{(N)}. \tag{2.6}$$

To determine S_N asymptotically, it is therefore sufficient to find $x_N^{(N)}$ for large N. For this purpose, we develop first the Wiener-Hopf procedure in a form suitable for iterations. In so doing, we will for convenience repeat some of the definitions and equations of Chapter X.

As a generalization of (2.5), consider the equation

$$\sum_{m=0}^{N} c_{n-m}x_m^{(N)} = y_n \tag{2.7}$$

for $0 \le n \le N$. We assume that $\sum_{n=-\infty}^{\infty} |c_n|$ converges so that

$$C(\xi) = \sum_{n=-\infty}^{\infty} c_n\xi^n \tag{2.8}$$

is continuous on the unit circle. We further assume that $\ln C(\xi)$ is continuous and periodic on the unit circle. As in Chapter X, we define

$$x_n^{(N)} = y_n = 0 \tag{2.9}$$

for $n < 0$ and for $n > N$

$$u_n = \begin{cases} \sum_{m=0}^{N} c_{N+n-m} x_m^{(N)} & \text{for } n > 0 \\ 0 & \text{for } n \leq 0 \end{cases} \tag{2.10}$$

and also

$$v_n = \begin{cases} \sum_{m=0}^{N} c_{-n-m} x_m^{(N)} & \text{for } n > 0 \\ 0 & \text{for } n \leq 0. \end{cases} \tag{2.11}$$

We further define, again as in Chapter X,

$$X(\xi) = \sum_{n=0}^{N} x_n^{(N)} \xi^n, \tag{2.12}$$

$$Y(\xi) = \sum_{n=0}^{N} y_n \xi^n, \tag{2.13}$$

$$U(\xi) = \sum_{n=1}^{\infty} u_n \xi^n, \tag{2.14}$$

and

$$V(\xi) = \sum_{n=1}^{\infty} v_n \xi^n. \tag{2.15}$$

It then follows from (2.7) that, for $|\xi| = 1$,

$$C(\xi)X(\xi) = Y(\xi) + U(\xi)\xi^N + V(\xi^{-1}). \tag{2.16}$$

Under the present assumptions, $C(\xi)$ has a unique factorization, up to a multiplicative constant, in the form

$$[C(\xi)]^{-1} = P(\xi)Q(\xi^{-1}) \tag{2.17}$$

for $|\xi| = 1$, such that $P(\xi)$ and $Q(\xi)$ are both analytic for $|\xi| < 1$, and continuous and nonzero for $|\xi| \leq 1$. Equation (2.16) can thus be rewritten in the form

$$\begin{aligned} &[P(\xi)]^{-1}X(\xi) - [Q(\xi^{-1})Y(\xi)]_+ - [Q(\xi^{-1})U(\xi)\xi^N]_+ \\ &\qquad = Q(\xi^{-1})V(\xi^{-1}) + [Q(\xi^{-1})Y(\xi)]_- + [Q(\xi^{-1})U(\xi)\xi^N]_-, \end{aligned} \tag{2.18}$$

again for $|\xi| = 1$, where the subscript $+$ $(-)$ means that we should expand the quantity in the brackets into a Laurent series and keep only those terms in which ξ is raised to a nonnegative (negative) power. We then apply the standard Wiener-Hopf argument by noticing that the left-hand side of (2.18) is analytic inside the unit circle, whereas the right-hand side is analytic outside the unit circle and furthermore approaches zero at infinity. Therefore

$$X(\xi) = P(\xi)\{[Q(\xi^{-1})Y(\xi)]_+ + [Q(\xi^{-1})U(\xi)\xi^N]_+\} \tag{2.19a}$$

and

$$V(\xi^{-1}) = -[Q(\xi^{-1})]^{-1}\{[Q(\xi^{-1})Y(\xi)]_- + [Q(\xi^{-1})U(\xi)\xi^N]_-\}. \tag{2.20a}$$

Similarly,

$$X(\xi^{-1})\xi^N = Q(\xi)\{[P(\xi^{-1})Y(\xi^{-1})\xi^N]_+ + [P(\xi^{-1})V(\xi)\xi^N]_+\} \tag{2.19b}$$

and

$$U(\xi^{-1}) = -[P(\xi^{-1})]^{-1}\{[P(\xi^{-1})Y(\xi^{-1})\xi^N]_- + [P(\xi^{-1})V(\xi)\xi^N]_-\}. \tag{2.20b}$$

These are the equations that we shall use. They are precisely equations (X.3.42) and (X.3.43).

We now specialize to the problem of the Ising model with $T > T_c$. In this case,

$$C(\xi) = \left[\frac{(1 - \alpha_1\xi)(1 - \alpha_2^{-1}\xi)}{(1 - \alpha_1\xi^{-1})(1 - \alpha_2^{-1}\xi^{-1})}\right]^{1/2}, \tag{2.21}$$

$$P(\xi) = [(1 - \alpha_1\xi)(1 - \alpha_2^{-1}\xi)]^{-1/2}, \tag{2.22}$$

and

$$Q(\xi) = [(1 - \alpha_1\xi)(1 - \alpha_2^{-1}\xi)]^{1/2}. \tag{2.23}$$

Moreover, a comparison of (2.5) with (2.7) shows that

$$Y(\xi) = 1. \tag{2.24}$$

We find $V(\xi)$ approximately by using (2.20a) with the $U(\xi)$ term neglected:

$$V(\xi^{-1}) \sim -[Q(\xi^{-1})]^{-1}[Q(\xi^{-1})]_- = [Q(\xi^{-1})]^{-1} - 1,$$

or

$$V(\xi) \sim [Q(\xi)]^{-1} - 1. \tag{2.25}$$

Equation (2.25) is then substituted into (2.19b) to give

$$X(\xi^{-1})\xi^N \sim Q(\xi)[P(\xi^{-1})Q(\xi)^{-1}\xi^N]_+. \tag{2.26}$$

The desired $x_N^{(N)}$ is found by setting $\xi = 0$ in (2.26):

$$x_N^{(N)} \doteq (2\pi i)^{-1}\oint d\xi\,\xi^{N-1}P(\xi^{-1})Q(\xi)^{-1}, \tag{2.27}$$

where the integration is around the unit circle. In (2.27), the symbol $\doteqdot$, as introduced in Chapter VII, means that, for $N \to \infty$ but T fixed, the right-hand side and the left-hand side have the same asymptotic expansion. More explicitly, by (2.22) and (2.23),

$$x_N^{(N)} \doteqdot \frac{1}{2\pi i}\oint d\xi \xi^{N-1}[(1-\alpha_1\xi)(1-\alpha_1\xi^{-1})(1-\alpha_2^{-1}\xi)(1-\alpha_2^{-1}\xi^{-1})]^{-1/2}, \quad (2.28a)$$

or

$$x_N^{(N)} \doteqdot -\frac{1}{2\pi}\int_0^{2\pi} d\theta e^{iN\theta}|(1-\alpha_1 e^{i\theta})(1-\alpha_2^{-1}e^{i\theta})|^{-1}. \quad (2.28b)$$

The error involved in (2.28) is exponentially small in N even when compared with $x_N^{(N)}$. In (2.28b), the minus sign on the right-hand side is due to the fact that, from (2.1), the square root under the integral of (2.28a) is taken to be negative at the point $\xi = -1$. Finally, the substitution of (2.4) and (2.28) in (2.6) gives

$$S_N \doteqdot -\frac{1}{2\pi i}\left[(1-\alpha_1^2)\left(1-\frac{1}{\alpha_2^2}\right)\left(1-\frac{\alpha_1}{\alpha_2}\right)^2\right]^{1/4}$$
$$\times \oint d\xi\xi^{N-1}\left[(1-\alpha_1\xi)\left(1-\frac{\alpha_1}{\xi}\right)\left(1-\frac{\xi}{\alpha_2}\right)\left(1-\frac{1}{\alpha_2\xi}\right)\right]^{-1/2}. \quad (2.29)$$

Equation (2.29) is the desired answer; it only remains to evaluate its right-hand side asymptotically for large N. This is straightforward but tedious. We deform the contour of integration around the branch cut from α_1 to $1/\alpha_2$ to get the result

$$S_N \doteqdot \frac{1}{\pi\alpha_2^N}\left[(1-\alpha_1^2)\left(1-\frac{1}{\alpha_2^2}\right)\left(1-\frac{\alpha_1}{\alpha_2}\right)^2\right]^{1/4}\int_{\alpha_1\alpha_2}^{1} d\xi_1\xi_1^{N-1}$$
$$\times\left[\left(1-\frac{\alpha_1\xi_1}{\alpha_2}\right)\left(1-\frac{\alpha_1\alpha_2}{\xi_1}\right)\left(1-\frac{\xi_1}{\alpha_2^2}\right)\left(\frac{1}{\xi_1}-1\right)\right]^{-1/2}. \quad (2.30)$$

From this point on, we can proceed in many slightly different ways. For example, the simplest thing to do is to expand the integrand of (2.30) about the point $\xi_1 = 1$ and then integrate term by term. We shall follow the procedure used in expanding similar integrals in Chapter VII, which is only slightly different. As in Sec. 5 of that chapter, let

$$x_1 = (1-\alpha_1/\alpha_2)^{-1}(1+\alpha_1/\alpha_2) = \cosh 2\beta E_1, \quad (2.31)$$

$$x_2 = (1-\alpha_1\alpha_2)^{-1}(1+\alpha_1\alpha_2) = \coth 2\beta E_2, \quad (2.32)$$

and

$$x_3 = \frac{\alpha_2^2+1}{\alpha_2^2-1}. \quad (2.33)$$

These three x's are related by

$$x_1x_2 + x_1x_3 - x_2x_3 = 1. \tag{2.34}$$

We use these three x's in (2.30); for example,

$$\left(1 - \frac{\alpha_1\xi_1}{\alpha_2}\right)^{-1/2} = \left(\frac{1 + x_1}{1 + \xi_1}\right)^{1/2}\left[1 + x_1\frac{1 - \xi_1}{1 + \xi_1}\right]^{-1/2}. \tag{2.35}$$

The result is

$$\begin{aligned} S_N \doteq\ & \pi^{-1}\alpha_2^{-N}\left(\frac{1 - \alpha_1^2}{1 - 1/\alpha_2^2}\right)^{1/4}\frac{1}{(1 - \alpha_1\alpha_2)^{1/2}}\,2^{3/2} \\ & \times \int_{\alpha_1\alpha_2}^{1} d\xi_1\,\frac{\xi_1^N}{(1 + \xi_1)^{3/2}(1 - \xi_1)^{1/2}}\,A_>\left(\frac{1 - \xi_1}{1 + \xi_1}\right), \end{aligned} \tag{2.36}$$

where [This $A_>$ is different from that of (VII.5.13)]

$$A_>(z) = [(1 + x_1z)(1 - x_2z)(1 + x_3z)]^{-1/2}. \tag{2.37}$$

If we expand $A_>(z)$ into a power series,

$$A_>(z) = \sum_{n=0}^{\infty} A_{n>}z^n, \tag{2.38}$$

then the first few coefficients are

$$\begin{aligned} A_{0>} &= 1, \\ A_{1>} &= -\tfrac{1}{2}(x_1 - x_2 + x_3), \\ A_{2>} &= \tfrac{3}{8}(x_1^2 + x_2^2 + x_3^2) - \tfrac{1}{4}(x_2x_3 - x_3x_1 + x_1x_2), \end{aligned}$$

and

$$\begin{aligned} A_{3>} = & -\tfrac{5}{16}(x_1^3 - x_2^3 + x_3^3) + \tfrac{3}{16}(x_1^2x_2 - x_1x_2^2 - x_2^2x_3 + x_2x_3^2 \\ & - x_3^2x_1 - x_3x_1^2) + \tfrac{1}{8}x_1x_2x_3. \end{aligned} \tag{2.39}$$

If we substitute (2.38) into (2.36) in order to integrate term by term, we can replace the lower limit of integration $\alpha_1\alpha_2$ by 0 without changing the asymptotic series:

$$\begin{aligned} S_N \doteq\ & \frac{1}{\pi\alpha_2^N}\left(\frac{1 - \alpha_1^2}{1 - \alpha_2^{-2}}\right)^{1/4}\frac{1}{(1 - \alpha_1\alpha_2)^{1/2}}\,N!\sum_{n=0}^{\infty} A_{n>}\,\frac{1}{2^n}\,\frac{\Gamma(n + \frac{1}{2})}{\Gamma(N + n + \frac{3}{2})} \\ & \times F(n + \tfrac{3}{2}, n + \tfrac{1}{2}; N + n + \tfrac{3}{2}; \tfrac{1}{2}). \end{aligned} \tag{2.40}$$

In (2.40), the sum over n is to be interpreted in the sense of asymptotic series, and we have used there Euler's integral representation of the hypergeometric function F, (VII.5.17). We may then use the series representation for F, (VII.5.19), and interchange the order of summations to get

$$S_N \doteq \frac{1}{\pi^{1/2}\alpha_2^N}\left(\frac{1-\alpha_1^2}{1-\alpha_2^{-2}}\right)^{1/4}\frac{1}{(1-\alpha_1\alpha_2)^{1/2}}N!\sum_{m=0}^{\infty}\frac{1}{\pi^{1/2}2^m}$$
$$\times\frac{\Gamma(m+\frac{3}{2})\Gamma(m+\frac{1}{2})}{\Gamma(N+m+\frac{3}{2})}\sum_{n=0}^{m}\frac{A_{n>}}{(m-n)!\,\Gamma(n+\frac{3}{2})}. \tag{2.41}$$

This is the desired answer.

For completeness we write down the first few terms:

$$S_N \sim \frac{1}{\pi^{1/2}\alpha_2^N}\left(\frac{1-\alpha_1^2}{1-\alpha_2^{-2}}\right)^{1/4}\frac{1}{(1-\alpha_1\alpha_2)^{1/2}}\frac{N!}{\Gamma(N+\frac{3}{2})}$$
$$\times\left\{1+\frac{3}{8}\frac{1+\frac{2}{3}A_{1>}}{N+\frac{3}{2}}+\frac{45}{64}\frac{\frac{1}{2}+\frac{2}{3}A_{1>}+(4/15)A_{2>}}{(N+\frac{3}{2})(N+\frac{5}{2})}\right.$$
$$+\frac{1575}{512}\frac{\frac{1}{6}+\frac{1}{3}A_{1>}+(4/15)A_{2>}+(8/105)A_{3>}}{(N+\frac{3}{2})(N+\frac{5}{2})(N+\frac{7}{2})}$$
$$\left.+\cdots\right\}, \tag{2.42}$$

or, more explicitly, as $N\to\infty$,

$$S_N \sim \frac{1}{(\pi N)^{1/2}\alpha_2^N}\left(\frac{1-\alpha_1^2}{1-\alpha_2^{-2}}\right)^{1/4}\frac{1}{(1-\alpha_1\alpha_2)^{1/2}}$$
$$\times\left[1+\frac{1}{4}\frac{A_{1>}}{N}+\frac{3}{16}\frac{A_{2>}-\frac{5}{6}}{N^2}+\frac{15}{64}\frac{A_{3>}-\frac{7}{6}A_{1>}}{N^3}+\cdots\right], \tag{2.43}$$

where $A_{1>}$, $A_{2>}$, and $A_{3>}$ are given by (2.39). These are the first four terms of the long-range correlation along the lattice sites above the critical temperature.

The asymptotic expansion of $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ is obtained from (2.43) by making the replacement (1.5). With that replacement

$$x_1\to 1, \qquad x_2\to 1$$

and

$$x_3\to x_3' = \frac{(\sinh 2\beta E_1\sinh 2\beta E_2)^{-2}+1}{(\sinh 2\beta E_1\sinh 2\beta E_2)^{-2}-1}. \tag{2.44}$$

Therefore, from (2.39),

$$\begin{aligned}
A_{0>} &\to 1,\\
A_{1>} &\to -\tfrac{1}{2}x_3',\\
A_{2>} &\to \tfrac{3}{8}x_3'^2+\tfrac{1}{2},\\
A_{3>} &\to \tfrac{1}{16}x_3'[-5x_3'^2-4].
\end{aligned} \tag{2.45}$$

Hence we have

$$\langle\sigma_{0,0}\sigma_{N,N}\rangle \sim \frac{1}{(\pi N)^{1/2}}\frac{[\sinh 2\beta E_1 \sinh 2\beta E_2]^N}{[1-(\sinh 2\beta E_1 \sinh 2\beta E_2)^2]^{1/4}}$$
$$\times\left\{1-\frac{1}{8}\frac{x_3'}{N}+\frac{1}{128}\frac{9x_3'^2-8}{N^2}\right.$$
$$\left.+\frac{5}{1024}\frac{x_3'(-15x_3'^2+16)}{N^3}+\cdots\right\}. \tag{2.46}$$

3. SPIN CORRELATIONS BELOW THE CRITICAL TEMPERATURE

In this section, we consider the somewhat more complicated case $T < T_c$. In view of (1.8), the logarithm of $\phi(\theta)$ is continuous and periodic in the present case. Accordingly, instead of (2.5), we study more directly here the equations

$$\sum_{m=0}^{N} a_{n-m}x_m^{(N)} = \delta_{n,0} \tag{3.1}$$

for $0 \le n \le N$. The solution of (3.1) is related to the correlation function S_N by

$$x_0^{(N)} = \frac{S_N}{S_{N+1}}. \tag{3.2}$$

In order to determine S_N from $x_0^{(N)}$, we need the known result of spontaneous magnetization (1.6) so that

$$S_N = \frac{[(1-\alpha_1^2)(1-\alpha_2^2)]^{1/4}}{(1-\alpha_1\alpha_2)^{1/2}}\prod_{n=N}^{\infty} x_0^{(n)}. \tag{3.3}$$

To calculate $x_0^{(N)}$ approximately for large N, we use the formalism developed in the last section, or more specifically Eqs. (2.19) and (2.20). By (1.3),

$$C(\xi) = \left[\frac{(1-\alpha_1\xi)(1-\alpha_2\xi^{-1})}{(1-\alpha_1\xi^{-1})(1-\alpha_2\xi)}\right]^{1/2}, \tag{3.4}$$

for $T < T_c$, so that

$$P(\xi) = \left(\frac{1-\alpha_2\xi}{1-\alpha_1\xi}\right)^{1/2}, \tag{3.5}$$

and

$$Q(\xi) = \left(\frac{1-\alpha_1\xi}{1-\alpha_2\xi}\right)^{1/2}. \tag{3.6}$$

Note that, both in this case and in the case treated in the last section,

$$P(\xi)Q(\xi) = 1. \tag{3.7}$$

The procedure to be followed is: (1) calculate $V(\xi)$ approximately from

(2.20*a*) with the $U(\xi)$ term neglected; (2) get $U(\xi)$ from (2.20*b*) with the $V(\xi)$ of step 1; and finally (3) compute $X(0)$ from (2.19*a*) with the $U(\xi)$ of step 2. We therefore see that the case $T < T_c$ is more complicated than $T > T_c$ in two respects: first, one more step is needed here to get $x_0^{(N)}$, and secondly, from (3.3) an infinite product of the $x_0^{(N)}$'s is required to obtain S_N.

Equations (2.24) and (2.25) still hold here. By (2.20*b*),

$$U(\xi^{-1}) \sim -[P(\xi^{-1})]^{-1}[P(\xi^{-1})Q(\xi)^{-1}\xi^N]_-. \tag{3.8}$$

For a function $F(\xi)$ given on the unit circle, let

$$[F(\xi)]'_+ = [F(\xi)]_+ - \frac{1}{2\pi i}\oint d\xi\,\frac{F(\xi)}{\xi}, \tag{3.9}$$

where the path of integration is around the unit circle. Then

$$[F(\xi)]'_+ = \frac{\xi}{2\pi i}\oint d\xi'\,\frac{F(\xi')}{\xi'(\xi'-\xi)}, \tag{3.10}$$

provided that the path of integration is indented outward near $\xi' = \xi$. With this notation, (3.8) can be rewritten as

$$U(\xi) \sim -[P(\xi)]^{-1}[P(\xi)Q(\xi^{-1})^{-1}\xi^{-N}]'_+. \tag{3.11}$$

The substitution of (3.11) into (2.19*a*) then gives

$$x_0^{(N)} = X(0) \doteqdot 1 - \frac{1}{2\pi i}\oint d\xi\xi^{N-1}Q(\xi^{-1})P(\xi)^{-1}[P(\xi)Q(\xi^{-1})^{-1}\xi^{-N}]'_+, \tag{3.12}$$

or, more explicitly,

$$x_0^{(N)} \doteqdot 1 + \frac{1}{(2\pi)^2}\oint d\xi\xi^N\left(\frac{1-\alpha_1\xi}{1-\alpha_2\xi}\right)^{1/2}\left(\frac{1-\alpha_1/\xi}{1-\alpha_2/\xi}\right)^{1/2}$$
$$\times\oint\frac{d\xi'}{(\xi'-\xi)\xi'^{N+1}}\left(\frac{1-\alpha_2\xi'}{1-\alpha_1\xi'}\right)^{1/2}\left(\frac{1-\alpha_2/\xi'}{1-\alpha_1/\xi'}\right)^{1/2}. \tag{3.13}$$

Again, the error involved in (3.13) is exponentially small in N compared with the double integral, or roughly of the order of α_2^{4N}. The double integral is of course roughly of the order α_2^{2N}. We finally substitute (3.13) in (3.3) to obtain, for large N,

$$\frac{(1-\alpha_1\alpha_2)^{1/2}}{[(1-\alpha_1^2)(1-\alpha_2^2)]^{1/4}}S_N$$
$$\doteqdot 1 + \sum_{n=N}^{\infty}(x_0^{(n)} - 1)$$
$$\doteqdot 1 + \frac{1}{(2\pi)^2}\oint d\xi\xi^N\left(\frac{1-\alpha_1\xi}{1-\alpha_2\xi}\right)^{1/2}\left(\frac{1-\alpha_1/\xi}{1-\alpha_2/\xi}\right)^{1/2}$$
$$\times\oint d\xi'\,\frac{1}{(\xi'-\xi)^2\xi'^N}\left(\frac{1-\alpha_2\xi'}{1-\alpha_1\xi'}\right)^{1/2}\left(\frac{1-\alpha_2/\xi'}{1-\alpha_1/\xi'}\right)^{1/2}. \tag{3.14}$$

In both (3.13) and (3.14), the path of integration for the variable ξ' is to be indented outward near $\xi' = \xi$. Equation (3.14) is the desired answer, but it remains to evaluate the right-hand side more explicitly for large N.

Since the authors are unable to find any elegant way of carrying out this evaluation, we shall proceed by brute force. We deform the contour of integration in the variable ξ around the branch cut from α_1 to α_2, that in the variable ξ' around the cut from $1/\alpha_2$ to $1/\alpha_1$, and change the variables

$$\xi = \alpha_2\xi_1,\ \xi' = 1/\alpha_2\xi_2, \tag{3.15}$$

and

$$\eta_1 = \frac{1-\xi_1}{1+\xi_1}, \qquad \eta_2 = \frac{1-\xi_2}{1+\xi_2}. \tag{3.16}$$

In terms of these variables and the x's of (2.31)–(2.33), we get

$$\begin{aligned} S_N \doteq{}& \frac{[(1-\alpha_1^2)(1-\alpha_2^2)]^{1/4}}{(1-\alpha_1\alpha_2)^{1/2}} \\ &\times \Bigg[1 + \frac{16}{\pi^2}\frac{\alpha_2^{2N+2}}{(1-\alpha_2^2)^2}\int_{\alpha_1/\alpha_2}^{1} d\xi_1 \int_{\alpha_1/\alpha_2}^{1} d\xi_2 \xi_1^N \xi_2^N \\ &\times \frac{(1-\xi_2)^{1/2}}{(1+\xi_1)^{3/2}(1-\xi_1)^{1/2}(1+\xi_2)^{5/2}} \\ &\times \frac{1}{(1 - x_3\eta_1 - x_3\eta_2 + \eta_1\eta_2)^2}\frac{A_<(\eta_1)}{A_<(\eta_2)}\Bigg], \end{aligned} \tag{3.17}$$

where [This $A_<$ is different from that of (VII.6.3)]

$$A_<(\eta) = \left[\frac{(1-\eta x_1)(1+\eta x_2)}{1-\eta x_3}\right]^{1/2}. \tag{3.18}$$

We need the series expansions

$$A_<(\eta) = \sum_{n=0}^{\infty} A_{n<}\eta^n, \tag{3.19}$$

$$\frac{1}{A_<(\eta)} = \sum_{n=0}^{\infty} \bar{A}_{n<}\eta^n, \tag{3.20}$$

and

$$\frac{1}{(1 - x_3\eta_1 - x_3\eta_2 + \eta_1\eta_2)^2} = \sum_{p,q=0}^{\infty} C_{pq}\eta_1^p\eta_2^q. \tag{3.21}$$

After substituting (3.19)–(3.21) in (3.17), we replace the lower limits of integration α_1/α_2 by zero to obtain

$$S_N \doteq \frac{[(1-\alpha_1^2)(1-\alpha_2^2)]^{1/4}}{(1-\alpha_1\alpha_2)^{1/2}}$$
$$\times \left[1 + \frac{2}{\pi}\frac{\alpha_2^{2N}}{N^2(1/\alpha_2-\alpha_2)^2}\right.$$
$$\left.\times \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\sum_{p=0}^{\infty}\sum_{q=0}^{\infty} N^{-m-n-p-q} A_{m<}\bar{A}_{n<} C_{pq}\mathscr{I}_{m+p}\mathscr{I}_{n+q+1}\right], \tag{3.22}$$

where, from (VII.5.18),

$$\mathscr{I}_n = \left(\frac{8N}{\pi}\right)^{1/2} N^n \int_0^1 d\xi\,\xi^N(1+\xi)^{-n-3/2}$$
$$= \left(\frac{N}{\pi}\right)^{1/2}(\tfrac{1}{2}N)^n \frac{\Gamma(N+1)\Gamma(n+\frac{1}{2})}{\Gamma(N+n+\frac{3}{2})} F(n+\tfrac{1}{2}, n+\tfrac{3}{2}; N+n+\tfrac{3}{2}; \tfrac{1}{2}). \tag{3.23}$$

Equation (3.22) gives the desired asymptotic behavior of S_N as $N \to \infty$ for $T < T_c$.

The first few terms are explicitly

$$S_N \sim \frac{[(1-\alpha_1^2)(1-\alpha_2^2)]^{1/4}}{(1-\alpha_1\alpha_2)^{1/2}}$$
$$\times \left\{1 + \frac{1}{2\pi N^2}\frac{\alpha_2^{2N}}{(1/\alpha_2-\alpha_2)^2}\left[1 + \frac{1}{2N}(-A_{1<} + 4x_3)\right.\right.$$
$$\left.\left. + \frac{3}{(2N)^2}\left(-A_{2<} + A_{1<}^2 - 2x_3A_{1<} + 6x_3^2 - \frac{13}{6}\right) + \cdots\right]\right\}, \tag{3.24}$$

where, by (3.19) and (3.18),

$$A_{1<} = \tfrac{1}{2}(-x_1 + x_2 + x_3), \tag{3.25}$$

and

$$A_{2<} = -\tfrac{1}{8}(x_1^2 + 2x_1x_2 + x_2^2 + 2x_1x_3 - 2x_2x_3 - 3x_3^2). \tag{3.26}$$

The asymptotic expansion of $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ is obtained from (3.24) by making the replacements (1.5) and (2.44). We find

$$\langle\sigma_{0,0}\sigma_{N,N}\rangle \sim [1 - (\sinh 2\beta E_1 \sinh 2\beta E_2)^{-2}]^{1/4}\{1 + (2\pi N^2)^{-1}$$
$$\times [\sinh 2\beta E_1 \sinh 2\beta E_2]^{-2(N+1)}$$
$$\times [(\sinh 2\beta E_1 \sinh 2\beta E_2)^{-2} - 1]^{-2}$$
$$\times [1 + \tfrac{7}{4}N^{-1}x_3' + \tfrac{1}{32}N^{-2}(117x_3'^2 - 40)]\}. \tag{3.27}$$

FUNCTIONS $\langle \sigma_{0,0}\, \sigma_{0,N} \rangle$ AND $\langle \sigma_{0,0}\, \sigma_{N,N} \rangle$ FOR LARGE N

4. $\langle \sigma_{0,0}\sigma_{N,N} \rangle$ AT $T = T_c$

Because of the discontinuity in $\phi(\theta)$ exhibited in (1.9), the expansion of $\langle \sigma_{0,0}\sigma_{0,N} \rangle$ when $T = T_c$ is more complicated than the two previous cases. However, when $T = T_c$, $\langle \sigma_{0,0}\sigma_{N,N} \rangle$ may not only be asymptotically expanded, but even be evaluated exactly in closed form.

When $T = T_c$, $\sinh 2\beta E_1 \sinh 2\beta E_2 = 1$ and we will write

$$S_N^{(0)} = \langle \sigma_{0,0}\sigma_{N,N} \rangle. \tag{4.1}$$

From Sec. 1 we find that $S_N^{(0)}$ is given as

$$S_N^{(0)} = \begin{vmatrix} a_0^{(0)} & a_{-1}^{(0)} & \cdots & a_{-N+1}^{(0)} \\ a_1^{(0)} & a_0^{(0)} & \cdots & a_{-N+2}^{(0)} \\ \vdots & \vdots & \vdots & \vdots \\ a_{N-1}^{(0)} & a_{N-2}^{(0)} & \cdots & a_0^{(0)} \end{vmatrix}, \tag{4.2}$$

where

$$a_n^{(0)} = \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{-in\theta}\phi^{(0)}(\theta) \tag{4.3}$$

with

$$\phi^{(0)}(\theta) = ie^{-i\theta/2}. \tag{4.4}$$

Consequently,

$$a_n^{(0)} = \frac{1}{\pi(n + \frac{1}{2})}. \tag{4.5}$$

Clearly, the value of $\langle \sigma_{0,0}\sigma_{N,N} \rangle$ at T_c is independent of E_1 and E_2.

Let M be the $N \times N$ matrix whose elements are, for $m, n = 0, \ldots, N - 1$,

$$M_{mn} = \tfrac{1}{2}\pi a_{m-n}^{(0)} = \frac{1}{2m - 2n + 1}. \tag{4.6}$$

Then

$$S_N^{(0)} = \det(2\pi^{-1}M) = (2\pi^{-1})^N \det M. \tag{4.7}$$

To evaluate $\det M$ we prove the following, more general theorem.

Theorem. If

$$M_{mn} = (\mu_m + \nu_n)^{-1} \tag{4.8}$$

and we let

$$\det_N M = \begin{vmatrix} \dfrac{1}{\mu_0 + \nu_0} & \dfrac{1}{\mu_0 + \nu_1} & \cdots & \dfrac{1}{\mu_0 + \nu_{N-1}} \\ \dfrac{1}{\mu_1 + \nu_0} & \dfrac{1}{\mu_1 + \nu_1} & \cdots & \dfrac{1}{\mu_1 + \nu_{N-1}} \\ \vdots & \vdots & \vdots & \vdots \\ \dfrac{1}{\mu_{N-1} + \nu_0} & \dfrac{1}{\mu_{N-1} + \nu_1} & \cdots & \dfrac{1}{\mu_{N-1} + \nu_{N-1}} \end{vmatrix}, \tag{4.9}$$

then

$$\det_N M = \frac{\prod_{0 \le m < n \le N-1} (\mu_m - \mu_n)(\nu_m - \nu_n)}{\prod_{m=0}^{N-1} \prod_{n=0}^{N-1} (\mu_m + \nu_n)}. \tag{4.10}$$

Proof. First of all, we observe that

$$\det_N M = \frac{P_N}{\prod_{m=0}^{N-1} \prod_{n=0}^{N-1} (\mu_m + \nu_n)}, \tag{4.11}$$

where P_N is a polynomial in $\mu_0, \mu_1, \ldots, \mu_{N-1}$ and $\nu_0, \nu_1, \ldots, \nu_{N-1}$ of degree $N^2 - N$. On the other hand, P_N is equal to zero if $\mu_m = \mu_n$ or $\nu_m = \nu_n$ for $m \neq n$. Therefore P_N is divisible by

$$\prod_{0 \le m < n \le N-1} (\mu_m - \mu_n)(\nu_m - \nu_n). \tag{4.12}$$

But the degree of this polynomial is $2[N(N-1)/2] = N^2 - N$. Thus P_N must equal the polynomial in (4.12) up to some multiplicative constant A_N which is independent of $\mu_0, \ldots, \mu_N$ and $\nu_0, \ldots, \nu_N$ but may depend on N. However, we may easily show that $A_N = 1$ for all N. Clearly, $A_1 = 1$. But if we multiply the last row of det M by μ_{N-1} and then allow first μ_{N-1} and then ν_{N-1} to approach ∞, we find

$$\mu_{N-1} \det_N M \to \det_{N-1} M. \tag{4.13}$$

On the other hand, in this same limit

$$\frac{\mu_{N-1} \prod_{0 \le m < n \le N-1} (\mu_m - \mu_n)(\nu_m - \nu_n)}{\prod_{m=0}^{N-1} \prod_{n=0}^{N-1} (\mu_m + \nu_n)} \to \frac{\prod_{0 \le m < n \le N-2} (\mu_m - \mu_n)(\nu_m - \nu_n)}{\prod_{m=0}^{N-2} \prod_{n=0}^{N-2} (\mu_m + \nu_n)}, \tag{4.14}$$

whence, by induction, it follows that $A_N = 1$ for all N, which proves the theorem.

For our application we set

$$\mu_m = 2m + 1 \qquad \text{and} \qquad \nu_n = -2n. \tag{4.15}$$

Then we immediately obtain from (4.7) and (4.10)

$$S_N^{(0)} = (2\pi^{-1})^N \frac{\prod_{0 \le m < n \le N-1} [2(m-n)][2(n-m)]}{\prod_{m=0}^{N-1} \prod_{n=0}^{N-1} [2(m-n)+1]}. \tag{4.16}$$

But

$$\prod_{m=0}^{N-1} \prod_{n=0}^{N-1} [2(m-n)+1] = \prod_{0 \le m < n \le N-1} [1 - 4(m-n)^2], \tag{4.17}$$

so we have the closed-form expression

$$S_N^{(0)} = \left(\frac{2}{\pi}\right)^N \prod_{0\le m<n\le N-1} \left[1 - \frac{1}{4(m-n)^2}\right]^{-1}$$

$$= \begin{cases} \dfrac{2}{\pi} & \text{if } N = 1, \\ (2\pi^{-1})^N \displaystyle\prod_{l=1}^{N-1} \left[1 - \frac{1}{4l^2}\right]^{l-N} & \text{if } N \ge 2. \end{cases} \tag{4.18}$$

When N is small we may use (4.18) directly to evaluate $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ at T_c. For example we have, as first disussed by Kaufman and Onsager,

$$\langle\sigma_{0,0}\sigma_{1,1}\rangle = \frac{2}{\pi} \sim 0.636{,}619{,}772,$$

$$\langle\sigma_{0,0}\sigma_{2,2}\rangle = \frac{16}{3\pi^2} \sim 0.540{,}379{,}646,$$

$$\langle\sigma_{0,0}\sigma_{3,3}\rangle = \frac{2048}{135\pi^3} \sim 0.489{,}267{,}722. \tag{4.19}$$

When N is large we must asymptotically expand (4.18). We first use a special case of the well-known identity

$$\frac{\sin \pi\delta}{\pi\delta} = \prod_{l=1}^{\infty} \left(1 - \frac{\delta^2}{l^2}\right) \tag{4.20}$$

to write

$$\frac{2}{\pi} = \prod_{l=1}^{\infty} \left(1 - \frac{1}{4l^2}\right). \tag{4.21}$$

Thus we find

$$\ln S_N^{(0)} = \sum_{l=1}^{N-1} l \ln\left(1 - \frac{1}{4l^2}\right) + N \sum_{l=N}^{\infty} \ln\left(1 - \frac{1}{4l^2}\right). \tag{4.22}$$

To express these series in terms of more familiar functions, write

$$\sum_{l=1}^{N-1} l \ln\left(1 - \frac{1}{4l^2}\right) = -\sum_{l=1}^{N-1} \frac{1}{4l} + \sum_{l=1}^{\infty} l\left[\ln\left(1 - \frac{1}{4l^2}\right) + \frac{1}{4l^2}\right]$$
$$- \sum_{l=N}^{\infty} l\left[\ln\left(1 - \frac{1}{4l^2}\right) + \frac{1}{4l^2}\right]. \tag{4.23}$$

It is now a simple matter to obtain the leading term in the asymptotic expansion of $S_N^{(0)}$. The definition of Euler's constant γ is

$$\gamma = \lim_{N\to\infty} \left\{\sum_{n=1}^{N} \frac{1}{n} - \ln N\right\}. \tag{4.24}$$

and γ is well known[2] to have approximately the value

$$\gamma \sim 0.577{,}215{,}665. \tag{4.25}$$

Furthermore, as $N \to \infty$,

$$N \sum_{l=N}^{\infty} \ln\left(1 - \frac{1}{4l^2}\right) \sim -N \sum_{l=N}^{\infty} \left(\frac{1}{4l^2}\right) \sim -\frac{N}{4} \int_N^{\infty} dl\, l^{-2} = \frac{1}{4}. \tag{4.26}$$

Therefore the leading term in the expansion of $\ln S_N^{(0)}$ is

$$\ln S_N^{(0)} \sim -\tfrac{1}{4} \ln N - \tfrac{1}{4}\gamma + \bar{A} - \tfrac{1}{4}, \tag{4.27}$$

where

$$\bar{A} = \sum_{l=1}^{\infty} l\left[\ln\left(1 - \frac{1}{4l^2}\right) + \frac{1}{4l^2}\right]. \tag{4.28}$$

The series for $\bar{A}$ cannot be evaluated exactly. In Appendix B we show that its value is approximately

$$\bar{A} = 0.006515177\cdots + \tfrac{1}{4} + \ln\left(\tfrac{3}{4}\right). \tag{4.29}$$

Thus as $N \to \infty$,

$$S_N^{(0)} \sim AN^{-1/4}, \tag{4.30}$$

where

$$A = 0.645002448\cdots. \tag{4.31}$$

Even when $N = 1$ this approximation agrees with the exact value of $S_1^{(0)}$ given in (4.19) to an accuracy of better than 2 percent.

The complete asymptotic expansion of $\ln S_N^{(0)}$ may also be obtained if we use the property of the function

$$\psi(z) = \Gamma'(z)/\Gamma(z) \tag{4.32}$$

that

$$\psi(N) = -\gamma + \sum_{n=1}^{N-1} \frac{1}{n}. \tag{4.33}$$

Thus

$$\ln S_N^{(0)} = -\tfrac{1}{4}\psi(N) - \tfrac{1}{4}\gamma + \bar{A} + N \sum_{l=N}^{\infty} \ln\left(1 - \frac{1}{4l^2}\right) - \sum_{l=N}^{\infty} l\left[\ln\left(1 - \frac{1}{4l^2}\right) + \frac{1}{4l^2}\right]. \tag{4.34}$$

2. A. Erdelyi, ed., *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), vol. 1, p. 1.

Expanding the logarithm and using the definition of the generalized zeta function

$$\zeta(s, \nu) = \sum_{n=0}^{\infty} (n + \nu)^{-s}, \tag{4.35}$$

we find

$$\begin{aligned}\ln S_N^{(0)} = &-\tfrac{1}{4}\psi(N) - \tfrac{1}{4}\gamma + \bar{A} - \tfrac{1}{4}N\zeta(2, N) \\ &+ \sum_{n=2}^{\infty} \frac{1}{n} 4^{-n}[\zeta(2n - 1, N) - N\zeta(2n, N)].\end{aligned} \tag{4.36}$$

The asymptotic expansions of $\psi(N)$ and $\zeta(n, N)$ are known to be[3]

$$\psi(N) \sim \ln N - (2N)^{-1} - \sum_{n=1}^{\infty} B_{2n} \frac{N^{-2n}}{2n} \tag{4.37}$$

and

$$\zeta(n, N) \sim \frac{N^{1-n}}{n-1} + \frac{1}{2}N^{-n} + \frac{1}{(n-1)!}\sum_{k=1}^{\infty} B_{2k} \frac{(n - 2 + 2k)!}{(2k)!} N^{-2k-n+1}, \tag{4.38}$$

where B_n, the well-known Bernoulli numbers, are defined by

$$\frac{z}{e^z - 1} = \sum_{n=0}^{\infty} B_n \frac{z^n}{n!}. \tag{4.39}$$

Substituting (4.37) and (4.38) in (4.36) we find

$$\ln S_N^{(0)} = -\tfrac{1}{4} \ln N - \tfrac{1}{4}(\gamma + 1) + \bar{A} + \sum_{n=1}^{\infty} A_n^{(0)} N^{-2n}, \tag{4.40}$$

where

$$A_n^{(0)} = \frac{1}{2}\frac{(2n - 1)!}{4^n} \sum_{k=0}^{n} \frac{B_{2k}(1 - 2k)4^k}{(2n - 2k + 2)!\,(2k)!}. \tag{4.41}$$

Since $B_0 = 1$, $B_2 = \frac{1}{6}$, and $B_4 = -\frac{1}{30}$, the first two $A_n^{(0)}$ are explicitly

$$A_1^{(0)} = -\frac{1}{64}$$

and

$$A_2^{(0)} = \frac{1}{256}. \tag{4.42}$$

Therefore we explicitly find that the first three terms in the asymptotic expansion of $S_N^{(0)}$ are

$$S_N^{(0)} = \langle\sigma_{0,0}\sigma_{N,N}\rangle_{T=T_c} = \frac{A}{N^{1/4}}\left(1 - \frac{1}{64}\cdot\frac{1}{N^2} + \frac{33}{8192}\cdot\frac{1}{N^4} + \cdots\right). \tag{4.43}$$

3. Reference 2, pp. 47, 48.

5. $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ AT $T = T_c$; LEADING TERM

When $T = T_c$ the function $\phi(\theta)$ of (1.3) specializes to

$$\phi(\theta) = ie^{-i\theta/2}\left(\frac{1 - \alpha_1 e^{i\theta}}{1 - \alpha_1 e^{-i\theta}}\right)^{1/2}, \tag{5.1}$$

with

$$\alpha_1 = z_{1c}^2. \tag{5.2}$$

Because (5.1) is discontinuous at $\theta = 0$, we cannot apply the procedures of Secs. 2 or 3. However, the discontinuity at $\theta = 0$ is of the same type as that studied in the previous section. Indeed, the ratio

$$\frac{\phi(\theta)}{\phi^{(0)}(\theta)} = \left(\frac{1 - \alpha_1 e^{i\theta}}{1 - \alpha_1 e^{-i\theta}}\right)^{1/2} \tag{5.3}$$

is a function which is analytic for $0 \leq \theta \leq 2\pi$. Furthermore, $S_N^{(0)}$ has just been calculated. Therefore to compute S_N it is sufficient to compute $S_N/S_N^{(0)}$. This ratio can easily be found by an application of (X.2.53), which is a generalization of Szegö's theorem. Note that while Szegö's theorem is proved rigorously in the previous chapter, no corresponding proof of (X.2.53) that is general enough for the present purpose exists.

To calculate the right-hand side of (X.2.53), we need to evaluate

$$g_n = \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{-in\theta} \ln\left[ie^{-i\theta/2}\left(\frac{1 - \alpha_1 e^{i\theta}}{1 - \alpha_1 e^{-i\theta}}\right)^{1/2}\right] \tag{5.4}$$

and

$$\bar{g}_n = \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{-in\theta} \ln ie^{-i\theta/2}. \tag{5.5}$$

This is easily done and we find [compare (X.4.6)]

$$g_n = \begin{cases} \dfrac{1}{2n} - \dfrac{1}{2n}\alpha_1^{|n|} & n \neq 0, \\ 0 & n = 0, \end{cases} \tag{5.6}$$

and

$$\bar{g}_n = \begin{cases} \dfrac{1}{2n} & n \neq 0, \\ 0 & n = 0. \end{cases} \tag{5.7}$$

Therefore we get from (X.2.53) that

$$\lim_{N\to\infty} \frac{S_N}{S_N^{(0)}} = \exp \sum_{n=1}^{\infty} n[g_{-n}g_n - \bar{g}_{-n}\bar{g}_n] = \left(\frac{1 + \alpha_1}{1 - \alpha_1}\right)^{1/4}. \tag{5.8}$$

Hence, using the expansion of $S_N^{(0)}$ given in the previous section, we conclude that the leading term in the asymptotic expansion of $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ at T_c is

$$S_N \sim \left(\frac{1+\alpha_1}{1-\alpha_1}\right)^{1/4} \frac{A}{N^{1/4}}, \tag{5.9}$$

with A given by (4.31).

6. $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ AT $T = T_c$; HIGHER-ORDER TERMS (I)

The computation of the previous section is sufficient only to give the leading term in the expansion of $S_N/S_N^{(0)}$ as $N \to \infty$. This is in contrast with the other expansions of this chapter, which could, in principle, be used to compute all terms in those expansions. Accordingly, we conclude this chapter with the study of the higher-order terms in $S_N/S_N^{(0)}$ as $N \to \infty$. The computation is extremely laborious. Moreover, the methods involved are not used in the remainder of this book. Therefore, while we include this calculation for completeness, we recommend that it be omitted on first reading.

In this section we obtain more information about the special case $\alpha_1 = 0$, $\alpha_2 = 1$.

Consider the inverse of the matrix M defined by (4.6). More precisely, let

$$L = \tfrac{1}{2}\pi M^{-1}; \tag{6.1}$$

then, by (4.10),

$$\begin{aligned} L_{pq} = \frac{1}{2}\frac{\pi(-1)^{p+q}}{\mu_q + \nu_p} &\left[\prod_{m=0}^{N}(\mu_m + \nu_p)\right]\left[\prod_{n=0}^{N}(\mu_q + \nu_n)\right]\left[\prod_{m=0}^{q-1}(\mu_q - \mu_m)\right]^{-1} \\ &\times \left[\prod_{m=q+1}^{N}(\mu_m - \mu_q)\right]^{-1}\left[\prod_{n=0}^{p-1}(\nu_p - \nu_n)\right]^{-1}\left[\prod_{n=p+1}^{N}(\nu_n - \nu_p)\right]^{-1}. \end{aligned} \tag{6.2}$$

With (4.15), (6.2) can be simplified to

$$\begin{aligned} L_{pq} &= \frac{1}{2}\pi\frac{1}{(2q-2p+1)2^{4N}}\frac{(2N-2p+1)!\,(2p)!\,(2N-2q)!\,(2q+1)!}{[(N-p)!\,p!\,(N-q)!\,q!]^2} \\ &= \frac{1}{2}\pi\frac{1}{(2q-2p+1)2^{2N}} \\ &\qquad\times\frac{(2N-2p+1)!!\,(2p-1)!!\,(2N-2q-1)!!\,(2q+1)!!}{(N-p)!\,p!\,(N-q)!\,q!} \\ &= \frac{2}{\pi}\frac{1}{2q-2p+1}\frac{\Gamma(N-p+\frac{3}{2})\Gamma(p+\frac{1}{2})\Gamma(N-q+\frac{1}{2})\Gamma(q+\frac{3}{2})}{(N-p)!\,p!\,(N-q)!\,q!}, \end{aligned} \tag{6.3}$$

where, for example,

$$(2p-1)!! = 1\cdot 3\cdot 5\cdot 7\cdots(2p-1). \tag{6.4}$$

As given by (6.1), L_{pq} is defined only for $0 \leq p \leq N$ and $0 \leq q \leq N$. Thus (6.3) may be used to extend the domain of definition for L_{pq} to all integers p and q. It is, however, immediately seen from (6.3) that with this extension

$$L_{pq} = 0 \tag{6.5}$$

unless $0 \leq p \leq N$ and $0 \leq q \leq N$. It is also interesting to note that

$$L_{N-q,N-p} = L_{pq}, \tag{6.6}$$

and that, for large N and fixed p and q,

$$L_{pq} \sim \frac{1}{2}\frac{2^{-p-q+1}}{2q-2p+1}\frac{(2p-1)!!\,(2q+1)!!}{p!\,q!}, \tag{6.7}$$

with an error of the order of N^{-1}. In view of (6.6), it is convenient to define the matrix operation $\star$ such that, for an $(N+1) \times (N+1)$ matrix $\mathscr{M}$,

$$(\mathscr{M}^{\star})_{qp} = \mathscr{M}_{N-p,N-q}. \tag{6.8}$$

Thus

$$M^{\star} = M \quad \text{and} \quad L^{\star} = L. \tag{6.9}$$

Finally, we proceed to compute the quantities

$$K_{pn} = \frac{2}{\pi}\sum_{m} L_{pm}M_{mn}. \tag{6.10}$$

By (6.5), $K_{pn} = 0$ unless $0 \leq p \leq N$; by (6.1),

$$K_{pn} = \delta_{p,n} \tag{6.11}$$

if $0 \leq p \leq N$ and $0 \leq n \leq N$. We are therefore interested in the case where $0 \leq p \leq N$ while either $n > N$ or $n < 0$. This in particular means $p \neq n$. Accordingly, for these ranges of values for p and n, by partial fraction

$$K_{pn} = \frac{1}{\pi^2}\frac{\Gamma(N-p+\frac{3}{2})\Gamma(p+\frac{1}{2})}{(N-p)!\,p!\,(p-n)}[pK^{(0)}(p) - nK^{(0)}(n)], \tag{6.12}$$

where

$$K^{(0)}(z) = \sum_{m=0}^{\infty}\frac{1}{m-z+\frac{1}{2}}\frac{\Gamma(m+\frac{1}{2})\Gamma(N-m+\frac{1}{2})}{(N-m)!\,m!}. \tag{6.13}$$

This sum for $K^{(0)}(z)$ can be carried out to yield[4]

$$K^{(0)}(z) = \pi(-1)^N\frac{\Gamma(z)\Gamma(\frac{1}{2}-z)}{\Gamma(-N+z)\Gamma(N-z+\frac{3}{2})}. \tag{6.14}$$

4. Reference 2, p. 79, Eq. 2.4(5).

Therefore, for $0 \le p \le N$ and $n > N$,

$$K_{pn} = \frac{1}{\pi(p-n)}\,\frac{\Gamma(N-p+\frac{3}{2})\Gamma(p+\frac{1}{2})n!\,\Gamma(n-N-\frac{1}{2})}{(N-p)!\,p!\,(n-N-1)!\,\Gamma(n+\frac{1}{2})}, \tag{6.15}$$

and, for $0 \le p \le N$ and $n < 0$,

$$K_{pn} = \frac{1}{\pi(p-n)}\,\frac{\Gamma(N-p+\frac{3}{2})\Gamma(p+\frac{1}{2})(N-n)!\,\Gamma(\frac{1}{2}-n)}{(N-p)!\,p!\,(-n-1)!\,\Gamma(N-n+\frac{3}{2})}. \tag{6.16}$$

Equations (6.11), (6.15), and (6.16) give K_{pn} in all cases.

We now turn our attention once more to the general case where α_1 is not necessarily zero.

7. $T = T_c$; HIGHER-ORDER TERMS (II)

In Sec. 4, we obtained in (4.43) the first three terms in the asymptotic expansion of $S_N^{(0)}$ at the critical temperature when $\alpha_1 = 0$. In this section we shall derive a result more accurate than (5.8), namely,

$$\frac{S_N}{S_N^{(0)}} = \left(\frac{1+\alpha_1}{1-\alpha_1}\right)^{1/4}\left[1 + \frac{1}{8}N^{-2}\frac{\alpha_1}{(1-\alpha_1)^2} + O(N^{-3})\right]. \tag{7.1}$$

Thus the generalization of (4.43) is, as $N \to \infty$,

$$S_N = AN^{-1/4}\left(\frac{1+\alpha_1}{1-\alpha_1}\right)^{1/4}\left\{1 + \frac{1}{8}N^{-2}\left[\frac{\alpha_1}{(1-\alpha_1)^2} - \frac{1}{8}\right] + O(N^{-3})\right\}. \tag{7.2}$$

Even though these results are rather simple, the actual calculation, to be presented below, is quite long.

The following two observations form the basis of the calculational procedure.

(1) Define

$$\begin{aligned} d_n &= \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{-in\theta}\frac{\phi(\theta)}{\phi^{(0)}(\theta)} \\ &= \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{-in\theta}\left(\frac{1-\alpha_1 e^{i\theta}}{1-\alpha_1 e^{-i\theta}}\right)^{1/2}, \end{aligned} \tag{7.3}$$

so that

$$a_{m-n} = \sum_{p=-\infty}^{\infty} a_{m-p}^{(0)}\, d_{p-n}, \tag{7.4}$$

where a_n and $a_n^{(0)}$ are given by (1.2) and (4.5) respectively. For large $|n|$, d_n is *exponentially small* in $|n|$.

(2) It is seen from (6.3) that, for large N and fixed p and q between 0 and N,

$$\begin{aligned} L_{pq} &= O(1), \\ L_{p,N-q} &= O(1), \\ L_{N-p,q} &= O(N^{-2}), \end{aligned}$$

and

$$L_{N-p,N-q} = O(1). \tag{7.5}$$

(A) Formulation of the Problem

Let $\mathscr{A}$ be the $(N + 1) \times (N + 1)$ matrix whose elements are, for $0 \leq m \leq N$ and $0 \leq n \leq N$,

$$\mathscr{A}_{mn} = a_{m-n}, \tag{7.6}$$

so that

$$S_{N+1} = \det \mathscr{A}. \tag{7.7}$$

By (4.5) and (6.1),

$$\mathscr{A}^{(0)} = 2\pi^{-1}M = L^{-1}. \tag{7.8}$$

Furthermore, it is clear from (1.1) that

$$S_N/S_{N+1} = (\mathscr{A}^{-1})_{00}, \tag{7.9}$$

where the right-hand side denotes the 00-th element of the $(N + 1) \times (N + 1)$ matrix $\mathscr{A}^{-1}$. Similarly, by (7.8),

$$S_N^{(0)}/S_{N+1}^{(0)} = L_{00}. \tag{7.10}$$

We propose to obtain (7.1) by calculating the quantity

$$\mathscr{R} = \frac{S_N}{S_{N+1}} \Big/ \frac{S_N^{(0)}}{S_{N+1}^{(0)}} = (\mathscr{A}^{-1})_{00}/L_{00}. \tag{7.11}$$

Let B be the $(N + 1) \times (N + 1)$ matrix

$$B = L\mathscr{A}, \tag{7.12}$$

so that

$$\mathscr{A}^{-1} = B^{-1}L. \tag{7.13}$$

If γ is the column matrix whose elements are

$$\gamma_n = \frac{L_{n0}}{L_{00}} = -\frac{1}{2\pi^{1/2}} \frac{\Gamma(n - \frac{1}{2})\Gamma(N - n + \frac{3}{2})N!}{n!\,(N - n)!\,\Gamma(N + \frac{3}{2})}, \tag{7.14}$$

then by (7.13) $\mathscr{R}$ can be expressed by

$$\mathscr{R} = (B^{-1}\gamma)_0, \tag{7.15}$$

where the right-hand side denotes the zeroth element of the column matrix $B^{-1}\gamma$.

We partition the matrix B as follows:

$$B = \begin{bmatrix} B^{(11)} & B^{(12)} \\ B^{(21)} & B^{(22)} \end{bmatrix}, \tag{7.16}$$

where the sizes of the four matrices $B^{(11)}$, $B^{(12)}$, $B^{(21)}$, and $B^{(22)}$ are respectively $N_1 \times N_1$, $N_1 \times N_2$, $N_2 \times N_1$, and $N_2 \times N_2$, with $N_1 + N_2 = N + 1$. We choose N_1 and N_2 to be roughly $\frac{1}{2}N$, the precise value being unimportant. A possible choice is, for example,

$$N_1 = N_2 = \tfrac{1}{2}(N + 1), \qquad \text{for } N \text{ odd},$$

and

$$N_1 = N_2 - 1 = \tfrac{1}{2}N, \qquad \text{for } N \text{ even}.$$

The inverse of B can be expressed in terms of these $B^{(ij)}$ by

$$B^{-1} = \begin{bmatrix} (B^{(11)} - B^{(12)}B^{(22)-1}B^{(21)})^{-1} & -B^{(11)-1}B^{(12)}(B^{(22)} - B^{(21)}B^{(11)-1}B^{(12)})^{-1} \\ -B^{(22)-1}B^{(21)}(B^{(11)} - B^{(12)}B^{(22)-1}B^{(21)})^{-1} & (B^{(22)} - B^{(21)}B^{(11)-1}B^{(12)})^{-1} \end{bmatrix}. \tag{7.17}$$

It is convenient to renumber the indices by introducing four matrices $\dot{B}^{(ij)}$:

$$\dot{B}^{(11)}_{mn} = B_{mn}, \qquad \text{for } 0 \le m < N_1,\ 0 \le n < N_1;$$

$$\dot{B}^{(12)}_{mn} = B_{m,N-n}, \qquad \text{for } 0 \le m < N_1,\ 0 \le n < N_2;$$

$$\dot{B}^{(21)}_{mn} = B_{N-m,n}, \qquad \text{for } 0 \le m < N_2,\ 0 \le n < N_1;$$

and

$$\dot{B}^{(22)}_{mn} = B_{N-m,N-n}, \qquad \text{for } 0 \le m < N_2,\ 0 \le n < N_2. \tag{7.18}$$

Similarly, we use two column matrices $\gamma^{(1)}$ and $\gamma^{(2)}$ defined by

$$\gamma^{(1)}_n = \gamma_n, \qquad \text{for } 0 \le n < N_1,$$

and

$$\gamma^{(2)}_n = \gamma_{N-n}, \qquad \text{for } 0 \le n < N_2. \tag{7.19}$$

Then, by (7.15) and (7.17), $\mathscr{R}$ can be expressed by

$$\mathscr{R} = [(\dot{B}^{(11)} - \dot{B}^{(12)}\dot{B}^{(22)-1}\dot{B}^{(21)})^{-1}\gamma^{(1)} - \dot{B}^{(11)-1}\dot{B}^{(12)}(\dot{B}^{(22)} - \dot{B}^{(21)}\dot{B}^{(11)-1}\dot{B}^{(12)})^{-1}\gamma^{(2)}]_0. \tag{7.20}$$

As seen from (6.3) for example, our expressions contain a rather large number of gamma functions. It is convenient to remove some of these by changing the $\dot{B}$'s slightly. Let

$$\bar{B}^{(11)}_{mn} = \frac{(N-m)!\,\Gamma(N-n+\frac{3}{2})}{\Gamma(N-m+\frac{3}{2})(N-n)!}\,\dot{B}^{(11)}_{mn},$$

$$\bar{B}^{(12)}_{mn} = \frac{N(N-m)!\,\Gamma(N-n+\frac{1}{2})}{\Gamma(N-m+\frac{3}{2})(N-n)!}\,\dot{B}^{(12)}_{mn},$$

$$\bar{B}^{(21)}_{mn} = \frac{N(N-m)!\,\Gamma(N-n+\frac{3}{2})}{\Gamma(N-m+\frac{1}{2})(N-n)!}\,\dot{B}^{(21)}_{mn},$$

and

$$\bar{B}^{(22)}_{mn} = \frac{(N-m)!\,\Gamma(N-n+\frac{1}{2})}{\Gamma(N-m+\frac{1}{2})(N-n)!}\,B^{(22)}_{mn}. \tag{7.21}$$

By (7.5) and (7.18), for large N but fixed m and n, all four $\bar{B}^{(ij)}_{mn}$ are of the order of magnitude 1. The substitution of (7.21) into (7.20) yields

$$\begin{aligned}\mathscr{R} = [(\bar{B}^{(11)} &- N^{-2}\bar{B}^{(12)}\bar{B}^{(22)-1}\bar{B}^{(21)})^{-1}\bar{\gamma}^{(1)} \\ &- N^{-2}\bar{B}^{(11)-1}\bar{B}^{(12)}(\bar{B}^{(22)} - N^{-2}\bar{B}^{(21)}\bar{B}^{(11)-1}\bar{B}^{(12)})^{-1}\bar{\gamma}^{(2)}]_0,\end{aligned} \tag{7.22}$$

where

$$\begin{aligned}\bar{\gamma}^{(1)}_n &= \frac{(N-n)!\,\Gamma(N+\frac{3}{2})}{\Gamma(N-n+\frac{3}{2})N!}\,\gamma^{(1)}_n \\ &= -\frac{1}{2\pi^{1/2}}\frac{\Gamma(n-\frac{1}{2})}{n!},\end{aligned} \tag{7.23}$$

and

$$\begin{aligned}\bar{\gamma}^{(2)}_n &= \frac{(N-n)!\,\Gamma(N+\frac{3}{2})}{\Gamma(N-n+\frac{1}{2})N!}\,\gamma^{(2)}_n \\ &= -\frac{1}{2\pi^{1/2}}\frac{N}{N-n-\frac{1}{2}}\frac{\Gamma(n+\frac{3}{2})}{n!}.\end{aligned} \tag{7.24}$$

Equation (7.22) is to be used for further development in this section. It only remains to write down the numerous $\bar{B}^{(ij)}_{mn}$ explicitly. By (7.12) and (7.4),

$$\begin{aligned}B_{mn} &= \sum_{q=0}^{N}\sum_{p=-\infty}^{\infty} L_{mq}a^{(0)}_{q-p}d_{p-n} \\ &= \sum_{p=-\infty}^{\infty} K_{mp}d_{p-n},\end{aligned} \tag{7.25}$$

where K_{mp} is defined by (6.10). Using (6.11), (6.15) and (6.16), we find

$$\begin{aligned}\bar{B}^{(11)}_{mn} = d'_{mn} &+ \frac{1}{\pi}\sum_{p=-\infty}^{-1}\frac{1}{m-p}\frac{\Gamma(m+\frac{1}{2})\Gamma(\frac{1}{2}-p)}{m!\,(-p-1)!}\,d'_{pn} \\ &+ \frac{1}{\pi}\sum_{p=N+1}^{\infty}\frac{1}{m-p}\frac{\Gamma(m+\frac{1}{2})p!\,\Gamma(p-N-\frac{1}{2})\Gamma(N-n+\frac{3}{2})}{m!\,(p-N-1)!\,\Gamma(p+\frac{1}{2})(N-n)!}\,d_{p-n};\end{aligned} \tag{7.26}$$

$$\begin{aligned}\bar{B}^{(12)}_{mn} = &-\frac{1}{\pi}\sum_{p=-\infty}^{-1}\frac{N}{N-m-p}\frac{\Gamma(m+\frac{1}{2})\Gamma(-p-\frac{1}{2})}{m!\,(-p-1)!}\,d''_{pn} \\ &+ \frac{N(N-m)!\,\Gamma(N-n+\frac{1}{2})}{\Gamma(N-m+\frac{3}{2})(N-n)!}\,d_{m+n-N} \\ &- \frac{1}{\pi}N\sum_{p=N+1}^{\infty}\frac{1}{N-m-p} \\ &\times \frac{\Gamma(m+\frac{1}{2})p!\,\Gamma(p-N+\frac{1}{2})\Gamma(N-n+\frac{1}{2})}{m!\,(p-N-1)!\,\Gamma(p+\frac{3}{2})(N-n)!}\,d_{-p+n};\end{aligned} \tag{7.27}$$

$$\bar{B}_{mn}^{(21)} = \frac{1}{\pi}\sum_{p=-\infty}^{-1}\frac{N}{N-m-p}\,\frac{\Gamma(m+\frac{3}{2})\Gamma(\frac{1}{2}-p)}{m!\,(-p-1)!}\,d'_{pn}$$
$$+\frac{N(N-m)!\,\Gamma(N-n+\frac{3}{2})}{\Gamma(N-m+\frac{1}{2})(N-n)!}\,d_{N-m-n}+\frac{1}{\pi}N\sum_{p=N+1}^{\infty}\frac{1}{N-m-p}$$
$$\times\frac{\Gamma(m+\frac{1}{2})p!\,\Gamma(p-N-\frac{1}{2})\Gamma(N-n+\frac{3}{2})}{m!\,(p-N-1)!\,\Gamma(p+\frac{1}{2})(N-n)!}\,d_{p-n}; \tag{7.28}$$

and

$$\bar{B}_{mn}^{(22)} = d''_{mn}-\frac{1}{\pi}\sum_{p=-\infty}^{-1}\frac{1}{m-p}\,\frac{\Gamma(m+\frac{3}{2})\Gamma(-p-\frac{1}{2})}{m!\,(-p-1)!}\,d''_{pn}$$
$$-\frac{1}{\pi}\sum_{p=N+1}^{\infty}\frac{1}{m-p}\,\frac{\Gamma(m+\frac{3}{2})p!\,\Gamma(p-N+\frac{1}{2})\Gamma(N-n+\frac{1}{2})}{m!\,(p-N-1)!\,\Gamma(p+\frac{3}{2})(N-n)!}$$
$$\times\, d_{-p+n}. \tag{7.29}$$

In (7.26)–(7.29), we have used the notation

$$d'_{pn}=\frac{(N-p)!\,\Gamma(N-n+\frac{3}{2})}{\Gamma(N-p+\frac{3}{2})(N-n)!}\,d_{p-n}$$

and

$$d''_{pn}=\frac{(N-p)!\,\Gamma(N-n+\frac{1}{2})}{\Gamma(N-p+\frac{1}{2})(N-n)!}\,d_{-p+n}. \tag{7.30}$$

(*B*) Asymptotic Expansion of $\mathscr{R}$

So far, no approximation has been made and (7.22) is exact. Since (7.26)–(7.29) are rather complicated, we restrict our attention to asymptotic expansions for large N. As d_n is exponentially small for large $|n|$, (7.26)–(7.29) are much simpler asymptotically. We need to keep only the first two terms in (7.26) and (7.29), and only the first term in (7.27) and (7.28):

$$\bar{B}_{mn}^{(11)} \doteq d'_{mn}+\frac{1}{\pi}\sum_{p=-\infty}^{-1}\frac{1}{m-p}\,\frac{\Gamma(m+\frac{1}{2})\Gamma(\frac{1}{2}-p)}{m!\,(-p-1)!}\,d'_{pn}, \tag{7.31}$$

$$\bar{B}_{mn}^{(12)} \doteq -\frac{1}{\pi}\sum_{p=-\infty}^{-1}\frac{N}{N-m-p}\,\frac{\Gamma(m+\frac{1}{2})\Gamma(-\frac{1}{2}-p)}{m!\,(-p-1)!}\,d''_{pn}, \tag{7.32}$$

$$\bar{B}_{mn}^{(21)} \doteq \frac{1}{\pi}\sum_{p=-\infty}^{-1}\frac{N}{N-m-p}\,\frac{\Gamma(m+\frac{3}{2})\Gamma(\frac{1}{2}-p)}{m!\,(-p-1)!}\,d'_{pn}, \tag{7.33}$$

and

$$\bar{B}_{mn}^{(22)} \doteq d''_{mn}-\frac{1}{\pi}\sum_{p=-\infty}^{-1}\frac{1}{m-p}\,\frac{\Gamma(m+\frac{3}{2})\Gamma(-\frac{1}{2}-p)}{m!\,(-p-1)!}\,d''_{pn}. \tag{7.34}$$

(Strictly speaking, (7.32) is not valid if m is close to N_1 and n close to N_2, and (7.33) is not valid if m is close to N_2 and n close to N_1. However, these elements of the matrices do not contribute to the asymptotic expansion of $\mathscr{R}$.)

Let $\tilde{d}'_{pn}$ and $\tilde{d}''_{pn}$ be respectively the asymptotic series for d'_{pn} and d''_{pn} for large N and fixed p and n. Thus $\tilde{d}'_{pn}$ and $\tilde{d}''_{pn}$ are defined, term by term, for all p and all n. Similarly, let $\tilde{B}^{(ij)}_{mn}$, $i = 1, 2$ and $j = 1, 2$, be the asymptotic series for $\bar{B}^{(ij)}_{mn}$, again for large N and fixed m and n. Thus $\tilde{B}^{(ij)}_{mn}$ is defined, term by term, for all $m \geq 0$ and all $n \geq 0$. We can accordingly form the infinite matrices $\tilde{B}^{(ij)}$, term by term, in powers of N^{-1}. The row and column indices for $\tilde{B}^{(ij)}$ each run from zero to infinity. In the same fashion, we define infinite column matrices $\tilde{\gamma}^{(i)}$ from the $\bar{\gamma}^{(i)}$ of (7.23) and (7.24), again as asymptotic series in N^{-1}. With the help of these infinite matrices and (7.22), we get asymptotically

$$\mathscr{R} \doteq \{(\tilde{B}^{(11)} - N^{-2}\tilde{B}^{(12)}\tilde{B}^{(22)-1}\tilde{B}^{(21)})^{-1}\tilde{\gamma}^{(1)} \\ - N^{-2}\tilde{B}^{(11)-1}\tilde{B}^{(12)}(\tilde{B}^{(22)} - N^{-2}\tilde{B}^{(21)}\tilde{B}^{(11)-1}\tilde{B}^{(12)})^{-1}\tilde{\gamma}^{(2)}\}_0. \tag{7.35}$$

(It is worthwhile to keep in mind that infinite matrices may not be associative.)

Let $\tilde{A}$ be the infinite matrix whose elements are

$$\tilde{A}_{mn} = a^{(0)}_{m-n} = 2/[\pi(2m - 2n + 1)] \tag{7.36}$$

for $m \geq 0$ and $n \geq 0$, and let $\tilde{A}^T$ be the transpose of $\tilde{A}$. We also define

$$\mathscr{B}^{(1)} = \tilde{A}\tilde{B}^{(11)} \tag{7.37}$$

and

$$\mathscr{B}^{(2)} = \tilde{A}^T\tilde{B}^{(22)}. \tag{7.38}$$

Therefore the required matrices $\tilde{B}^{(11)-1}$ and $\tilde{B}^{(22)-1}$ are

$$\tilde{B}^{(11)-1} = \mathscr{B}^{(1)-1}\tilde{A}, \tag{7.39}$$

and

$$\tilde{B}^{(22)-1} = \mathscr{B}^{(2)-1}\tilde{A}^T. \tag{7.40}$$

We proceed to calculate the elements of $\mathscr{B}^{(1)}$ and $\mathscr{B}^{(2)}$. Since, for $p < 0$,

$$\sum_{q=0}^{\infty} \frac{1}{(m - q + \frac{1}{2})(q - p)} \frac{\Gamma(q + \frac{1}{2})}{q!} \\ = \frac{1}{m - p + \frac{1}{2}} \sum_{q=0}^{\infty} \left(\frac{1}{m - q + \frac{1}{2}} + \frac{1}{q - p}\right) \frac{\Gamma(q + \frac{1}{2})}{q!} \\ = \frac{\pi}{m - p + \frac{1}{2}} \frac{\Gamma(-p)}{\Gamma(\frac{1}{2} - p)}, \tag{7.41}$$

we must have

$$\mathscr{B}^{(1)}_{mn} = \frac{2}{\pi}\sum_{p=0}^{\infty}\frac{1}{2m-2p+1}\,\tilde{d}'_{pn} + \frac{2}{\pi}\sum_{p=-\infty}^{-1}\frac{1}{2m-2p+1}\,\tilde{d}'_{pn}$$

$$= \frac{2}{\pi}\sum_{p=-\infty}^{\infty}\frac{1}{2m-2p+1}\tilde{d}'_{pn}. \tag{7.42}$$

Similarly,

$$\mathscr{B}^{(2)}_{mn} = -\frac{2}{\pi}\sum_{p=-\infty}^{\infty}\frac{1}{2m-2p-1}\,\tilde{d}''_{pn}. \tag{7.43}$$

Both (7.42) and (7.43) are to be understood in the sense of term-by-term equality for each power of N^{-1}.

A very similar calculation yields

$$(\tilde{A}\tilde{\gamma}^{(1)})_n = \delta_{n,0}. \tag{7.44}$$

Unlike (7.42) and (7.43), (7.44) does not involve N and hence is exact. With this result (7.35) can be written alternatively in the form

$$\mathscr{R} \doteq \{(1 - N^{-2}\tilde{B}^{(11)-1}\tilde{B}^{(12)}\tilde{B}^{(22)-1}\tilde{B}^{(21)})^{-1}\mathscr{B}^{(1)-1}\}_{00} - N^{-2}$$

$$\times\,\{\tilde{B}^{(11)-1}\tilde{B}^{(12)}(1 - N^{-2}\tilde{B}^{(22)-1}\tilde{B}^{(21)}\tilde{B}^{(11)-1}\tilde{B}^{(12)})^{-1}\tilde{B}^{(22)-1}\tilde{\gamma}^{(2)}\}_0. \tag{7.45}$$

We have kept the entire asymptotic series so far. From here on, we shall keep only enough terms to get (7.1). For this more limited purpose, we write

$$\mathscr{R} \sim \mathscr{R}_1 + \mathscr{R}_2 + \mathscr{R}_3, \tag{7.46}$$

where

$$\mathscr{R}_1 = (\mathscr{B}^{(1)-1})_{00}, \tag{7.47}$$

$$\mathscr{R}_2 = N^{-2}\{\tilde{B}^{(11)-1}\tilde{B}^{(12)}\tilde{B}^{(22)-1}\tilde{B}^{(21)}\mathscr{B}^{(1)-1}\}_{00}, \tag{7.48}$$

and

$$\mathscr{R}_3 = -N^{-2}\{\tilde{B}^{(11)-1}\tilde{B}^{(12)}\tilde{B}^{(22)-1}\tilde{\gamma}^{(2)}\}_0. \tag{7.49}$$

We need to calculate each of these three $\mathscr{R}$'s to the accuracy N^{-3} for large N.

It is useful to note, in connection with (7.42) and (7.43), that it follows from (7.30) that

$$\tilde{d}'_{pn} = d_{p-n}[1 + \tfrac{1}{2}\bar{N}^{-1}(p-n) + O(N^{-2})],$$

and

$$\tilde{d}''_{pn} = d_{-p+n}[1 - \tfrac{1}{2}\bar{N}^{-1}(p-n) + O(N^{-2})], \tag{7.50}$$

where

$$\bar{N} = N + O(1). \tag{7.51}$$

We therefore define an infinite matrix $\mathscr{B}$, for $m \geq 0$ and $n \geq 0$, by

$$\mathscr{B}_{mn} = \frac{2}{\pi} \sum_{p=-\infty}^{\infty} \frac{1}{2m - 2p + 1} d_{p-n}[1 + \tfrac{1}{2}\bar{N}^{-1}(p - n)]. \tag{7.52}$$

Thus, to order N^{-1},

$$\mathscr{B}^{(1)} \sim \mathscr{B} \quad \text{and} \quad \mathscr{B}^{(2)} \sim \mathscr{B}^{T}. \tag{7.53}$$

This approximation (7.53) may be used in (7.48) and (7.49) for the purposes of obtaining $\mathscr{R}_2$ and $\mathscr{R}_3$, but is not accurate enough for $\mathscr{R}_1$ as given by (7.47).

(*C*) Approximate Calculation of $\mathscr{B}^{-1}$

Let

$$\mathscr{S} = \mathscr{B}^{-1}. \tag{7.54}$$

Since, by (7.52), $\mathscr{B}_{mn}$ depends only on $m - n$, we may compute $\mathscr{S}$ again by the method of Wiener and Hopf. Define $C(\xi)$ for $|\xi| = 1$ such that

$$\mathscr{B}_{mn} = \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-i(m-n)\theta} C(e^{i\theta}), \tag{7.55}$$

then

$$C(\xi) = \frac{i}{\xi^{1/2}} \left(\frac{1 - \alpha_1\xi}{1 - \alpha_1/\xi}\right)^{1/2} \left[1 - \frac{\alpha_1}{4\bar{N}} \frac{\xi - 2\alpha_1 + 1/\xi}{(1 - \alpha_1\xi)(1 - \alpha_1/\xi)}\right]. \tag{7.56}$$

Let

$$\begin{aligned} \alpha_1' = \frac{1}{2\alpha_1} \frac{1}{1 + \frac{1}{4}\bar{N}^{-1}} (1 &+ \alpha_1^2(1 + \tfrac{1}{2}\bar{N}^{-1}) \\ &- \{[1 + \alpha_1^2(1 + \tfrac{1}{2}\bar{N}^{-1})]^2 - 4\alpha_1^2(1 + \tfrac{1}{4}\bar{N}^{-1})^2\}^{1/2}), \end{aligned} \tag{7.57}$$

then

$$C(\xi) = \frac{i}{\xi^{1/2}} \left(\frac{1 - \alpha_1\xi}{1 - \alpha_1/\xi}\right)^{1/2} \mathscr{C} \left(\frac{1 - \alpha_1'\xi}{1 - \alpha_1'/\xi}\right) \left(\frac{\xi - \alpha_1'}{\xi - \alpha_1}\right), \tag{7.58}$$

where

$$\mathscr{C} = \alpha_1(1 + \tfrac{1}{4}\bar{N}^{-1})/\alpha_1'. \tag{7.59}$$

Suppose that we define P and Q on the basis of (2.17) using this $C(\xi)$ of (7.58), then one possible choice is

$$P(\xi) = (1 - \xi)^{1/2} \frac{(1 - \alpha_1\xi)^{1/2}}{1 - \alpha_1'\xi}, \tag{7.60}$$

and

$$Q(\xi) = \mathscr{C}^{-1} \frac{1}{(1 - \xi)^{1/2}} \frac{(1 - \alpha_1\xi)^{3/2}}{1 - \alpha_1'\xi}. \tag{7.61}$$

When $\bar{N}\to\infty$, the constant $\mathscr{C}$ is found to be

$$\mathscr{C} = 1 - \frac{1}{16}\frac{\alpha_1^2}{1-\alpha_1^2}\bar{N}^{-2} - \frac{1}{32}\frac{\alpha_1^4}{(1-\alpha_1^2)^2}\bar{N}^{-3} + O(N^{-4}). \tag{7.62}$$

By (7.54), the elements of the matrix $\mathscr{S}$ satisfy

$$\sum_{m=0}^{\infty}\mathscr{B}_{pm}\mathscr{S}_{mn} = \delta_{p,n} \tag{7.63}$$

and

$$\sum_{n=0}^{\infty}\mathscr{S}_{mn}\mathscr{B}_{np} = \delta_{m,p}. \tag{7.64}$$

Both of these equations can be solved by the method of Wiener and Hopf and the results are, using the notation of Sec. 2 with (7.60) and (7.61),

$$\sum_{m=0}^{\infty}\mathscr{S}_{mn}\xi^m = \mathscr{C}^{-1}(1-\xi)^{1/2}\frac{(1-\alpha_1\xi)^{1/2}}{1-\alpha_1'\xi}\left[\frac{\xi^n}{(\xi-1)^{1/2}}\frac{(\xi-\alpha_1)^{3/2}}{\xi-\alpha_1'}\right]_+ \tag{7.65}$$

and

$$\sum_{n=0}^{\infty}\mathscr{S}_{mn}\xi^n = \mathscr{C}^{-1}\frac{1}{(1-\xi)^{1/2}}\frac{(1-\alpha_1\xi)^{3/2}}{1-\alpha_1'\xi}\left[\xi^m(\xi-1)^{1/2}\frac{(\xi-\alpha_1)^{1/2}}{\xi-\alpha_1'}\right]_+. \tag{7.66}$$

Equations (7.65) and (7.66) are of course merely different versions of the same formula. A more symmetrical way to write this result is as follows. Let

$$P(\xi) = \sum_{n=0}^{\infty}p_n\xi^n \qquad\text{and}\qquad Q(\xi) = \sum_{n=0}^{\infty}q_n\xi^n \tag{7.67}$$

for $|\xi| < 1$; then

$$\mathscr{S}_{mn} = \sum_{j=0}^{\min(m,n)}p_{m-j}q_{n-j}. \tag{7.68}$$

In particular, it follows from (7.62) that

$$\mathscr{S}_{00} = \mathscr{C}^{-1} = 1 + \frac{1}{16}\frac{\alpha_1^2}{1-\alpha_1^2}\bar{N}^{-2} + \frac{1}{32}\frac{\alpha_1^4}{(1-\alpha_1^2)^2}\bar{N}^{-3} + O(N^{-4}). \tag{7.69}$$

(*D*) Approximate Calculation of $\mathscr{R}_1$

In order to obtain $\mathscr{R}_1$ of (7.47) to the accuracy N^{-3}, we need a formula for $\tilde{d}'_{pn}$ more accurate than (7.50). Since, for $z\to\infty$,

$$\frac{\Gamma(z+\frac{3}{2})}{\Gamma(z+1)} = (z+\tfrac{3}{4})^{1/2}\left[1 + \frac{1}{64}\frac{1}{(z+\frac{3}{4})^2} + O(z^{-4})\right], \tag{7.70}$$

we have from (7.30), for $N \to \infty$,

$$d'_{pn} = d_{p-n}\left(\frac{N + \frac{3}{4} - n}{N + \frac{3}{4} - p}\right)^{1/2}[1 + \tfrac{1}{32}N^{-3}(n - p) + O(N^{-4})]$$

$$= d_{p-n}\left(\frac{\bar{N} - n}{\bar{N} - p}\right)^{1/2}[1 + O(N^{-4})], \tag{7.71}$$

provided that

$$\bar{N} = N + \tfrac{3}{4} + \tfrac{1}{16}N^{-1}. \tag{7.72}$$

On the other hand, note that the term $\bar{N}^{-1}$ is missing on the right-hand side of (7.69). Thus it is sufficient, for the purpose of obtaining (7.1), to use

$$\bar{N} = N + \tfrac{3}{4}. \tag{7.73}$$

By (7.71), (7.42), and (7.52), we have, to the required accuracy,

$$\mathscr{B}^{(1)} \sim \mathscr{B} + \mathscr{B}', \tag{7.74}$$

where

$$\mathscr{B}'_{mn} = \frac{2}{\pi}\sum_{p=-\infty}^{\infty}\frac{1}{2m - 2p + 1}\, d_{p-n}(p - n)\tfrac{1}{8}\bar{N}^{-2}$$

$$\times\ [(3p + n) + \tfrac{1}{2}\bar{N}^{-1}(5p^2 + 2pn + n^2)]. \tag{7.75}$$

Therefore, the required $\mathscr{R}_1$ is

$$\mathscr{R}_1 \sim \mathscr{S}_{00} - \{(\mathscr{S}\mathscr{B}')\mathscr{S}\}_{00}. \tag{7.76}$$

Since $\mathscr{S}_{00}$ is given by (7.69), we concentrate on the second term here.

Let

$$\mathscr{T}_p = \frac{2}{\pi}\sum_{n=0}^{\infty}\frac{\mathscr{S}_{0n}}{(2n - 2p + 1)} \tag{7.77}$$

for all integers p, then

$$\mathscr{R}_1 \sim \mathscr{S}_{00} - \tfrac{1}{8}\bar{N}^{-2}\sum_{p=-\infty}^{\infty}\sum_{m=0}^{\infty}\mathscr{T}_p d_{p-m}(p - m)$$

$$\times\ [(3p + m) + \tfrac{1}{2}\bar{N}^{-1}(5p^2 + 2pm + m^2)]\mathscr{S}_{m0}. \tag{7.78}$$

Since, by (7.66), the generating function for $\mathscr{S}_{0n}$ is

$$\sum_{n=0}^{\infty}\mathscr{S}_{0n}\xi^n = \mathscr{C}^{-1}\frac{1}{(1 - \xi)^{1/2}}\frac{(1 - \alpha_1\xi)^{3/2}}{1 - \alpha'_1\xi}, \tag{7.79}$$

$\mathscr{T}_p$ is generated by

$$\sum_{p=-\infty}^{\infty}\mathscr{T}_p\xi^p = \mathscr{C}^{-1}\left(\frac{\xi}{\xi - 1}\right)^{1/2}\frac{(1 - \alpha_1\xi)^{3/2}}{1 - \alpha'_1\xi}. \tag{7.80}$$

The point of greatest importance here is that, whereas the right-hand side of (7.79) has a branch cut from 1 to infinity, the right-hand side of (7.80) is *analytic in the region*

$$1 < |\xi| < 1/\alpha_1'. \tag{7.81}$$

Accordingly,

$$\mathscr{T}_p \to 0 \tag{7.82}$$

exponentially as $p \to +\infty$, and

$$\mathscr{T}_{-p} = (2\pi i\mathscr{C})^{-1} \oint_- d\xi\xi^{-p-1}\xi^{-1/2}(1-\xi)^{-1/2}(\xi-\alpha_1)^{3/2}(\xi-\alpha_1')^{-1}, \tag{7.83}$$

where $\oint_-$ denotes a contour integral in the counterclockwise direction along a circular path of radius between α_1' and 1. Note that the integrand in (7.83) is positive for $\alpha_1' < \xi < 1$.

With (7.65) and (7.83), the evaluation of $\mathscr{R}_1$ by (7.78) is straightforward but tedious. By (7.50), it is convenient to rewrite (7.78) in the form

$$\begin{aligned}\mathscr{R}_1 \sim \mathscr{S}_{00} - \tfrac{1}{8}\bar{N}^{-2} \sum_{p=-\infty}^{\infty} \sum_{m=0}^{\infty} \mathscr{T}_p\{d_{p-m}[1 + \tfrac{1}{2}\bar{N}^{-1}(p-m)]\} \\ \times \{(p-m)[(3p+m) + \bar{N}^{-1}(p+m)^2]\}\mathscr{S}_{m0}.\end{aligned} \tag{7.84}$$

Let

$$\begin{aligned}\mathscr{G}_1(\xi) &= \xi^{-1/2}(1-\xi)^{-1/2}(\xi-\alpha_1)^{3/2}(\xi-\alpha_1')^{-1} \\ &= \sum_{p=-\infty}^{\infty} \mathscr{C}\mathscr{T}_{-p}\xi^p,\end{aligned} \tag{7.85}$$

$$\begin{aligned}\mathscr{G}_2(\xi) &= \xi^{1/2}(1-\alpha_1\xi)^{-1/2}(1-\alpha_1'\xi)(\xi-\alpha_1)^{-3/2}(\xi-\alpha_1') \\ &= \sum_{p=-\infty}^{\infty} d_p(1+\tfrac{1}{2}\bar{N}^{-1}p)\xi^p,\end{aligned} \tag{7.86}$$

and

$$\begin{aligned}\mathscr{G}_3(\xi) &= (1-\xi)^{1/2}(1-\alpha_1\xi)^{1/2}(1-\alpha_1'\xi)^{-1} \\ &= \sum_{m=0}^{\infty} \mathscr{C}\mathscr{S}_{m0}\xi^m.\end{aligned} \tag{7.87}$$

Then (7.84) is equivalent to

$$\begin{aligned}\mathscr{R}_1 \sim \mathscr{S}_{00} - \tfrac{1}{8}\bar{N}^{-2}\frac{1}{2\pi i}\oint_- \frac{d\xi}{\xi} \\ \times [(2\mathscr{G}_1''\mathscr{G}_2\mathscr{G}_3 + \mathscr{G}_1\mathscr{G}_2''\mathscr{G}_3) - \tfrac{1}{3}\bar{N}^{-1}(4\mathscr{G}_1'''\mathscr{G}_2\mathscr{G}_3 + \mathscr{G}_1\mathscr{G}_2'''\mathscr{G}_3)],\end{aligned} \tag{7.88}$$

where each prime means $\xi\, d/d\xi$. In obtaining (7.88), we have made use of the fact that $\mathscr{G}_3(\xi)$ is analytic inside the unit circle. The various functions have been chosen in such a way that

$$\mathscr{G}_1(\xi)\mathscr{G}_2(\xi)\mathscr{G}_3(\xi) = 1. \tag{7.89}$$

Because of (7.89), the evaluation of the right-hand side of (7.88) is not difficult with the help of the formulas

$$\oint_{-} (d\xi/\xi)\mathscr{G}_i^{-1}\mathscr{G}_i'' = \oint_{-} \xi\, d\xi(d \ln \mathscr{G}_i/d\xi)^2,$$

and

$$\oint_{-} (d\xi/\xi)\mathscr{G}_i^{-1}\mathscr{G}_i''' = \oint_{-} \xi^2\, d\xi(d \ln \mathscr{G}_i/d\xi)^3, \tag{7.90}$$

for $i = 1, 2$. By (7.62) and (7.73), the result for $\mathscr{R}_1$ is

$$\begin{aligned}\mathscr{R}_1 &= 1 - \frac{1}{8}\bar{N}^{-2}\frac{\alpha_1}{1-\alpha_1} + \frac{1}{16}\bar{N}^{-3}\alpha_1\frac{1+2\alpha_1}{(1-\alpha_1)^2} + O(N^{-4}) \\ &= 1 - \frac{1}{8}N^{-2}\frac{\alpha_1}{1-\alpha_1} + \frac{1}{16}N^{-3}\alpha_1\frac{4-\alpha_1}{(1-\alpha_1)^2} + O(N^{-4}).\end{aligned} \tag{7.91}$$

(*E*) Approximate Calculation of $\mathscr{R}_3$

Let

$$\rho_n = -\frac{1}{2\pi^{1/2}}\frac{N}{N-n+\frac{1}{2}}\frac{\Gamma(n+\frac{1}{2})}{n!}, \tag{7.92}$$

and

$$\tau_n = \frac{2}{\pi^{1/2}}\sum_{p=-\infty}^{-1}\frac{1}{(-p-1)!}\Gamma(-p-\tfrac{1}{2})[1+N^{-1}(p+\tfrac{1}{2})]\tilde{d}''_{pn}; \tag{7.93}$$

then by (7.32), to the required accuracy, for fixed $m \geq 0$ and $n \geq 0$,

$$\bar{B}^{(12)}_{mn} \sim \rho_m\tau_n. \tag{7.94}$$

Let ρ be the infinite column matrix with elements ρ_n, and τ be the infinite row matrix with elements τ_n; then by (7.49)

$$\mathscr{R}_3 \sim -N^{-2}\mathscr{R}_3'\mathscr{R}_3'', \tag{7.95}$$

where

$$\mathscr{R}_3' = (\tilde{B}^{(11)-1}\rho)_0 \tag{7.96}$$

and

$$\mathscr{R}_3'' = \tau\tilde{B}^{(22)-1}\tilde{\gamma}^{(2)}. \tag{7.97}$$

Because of (7.96), for the purpose of computing $\mathscr{R}_3$, we need, by (7.39), (7.53), and (7.54),

$$(\tilde{B}^{(11)-1})_{0n} = \sum_{m=0}^{\infty}(\mathscr{B}^{(1)-1})_{0m}a^{(0)}_{m-n} \sim \sum_{m=0}^{\infty}\mathscr{S}_{0m}a^{(0)}_{m-n}. \tag{7.98}$$

Accordingly, by (7.66), $(\tilde{B}^{(11)-1})_{0n}$ are generated approximately by

$$\sum_{n=-\infty}^{\infty}(\tilde{B}^{(11)-1})_{0n}\xi^n \sim \left(\frac{\xi}{\xi-1}\right)^{1/2}\frac{(1-\alpha_1\xi)^{3/2}}{1-\alpha_1'\xi}. \tag{7.99}$$

We note that the right-hand side of (7.99) is analytic in the region (7.81). On the other hand, ρ_n are generated by, also approximately,

$$\sum_{n=0}^{\infty}\rho_n\xi^n \sim -\frac{1}{2}\frac{1-N^{-1}}{(1-\xi)^{1/2}}\left(1+\frac{1}{2}\frac{N^{-1}}{1-\xi}\right), \tag{7.100}$$

which is analytic in the unit circle. A straightforward calculation from (7.96), (7.99), and (7.100) then gives

$$\mathscr{R}_3' \sim -\frac{1}{2}(1-N^{-1})\frac{1}{2\pi i}\oint_+\frac{d\xi}{\xi-1}\frac{(1-\alpha_1\xi)^{3/2}}{1-\alpha_1'\xi}\left(1+\frac{1}{2}N^{-1}\frac{\xi}{\xi-1}\right), \tag{7.101}$$

where $\oint_+$ denotes a contour integration in the counterclockwise direction along a circular path lying in the region (7.81), and hence

$$\mathscr{R}_3' \sim -\tfrac{1}{2}(1-\alpha_1)^{1/2}(1-\tfrac{1}{2}N^{-1}) \tag{7.102}$$

as $N \to \infty$ with an error of order N^{-2}.

We proceed to calculate $\mathscr{R}_3''$. By (7.97), (7.40), and (7.53),

$$\mathscr{R}_3'' \sim (\tau\mathscr{S}^T\tilde{A}^T)\tilde{\gamma}^{(2)}. \tag{7.103}$$

It follows from (7.50) and (7.93) that the τ_n are generated approximately by

$$\sum_{n=-\infty}^{\infty}\tau_n\xi^{-n} \sim 2\frac{\xi}{(1-\xi)^{1/2}(1-\alpha_1\xi)^{3/2}}\frac{(1-\alpha_1'\xi)(1-\alpha_1'/\xi)}{(1-\alpha_1/\xi)^{1/2}} \times\left(1-\frac{1}{2}N^{-1}\frac{1}{1-\xi}\right). \tag{7.104}$$

Hence, by (7.66), (7.60), and (7.67), for $|\zeta| \le 1$,

$$\begin{aligned}\sum_{n=0}^{\infty}(\tau\mathscr{S}^T)_n\zeta^n &\sim \frac{1}{\pi i}\oint_-\frac{d\xi}{1-\xi}\frac{1-\alpha_1'/\xi}{(1-\alpha_1/\xi)^{1/2}}\left(1-\frac{1}{2}N^{-1}\frac{1}{1-\xi}\right)\\ &\quad\times\sum_{n=0}^{\infty}\zeta^n\sum_{m=0}^{\infty}\rho_m\xi^{n-m}\\ &=\frac{1}{\pi i}\oint_-\frac{d\xi}{1-\xi}\frac{1-\alpha_1'/\xi}{(1-\alpha_1/\xi)^{1/2}}\left(1-\frac{1}{2}N^{-1}\frac{1}{1-\xi}\right)\\ &\quad\times\frac{(1-\zeta)^{1/2}(1-\alpha_1\zeta)^{1/2}}{(1-\xi\zeta)(1-\alpha_1'\zeta)}\\ &=\frac{2}{(1-\zeta)^{1/2}}\left[\frac{1-\alpha_1'}{(1-\alpha_1)^{1/2}}\frac{(1-\alpha_1\zeta)^{1/2}}{1-\alpha_1'\zeta}-1\right.\\ &\quad\left.-\frac{1}{2}N^{-1}\frac{\zeta}{1-\zeta}\right].\end{aligned} \tag{7.105}$$

On the other hand, by (7.24), $\tilde{\gamma}_n^{(2)}$ are generated approximately by

$$\sum_{n=0}^{\infty} \tilde{\gamma}_n^{(2)} \xi^{-n} \sim -\frac{1}{4}(1 - N^{-1})\left(\frac{\xi}{\xi - 1}\right)^{3/2}\left(1 + \frac{3}{2}N^{-1}\frac{\xi}{\xi - 1}\right) \tag{7.106}$$

for $|\xi| > 1$. The substitution of (7.105) and (7.106) in (7.103) gives, after some algebraic simplication very similar to that encountered previously,

$$\mathscr{R}_3'' \sim \frac{1}{4}\frac{\alpha_1}{1 - \alpha_1}\left(1 + \frac{1}{2}N^{-1}\frac{1 + 2\alpha_1}{1 - \alpha_1}\right). \tag{7.107}$$

And the substitution of (7.102) and (7.107) in (7.95) yields

$$\mathscr{R}_3 \sim \frac{1}{8}N^{-2}\frac{\alpha_1}{(1 - \alpha_1)^{1/2}}\left(1 + \frac{3}{2}N^{-1}\frac{\alpha_1}{1 - \alpha_1}\right), \tag{7.108}$$

again for $N \to \infty$ with an error of order N^{-4}.

(*F*) Approximate Calculation of $\mathscr{R}_2$

Let

$$\bar{\tau}_n = -\frac{2}{\pi^{1/2}}\sum_{p=-\infty}^{-1}\frac{1}{(-p - 1)!}\Gamma(\tfrac{1}{2} - p)[1 + N^{-1}(p - \tfrac{1}{2})]\tilde{d}'_{pn}, \tag{7.109}$$

which is similar to (7.93); then, by (7.33) and (7.24), we get to the required accuracy, for fixed $m \geq 0$ and $n \geq 0$,

$$\bar{B}_{mn}^{(21)} \sim \bar{\gamma}_m^{(2)}\bar{\tau}_n. \tag{7.110}$$

The substitution of (7.110) in (7.48) gives, because of (7.49),

$$\mathscr{R}_2 \sim -\mathscr{R}_3(\bar{\tau}\mathscr{B}^{(1)-1})_0, \tag{7.111}$$

where $\bar{\tau}$, like τ, is an infinite row matrix whose elements are the $\bar{\tau}_n$ of (7.109) for $n \geq 0$.

The computation of $(\bar{\tau}\mathscr{B}^{(1)-1})_0$ is again based on the method of generating functions and contains no new feature. The result is

$$(\bar{\tau}\mathscr{B}^{(1)-1})_0 \sim 1 - \frac{1}{(1 - \alpha_1)^{1/2}} + N^{-1}\frac{\alpha_1}{(1 - \alpha_1)^{3/2}}. \tag{7.112}$$

When (7.112) is used together with (7.108) in (7.111), we get

$$\begin{aligned}\mathscr{R}_2 + \mathscr{R}_3 &\sim \mathscr{R}_3\left[\frac{1}{(1 - \alpha_1)^{1/2}} - N^{-1}\frac{\alpha_1}{(1 - \alpha_1)^{3/2}}\right] \\ &\sim \frac{1}{8}N^{-2}\frac{\alpha_1}{1 - \alpha_1}\left(1 + \frac{1}{2}N^{-1}\frac{\alpha_1}{1 - \alpha_1}\right).\end{aligned} \tag{7.113}$$

All square roots have disappeared.

FUNCTIONS $\langle\sigma_{0,0}\,\sigma_{0,N}\rangle$ AND $\langle\sigma_{0,0}\,\sigma_{N,N}\rangle$ FOR LARGE N

(G) Final Result

It only remains to substitute (7.91) and (7.113) in (7.46) to find that, as $N \to \infty$,

$$\mathscr{R} = 1 + \frac{1}{4} N^{-3} \frac{\alpha_1}{(1 - \alpha_1)^2} + O(N^{-4}). \tag{7.114}$$

It is difficult not to be impressed by the remarkable amount of cancellation. We now recall the definition of $\mathscr{R}$ as given by (7.11) and we find that

$$\frac{S_N}{S_N^{(0)}} = \text{const}\left[1 + \frac{1}{8} N^{-2} \frac{\alpha_1}{(1 - \alpha_1)^2} + O(N^{-3})\right] \tag{7.115}$$

for $N \to \infty$. The multiplicative constant is then found to be

$$\left(\frac{1 + \alpha_1}{1 - \alpha_1}\right)^{1/4} \tag{7.116}$$

on the basis of (5.8). The required result (7.1) is just (7.115) with (7.116).

CHAPTER XII
Asymptotic Expansion of $\langle \sigma_{0,0}\sigma_{M,N} \rangle$

1. INTRODUCTION[1]

In the previous chapter we studied for fixed T the asymptotic behavior of $\langle \sigma_{0,0}\sigma_{0,N} \rangle$ and $\langle \sigma_{0,0}\sigma_{N,N} \rangle$ as $N \to \infty$. In this chapter we shall give the asymptotic form of the correlation function $\langle \sigma_{0,0}\sigma_{M,N} \rangle$ for arbitrary M and N when $M^2 + N^2$ is large. Since the case $M = 0$ or $N = 0$ is already treated in Chapter XI, we shall, without loss of generality, assume both M and N to be positive. As in Chapter XI, we have to treat the three cases $T < T_c$, $T > T_c$, and $T = T_c$, separately. We shall, however, give the asymptotic form of the correlation function only for the cases $T < T_c$ and $T > T_c$, where the results in Chapter XI can be regarded as a special case of those here. The asymptotic form of $\langle \sigma_{0,0}\sigma_{M,N} \rangle$ for arbitrary M and N at $T = T_c$ cannot be given because it is not known.

The computations involved in this chapter are more complicated than the corresponding calculations for $T < T_c$ and $T > T_c$ of the previous chapter. The reason is that the correlation function cannot be expressed as a Toeplitz determinant. Furthermore, the final expressions of $\langle \sigma_{0,0}\sigma_{M,N} \rangle$ for $T < T_c$ and $T > T_c$ are quite messy.

We conclude this chapter with a discussion of the more qualitative aspects of the correlation function computed in this and the previous chapter. In particular, we make comparisons with the boundary correlation functions of Chapter VII and speculate about some of those aspects of the correlation functions we have been unable to compute explicitly, such as the behavior of the magnetic susceptibility as $T \to T_c$.

1. This chapter is based on the work of H. Cheng and T. T. Wu, *Phys. Rev.* **164**, 719 (1967).

2. THE CORRELATION $\langle\sigma_{0,0}\sigma_{M,N}\rangle$

Let us consider a two-dimensional Ising lattice with $2\mathscr{M} \times 2\mathscr{N}$ lattice sites. The lattice sites at the boundary are assumed to join in such a way that $(0, -\mathscr{N}+1)$ and $(M, \mathscr{N})$ are nearest neighbors. More precisely, we assume $\mathscr{M}$ to be a multiple of M, and take the Hamiltonian to be

$$-E_1 \sum_{m=-\mathscr{M}+1}^{\mathscr{M}} \left[\sigma_{m,-\mathscr{N}+1}\sigma_{m+M,\mathscr{N}} + \sum_{n=-\mathscr{N}+1}^{\mathscr{N}-1} \sigma_{m,n}\sigma_{m,n+1}\right] - E_2 \sum_{m=-\mathscr{M}+1}^{\mathscr{M}} \sum_{n=-\mathscr{N}+1}^{\mathscr{N}} \sigma_{m,n}\sigma_{m+1,n}, \tag{2.1}$$

where we remind the reader that without loss of generality E_1 and E_2 have been taken to be positive. In (2.1), $\sigma_{m,n}$ is to be interpreted as $\sigma_{m-2\mathscr{M},n}$ when $m > \mathscr{M}$.

Note that our Hamiltonian as given by (2.1) is *dependent* on M. That is, we are here proposing to calculate the spin-spin correlation function $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ with a Hamiltonian which varies with M. Strictly speaking, this is not the Ising model. However, the dependence on M comes from the boundary terms only. It is our hope that, as $\mathscr{M}, \mathscr{N} \to \infty$, the "boundary effects" vanish, and that the correlation function we obtain agrees with that of the Ising model. It is inconceivable to us that such artificial alteration of the Hamiltonian is inherently necessary for the analysis of the Ising model. In other words, we believe the present difficulty with the boundary effects to be entirely due to imperfections in our calculational procedure. Unfortunately, despite all of our efforts, we have not been able to find a simpler method.

In order to understand this particular way of joining the boundaries, we evaluate the free energy for the Ising model on the basis of (2.1) and verify that there is no dependence on M in the limit $\mathscr{M} \to \infty$ and $\mathscr{N} \to \infty$. The partition function Z is given by

$$Z^2 = (2\cosh\beta E_1 \cosh\beta E_2)^{8\mathscr{M}\mathscr{N}} \det A, \tag{2.2}$$

where A is the same matrix as the one given by (VIII.2.3) except that here

$$A(m+M, \mathscr{N}; m, -\mathscr{N}+1) = \begin{bmatrix} 0 & z_1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \tag{2.3}$$

$$A(m, -\mathscr{N}+1; m+M, \mathscr{N}) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ -z_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \tag{2.4}$$

and

$$A(m, -\mathcal{N}+1; m, \mathcal{N}) = A(m, \mathcal{N}; m, -\mathcal{N}+1) = 0. \tag{2.5}$$

The value of det A can be found in the following way. Define the $4M \times 4M$ matrices $\bar{A}(\bar{m}, n; \bar{m}', n')$, where $\bar{m}, \bar{m}' = -M^{-1}\mathcal{M} + 1, -M^{-1}\mathcal{M} + 2, \ldots, M^{-1}\mathcal{M} - 1, M^{-1}\mathcal{M}$ and $n, n' = -\mathcal{N} + 1, \ldots, \mathcal{N} - 1, \mathcal{N}$, by the matrix elements, with $j, j' = 0, 1, \ldots, M - 1$,

$$[\bar{A}(\bar{m}, n; \bar{m}', n')]_{j,j'} = A(M\bar{m} + j, n; M\bar{m}' + j', n'). \tag{2.6}$$

Note that both sides of (2.6) are 4×4 matrices. We shall order these $4M \times 4M$ matrices $\bar{A}$ by the index

$$l = n - 2\mathcal{N}\bar{m}, \tag{2.7}$$

which runs from $-2M^{-1}\mathcal{M}\mathcal{N} - \mathcal{N} + 1$ to $2M^{-1}\mathcal{M}\mathcal{N} - \mathcal{N}$. Because of these limits, it is convenient to extend l periodically. With this convention, by (2.1) $\bar{A}(\bar{m}, n; \bar{m}', n')$ really depends only on $l - l'$; that is,

$$\bar{A}(\bar{m}, n; \bar{m}', n') = \bar{A}_{l-l'}, \tag{2.8}$$

with

$$\bar{A}_{l+P} = \bar{A}_l, \tag{2.9}$$

where $P = 4M^{-1}\mathcal{M}\mathcal{N}$. By rearrangement of the rows and columns, the original matrix A can be written

$$\begin{bmatrix} \bar{A}_0 & \bar{A}_1 & \bar{A}_2 & \cdots & \bar{A}_{P-1} \\ \bar{A}_{-1} & \bar{A}_0 & \bar{A}_1 & \cdots & \bar{A}_{P-2} \\ \bar{A}_{-2} & \bar{A}_{-1} & \bar{A}_0 & \cdots & \bar{A}_{P-3} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \bar{A}_{-P+1} & \bar{A}_{-P+2} & \bar{A}_{-P+3} & \cdots & \bar{A}_0 \end{bmatrix}. \tag{2.10}$$

By (2.9) this is a cyclic matrix. Thus its determinant is easily found to be

$$\det A = \prod_{l=0}^{P-1} \det \lambda^{(l)}, \tag{2.11}$$

where $\lambda^{(l)}$ is the $4M \times 4M$ matrix

$$\lambda^{(l)} = \sum_{l'=0}^{P-1} A_{l'} \exp(i2\pi l l'/P). \tag{2.12}$$

It remains to evaluate det $\lambda^{(l)}$. Equation (2.12) is more explicitly

$$(\lambda^{(l)})_{jj'} = \sum_{n'=-\mathcal{N}+1}^{\mathcal{N}} \sum_{\bar{m}'=-M^{-1}\mathcal{M}+1}^{M^{-1}\mathcal{M}} A(M\bar{m}' + j, n'; j', 0) \times \exp[2\pi i l(n' - 2\mathcal{N}\bar{m}')/P]. \tag{2.13}$$

Since $A(\alpha, \beta; \alpha', \beta')$ depends only on $\alpha - \alpha'$ and $\beta - \beta'$, $\lambda^{(l)}$ is a Toeplitz matrix. Therefore we may define

$$(\lambda^{(l)})_{jj'} = \lambda^{(l)}_{j-j'}, \tag{2.14}$$

Furthermore, from (2.13), we have

$$\lambda^{(l)}_{-j} = \lambda^{(l)}_{M-j} \exp(-i\theta), \tag{2.15}$$

where

$$\theta = \pi Ml/\mathscr{M}. \tag{2.16}$$

The matrix $\lambda^{(l)}$ can therefore be written

$$\begin{bmatrix} \lambda^{(l)}_0 & \lambda^{(l)}_1 & \lambda^{(l)}_2 & \cdots & \lambda^{(l)}_{M-1} \\ e^{-i\theta}\lambda^{(l)}_{M-1} & \lambda^{(l)}_0 & \lambda^{(l)}_1 & \cdots & \lambda^{(l)}_{M-2} \\ e^{-i\theta}\lambda^{(l)}_{M-2} & e^{-i\theta}\lambda^{(l)}_{M-1} & \lambda^{(l)}_0 & \cdots & \lambda^{(l)}_{M-3} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ e^{-i\theta}\lambda^{(l)}_1 & e^{-i\theta}\lambda^{(l)}_2 & e^{-i\theta}\lambda^{(l)}_3 & \cdots & \lambda^{(l)}_0 \end{bmatrix}. \tag{2.17}$$

This Toeplitz matrix is neither cyclic nor near-cyclic. However, the technique used in Sec. 6 of Chapter IV to evaluate the determinant of a cyclic and of a nearly cyclic matrix may still be applied and we find that

$$\det \lambda^{(l)} = \prod_{j=0}^{M-1} \det \lambda^{(l)}(j) \tag{2.18}$$

where

$$\lambda^{(l)}(j) = \sum_{j'=0}^{M-1} \lambda^{(l)}_{j'} \exp[i(2\pi j - \theta)j'/M]. \tag{2.19}$$

Substituting (2.13) and (2.14) in (2.19), and taking care of the fact that $A(\alpha, \beta; \alpha', \beta')$ is nonzero only when (α, β) and (α', β') are either the same or nearest neighbors, we get

$$\begin{aligned} \lambda^{(l)}(j) = \sum_{j'=0}^{M-1} \sum_{n'=-\mathscr{N}+1}^{\mathscr{N}} \sum_{\bar{m}'=-M^{-1}\mathscr{M}+1}^{M^{-1}\mathscr{M}} & A(M\bar{m}' + j', n'; 0, 0) \\ & \times \exp[2\pi il(n' - 2\mathscr{N}\bar{m}')/P + i(2\pi j - \theta)j'/M] \\ = {} & A(0, 0; 0, 0) + A(1, 0; 0, 0) \exp[i(2\pi j - \theta)/M] \\ & + A(-1, 0; 0, 0) \exp[-i(2\pi j - \theta)/M] \\ & + A(0, 1; 0, 0) \exp(2\pi il/P) + A(0, -1; 0, 0) \exp(-2\pi il/P). \end{aligned} \tag{2.20}$$

From (2.20), we may make the explicit evaluation

$$\begin{aligned} \det \lambda^{(l)}(j) = {} & (1 + z_1^2)(1 + z_2^2) - 2z_2(1 - z_1^2) \cos(2\pi j/M - \pi l/\mathscr{M}) \\ & - 2z_1(1 - z_2^2) \cos(2\pi l/P). \end{aligned} \tag{2.21}$$

From (2.2), (2.11), (2.18) and (2.21), the free energy per spin is given by

$$F = -kT(4\mathscr{M}\mathscr{N})^{-1}\ln Z = -kT\ln(2\cosh\beta E_1\cosh\beta E_2)$$
$$-\,kT(8\mathscr{M}\mathscr{N})^{-1}\sum_{l=0}^{P-1}\sum_{j=0}^{M-1}\ln[(1+z_1^2)(1+z_2^2)$$
$$-\,2z_2(1-z_1^2)\cos(2\pi j/M - \pi l/\mathscr{M}) - 2z_1(1-z_2^2)\cos(2\pi l/P)]. \tag{2.22}$$

In the limit $\mathscr{M}, \mathscr{N}\to\infty$, (2.22) becomes

$$F = -kT\ln(2\cosh\beta E_1\cosh\beta E_2)$$
$$-\,\frac{kT}{8\pi^2}\int_{-\pi}^{\pi}d\phi_1\int_{-\pi}^{\pi}d\phi_2\ln[(1+z_1^2)(1+z_2^2)$$
$$-\,2z_2(1-z_1^2)\cos\phi_1 - 2z_1(1-z_2^2)\cos\phi_2]. \tag{2.23}$$

Note that M does not appear in (2.23).

Having verified that the particular way of joining the boundaries does not affect the thermodynamic properties of the system, we turn our attention to the correlation $\langle\sigma_{0,0}\sigma_{M,N}\rangle$. From the lattice site $(0, 0)$ we may arrive at the lattice site (M, N) by the following sequence: $(0, 0)$, $(0, -1), (0, -2), \ldots, (0, -\mathscr{N}+1), (M, \mathscr{N}), (M, \mathscr{N}-1), \ldots, (M, N+1)$, (M, N). It is convenient to designate

$(0, 0)L, (0, -1)L, \ldots, (0, -\mathscr{N}+2)L, (0, -\mathscr{N}+1)L$ by ①,

$(0, -1)R, (0, -2)R, \ldots, (0, -\mathscr{N}+1)R, (0, -\mathscr{N})R$ by ②,

$(M, N)R, (M, N+1)R, \ldots, (M, \mathscr{N}-2)R, (M, \mathscr{N}-1)R$ by ③,

and

$(M, N+1)L, (M, N+2)L, \ldots, (M, \mathscr{N}-1)L, (M, \mathscr{N})L$ by ④, (2.24)

where $(0, -\mathscr{N})R$ is defined to be $(0, \mathscr{N})R$ for the sake of symmetry. With the choice of such a sequence of lattice sites, we can follow the procedure of Chapter VIII to express $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ in terms of Pfaffians:

$$\langle\sigma_{0,0}\sigma_{M,N}\rangle = \pm\lim_{\mathscr{M},\mathscr{N}\to\infty} z_1^{2\mathscr{N}-N}\,\mathrm{Pf}(y^{-1}+Q)\,\mathrm{Pf}(y) \tag{2.25}$$

where the sign on the right-hand side should be chosen so that the correlation is positive. In (2.25),

$$y = \left(\frac{1}{z_1} - z_1\right)\begin{array}{c} \\ ① \\ ② \\ ③ \\ ④ \end{array}\begin{array}{c} \begin{array}{cccc} ① & ② & ③ & ④ \end{array} \\ \begin{bmatrix} 0 & -I & 0 & 0 \\ I & 0 & 0 & 0 \\ 0 & 0 & 0 & I \\ 0 & 0 & -I & 0 \end{bmatrix} \end{array}, \tag{2.26}$$

$$y^{-1}+Q=\frac{1}{1-z_1^2}\begin{array}{c|cccc} & ① & ② & ③ & ④ \\ \hline ① & 0 & \bar S & \bar T & \bar U \\ ② & -\bar S^T & 0 & -\bar U & \bar V \\ ③ & -\bar T & \bar U & 0 & -\bar S \\ ④ & -\bar U & -\bar V & \bar S^T & 0 \end{array}, \tag{2.27}$$

where $\bar S^T$ is the transpose of $\bar S$. In (2.27), the elements of the finite matrices $\bar S$, $\bar T$, $\bar U$, and $\bar V$ have the following limiting values, called $S_{mn},\ldots$, as $\mathscr{M}\to\infty$ and $\mathscr{N}\to\infty$ for fixed $m, n = 0, 1, 2, \ldots$:

$$S_{mn} = (1-z_1^2)A^{-1}(0,0;0,m-n-1)_{LR}+z_1\delta_{m,n}, \tag{2.28}$$

$$T_{mn} = (1-z_1^2)A^{-1}(0,0;M,N+m+n)_{LR} \tag{2.29}$$

$$U_{mn} = (1-z_1^2)A^{-1}(0,0;M,N+m+n+1)_{LL} \tag{2.30}$$

and

$$V_{mn} = -(1-z_1^2)A^{-1}(0,0;M,-N-m-n-2)_{LR}, \tag{2.31}$$

with

$$A^{-1}(0,0;l_1,l_2)_{LR} = -\frac{1}{4\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}d\phi_1\,d\phi_2\exp(-il_1\phi_1-il_2\phi_2)\frac{1}{\Delta(\phi_1,\phi_2)} \times[1-z_2^2-z_1(1+z_2^2+2z_2\cos\phi_1)\exp(-i\phi_2)], \tag{2.32}$$

$$A^{-1}(0,0;l_1,l_2)_{LL} = -\frac{1}{4\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}d\phi_1\,d\phi_2\exp(-il_1\phi_1-il_2\phi_2)\frac{1}{\Delta(\phi_1,\phi_2)} \times(2iz_2\sin\phi_1), \tag{2.33}$$

and

$$\Delta(\phi_1,\phi_2) = (1+z_1^2)(1+z_2^2)-2z_2(1-z_1^2)\cos\phi_1-2z_1(1-z_2^2)\cos\phi_2. \tag{2.34}$$

Note that S_{mn} is the same as the a_{m-n} of (VIII.2.29).

From (2.26) we have

$$\mathrm{Pf}\,(y) = (z_1^{-1}-z_1)^{2\mathscr{N}-N}, \tag{2.35}$$

thus (2.25) becomes

$$\langle\sigma_{0,0}\sigma_{M,N}\rangle = \pm\lim_{\mathscr{M},\mathscr{N}\to\infty}(1-z_1^2)^{2\mathscr{N}-N}\,\mathrm{Pf}\,(y^{-1}+Q)$$

$$= \lim_{\mathscr{M},\mathscr{N}\to\infty}\begin{vmatrix} 0 & \bar S & \bar T & \bar U \\ -\bar S^T & 0 & -\bar U & \bar V \\ -\bar T & \bar U & 0 & -\bar S \\ -\bar U & -\bar V & \bar S^T & 0 \end{vmatrix}^{1/2}. \tag{2.36}$$

We are therefore left with the evaluation of the determinant on the right-hand side of (2.36).

3. SPIN CORRELATIONS BELOW THE CRITICAL TEMPERATURE

To obtain the asymptotic form of the correlation function $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ for $T < T_c$, we first consider $f_{MN}(\mathscr{M}, \mathscr{N})$, which is the ratio of the expectation value of $\langle\sigma_{0,0}\sigma_{M,N+1}\rangle_{\mathscr{M},\mathscr{N}}$ for finite $\mathscr{M}$ and $\mathscr{N}$ to that of $\langle\sigma_{0,0}\sigma_{M,N}\rangle_{\mathscr{M},\mathscr{N}}$ for the same $\mathscr{M}$ and $\mathscr{N}$. More precisely,

$$f_{MN}^2(\mathscr{M}, \mathscr{N}) = \frac{\begin{vmatrix} 0 & \bar{S} & \bar{T}\sim & \bar{U}\sim \\ -\bar{S}^T & 0 & -\bar{U}\sim & \bar{V}\sim \\ -\sim\bar{T} & \sim\bar{U} & 0 & -\sim\bar{S}\sim \\ -\sim\bar{U} & -\sim\bar{V} & (\sim\bar{S}\sim)^T & 0 \end{vmatrix}}{\begin{vmatrix} 0 & \bar{S} & \bar{T} & \bar{U} \\ -\bar{S}^T & 0 & -\bar{U} & \bar{V} \\ -\bar{T} & \bar{U} & 0 & -\bar{S} \\ -\bar{U} & -\bar{V} & \bar{S}^T & 0 \end{vmatrix}}, \tag{3.1}$$

where the left (right) $\sim$ signifies the deletion of the first row (column) of the matrix. As in Chapter XI, consider the linear equations

$$\begin{bmatrix} 0 & \bar{S} & \bar{T} & \bar{U} \\ -\bar{S}^T & 0 & -\bar{U} & \bar{V} \\ -\bar{T} & \bar{U} & 0 & -\bar{S} \\ -\bar{U} & -\bar{V} & \bar{S}^T & 0 \end{bmatrix} \begin{bmatrix} \bar{x}_1 & \bar{x}_1' \\ \bar{x}_2 & \bar{x}_2' \\ \bar{x}_3 & \bar{x}_3' \\ \bar{x}_4 & \bar{x}_4' \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ \bar{\delta} & 0 \\ 0 & \bar{\delta} \end{bmatrix}, \tag{3.2}$$

where

$$\bar{\delta} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \tag{3.3}$$

the number of elements being $\mathscr{N} - N$. Application of Jacobi's theorem (IV.2.13a) to (3.1) and (3.2) gives

$$f_{MN}^2(\mathscr{M}, \mathscr{N}) = \bar{x}_{30}\bar{x}_{40}' - \bar{x}_{30}'\bar{x}_{40}. \tag{3.4}$$

where $\bar{x}_{30}$, for example, denotes the first element of the column matrix $\bar{x}_3$. Moreover, $\bar{x}_{30}$ and $\bar{x}'_{40}$ are zero because the diagonal cofactor of an antisymmetric matrix vanishes.

At this stage, we take the limit $\mathscr{M} \to \infty$ and $\mathscr{N} \to \infty$. Let

$$f_{MN} = \lim_{\mathscr{M},\mathscr{N} \to \infty} f_{MN}(\mathscr{M}, \mathscr{N}), \tag{3.5}$$

or

$$f_{MN} = \frac{\langle\sigma_{0,0}\sigma_{M,N+1}\rangle}{\langle\sigma_{0,0}\sigma_{M,N}\rangle}. \tag{3.6}$$

By (2.28–2.31) consider the infinite system of linear equations

$$\begin{bmatrix} 0 & S & T & U \\ -S^T & 0 & -U & V \\ -T & U & 0 & -S \\ -U & -V & S^T & 0 \end{bmatrix} \begin{bmatrix} x_1 & x'_1 \\ x_2 & x'_2 \\ x_3 & x'_3 \\ x_4 & x'_4 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ \delta & 0 \\ 0 & \delta \end{bmatrix}, \tag{3.7}$$

when δ is the infinite column matrix

$$\delta = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{bmatrix}. \tag{3.8}$$

It then follows from (3.4) and (3.5) that

$$f_{MN}^2 = x_{30}x'_{40} - x'_{30}x_{40} = -x'_{30}x_{40}. \tag{3.9}$$

Once f_{MN} is known, the correlation function, in the limit $\mathscr{M} \to \infty$ and $\mathscr{N} \to \infty$ can be expressed as

$$\langle\sigma_{0,0}\sigma_{M,N}\rangle = S_\infty \left[\prod_{n=N}^{\infty} f_{Mn}\right]^{-1}, \tag{3.10}$$

where, from (X.4.9),

$$S_\infty = [1 - (\sinh 2\beta E_1 \sinh 2\beta E_2)^{-2}]^{1/4} \tag{3.11}$$

is the square of the spontaneous magnetization.

We now need to evaluate x_3, x'_3, x_4 and x'_4 when $M^2 + N^2$ is large. We observe that, for large $M^2 + N^2$, the elements of S are of the order of unity while those of T, U, and V are exponentially small. Series expansion in T, U, and V gives

$$\begin{bmatrix} 0 & S & T & U \\ -S^T & 0 & -U & V \\ -T & U & 0 & -S \\ -U & -V & S^T & 0 \end{bmatrix}^{-1}$$

$$= \begin{bmatrix} 0 & -(S^T)^{-1} & 0 & 0 \\ S^{-1} & 0 & 0 & 0 \\ 0 & 0 & 0 & (S^T)^{-1} \\ 0 & 0 & -S^{-1} & 0 \end{bmatrix}$$

$$- \begin{bmatrix} 0 & -(S^T)^{-1} & 0 & 0 \\ S^{-1} & 0 & 0 & 0 \\ 0 & 0 & 0 & (S^T)^{-1} \\ 0 & 0 & -S^{-1} & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & T & U \\ 0 & 0 & -U & V \\ -T & U & 0 & 0 \\ -U & -V & 0 & 0 \end{bmatrix}$$

$$\times \begin{bmatrix} 0 & -(S^T)^{-1} & 0 & 0 \\ S^{-1} & 0 & 0 & 0 \\ 0 & 0 & 0 & (S^T)^{-1} \\ 0 & 0 & -S^{-1} & 0 \end{bmatrix}$$

$$+ \begin{bmatrix} 0 & -(S^T)^{-1} & 0 & 0 \\ S^{-1} & 0 & 0 & 0 \\ 0 & 0 & 0 & (S^T)^{-1} \\ 0 & 0 & -S^{-1} & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & T & U \\ 0 & 0 & -U & V \\ -T & U & 0 & 0 \\ -U & -V & 0 & 0 \end{bmatrix}$$

$$\times \begin{bmatrix} 0 & -(S^T)^{-1} & 0 & 0 \\ S^{-1} & 0 & 0 & 0 \\ 0 & 0 & 0 & (S^T)^{-1} \\ 0 & 0 & -S^{-1} & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & T & U \\ 0 & 0 & -U & V \\ -T & U & 0 & 0 \\ -U & -V & 0 & 0 \end{bmatrix}$$

$$\times \begin{bmatrix} 0 & -(S^T)^{-1} & 0 & 0 \\ S^{-1} & 0 & 0 & 0 \\ 0 & 0 & 0 & (S^T)^{-1} \\ 0 & 0 & -S^{-1} & 0 \end{bmatrix} + \cdots. \tag{3.12}$$

In particular,

$$\begin{bmatrix} x_{30} & x'_{30} \\ x_{40} & x'_{40} \end{bmatrix} = \begin{bmatrix} 0 & 0 & \delta^T & 0 \\ 0 & 0 & 0 & \delta^T \end{bmatrix} \begin{bmatrix} 0 & S & T & U \\ -S^T & 0 & -U & V \\ -T & U & 0 & -S \\ -U & -V & S^T & 0 \end{bmatrix}^{-1} \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ \delta & 0 \\ 0 & \delta \end{bmatrix}$$

$$= \begin{bmatrix} 0 & \delta^T S^{-1}\delta \\ -\delta^T S^{-1}\delta & 0 \end{bmatrix}$$

$$+ \begin{bmatrix} \delta^T(S^T)^{-1}[VS^{-1}U - U(S^T)^{-1}V]S^{-1}\delta & -\delta^T(S^T)^{-1}[VS^{-1}T + U(S^T)^{-1}U](S^T)^{-1}\delta \\ \delta^T S^{-1}[US^{-1}U + T(S^T)^{-1}V]S^{-1}\delta & -\delta^T S^{-1}[US^{-1}T - T(S^T)^{-1}U](S^T)^{-1}\delta \end{bmatrix}$$

$$+ \cdots. \tag{3.13}$$

The diagonal elements in this expression vanish, as they must. The substitution of (3.13) in (3.9) gives

$$f_{MN} \doteqdot \delta^T S^{-1}\delta - \delta^T S^{-1}[US^{-1}U + T(S^T)^{-1}V]S^{-1}\delta, \tag{3.14}$$

where, as in Chapter XI, $\doteqdot$ means that the right- and left-hand sides have the same asymptotic expansion in the limit $M^2 + N^2 \to \infty$ for fixed T ($< T_c$ in this case). The terms neglected in (3.14) are smaller than those retained by an exponential factor. We proceed to calculate the right-hand side of (3.14) asymptotically.

From (2.28) and (2.32), we may get

$$S_{mn} = \frac{1}{2\pi}\int_0^{2\pi} \phi(\theta)e^{-i(n-m)\theta}\,d\theta, \tag{3.15}$$

where, as in (VIII.2.30),

$$\phi(\theta) = \left[\frac{(1-\alpha_1 e^{i\theta})(1-\alpha_2 e^{-i\theta})}{(1-\alpha_1 e^{-i\theta})(1-\alpha_2 e^{i\theta})}\right]^{1/2}, \tag{3.16}$$

$$\alpha_1 = z_1\frac{1-z_2}{1+z_2} \quad \text{and} \quad \alpha_2 = z_1^{-1}\frac{1-z_2}{1+z_2}. \tag{3.17}$$

As discussed in Sec. 7(C) of Chapter XI, the method of Wiener-Hopf can be applied to obtain the matrix elements of S^{-1} by solving the equation

$$\sum_{l=0}^{\infty} S_{ml}(S^{-1})_{ln} = \delta_{m,n}. \tag{3.18}$$

The result is

$$(S^{-1})_{mn} = -\frac{1}{4\pi^2}\oint d\xi\,\frac{1}{\xi^{n+1}}\left(\frac{1-\alpha_2\xi}{1-\alpha_1\xi}\right)^{1/2}\oint d\xi'\,\frac{\xi'^m}{\xi'-\xi}\left(\frac{1-\alpha_1/\xi'}{1-\alpha_2/\xi'}\right)^{1/2}, \tag{3.19}$$

where the contours of integration are the unit circles, except that the one for ξ' is to be indented outward near $\xi' = \xi$. In particular,

$$\delta^T S^{-1} \delta = (S^{-1})_{00} = 1, \tag{3.20}$$

$$(S^{-1})_{m0} = \frac{1}{2\pi i} \oint d\xi \xi^{m-1} \left(\frac{1 - \alpha_1/\xi}{1 - \alpha_2/\xi} \right)^{1/2}, \tag{3.21}$$

and

$$(S^{-1})_{0n} = \frac{1}{2\pi i} \oint d\xi \frac{1}{\xi^{n+1}} \left(\frac{1 - \alpha_2 \xi}{1 - \alpha_1 \xi} \right)^{1/2}. \tag{3.22}$$

Substituting (2.29–2.33) and (3.19–3.22) in (3.14), we get, after performing the matrix multiplication,

$$\begin{aligned} f_{MN}^2 \doteqdot 1 &+ \frac{1}{8\pi^4} (1 - z_1^2)^2 \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} d\phi_1 \, d\phi_2 \, d\phi_3 \, d\phi_4 \\ &\times \exp[-iM(\phi_1 + \phi_3) - i(N + 1)(\phi_2 + \phi_4)] \\ &\times \Bigg\{ [(1 - z_2^2) e^{i\phi_2} - z_1(1 + z_2^2 + 2z_2 \cos \phi_1)] \\ &\qquad \times [(1 - z_2^2) e^{-i\phi_4} - z_1(1 + z_2^2 + 2z_2 \cos \phi_3)] \\ &\qquad \times \frac{(1 - \alpha_2 e^{-i\phi_2})(1 - \alpha_1 e^{-i\phi_4})}{(1 - \alpha_2 e^{-i\phi_4})(1 - \alpha_1 e^{-i\phi_2})} + 4z_2^2 \sin \phi_1 \sin \phi_3 \Bigg\} \\ &\qquad \times \frac{1}{1 - e^{-i(\phi_2 + \phi_4)}} \frac{1}{\Delta(\phi_1, \phi_2) \Delta(\phi_3, \phi_4)}. \end{aligned} \tag{3.23}$$

Equation (3.23) can be simplified considerably if we substitute

$$\cos \phi_1 = \tfrac{1}{2}[z_2(1 - z_1^2)]^{-1}[(1 + z_1^2)(1 + z_2^2) - 2z_1(1 - z_2^2) \cos \phi_2] \tag{3.24}$$

and

$$\cos \phi_3 = \tfrac{1}{2}[z_2(1 - z_1^2)]^{-1}[(1 + z_1^2)(1 + z_2^2) - 2z_1(1 - z_2^2) \cos \phi_4] \tag{3.25}$$

in the brackets. These substitutions are justified since the region where $\Delta(\phi_1, \phi_2)$ and $\Delta(\phi_3, \phi_4)$ are zero is exactly the region which contributes to the integral. We then obtain

$$\begin{aligned} f_{MN}^2 \doteqdot 1 &- \frac{1}{\pi^4} (1 - z_1^2)^2 z_2^2 \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} d\phi_1 \, d\phi_2 \, d\phi_3 \, d\phi_4 \\ &\times \frac{\exp[-iM(\phi_1 + \phi_3) - iN(\phi_2 + \phi_4)]}{e^{i(\phi_2 + \phi_4)} - 1} \\ &\times \frac{\sin^2 \frac{1}{2}(\phi_1 - \phi_3)}{(a - \gamma_1 \cos \phi_1 - \gamma_2 \cos \phi_2)(a - \gamma_1 \cos \phi_3 - \gamma_2 \cos \phi_4)}. \end{aligned} \tag{3.26}$$

where

$$a = (1 + z_1^2)(1 + z_2^2),$$

$$\gamma_1 = 2z_2(1 - z_1^2),$$

and

$$\gamma_2 = 2z_1(1 - z_2^2). \tag{3.27}$$

Substituting (3.26) in (3.10), we get

$$\begin{aligned}\langle\sigma_{0,0}\sigma_{M,N}\rangle \\ \doteqdot S_\infty\Big\{1 &- \frac{1}{2}\frac{\gamma_1^2}{16\pi^4}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} d\phi_1\,d\phi_2\,d\phi_3\,d\phi_4 \\ &\times \exp\left[-iM(\phi_1 + \phi_3) - iN(\phi_2 + \phi_4)\right] \\ &\times \frac{\sin^2\frac{1}{2}(\phi_1 - \phi_3)}{\sin^2\frac{1}{2}(\phi_2 + \phi_4)} \\ &\times \frac{1}{(a - \gamma_1\cos\phi_1 - \gamma_2\cos\phi_2)(a - \gamma_1\cos\phi_3 - \gamma_2\cos\phi_4)}\Big\}. \end{aligned} \tag{3.28}$$

Equation (3.28) is the desired result. However, the form as it stands is not symmetric under interchange of M and N and of γ_1 and γ_2. It is trivial to recover this symmetry by observing that if we carry out the integrations over ϕ_2 and ϕ_4 the multiple integral in (3.28) is equal to the residue at

$$a - \gamma_1\cos\phi_1 - \gamma_2\cos\phi_2 = 0, \quad \text{and} \quad a - \gamma_1\cos\phi_3 - \gamma_2\cos\phi_4 = 0. \tag{3.29}$$

From (3.29), we obtain

$$\begin{aligned}\gamma_1 &\sin\tfrac{1}{2}(\phi_1 - \phi_3)\sin\tfrac{1}{2}(\phi_1 + \phi_3) \\ &+ \gamma_2\sin\tfrac{1}{2}(\phi_2 - \phi_4)\sin\tfrac{1}{2}(\phi_2 + \phi_4) = 0.\end{aligned} \tag{3.30}$$

Making use of (3.30), we may write (3.28) in the symmetric form

$$\begin{aligned}\langle\sigma_{0,0}\sigma_{M,N}\rangle \\ \doteqdot S_\infty\Big\{1 &+ \frac{1}{2}\frac{\gamma_1\gamma_2}{16\pi^4}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} d\phi_1\,d\phi_2\,d\phi_3\,d\phi_4 \\ &\times \exp\left[1 - iM(\phi_1 + \phi_3) - iN(\phi_2 + \phi_4)\right] \\ &\times \frac{\sin\frac{1}{2}(\phi_1 - \phi_3)\sin\frac{1}{2}(\phi_2 - \phi_4)}{\sin\frac{1}{2}(\phi_1 + \phi_3)\sin\frac{1}{2}(\phi_2 + \phi_4)} \\ &\times \frac{1}{(a - \gamma_1\cos\phi_1 - \gamma_2\cos\phi_2)(a - \gamma_1\cos\phi_3 - \gamma_2\cos\phi_4)}\Big\}. \end{aligned} \tag{3.31}$$

The asymptotic evaluation of the right-hand side of (3.31) is rather tedious. After integration over ϕ_2 and ϕ_4, (3.31) becomes

$$\langle\sigma_{0,0}\sigma_{M,N}\rangle$$

$$\doteqdot S_\infty\left\{1 - \frac{\gamma_1}{8\pi^2\gamma_2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} d\phi_1\, d\phi_3 \exp\left[-iM(\phi_1+\phi_3) - iN(\phi_2+\phi_4)\right]\right.$$

$$\left.\times \frac{\sin\frac{1}{2}(\phi_1-\phi_3)\sin\frac{1}{2}(\phi_2-\phi_4)}{\sin\phi_2 \sin\phi_4 \sin\frac{1}{2}(\phi_1+\phi_3)\sin\frac{1}{2}(\phi_2+\phi_4)}\right\}, \tag{3.32}$$

where ϕ_2 and ϕ_4 are related to ϕ_1 and ϕ_3 by (3.29). To make the integral in (3.32) more symmetric, let us introduce the variables u and v:

$$\gamma_1\cosh\psi_1 = \frac{a}{2} + u, \qquad \gamma_1\cosh\psi_3 = \frac{a}{2} + v, \tag{3.33}$$

where

$$\psi_n = i\phi_n, \qquad n = 1, 2, 3, 4.$$

Then (3.29) gives

$$\gamma_2\cosh\psi_2 = \frac{a}{2} - u, \qquad \gamma_2\cosh\psi_4 = \frac{a}{2} - v. \tag{3.34}$$

With the variables u and v, (3.32) is reduced to

$$\langle\sigma_{0,0}\sigma_{M,N}\rangle \doteqdot S_\infty\left\{1 - \frac{1}{8\pi^2\gamma_1\gamma_2}\int\int du\, dv \exp\left[-M(\psi_1+\psi_3)\right.\right.$$

$$\left. - N(\psi_2+\psi_4)\right]$$

$$\left.\times \frac{\sinh\frac{1}{2}(\psi_1-\psi_3)\sinh\frac{1}{2}(\psi_2-\psi_4)}{\sinh\frac{1}{2}(\psi_1+\psi_3)\sinh\frac{1}{2}(\psi_2+\psi_4)}\left(\prod_{i=1}^{4}\sinh\psi_i\right)^{-1}\right\}. \tag{3.35}$$

The saddle point is easily found to be

$$\psi_1 = \psi_3 = \theta_1, \qquad \psi_2 = \psi_4 = \theta_2, \tag{3.36}$$

where

$$\cosh\theta_1 = \frac{(M^2/\gamma_1)(a^2-\gamma_2^2) + N^2\gamma_1}{aM^2 + [M^2N^2a^2 + (M^2-N^2)(M^2\gamma_2^2 - N^2\gamma_1^2)]^{1/2}},$$

and

$$\cosh\theta_2 = \frac{(N^2/\gamma_2)(a^2-\gamma_1^2) + M^2\gamma_2}{aN^2 + [M^2N^2a^2 + (M^2-N^2)(M^2\gamma_2^2 - N^2\gamma_1^2)]^{1/2}}. \tag{3.37}$$

Here a, γ_1, and γ_2 are given by (3.27). Note that θ_1 and θ_2 are both positive when M and N are positive.

We shall expand the integrand of (3.35) in the neighborhood of the saddle point. From (3.33) we have

$$\frac{d\psi_1}{du}=\frac{1}{\gamma_1\sinh\psi_1}, \tag{3.38}$$

$$\frac{d^2\psi_1}{du^2}=-\frac{\text{co h}\,\psi_1}{\gamma_1^2\sinh^3\psi_1}, \tag{3.39}$$

$$\frac{d^3\psi_1}{du^3}=\frac{3+2\sinh^2\psi_1}{\gamma_1^3\sinh^5\psi_1}, \tag{3.40}$$

$$\frac{d^4\psi_1}{du^4}=-\frac{3\cosh\psi_1(5+2\sinh^2\psi_1)}{\gamma_1^4\sinh^7\psi_1}, \tag{3.41}$$

and similarly for the derivatives of ψ_3 with respect to v. The derivatives of ψ_2, for example, can be obtained from (3.38–3.41) by the replacements

$$u\to-u,\qquad \psi_1\to\psi_2,\qquad \gamma_1\to\gamma_2.$$

Writing

$$\xi=u-u_0,\qquad \eta=v-v_0, \tag{3.42}$$

where u_0 and v_0 are the values of u and v at the saddle point, we have, in the neighborhood of the point,

$$\begin{aligned}&\sinh\tfrac{1}{2}(\psi_1-\psi_3)\\&\quad\sim\frac{\xi-\eta}{2\gamma_1\sinh\theta_1}\left[1-\frac{(\xi+\eta)\cosh\theta_1}{2\gamma_1\sinh^2\theta_1}+\frac{(4+3\sinh^2\theta_1)(\xi+\eta)^2}{8\gamma_1^2\sinh^4\theta_1}\right.\\&\qquad\left.-\frac{\xi\eta\cosh^2\theta_1}{2\gamma_1^2\sinh^4\theta_1}\right],\end{aligned} \tag{3.43}$$

$$\begin{aligned}&\sinh\tfrac{1}{2}(\psi_2-\psi_4)\\&\quad\sim-\frac{\xi-\eta}{2\gamma_2\sinh\theta_2}\left[1+\frac{(\xi+\eta)\cosh\theta_2}{2\gamma_2\sinh^2\theta_2}+\frac{(4+3\sinh^2\theta_2)(\xi+\eta)^2}{8\gamma_2^2\sinh^4\theta_2}\right.\\&\qquad\left.-\frac{\xi\eta\cosh^2\theta_2}{2\gamma_2^2\sinh^4\theta_2}\right],\end{aligned} \tag{3.44}$$

$$\begin{aligned}&\frac{1}{\sinh\tfrac{1}{2}(\psi_1+\psi_3)}\\&\quad\sim\frac{1}{\sinh\theta_1}\left[1-\frac{(\xi+\eta)\cosh\theta_1}{2\gamma_1\sinh^2\theta_1}+\frac{(3\sinh^2\theta_1+4)(\xi+\eta)^2}{8\gamma_1^2\sinh^4\theta_1}\right.\\&\qquad\left.-\frac{\xi\eta\cosh^2\theta_1}{2\gamma_1^2\sinh^4\theta_1}\right],\end{aligned} \tag{3.45}$$

$$\frac{1}{\sinh \frac{1}{2}(\psi_2 + \psi_4)}$$
$$\sim \frac{1}{\sinh \theta_2}\left[1 + \frac{(\xi + \eta)\cosh \theta_2}{2\gamma_2 \sinh^2 \theta_2} + \frac{(3\sinh^2 \theta_2 + 4)(\xi + \eta)^2}{8\gamma_2^2 \sinh^4 \theta_2} - \frac{\xi\eta \cosh^2 \theta_2}{2\gamma_2^2 \sinh^4 \theta_2}\right], \tag{3.46}$$

$$\left(\prod_{n=1}^{4} \sinh \psi_n\right)^{-1}$$
$$\sim \frac{1}{\sinh^2 \theta_1 \sinh^2 \theta_2}\left\{1 + \left[\frac{\cosh \theta_2}{\gamma_2 \sinh^2 \theta_2} - \frac{\cosh \theta_1}{\gamma_1 \sinh^2 \theta_1}\right](\xi + \eta) + \left[\frac{3 + 2\sinh^2 \theta_1}{2\gamma_1^2 \sinh^4 \theta_1} + \frac{3 + 2\sinh^2 \theta_2}{2\gamma_2^2 \sinh^4 \theta_2} - \frac{\cosh \theta_1 \cosh \theta_2}{\gamma_1\gamma_2 \sinh^2 \theta_1 \sinh^2 \theta_2}\right](\xi + \eta)^2 - \left[\frac{2 + \sinh^2 \theta_1}{\gamma_1^2 \sinh^4 \theta_1} + \frac{2 + \sinh^2 \theta_2}{\gamma_2^2 \sinh^4 \theta_2}\right]\xi\eta\right\}, \tag{3.47}$$

and

$$\exp\left[-M(\psi_1 + \psi_3) - N(\psi_2 + \psi_4)\right]$$
$$\sim \exp(-2M\theta_1 - 2N\theta_2) \times \exp\left\{\left[\frac{M\cosh \theta_1}{2\gamma_1^2 \sinh^3 \theta_1} + \frac{N\cosh \theta_2}{2\gamma_2^2 \sinh^3 \theta_2}\right](\xi^2 + \eta^2)\right\}$$
$$\times \left\{1 - \left[\frac{(3 + 2\sinh^2 \theta_1)M}{\gamma_1^3 \sinh^5 \theta_1} - \frac{(3 + 2\sinh^2 \theta_2)N}{\gamma_2^3 \sinh^5 \theta_2}\right]\frac{\xi^3 + \eta^3}{6} + \left[\frac{\cosh \theta_1(5 + 2\sinh^2 \theta_1)M}{\gamma_1^4 \sinh^7 \theta_1} + \frac{\cosh \theta_2(5 + 2\sinh^2 \theta_2)N}{\gamma_2^4 \sinh^7 \theta_2}\right] \times \frac{\xi^4 + \eta^4}{8} + \left[\frac{(3 + 2\sinh^2 \theta_1)M}{\gamma_1^3 \sinh^5 \theta_1} - \frac{(3 + 2\sinh^2 \theta_2)N}{\gamma_2^3 \sinh^5 \theta_2}\right]^2 \times \frac{(\xi^3 + \eta^3)^2}{72}\right\}. \tag{3.48}$$

We also have

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy (x - y)^2 \exp(-ax^2 - ay^2) \times [1, (x + y)^2, xy, x^4 + y^4, (x + y)(x^3 + y^3), (x^3 + y^3)^2] = \frac{\pi}{a^2}\left(1, \frac{1}{a}, -\frac{1}{2a}, \frac{9}{2a^2}, \frac{3}{a^2}, \frac{51}{4a^3}\right). \tag{3.49}$$

Substituting (3.43–3.48) in (3.35), putting $\xi = iy$, $\eta = ix$, and making use of (3.49), we may obtain the final result that, when $T < T_c$,

$$\begin{aligned}\langle\sigma_{0,0}\sigma_{M,N}\rangle \sim \left[1 - \frac{1}{(\sinh 2\beta E_1 \sinh 2\beta E_2)^2}\right]^{1/4} \\ \times \Bigg\{1 + \frac{\exp(-2M\theta_1 - 2N\theta_2)}{8\pi(M\sinh\theta_1\cosh\theta_2 + N\cosh\theta_1\sinh\theta_2)^2} \\ \times \Bigg[\!\!\Bigg[1 - \frac{1}{12}\frac{1}{(M\tanh\theta_1 + N\tanh\theta_2)^3} \\ \times \Bigg[21M^2\tanh^2\theta_1(1 + 2\tanh^2\theta_2) + 21N^2\tanh^2\theta_2 \\ \times (1 + 2\tanh^2\theta_1) - \tanh^3\theta_1\tanh\theta_2(3 - 17\tanh^2\theta_2)\frac{M^3}{N} \\ - \tanh^3\theta_2\tanh\theta_1(3 - 17\tanh^2\theta_1)\frac{N^3}{M} \\ + 2MN\tanh\theta_1\tanh\theta_2(21 + 12\tanh^2\theta_1 + 12\tanh^2\theta_2 \\ - 17\tanh^2\theta_1\tanh^2\theta_2)\Bigg] + \cdots\Bigg]\!\!\Bigg]\Bigg\},\end{aligned} \qquad (3.50)$$

4. SPIN CORRELATIONS ABOVE THE CRITICAL TEMPERATURE

We next turn our attention to the case $T > T_c$. Even in the special case treated in Chapter XI, it is necessary to modify the Toeplitz determinant. We accordingly define

$$D(M, N; \mathscr{M}, \mathscr{N}) = \begin{array}{c} \\ ① \\ ②' \\ ③ \\ ④' \end{array}\!\!\begin{array}{c} \begin{array}{cccc} ① & ②' & ③ & ④' \end{array} \\ \begin{bmatrix} 0 & \bar{S}\approx & \bar{T} & \bar{U}\approx \\ -\approx\bar{S}^T & 0 & -\approx U & \approx V\approx \\ -\bar{T} & \bar{U}\approx & 0 & -\bar{S}\approx \\ -\approx\bar{U} & -\approx V\approx & \approx\bar{S}^T & 0 \end{bmatrix} \end{array}, \qquad (4.1)$$

where the right (left) $\approx$ signifies the addition of a column (row) to the matrix, making use of the points $(0, 0)R$ and $(M, N)L$ in addition to those of (2.24); that is, we designate

$(0, 0)R, (0, -1)R, (0, -2)R, \ldots, (0, -\mathscr{N} + 1)R, (0, -\mathscr{N})R$ by ②′,

and

$(M, N)L, (M, N + 1)L, (M, N + 2)L, \ldots, (M, \mathscr{N} - 1)L, (M, \mathscr{N})L$ by ④′. (4.2)

We consider the ratio

$$r(M,N;\mathcal{M},\mathcal{N}) = [D(M,N;\mathcal{M},\mathcal{N})]^{-1} \begin{array}{c c} & \begin{array}{cccc} ① & ② & ③ & ④ \end{array} \\ \begin{array}{c} ① \\ ② \\ ③ \\ ④ \end{array} & \begin{bmatrix} 0 & \bar{S} & \bar{T} & \bar{U} \\ -\bar{S}^T & 0 & -\bar{U} & \bar{V} \\ -\bar{T} & \bar{U} & 0 & -\bar{S} \\ -\bar{U} & -\bar{V} & \bar{S}^T & 0 \end{bmatrix} \end{array}, \tag{4.3}$$

and consider the linear equations, analogous to (3.2),

$$\begin{bmatrix} 0 & \bar{S}\approx & \bar{T} & \bar{U}\approx \\ -\approx\bar{S}^T & 0 & -\approx\bar{U} & \approx\bar{V}\approx \\ -\bar{T} & \bar{U}\approx & 0 & -\bar{S}\approx \\ -\approx\bar{U} & -\approx\bar{V}\approx & \approx\bar{S}^T & 0 \end{bmatrix} \begin{bmatrix} \bar{x}_1 & \bar{x}_1' \\ \bar{x}_2 & \bar{x}_2' \\ \bar{x}_3 & \bar{x}_3' \\ \bar{x}_4 & \bar{x}_4' \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ \delta' & 0 \\ 0 & 0 \\ 0 & \delta'' \end{bmatrix}, \tag{4.4}$$

where

$$\delta' = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \qquad \delta'' = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \tag{4.5}$$

the number of elements being $\mathcal{N} + 1$ for δ', and $\mathcal{N} - N + 1$ for δ'' [compare (3.3)]. Again application of Jacobi's theorem (IV.2.13*a*) to (4.3) and (4.4) gives

$$r(M,N;\mathcal{M},\mathcal{N}) = \bar{x}_{20}\bar{x}_{40}' - \bar{x}_{20}'\bar{x}_{40}. \tag{4.6}$$

Consider the limit $\mathcal{M}, \mathcal{N} \to \infty$. First, the ratio

$$\frac{D(M, N+1;\mathcal{M},\mathcal{N})}{D(M,N;\mathcal{M},\mathcal{N})}$$

can be obtained by solving a system of linear equations. Since the index of the kernel that generates the matrix

$$\tilde{S} = \lim_{\mathcal{M},\mathcal{N}\to\infty} \bar{S}\approx \tag{4.7}$$

is zero, the procedure of Sec. 3 can be applied to show that the quantity

$$1 - \lim_{\mathcal{M},\mathcal{N}\to\infty} \frac{D(M, N+1;\mathcal{M},\mathcal{N})}{D(M,N;\mathcal{M},\mathcal{N})} \tag{4.8}$$

is exponentially small as $M^2 + N^2$ is large. Thus

$$D(M) = \lim_{N\to\infty} \lim_{\mathcal{M},\mathcal{N}\to\infty} D(M,N;\mathcal{M},\mathcal{N}) \tag{4.9}$$

exists, and by (4.3) and (2.36)

$$\langle\sigma_{0,0}\sigma_{M,N}\rangle \doteqdot [D(M)r(M,N)]^{1/2}, \tag{4.10}$$

where

$$r(M,N) = \lim_{\mathscr{M},\mathscr{N}\to\infty} r(M,N;\mathscr{M},\mathscr{N}). \tag{4.11}$$

In order to compute $r(M,N)$, consider the infinite system of linear equations

$$\begin{bmatrix} 0 & \tilde{S} & T & \tilde{U} \\ -\tilde{S}^T & 0 & -\tilde{U} & \tilde{V} \\ -T & \tilde{U} & 0 & -\tilde{S} \\ -\tilde{U} & -\tilde{V} & \tilde{S}^T & 0 \end{bmatrix} \begin{bmatrix} x_1 & x_1' \\ x_2 & x_2' \\ x_3 & x_3' \\ x_4 & x_4' \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ \delta & 0 \\ 0 & 0 \\ 0 & \delta \end{bmatrix}, \tag{4.12}$$

where

$$\tilde{U} = \lim_{\mathscr{M},\mathscr{N}\to\infty} \bar{U}\approx,$$

and

$$\tilde{V} = \lim_{\mathscr{M},\mathscr{N}\to\infty} \approx\bar{V}\approx. \tag{4.13}$$

Both (4.7) and (4.13) hold for each fixed matrix element. With (4.12), it follows from (4.6) and (4.11) that

$$r(M,N) = x_{20}x_{40}' - x_{20}'x_{40}. \tag{4.14}$$

As before, we may obtain the asymptotic expansions of x_{20}, x_{20}', x_{40}, and x_{40}' by expanding the inverse matrix in a perturbation series (3.12):

$$x_2 = x_4' = 0,$$

and

$$x_2' = -x_4 = -\tilde{S}^{-1}T(\tilde{S}^T)^{-1}\delta, \tag{4.15}$$

to first order in T, $\tilde{U}$ and $\tilde{V}$. The terms neglected in (4.15) are exponentially smaller than those retained as $M^2 + N^2 \to \infty$. The substitution of (4.15) in (4.14) gives

$$r(M,N) \doteqdot [\delta^T\tilde{S}^{-1}T(\tilde{S}^T)^{-1}\delta]^2. \tag{4.16}$$

To obtain the matrix $\tilde{S}^{-1}$, we solve the equations

$$\sum_{l=0}^{\infty} b_{n-l}(\tilde{S}^{-1})_{lm} = \delta_{n,m} \tag{4.17}$$

for $n \geq 0$ [see Sec. 2 of Chapter XI]. The solution is

$$(\tilde{S}^{-1})_{lm} = -\frac{1}{4\pi^2}\oint \frac{\xi^{-m-1}}{[(1-\alpha_1\xi)(1-\xi/\alpha_2)]^{1/2}}\,d\xi \oint \frac{(1-\alpha_1/\xi')^{1/2}}{\xi'-\xi}\,\xi'^{l}\,d\xi', \tag{4.18}$$

where the contours of integration are the unit circles, except that the one for ξ' is to be indented outward near $\xi' = \xi$. In particular

$$(\tilde{S}^{-1})_{0m} = \frac{1}{2\pi i}\oint \frac{\xi^{-m-1}}{[(1-\alpha_1\xi)(1-\xi/\alpha_2)]^{1/2}}\,d\xi. \tag{4.19}$$

From (2.29), (4.16) and (4.19), we obtain

$$\begin{aligned} r(M, N) \doteq \Bigg[\frac{1-z_1^2}{4\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} d\phi_1\,d\phi_2\,\frac{\exp(-iM\phi_1 - iN\phi_2)}{a - \gamma_1\cos\phi_1 - \gamma_2\cos\phi_2} \\ \times \frac{1 - z_2^2 - z_1(1 + z_2^2 + 2z_2\cos\phi_1)e^{-i\phi_2}}{(1-\alpha_1 e^{-i\phi_2})(1 - e^{-i\phi_2}/\alpha_2)}\Bigg]^2. \end{aligned} \tag{4.20}$$

If we set

$$\cos\phi_1 = (a - \gamma_2\cos\phi_2)/\gamma_1,$$

(4.20) takes the form

$$r(M, N) \doteq (1 - z_2^2)^2 F_{M,N}^2, \tag{4.21}$$

where

$$F_{M,N} = \frac{1}{4\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} d\phi_1\,d\phi_2\,\frac{e^{-iM\phi_1 - iN\phi_2}}{a - \gamma_1\cos\phi_1 - \gamma_2\cos\phi_2}. \tag{4.22}$$

It follows from (4.10) and (4.21) that

$$\langle\sigma_{0,0}\sigma_{M,N}\rangle \doteq DF_{M,N}, \tag{4.23}$$

where

$$D = [D(M)]^{1/2}(1 - z_2^2)$$

is independent of M, as $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ should be symmetric with respect to the interchange of M, z_1 and N, z_2. The value of D will be obtained by comparing the asymptotic behavior of (4.23) in the special case $M = 0$ with the asymptotic form of $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ given in (2.43) of Chapter XI.

To derive the asymptotic form of $F_{M,N}$ when $M^2 + N^2$ is large we rewrite (4.22) as

$$\begin{aligned} F_{M,N} &= \int_0^{\infty} dx e^{-ax}\,\frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi_1 e^{-iM\phi_1 + x\gamma_1\cos\phi_1}\,\frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi_2 e^{-iN\phi_2 + x\gamma_2\cos\phi_2} \\ &= \int_0^{\infty} dx e^{-ax} I_M(x\gamma_1) I_N(x\gamma_2), \end{aligned} \tag{4.24}$$

where we have used the definition of the modified Bessel function of the first kind,

$$I_n(z) = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi e^{-in\phi + z\cos\phi}. \tag{4.25}$$

ASYMPTOTIC EXPANSION OF $\langle\sigma_{0,0}\,\sigma_{M,N}\rangle$

When n is large the asymptotic expansion of $I_n(z)$ is well known. Since we will be content with the first two terms in the expansion of $F_{M,N}$, we replace $I_n(z)$ in (4.24) by the first two terms of this asymptotic expansion,[2]

$$I_n(z) \sim \exp\,[(n^2 + z^2)^{1/2} - n\sinh^{-1}(n/z)](2\pi)^{-1/2}(n^2 + z^2)^{-1/4} \times [1 - (24n)^{-1}(1 + z^2/n^2)^{-3/2}(2 - 3z^2/n^2)], \tag{4.26}$$

and obtain

$$\begin{aligned} F_{M,N} \sim \frac{1}{2\pi}\int_0^\infty dx\,\exp\Big[-ax + (M^2 + \gamma_1^2x^2)^{1/2} - M\sinh^{-1}\left(\frac{M}{\gamma_1 x}\right) \\ + (N^2 + \gamma_2^2x^2)^{1/2} - N\sinh^{-1}\left(\frac{N}{\gamma_2 x}\right)\Big] \\ \times \frac{1}{[(M^2 + \gamma_1^2x^2)(N^2 + \gamma_2^2x^2)]^{1/4}} \\ \times \left[1 - \frac{2 - 3\gamma_1^2x^2/M^2}{24M(1 + \gamma_1^2x^2/M^2)^{3/2}} - \frac{2 - 3\gamma_2^2x^2/N^2}{24N(1 + \gamma_2^2x^2/N^2)^{3/2}}\right]. \end{aligned} \tag{4.27}$$

We shall evaluate (4.27) by the saddle-point method. Let us define

$$g(x) = ax - (M^2 + \gamma_1^2x^2)^{1/2} - (N^2 + \gamma_2^2x^2)^{1/2} + M\sinh^{-1}(M/\gamma_1 x) + N\sinh^{-1}(N/\gamma_2 x). \tag{4.28}$$

The derivative of $g(x)$ is given by

$$g^{(1)}(x) = a - x^{-1}(M^2 + \gamma_1^2x^2)^{1/2} - x^{-1}(N^2 + \gamma_2^2x^2)^{1/2}. \tag{4.29}$$

The saddle point x_0 at which $g^{(1)}(x)$ vanishes will now be determined. It is convenient to adopt the following notation:

$$\theta_1 = \sinh^{-1}\frac{M}{\gamma_1 x_0}, \qquad \theta_2 = \sinh^{-1}\frac{N}{\gamma_2 x_0}. \tag{4.30}$$

It follows from (4.30) that

$$\gamma_1 N\sinh\theta_1 = \gamma_2 M\sinh\theta_2. \tag{4.31}$$

From (4.29) and (4.30) we have

$$\gamma_1\cosh\theta_1 + \gamma_2\cosh\theta_2 = a. \tag{4.32}$$

Solving (4.31) and (4.32), we may obtain θ_1 and θ_2 which are explicitly given in (3.37). The saddle point x_0 is given by

$$\begin{aligned} x_0 = \{a^2(M^2 + N^2) - (M^2 - N^2)(\gamma_1^2 - \gamma_2^2) \\ + 2a[M^2N^2a^2 + (M^2 - N^2)(M^2\gamma_2^2 - N^2\gamma_1^2)]^{1/2}\}^{1/2} \\ \times [a^2 - (\gamma_1 + \gamma_2)^2]^{-1/2}[a^2 - (\gamma_1 - \gamma_2)^2]^{-1/2}. \end{aligned} \tag{4.33}$$

2. A. Erdelyi, ed., *Higher Transcendental Functions* (McGraw Hill, New York, 1953), vol. II, p. 86.

The higher derivatives of $g(x)$ at the saddle point are given by

$$g^{(2)}(x_0) = (M \tanh\theta_1 + N \tanh\theta_2)x_0^{-2},$$

$$g^{(3)}(x_0) = x_0^{-3}[M \tanh^3\theta_1 + N \tanh^3\theta_2 - 3(M \tanh\theta_1 + N \tanh\theta_2)],$$

and

$$\begin{aligned} g^{(4)}(x_0) = {} & 3x_0^{-4}[M \tanh^5\theta_1 + N \tanh^5\theta_2 - 3(M \tanh^3\theta_1 + N \tanh^3\theta_2) \\ & + 4(M \tanh\theta_1 + N \tanh\theta_2)]. \end{aligned} \tag{4.34}$$

Expanding the integrand of (4.27) about x_0, and setting $\xi = x - x_0$, we get

$$\begin{aligned} F_{M,N} \sim {} & \frac{1}{2\pi} \frac{1}{[(M^2 + \gamma_1^2 x_0^2)(N^2 + \gamma_2^2 x_0^2)]^{1/4}} \\ & \times \exp(-M\theta_1 - N\theta_2) \int_{-\infty}^{\infty} d\xi \exp[-\tfrac{1}{2}g^{(2)}(x_0)\xi^2] \\ & \times \left[1 - \frac{1}{6} g^{(3)}(x_0)\xi^3 - \frac{g^{(4)}(x_0)\xi^4}{24} + \frac{1}{72}[g^{(3)}(x_0)]^2\xi^6\right] \\ & \times \left[1 - \frac{1}{2x_0}(2 - \tanh^2\theta_1 - \tanh^2\theta_2)\xi \right. \\ & \quad + \frac{1}{8x_0^2}(8 - 10 \tanh^2\theta_1 - 10 \tanh^2\theta_2 \\ & \quad \left. + 2 \tanh^2\theta_1 \tanh^2\theta_2 + 5 \tanh^4\theta_1 + 5 \tanh^4\theta_2)\xi^2\right] \\ & \times \left[1 - \frac{2 - 3\gamma_1^2 x_0^2/M^2}{24M(1 + \gamma_1^2 x_0^2/M^2)^{3/2}} - \frac{2 - 3\gamma_2^2 x_0^2/N^2}{24N(1 + \gamma_2^2 x_0^2/N^2)^{3/2}}\right]. \end{aligned} \tag{4.35}$$

Now we have

$$\int_{-\infty}^{\infty} d\xi\, e^{-a\xi^2}(1, \xi^2, \xi^4, \xi^6) = \left(\frac{a}{\pi}\right)^{1/2}\left(1, \frac{1}{2a}, \frac{3}{4a^2}, \frac{15}{8a^3}\right). \tag{4.36}$$

From (4.35) and (4.36) we obtain

$$\begin{aligned} F_{M,N} \sim {} & \frac{1}{(2\pi\gamma_1\gamma_2)^{1/2}(M \sinh\theta_1 \cosh\theta_2 + N \cosh\theta_1 \sinh\theta_2)^{1/2}} \\ & \times \exp(-M\theta_1 - N\theta_2)\left\{1 - \frac{1}{24(M \tanh\theta_1 + N \tanh\theta_2)^3}\right. \\ & \times \left[3M^2 \tanh^2\theta_1(1 + \tanh^2\theta_2) + 3N^2 \tanh^2\theta_2(1 + \tanh^2\theta_1)\right. \\ & - \tanh^3\theta_1 \tanh\theta_2(3 - 5 \tanh^2\theta_2)M^3/N \\ & - \tanh^3\theta_2 \tanh\theta_1(3 - 5 \tanh^2\theta_1)N^3/M + 2 \tanh\theta_1 \tanh\theta_2 \\ & \left. \times MN(3 + 3 \tanh^2\theta_1 + 3 \tanh^2\theta_2 - 5 \tanh^2\theta_1 \tanh^2\theta_2)\right] \\ & \left. + \cdots \right\}. \end{aligned} \tag{4.37}$$

We may now substitute (4.37) in (4.23). Let $M \to 0$ and compare the resulting expression with (XI.2.43). One then obtains

$$D = (\gamma_1\gamma_2)^{-1/2}[(\sinh 2\beta E_1 \sinh 2\beta E_2)^{-2} - 1]^{1/4}. \tag{4.38}$$

Thus we have the final result that for $T > T_c$, if $M^2 + N^2$ is large,

$$\begin{aligned}
\langle\sigma_{0,0}\sigma_{M,N}\rangle \\
&\sim (2\pi)^{-1/2}[(\sinh 2\beta E_1 \sinh 2\beta E_2)^{-2} - 1]^{1/4} \\
&\times (M \sinh\theta_1 \cosh\theta_2 + N\cosh\theta_1 \sinh\theta_2)^{-1/2} \\
&\times \exp(-M\theta_1 - N\theta_2)\{1 - (24)^{-1}(M\tanh\theta_1 + N\tanh\theta_2)^{-3} \\
&\times [3M^2\tanh^2\theta_1(1 + \tanh^2\theta_2) + 3N^2\tanh^2\theta_2(1 + \tanh^2\theta_1) \\
&- \tanh^3\theta_1 \tanh\theta_2(3 - 5\tanh^2\theta_2)M^3/N \\
&- \tanh^3\theta_2 \tanh\theta_1(3 - 5\tanh^2\theta_1)N^3/M \\
&+ 2\tanh\theta_1 \tanh\theta_2\, MN(3 + 3\tanh^2\theta_1 + 3\tanh^2\theta_2 \\
&- 5\tanh^2\theta_1\tanh^2\theta_2)] + \cdots\}.
\end{aligned} \tag{4.39}$$

5. DISCUSSION

The calculations of this and the preceding chapter have been involved. Furthermore, they do not give us as complete information as we obtained for the boundary. It is, therefore, useful to conclude these two chapters[3] with a discussion of those aspects of the correlation function we have not computed and with a comparison with the boundary properties.

(*A*) Monotonicity

Perhaps the most elementary property which we expect the correlation function in Onsager's lattice to possess is that of monotonicity. More

3. For specialists, as opposed to neophytes, we wish to make an additional remark. The correlation function $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ can be expressed as

$$M^2 + \int_0^{\Lambda_1} d\Lambda |\langle 0|\sigma|\Lambda\rangle|^2(\Lambda/\Lambda_0)^N G(\Lambda),$$

where Λ are the eigenvalues of the transfer matrix [H. A. Kramers and G. H. Wannier, *Phys. Rev.* **60**, 252 (1941)], Λ_0 is the maximum eigenvalue, and $G(\Lambda)$ is the density of eigenvalues. It has been shown by Onsager [*Phys. Rev.* **65**, 117 (1944)] that, for $T \neq T_c$, Λ_1 is less than Λ_0, that is, there is a gap in the spectrum of the transfer matrix, and that, near Λ_1, $G(\Lambda) \sim (\Lambda_1 - \Lambda)^{-1/2}$. This inverse-square-root behavior, together with the fact that the right-hand side of (XI.2.43) contains a factor $N^{-1/2}$, implies that $\lim_{\Lambda\to\Lambda_1}\langle 0|\sigma|\Lambda\rangle \neq 0$. So far as we know, (XI.2.43) or a similar formula such as (4.39) is an essential ingredient in deriving this result that $\lim_{\Lambda\to\Lambda_1}\langle 0|\sigma|\Lambda\rangle$ does not vanish for $T > T_c$. We emphasize that, in view of the observation that the right-hand side of (XI.3.24) has a factor N^{-2} instead of $N^{-1/2}$, the nonvanishing of this limiting value is by no means obvious.

precisely, we expect that, if E_1, E_2, M, and N are positive,

$$\langle\sigma_{0,0}\sigma_{M,N}\rangle \geq \langle\sigma_{0,0}\sigma_{M,N+1}\rangle \tag{5.1a}$$

and

$$\langle\sigma_{0,0}\sigma_{M,N}\rangle \geq \langle\sigma_{0,0}\sigma_{M+1,N}\rangle. \tag{5.1b}$$

From (3.50) and (4.39) we know that these inequalities are satisfied for sufficiently large $M^2 + N^2$ if $T \neq T_c$. By an extension of the Wiener-Hopf technique used in the asymptotic expansion of $\langle\sigma_{0,0}\sigma_{0,N}\rangle$ for $T > T_c$ and $T < T_c$, Hartwig and Fisher[4] have proved the special case of (5.1) that, for every positive N,

$$\langle\sigma_{0,0}\sigma_{0,N}\rangle \geq \langle\sigma_{0,0}\sigma_{0,N+1}\rangle \tag{5.2a}$$

and

$$\langle\sigma_{0,0}\sigma_{N,N}\rangle \geq \langle\sigma_{0,0}\sigma_{N+1,N+1}\rangle. \tag{5.2b}$$

However, a proof that the general case (5.1) holds for all N and M which are not necessarily large does not yet exist.

(*B*) Anisotropy

Let **r** be the vector (N, M). The length of this vector is

$$r = (M^2 + N^2)^{1/2}$$

and it makes an angle θ with the horizontal axis. If we consider the limit $r \to \infty$ with θ fixed we have seen from (4.39) and (3.50) that

$$\langle\sigma_{0,0}\sigma_{M,N}\rangle \sim \frac{f_>(\theta)}{r^{1/2}} e^{-r/\xi_>(\theta)} \qquad \text{for } T > T_c \tag{5.3a}$$

and

$$\langle\sigma_{0,0}\sigma_{M,N}\rangle \sim M^2 + \frac{f_<(\theta)}{r^2} e^{-r/\xi_<(\theta)} \qquad \text{for } T < T_c, \tag{5.3b}$$

where $f_>(\theta)$, $f_<(\theta)$, $\xi_>(\theta)$, and $\xi_<(\theta)$ are known functions of θ. It is natural to ask if there are any cases in which $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ is isotropic in the sense that $\xi(\theta)$ is independent of θ. However, it is easily seen from (3.50) and (4.39) that there are no values for E_1 and E_2 (other than $E_1 = E_2 = 0$) for which $\xi_>(\theta)$ and $\xi_<(\theta)$ are independent of θ. Therefore, not even for $E_1 = E_2$ are the correlation functions isotropic if $T \neq T_c$.

The case at $T = T_c$, however, is somewhat different. Indeed, we do not explicitly know how $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ behaves at $T = T_c$ except when

4. R. E. Hartwig and M. E. Fisher, *Arch. Rational Mech. Anal.* **32**, 190 (1969).

$M = 0$, $N = 0$, or $M = N$. In these cases the leading term of the $N \to \infty$ expansion is

$$\langle\sigma_{0,0}\sigma_{M,N}\rangle \sim A(\theta)r^{-1/4}, \tag{5.4}$$

and we find it inconceivable that (5.4) can be other than correct for all θ. That being the case, this condition for "asymptotic isotropy" is that $A(\theta)$ is independent of θ. From an examination of (XI.5.9) it is clear that $A(0)$ and $A(90°)$ will not be equal unless $E_1 = E_2$. When this condition holds we find that

$$\alpha_1 = 3 - 2\sqrt{2} \tag{5.5}$$

and

$$\langle\sigma_{0,0}\sigma_{0,N}\rangle \sim 2^{1/8}AN^{-1/4}. \tag{5.6}$$

Therefore

$$\langle\sigma_{0,0}\sigma_{0,2^{1/2}N}\rangle \sim AN^{-1/4}, \tag{5.7}$$

which is identical with the leading term of $\langle\sigma_{0,0}\sigma_{N,N}\rangle$ given by (XI.4.30). On the basis of this equality we conjecture that, when $T = T_c$ and $E_1 = E_2$, $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ is asymptotically isotropic. More precisely, we conjecture that $A(\theta) = 2^{1/8}A$ for all θ.

(*C*) Comparison with Boundary Correlations

We have found in (VII.5.29) and (VII.6.11) that, for large N,

$$\mathfrak{S}_{1,1}(N) \sim \frac{C_>}{N^{3/2}}\,e^{-N/\xi_{b>}} \qquad \text{if } T > T_c \tag{5.8a}$$

and

$$\mathfrak{S}_{1,1}(N) \sim \mathfrak{M}_1^2 + \frac{C_<}{N^{3/2}}\,e^{-N/\xi_{b<}} \qquad \text{if } T < T_c. \tag{5.8b}$$

Several comparisons should be noted. First of all

$$\xi_{b>} = \xi_>(0) = \ln \alpha_2. \tag{5.9}$$

However

$$\xi_{b<} = \tfrac{1}{2}\xi_<(0) = -\ln \alpha_2. \tag{5.10}$$

Furthermore, for the boundary, the powers of N multiplying the exponentials are the same for $T > T_c$ and $T < T_c$, whereas for the bulk, the powers of r multiplying the exponentials are different. These qualitative differences between the bulk and the boundary are not understood in detail.

(*D*) T Near T_c

The asymptotic expansion (XI.2.43), (XI.2.46), (XI.3.24), (XI.3.27) and (3.50) and (4.39) hold as $M^2 + N^2 \to \infty$ at fixed temperatures $T \neq T_c$. However, from, say, (XI.2.43) and (XI.3.24) we see that, in order to assume that the second term of the expansion is much smaller than the first, we must require that

$$N \gg |x_3| \tag{5.11}$$

or, equivalently, that

$$N \gg |1 - T/T_c|^{-1}. \tag{5.12}$$

More generally, we see from (3.50) and (4.39) that in order for the asymptotic expansion of $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ for $T \neq T_c$ to be valid we must not only have $(M^2 + N^2)^{1/2} \gg 1$ but also

$$(M^2 + N^2)^{1/2} \gg |1 - T/T_c|^{-1}. \tag{5.13}$$

Therefore these expansions give us little information about $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ when the inequality (5.13) fails to hold.

A similar situation has already been encountered when we studied the boundary correlation functions. There also the asymptotic expansion of $\mathfrak{S}_{1,1}(N)$ derived for $N \gg 1$ and T fixed and not equal to T_c is valid only if $N \gg |1 - T/T_c|^{-1}$. However, for the boundary we were able to derive an approximation for $\mathfrak{S}_{1,1}(N)$ which would connect the region $N \gg |1 - T/T_c|^{-1}$ and $T \sim T_c$ with $N \gg 1$ and $T = T_c$. To derive such an interpolating approximation we considered the limit where $N \to \infty$, $T \to T_c$, but

$$t = N(\alpha_2 - 1) = N\beta_c[E_1(1/z_{1c} - z_{1c}) + 2E_2](T/T_c - 1) \tag{5.14}$$

is fixed. In this limit,

$$N[\mathfrak{S}_{1,1}(N) - \mathfrak{M}_1^2] \to f(t). \tag{5.15}$$

Therefore, when $T \sim T_c$ and $N \gg 1$,

$$\mathfrak{S}_{1,1}(N) - \mathfrak{M}_1^2 \sim f(t)/N \tag{5.16}$$

and, from Sec. 8(*C*) in Chapter VII, we see that $f(t)$ has the properties

(1) $f(0) = \pi^{-1}|z_{2c}|^{-1}$, $\qquad$ (5.17)

and

(2) as $|t| \to \infty$,

$$f(t) \to |z_{2c}|^{-1}(2\pi|t|)^{-1/2}e^{-|t|}. \tag{5.18}$$

In particular, we note that property (2) indicates that, if $T \sim T_c$ and $N \gg |1 - T/T_c|^{-1}$,

$$\mathfrak{S}_{1,1}(N) - \mathfrak{M}_1^2 \sim |z_{2c}|^{-1}(2\pi N^3|\alpha_2 - 1|)^{-1/2}e^{-N|1-\alpha_2|}. \tag{5.19}$$

This expression is identical with that obtained by making the approximation $T \sim T_c$ in the asymptotic expansions (VII.5.29) and (VII.6.11).

It would be most desirable if an interpolation formula of this kind could be found for $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ such that if

$$t = (M^2 + N^2)^{1/2}(T/T_c - 1) \tag{5.20}$$

is fixed, then for $M^2 + N^2 \to \infty$,

$$(M^2 + N^2)^{1/8}[\langle\sigma_{0,0}\sigma_{M,N}\rangle - M^2] \to f(t, \theta). \tag{5.21}$$

Such an $f(t, \theta)$ should have properties similar to properties (1) and (2) of $f(t)$, namely,

(1′) $f(0, \theta)$ should be that positive function of θ such that, at T_c, $\langle\sigma_{0,0}\sigma_{M,N}\rangle \sim f(0, \theta)/(M^2 + N^2)^{1/8}$; from the previous chapter we have the explicit information that

$$f(0, 0) = \left(\frac{1 + z_{1c}^2}{1 - z_{1c}^2}\right)^{1/4} A, \tag{5.22a}$$

$$f(0, 45^\circ) = 2^{1/8}A, \tag{5.22b}$$

and

$$f(0, 90^\circ) = \left(\frac{1 + z_{2c}^2}{1 - z_{2c}^2}\right)^{1/4} A; \tag{5.22c}$$

(2′) as $t \to +\infty$,

$$\begin{aligned} f(t, \theta) \to\, & (2\pi)^{-1/2}K_1K_2[t(\gamma_1^{-1}\sin^2\theta + \gamma_2^{-1}\cos^2\theta)]^{-1/4} \\ & \times \exp[-tK_2(\gamma_1^{-1}\sin^2\theta + \gamma_2^{-1}\cos^2\theta)^{1/2}], \end{aligned} \tag{5.23a}$$

and as $t \to -\infty$,

$$\begin{aligned} f(t, \theta) \to\, & (8\pi)^{-1}K_1K_2^{\frac{1}{4}}|t|^{-7/4}(\gamma_1^{-1}\sin^2\theta + \gamma_2^{-1}\cos^2\theta)^{-1} \\ & \times \exp[-|t|2K_2(\gamma_1^{-1}\sin^2\theta + \gamma_2^{-1}\cos^2\theta)^{1/2}], \end{aligned} \tag{5.23b}$$

where

$$K_1 = [4\beta_c(E_1 \coth 2\beta_cE_1 + E_2 \coth 2\beta_cE_2)]^{1/4} \tag{5.24a}$$

and

$$K_2 = 2\sqrt{2}\beta_c[E_1(1 - z_{1c}) + E_2(1 - z_{2c})]. \tag{5.24b}$$

These formulas are obtained by making the approximation $T \sim T_c$ in (3.50) and (4.39). We note in particular that if $E_1 = E_2$ these limiting forms do not depend on θ.

The interpolating function $f(t, \theta)$ is closely related to the behavior of the magnetic susceptibility at $H = 0$ near T_c. As we discussed in Chapter II, the magnetic susceptibility of Onsager's lattice is expressible in terms of the spin correlation function as

$$\chi = \frac{\partial M}{\partial H}\bigg|_{H=0} = \beta \lim_{H\to 0} \lim_{\substack{\mathscr{M}\to\infty \\ \mathscr{N}\to\infty}} \frac{1}{(2\mathscr{M})(2\mathscr{N})} \sum_{M=-\mathscr{M}+1}^{\mathscr{M}} \sum_{M'=-\mathscr{M}+1}^{\mathscr{M}}$$
$$\times \sum_{N=-\mathscr{N}+1}^{\mathscr{N}} \sum_{N'=-\mathscr{N}+1}^{\mathscr{N}} [\langle \sigma_{M,N}\sigma_{M',N'}\rangle - S_\infty]$$
$$= \beta \sum_{M=-\infty}^{\infty} \sum_{N=-\infty}^{\infty} [\langle \sigma_{0,0}\sigma_{M,N}\rangle - S_\infty]. \tag{5.25}$$

We have been able to derive only asymptotic expansions for $\langle \sigma_{0,0}\sigma_{M,N}\rangle$, so we cannot hope to use (5.25) to compute χ exactly.

However, if we omit a fixed, finite number of terms from the sum we will only decrease χ by a function which is continuous at T_c. Therefore we see immediately that, at T_c,

$$\chi > 4\beta \sum_{M=M_0}^{\infty} \sum_{N=N_0}^{\infty} \frac{f(0,\theta)}{(M^2+N^2)^{1/8}} + 2\beta \sum_{M=-M_0+1}^{M_0-1} \sum_{N=N_0}^{\infty} \frac{f(0,\theta)}{(M^2+N^2)^{1/8}}$$
$$+ 2\beta \sum_{N=-N_0+1}^{N_0-1} \sum_{M=M_0}^{\infty} \frac{f(0,\theta)}{(M^2+N^2)^{1/8}}$$
$$> 4\beta \min_\theta [f(0,\theta)] \sum_{M=M_0}^{\infty} \sum_{N=N_0}^{\infty} \frac{1}{(M^2+N^2)^{1/8}}. \tag{5.26}$$

This last series clearly diverges. Such a divergence when $T = T_c$ is, of course, not unexpected. However, a knowledge of the interpolating function $f(t, \theta)$ will let us compute important information about how χ diverges.

Consider first the boundary. Then

$$\frac{\chi}{\beta} = 2 \sum_{N=N_0}^{\infty} \frac{f(t)}{N} + O(1) = 2 \sum_{N=N_0}^{\infty} \frac{f[N(\alpha_2 - 1)]}{N} + O(1)$$
$$= 2\int_{N_0}^{\infty} dN \frac{f[N(\alpha_2 - 1)]}{N} + O(1)$$
$$= 2\int_{N_0|\alpha_2 - 1|}^{\infty} dt \frac{f(t)}{t} + O(1). \tag{5.27}$$

This integral converges as $t \to \infty$ because of property (2) but diverges as $t \to 0$. Thus

$$\frac{\chi}{\beta} = -2f(0) \ln N_0|\alpha_2 - 1| + O(1)$$
$$= -\frac{2}{\pi|z_{2c}|} \ln \left|1 - \frac{T}{T_c}\right| + O(1), \tag{5.28}$$

where we have used the value of $f(0)$ given by (5.17). This expression for χ is exactly the same as that derived in (VI.5.38). Therefore, for the boundary, mere knowledge of the form of the $T \sim T_c$ expansion plus the knowledge of the asymptotic behavior of $\mathfrak{S}_{1,1}(N)$ at $T = T_c$ is sufficient to compute χ.

Consider now the bulk where the behavior of χ near T_c has not yet been discovered. Using the form of the interpolating function (5.21) we have

$$\chi = 4\beta|1 - T/T_c|^{1/4}\int_0^{\pi/2} d\theta \int_{r_0}^{\infty} dr\, r \frac{f[r(T/T_c - 1), \theta]}{[r|T/T_c - 1|]^{1/4}}[1 + O(1)]$$

$$= 4|1 - T/T_c|^{-7/4}\int_0^{\pi/2} d\theta \int_{r_0|1-T/T_c|}^{\infty} dt t^{3/4} f[\operatorname{sgn}(T - T_c)t, \theta][1 + O(1)]. \quad (5.29)$$

At $T \to T_c$ the lower limit of t integration may be replaced by zero since the integral converges at zero. The error introduced vanishes at $T = T_c$ and therefore does not affect the coefficient of $|1 - T/T_c|^{-7/4}$. Accordingly, we find that the most divergent term in χ as $T \to T_c$ is

$$\chi \sim c^+|1 - T/T_c|^{-7/4} \qquad \text{if } T \to T_c^+$$

and

$$\chi \sim c^-|1 - T/T_c|^{-7/4} \qquad \text{if } T \to T_c^- \quad (5.30)$$

where

$$c^+ = 4\beta_c \int_0^{\pi/2} d\theta \int_0^{\infty} dt t^{3/4} f(t, \theta)$$

and

$$c^- = 4\beta_c \int_0^{\pi/2} d\theta \int_0^{\infty} dt t^{3/4} f(-t, \theta). \quad (5.31)$$

In contrast to the boundary, where $f(t) = f(-t)$,

$$f(-t, \theta) \neq f(t, \theta). \quad (5.32)$$

More specifically, we know from property (2) that, as $t \to \infty$,

$$f(-t, \theta)/f(t, \theta) \to 0. \quad (5.33)$$

Therefore we make the obvious conjecture that not only asymptotically, but for all t,

$$f(-t, \theta) \leq f(t, \theta). \quad (5.34)$$

An immediate consequence of the conjecture (5.34) is

$$c^+ > c^-. \quad (5.35)$$

It is impossible to use this approach to obtain more exact information about χ than that contained in (5.30) and (5.35) without having more information about $f(t, \theta)$. It is possible, however, to make numerical studies of χ by use of series expansions. This has been done when $E_1 = E_2$ for $T < T_c$ by Baker[5] and for $T > T_c$ by Essam and Fisher.[6] They obtain

$$c^+ \sim 0.96272, \qquad c^- = 0.0262 \pm 0.0006. \tag{5.36}$$

(It is not clear from the published work how the estimate of error on c^- is obtained, and no estimate of error on c^+ is given.)

In contrast to the boundary case, where all diverging terms in χ are exhibited by (5.28), the divergences exhibited by (5.30) for the bulk are not quite the whole story. It is possible, as we did for the boundary, to consider the correction term to the formula

$$\langle \sigma_{0,0}\sigma_{M,N} \rangle - M^2 \sim \frac{f(t, \theta)}{(M^2 + N^2)^{1/8}}. \tag{5.37}$$

An obvious guess at the first correction to this formula is

$$\langle \sigma_{0,0}\sigma_{M,N} \rangle - M^2 \sim \frac{f(t, \theta)}{(M^2 + N^2)^{1/8}} + \frac{f_1(t, \theta)}{(M^2 + N^2)^{5/8}}, \tag{5.38}$$

where we speculate on the basis of the $T = T_c$ expansions of $\langle \sigma_{0,0}\sigma_{0,N} \rangle$ and $\langle \sigma_{0,0}\sigma_{N,N} \rangle$ that

$$f_1(0, \theta) = 0. \tag{5.39}$$

However, if $t \neq 0$, $f_1(t, \theta)$ should not vanish. This correction term leads to an additional term in χ which diverges as $|1 - T/T_c|^{-3/4}$. Finally, in addition to these two diverging terms there will be a term of $O(1)$. There is no reason that this constant must be the same above and below T_c. Therefore, we conclude that if $T \gtrsim T_c$

$$\chi = c^+|1 - T/T_c|^{-7/4} + c_1^+|1 - T/T_c|^{-3/4} + c_2^+ + o(1) \tag{5.40a}$$

and if $T \lesssim T_c$

$$\chi = c^-|1 - T/T_c|^{-7/4} + c_1^-|1 - T/T_c|^{-3/4} + c_2^- + o(1). \tag{5.40b}$$

Since the contribution to (5.25) from $|M| \leq M_0$ and $|N| \leq N_0$ is continuous at T_c, the difference between c_2^+ and c_2^- can be found from a sufficiently detailed computation of the asymptotic behavior of $\langle \sigma_{0,0}\sigma_{M,N} \rangle$ for $T \sim T_c$.

5. G. A. Baker, *Phys. Rev.* **124**, 768 (1961).
6. J. W. Essam and M. E. Fisher, *J. Chem. Phys.* **38**, 802 (1963).

CHAPTER XIII
Boundary Hysteresis and Spin Probability Functions

1. INTRODUCTION[1]

When $E_1 > 0$, $E_2 > 0$, and $T < T_c$ the magnetization $M(H)$ is discontinuous at $H = 0$. In the bulk, beyond the remark made in the last chapter that if $T \neq T_c$, $\chi = \partial M/\partial H|_{H=0}$ is finite, we are unable to say much more about the behavior of $M(H)$ as a function of H near $H = 0$. For the boundary magnetization $\mathfrak{M}_1(\mathfrak{H})$, however, the situation is quite different. We discovered in Sec. 5 of Chapter VI an explicit formula for $\mathfrak{M}_1(\mathfrak{H})$. From this representation we have found for $T < T_c$ that, though $\mathfrak{M}_1(\mathfrak{H})$ is discontinuous at $\mathfrak{H} = 0$, all derivatives of $\mathfrak{M}_1(\mathfrak{H})$ remain finite as $\mathfrak{H} \to 0^+$. Moreover, $\mathfrak{M}_1(\mathfrak{H})$ could be analytically continued from $\mathfrak{H} > 0$ to $\mathfrak{H} < 0$ in such a way that if $\mathfrak{M}_1(\mathfrak{H})$ and its analytic continuation are considered together, the resulting two-valued function of $\mathfrak{H}$ has a loop that is reminiscent of a hysteresis behavior. In this chapter, we investigate the physical meaning of this mathematical result in detail. For this purpose, we study $P(\bar{\sigma}; \mathfrak{H})$, the probability that in a magnetic field $\mathfrak{H}$ the average boundary spin has the value $\bar{\sigma}$.

Consider an Ising model in which $\bar{\mathcal{N}}$ spins interact with a magnetic field of strength H. (In practice, $\bar{\mathcal{N}}$ will usually be $\mathcal{N}$ or $\mathcal{M}\mathcal{N}$.) Denote the spin variable of the jth site that interacts with H by σ_j. Let $\delta(x)$ denote the Kronecker delta of the discrete variable x and assume that $\bar{\sigma}$ is such that $|\frac{1}{2}\bar{\mathcal{N}}\bar{\sigma}|$ is an integer not larger than $\frac{1}{2}\bar{\mathcal{N}}$. Then $P(\bar{\sigma}; H)$, the probability that the average spin of those $\bar{\mathcal{N}}$ spins is $\bar{\sigma}$, is

$$P(\bar{\sigma}; H) = \left\langle \delta\left(\sum_{j=1}^{\bar{\mathcal{N}}} \sigma_j - \bar{\mathcal{N}}\bar{\sigma} \right) \right\rangle. \tag{1.1}$$

1. This chapter is based on the work of B. M. McCoy and T. T. Wu, *Phys. Rev.* **162**, 436 (1967), **174**, 546 (1968).

The Kronecker delta can be written

$$\delta(x) = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta e^{ix\theta}, \tag{1.2}$$

and we substitute this representation in (1.1) to find

$$\begin{aligned} P(\bar{\sigma}; H) &= \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta \left\langle \exp\left[i\theta\left(\sum_{j=1}^{\bar{\mathcal{N}}} \sigma_j - \bar{\mathcal{N}}\bar{\sigma}\right)\right]\right\rangle \\ &= Z(H)^{-1}\frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta \sum_{\sigma=\pm 1} \\ &\quad \times \exp\left[-\beta\mathscr{E}(H=0) + \beta H \sum_{j=1}^{\bar{\mathcal{N}}} \sigma_j + i\theta \sum_{j=1}^{\bar{\mathcal{N}}} \sigma_j - i\theta\bar{\mathcal{N}}\bar{\sigma}\right] \\ &= Z(H)^{-1} e^{\beta H \bar{\mathcal{N}}\bar{\sigma}} \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta \exp\left(-i\theta\bar{\mathcal{N}}\bar{\sigma}\right) Z(i\beta^{-1}\theta), \end{aligned} \tag{1.3}$$

where $Z(H)$ is the partition function of the system in the presence of the magnetic field H. The rest of this chapter will be devoted to consequences of this formula. Formula (1.3) is an exact result which is valid even for a finite lattice of $\mathcal{M}$ rows and $\mathcal{N}$ columns. We will discuss the relation between the cases $\mathcal{M}$ and $\mathcal{N}$ finite and $\mathcal{M} \to \infty$ and $\mathcal{N} \to \infty$ in detail in Sec. 4.

In the thermodynamic limit the free energy is defined as

$$-\frac{1}{\beta} \lim_{\substack{\mathcal{M}\to\infty \\ \mathcal{N}\to\infty}} \frac{1}{\mathcal{M}\mathcal{N}} \ln Z(H). \tag{1.4}$$

Therefore, for a large system (at least for some purposes), we may write

$$Z(H) \sim e^{-\beta\bar{\mathcal{N}}F(H)} Z(0), \tag{1.5}$$

where $F(H)$ is that part of the free energy that depends on H and obeys $F(0) = 0$. Therefore, we write (1.3) as

$$P(\bar{\sigma}; H) \sim e^{\beta\bar{\mathcal{N}}[H\bar{\sigma} + F(H)]} \frac{\beta}{2\pi i}\int_{-i\pi/\beta}^{i\pi/\beta} d\xi \exp\{-\bar{\mathcal{N}}\beta[\xi\bar{\sigma} + F(\xi)]\}. \tag{1.6}$$

If in addition to the assumption that $\mathcal{M}$ and $\mathcal{N}$ are large, we also assume that $\bar{\mathcal{N}}$ is large, we may approximate (1.6) by the method of steepest descents. The point of steepest descent is determined from

$$\bar{\sigma} = -F'(\xi_0) = M(\xi_0). \tag{1.7}$$

(This equation must be used with caution if $T < T_c$ and $|\bar{\sigma}| < M(0^+)$. We return to this point in Sec. 2.) On the assumption that $F(H)$ has a sufficiently large range of analyticity that we can deform the contour to the steepest-descents path, and if $\chi(\xi_0) = -F''(\xi_0)$ exists, we find that

$$P(\bar{\sigma}; H) \sim [\beta/\chi(\xi_0)\mathcal{N}2\pi]^{1/2} \exp\{\mathcal{N}[W(\bar{\sigma}) + \beta(H\bar{\sigma} + F(H))]\}, \tag{1.8}$$

where

$$W(\bar{\sigma}) = -\beta[\xi_0\bar{\sigma} + F(\xi_0)]. \tag{1.9}$$

In the case of large $\mathcal{N}$ it is more convenient to consider the probability density function $p(\bar{\sigma}, H)$ which is defined as the probability that the average boundary spin will be found in the interval $d\bar{\sigma}$ centered about $\bar{\sigma}$. Since, in the interval $-1 \le \bar{\sigma} \le 1$, $\bar{\sigma}$ may take on $\mathcal{N} + 1$ distinct values we find for large $\mathcal{N}$

$$p(\bar{\sigma}, H) = \tfrac{1}{2}\mathcal{N}P(\bar{\sigma}; H). \tag{1.10}$$

Just as the probability function $P(\bar{\sigma}; H)$ satisfies

$$\sum_{\sigma=-1}^{1} P(\bar{\sigma}; H) = 1, \tag{1.11a}$$

the density function $p(\bar{\sigma}, H)$ satisfies, as $\mathcal{N} \to \infty$,

$$\int_{-1}^{1} d\bar{\sigma} p(\bar{\sigma}, H) = 1. \tag{1.11b}$$

We will show in detail in the next section that $P(\bar{\sigma}; 0)$ has its maxima at 0 if $T \ge T_c$ and $\pm M(0^+)$ if $T < T_c$ and that near these maxima $P(\bar{\sigma}; 0)$ behaves as a Gaussian if $T \ne T_c$. At T_c, $\chi(\xi_0)$ will not exist and the Gaussian form in (1.8) breaks down. What replaces the Gaussian will be computed in Sec. 3 from (1.3).

The approximation (1.8) expresses P in terms of the free energy and not the partition function. When $T > T_c$ such an approximation is quite accurate. However, it must be recalled that the partition function for a lattice of $\mathcal{M}$ rows and $\mathcal{N}$ columns contains more information than does the free energy per particle. This information becomes important if we wish to study in detail the behavior of the spin probability function when $T < T_c$ and $-M(0^+) < \bar{\sigma} < M(0^+)$. This case is studied in Secs. 4 and 5, where we consider the dependence of the spin probability function on: (1) the way in which the $\mathcal{M} \to \infty$, $\mathcal{N} \to \infty$ limit is attained, and (2) the modification caused by boundary conditions. In Sec. 4 we also study the behavior of the magnetization of the Jth row of the half-plane Onsager lattice. This proves necessary for a complete physical interpretation of the boundary hysteresis phenomena.

Before applying these formulas, we find it useful to give a heuristic argument why the distribution $p(\bar{\sigma}, 0)$ [which will be abbreviated $p(\bar{\sigma})$] can be approximated by a Gaussian when $T \ne T_c$ and $\bar{\sigma}$ is close enough to M. For definiteness, we consider the case $\bar{\mathcal{N}} = \mathcal{N}\mathcal{M}$ (H interacts with all spins). Define the nth moment of $p(\bar{\sigma})$ by

$$\langle \bar{\sigma}^n \rangle = \bar{\mathcal{N}}^{-n} \sum \langle \sigma_j \sigma_k \cdots \sigma_l \rangle_{\mathcal{M},\mathcal{N}}, \tag{1.12}$$

where there are n σ's in the product and the sum is over all lattice sites. If n is odd, this moment vanishes by symmetry. If n is 2 we note that in Onsager's lattice with periodic boundary condition when $j^2 + k^2$, $\mathcal{M}$, and $\mathcal{N}$ are all large

$$\langle \sigma_{0,0} \sigma_{j,k} \rangle_{\mathcal{M},\mathcal{N}} \sim M^2, \tag{1.13}$$

where M is the spontaneous magnetization.

When $(j^2 + k^2)^{1/2}$ is of the order of $\mathcal{M}$ or $\mathcal{N}$ the validity of (1.13) depends on the boundary condition (see Sec. 5) but is expected to be a general property of most lattices. In that case we have for even n

$$\lim_{\bar{\mathcal{N}} \to \infty} \langle \bar{\sigma}^n \rangle = M^n. \tag{1.14}$$

This means that $p(\bar{\sigma})$ consists of two sharp spikes, one at each of the two values of the spontaneous magnetization.

To obtain further information about the structure of these spikes, we define a new average $\langle\ \rangle_{1/2}$ and a new operator,

$$\rho_j = \sigma_j - M, \tag{1.15}$$

and consider only those states which lead to $\langle \rho_j \rangle_{1/2} = 0$. Loosely speaking, we are averaging over the half of the states which have a spontaneous magnetization of $+M$. For this special class of states, we may systematically define the functions $f_{ijk\ldots}$ as follows:

$$\langle \rho_i \rho_j \rangle_{1/2} = \langle \rho_i \rangle_{1/2} \langle \rho_j \rangle_{1/2} + f_{ij} = f_{ij}, \tag{1.16}$$

$$\langle \rho_i \rho_j \rho_k \rangle_{1/2} = f_{ijk}, \tag{1.17}$$

$$\langle \rho_i \rho_j \rho_k \rho_l \rangle_{1/2} = f_{ij} f_{kl} + f_{ik} f_{jl} + f_{il} f_{jk} + f_{ijkl}. \tag{1.18}$$

The $f_{ij\ldots}$ are totally symmetric functions of their indices and are constructed so that when any two indices refer to points widely separated in space $f_{ij\ldots}$ goes to zero. In terms of these functions, we may expand the moments of $p(\bar{\sigma})$ as a series in $\bar{\mathcal{N}}^{-1}$. It is a simple counting problem to verify that

$$\begin{aligned} \langle \bar{\rho}^{2n} \rangle_{1/2} &= \bar{\mathcal{N}}^{-2n} \sum \langle \rho_i \rho_j \cdots \rho_l \rangle_{1/2} \\ &= (2n-1)(2n-3) \cdots 3 \bar{\mathcal{N}}^{-2n} \left(\sum f_{ij} \right)^n + O(\bar{\mathcal{N}}^{-n-1}) \\ &= (2n-1)(2n-3) \cdots 3 \bar{\mathcal{N}}^{-n} \left(\sum f_{0j} \right)^n + O(\bar{\mathcal{N}}^{-n-1}), \end{aligned} \tag{1.19}$$

where the last equation is valid only in a translationally invariant lattice and the $O(\mathcal{N}^{-n-1})$ term is absent if $n = 1$. Similarly,

$$\begin{aligned}\langle\bar{\rho}^{2n+1}\rangle_{1/2} &= \mathcal{N}^{-2n-1}\sum\langle\rho_i\rho_j\cdots\rho_l\rangle_{1/2}\\ &= (2n+1)2n(2n-1)(3!)^{-1}(2n-3)(2n-5)\cdots\\ &\cdots 3\left(\mathcal{N}^{-3}\sum f_{ijk}\right)\left(\mathcal{N}^{-2}\sum f_{ij}\right)^{n-1} + O(\mathcal{N}^{-n-2}).\end{aligned} \tag{1.20}$$

The leading terms in (1.19) are the even moments of a Gaussian of width $(\mathcal{N}^{-1}\sum_j f_{0j})^{1/2}$ centered at $\bar{\rho} = 0$. To this order, the odd moments (1.20) are zero. Therefore, if $T \neq T_c$ (so $\sum_j f_{0j}$ converges) and $\bar{\sigma}$ is close enough to $\pm M$, $p(\bar{\sigma}, 0)$ is well approximated by a Gaussian. However, the important question of how close to M one must go before Gaussian behavior is obtained cannot be answered from this analysis. Finally, we may make connection with the general formula (1.8) by remarking that if we make a complete asymptotic evaluation of the integral in (1.8) and compute the moments of the resulting $p(\bar{\sigma}, 0)$ about $+M$, we will obtain exactly the expansions (1.19) and (1.20).

2. BOUNDARY HYSTERESIS: A CRUDE INTERPRETATION

The discussion of $p(\bar{\sigma})$ just given, which allows us to conclude that, for $T < T_c$, $p(\bar{\sigma})$ consists of two sharp spikes, may be carried over to the case of the boundary as well. However, for the case in which the field $\mathfrak{H}$ interacts with the $2\mathcal{N}$ spins of the boundary, $\mathfrak{F}(\mathfrak{H})$ is known from Chapter VI. Therefore we may use (1.8) or, more generally, (1.3) to compute the boundary spin probability density $p(\bar{\sigma})$ more explicitly.

It is clear if $T > T_c$ how to apply (1.8). However, if $T < T_c$, it is not obvious in general how (1.7) may be satisfied. We are not in a position to answer this generally, but for the boundary we can give an explicit answer: if

$$0 \leq \bar{\sigma} \leq \mathfrak{M}_1(0^+), \tag{2.1}$$

then the point of steepest descent is shifted to the analytic continuation of $\mathfrak{M}_1$. That is, (1.8) is still valid provided that we note that the point of steepest descent is now at

$$\bar{\sigma} = \mathfrak{M}_1^c(\xi). \tag{2.2}$$

Thus, for (2.1), (1.9) takes the form

$$W = W(\mathfrak{M}_1^c) = -\beta(\mathfrak{H}\mathfrak{M}_1^c + \mathfrak{F}^c), \tag{2.3}$$

where $\mathfrak{F}^c$ is the analytic continuation of $\mathfrak{F}$. For simplicity, we shall use

(1.9), with $0 \le \mathfrak{M}_1 \le 1$, to mean both (1.9) and (2.3). In particular, differentiation with respect to $\mathfrak{M}_1$ gives

$$\partial W/\partial \mathfrak{M}_1 = -\beta \mathfrak{H}. \tag{2.4}$$

Thus

$$W = W' = 0 \tag{2.5}$$

at $\mathfrak{H} = 0$, that is, $\mathfrak{M}_1 = \mathfrak{M}_1(0^+)$. In other words, the distribution does have a maximum at $\bar{\sigma} = \mathfrak{M}_1(0^+)$. The curve $W(\bar{\sigma})$ is plotted in Fig. 13.1. Note the discontinuity of $W'(\bar{\sigma})$ at $\bar{\sigma} = 0$, as given by (2.4).

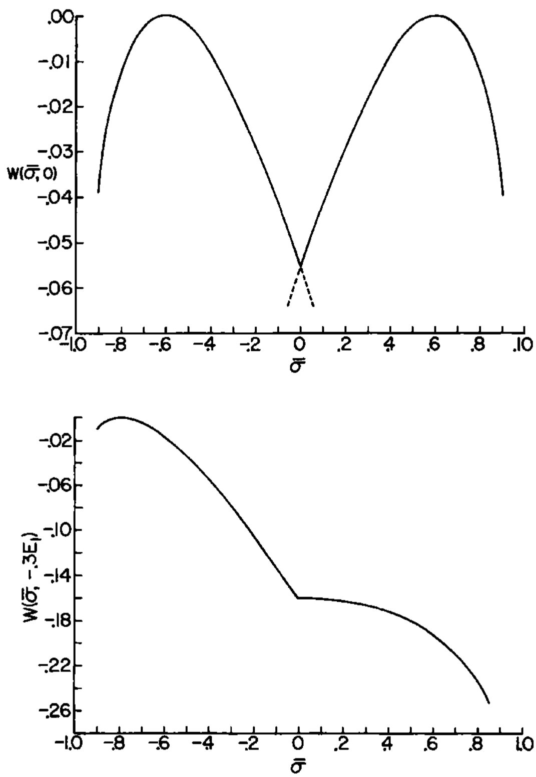


Fig. 13.1. (*a*) The function $W(\bar{\sigma}, 0)$ plotted for $E_1/k = E_2/k = 1$ and $T = 0.9T_c$; (*b*) the function $W(\bar{\sigma}, \mathfrak{H})$ plotted for $\mathfrak{H} = -0.3E_1$, $E_1/k = E_2/k = 1$, and $T = 0.9T_c$; at this value of $\mathfrak{H}$ the secondary maximum has just reached $\bar{\sigma} = 0$.

When a magnetic field is present, we still define

$$W(\bar{\sigma}, \mathfrak{H}) = \lim_{\mathcal{N} \to \infty} (2\mathcal{N})^{-1} \ln \lim_{\mathcal{M} \to \infty} P(\bar{\sigma}; \mathfrak{H}). \tag{2.6}$$

This is very simply related to $W(\bar{\sigma}) = W(\bar{\sigma}, 0)$ from (1.8) as

$$W(\bar{\sigma}, \mathfrak{H}) = W(\bar{\sigma}) + \beta\mathfrak{H}\bar{\sigma} - \text{const}, \tag{2.7}$$

where the constant, which is independent of $\bar{\sigma}$, is determined by the condition

$$\max_{-1 \leqslant \bar{\sigma} \leqslant 1} W(\bar{\sigma}, \mathfrak{H}) = 0. \tag{2.8}$$

With reference to Fig. 13.1, we see that, for $|\mathfrak{H}|$ not too large, $W(\bar{\sigma}, \mathfrak{H})$ has two maxima, located at $\bar{\sigma}_r$ and $\bar{\sigma}_l$, say, with $\bar{\sigma}_r > \bar{\sigma}_l$. For $\mathfrak{H} > 0$, the right-hand maximum at $\bar{\sigma}_r$ is larger, whereas for $\mathfrak{H} < 0$, the left-hand maximum at $\bar{\sigma}_l$ is larger. For $\mathfrak{H} > 0$, by (2.4) and (2.7), $\bar{\sigma}_r$ is located at the point where

$$\mathfrak{M}_1(\mathfrak{H}) = \bar{\sigma}_r. \tag{2.9}$$

Similarly, for $\mathfrak{H} < 0$ and $|\mathfrak{H}|$ sufficiently small, $\bar{\sigma}_r$ satisfies

$$\mathfrak{M}_1^c(\mathfrak{H}) = \bar{\sigma}_r. \tag{2.10}$$

However, as seen from Fig. 13.1, the right-hand maximum *disappears* after $\bar{\sigma}_r$ reaches 0. For values of $\mathfrak{H}$ such that $\mathfrak{M}_1^c(\mathfrak{H}) \leq 0$, $W(\bar{\sigma}, \mathfrak{H})$ has only one maximum.

A possible physical interpretation of this mathematical result is as follows. For a system in thermodynamic equilibrium, with $T < T_c$ and $\mathfrak{H} \neq 0$, the average value of the boundary spin is almost certainly close to $\mathfrak{M}_1$; these are stable states. As $\mathfrak{H}$ is reduced from a small positive value to a small negative value, this average value changes sign. Since it is difficult to make transition between states of these opposite values of average boundary spin, it takes a very long time to reach thermodynamic

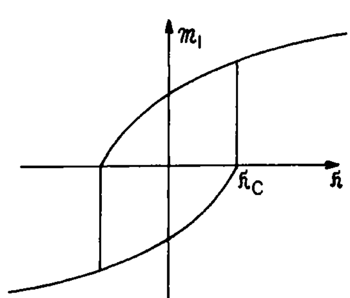


Fig. 13.2. Schematic plot of $\mathfrak{M}_1(\mathfrak{H})$ and $\mathfrak{M}_1^c(\mathfrak{H})$ indicating a hysteresis loop that stops at $\mathfrak{M}_1^c(\mathfrak{H}) = 0$.

equilibrium even after $\mathfrak{H}$ is made negative. For a time (short compared with the time needed to approach this equilibrium), the average value of the boundary spins for the system refuses to change sign; instead, it follows the position of the lesser maximum.

This argument allows us to conclude that as $\mathfrak{H}$ is decreased from ∞ the boundary magnetization will follow $\mathfrak{M}_1(\mathfrak{H})$ and its analytic continuation $\mathfrak{M}_1^c(\mathfrak{H})$ as long as $\mathfrak{M}_1^c(\mathfrak{H})$ is positive (see Fig. 13.2). However, no conclusion can be reached on the basis of these considerations about the region where $\mathfrak{M}_1^c(\mathfrak{H}) < 0$. To gain further insight into the significance of this region we need the more elaborate considerations of Sec. 4.

3. CRITICAL ISOTHERM

When $T \neq T_c$ it is straightforward to make explicit the Gaussian nature of $p(\bar{\sigma})$ where $\bar{\sigma}$ is near its maximum at $M(0^+)$. We may expand

$$\bar{\sigma} = M(\xi_0) \sim M(0^+) + \chi(0^+)\xi_0 + \cdots, \tag{3.1}$$

so

$$[\bar{\sigma} - M(0^+)]/\chi(0) \sim \xi_0. \tag{3.2}$$

Thus

$$F(\xi_0) \sim -\xi_0 M(0^+) - \tfrac{1}{2}\xi_0^2\chi(0) + \cdots \sim -\tfrac{1}{2}[\bar{\sigma}^2 - M^2(0^+)]/\chi(0) \tag{3.3}$$

and we find

$$p(\bar{\sigma}) \sim \mathcal{N}\frac{\epsilon_T}{2}\left[\frac{\beta}{\chi(0)2\mathcal{N}\pi}\right]^{1/2}\exp\left\{-\mathcal{N}\beta\frac{[\bar{\sigma} - M(0^+)]^2}{2\chi(0)}\right\}, \tag{3.4}$$

where

$$\epsilon_T = \begin{cases} 1 & \text{if } T < T_c \\ 2 & \text{if } T > T_c. \end{cases} \tag{3.5}$$

This factor 2 which ϵ_T accounts for is not computed from (1.9) but is required from the normalization condition (1.11b) and the remark that, for $H = 0$ and $T < T_c$, $p(\bar{\sigma})$ has *two* maxima.

If $T = T_c$ and $H = 0$, (3.4) breaks down since $\chi(0)$ diverges at T_c. This divergence indicates that $p(\bar{\sigma})$ no longer has a Gaussian form.

Consider first the situation on the boundary for T near T_c and $\bar{\sigma}$ small. Recall from (VI.5.35) and (VI.5.36) that if $T < T_c$

$$\mathfrak{M}_1 \sim \left(\frac{1 - \alpha_2}{|z_2|}\right)^{1/2}\operatorname{sgn} z - \frac{2}{\pi}\frac{z}{|z_2|}\ln(1 - \alpha_2 + z^2), \tag{3.6a}$$

and that if $T > T_c$

$$\mathfrak{M}_1 \sim -\frac{2}{\pi}\frac{z}{|z_2|}\ln\left(1 - \frac{1}{\alpha_2} + z^2\right). \tag{3.6b}$$

Then from (1.9)

$$W(\bar{\sigma}) \sim \frac{1}{\pi}\frac{z^2}{|z_2|}\ln(|1-\alpha_2| + z^2), \tag{3.7}$$

where z is considered to be a parameter that, following (1.7), is to be found from

$$\bar{\sigma} = \left[\frac{1-\alpha_2}{|z_2|}\right]^{1/2} \operatorname{sgn} z - \frac{2}{\pi}\frac{z}{|z_2|}\ln(1-\alpha_2+z^2) \tag{3.8}$$

if $T \leq T_c$ and from

$$\bar{\sigma} = -\frac{2}{\pi}\frac{z}{|z_2|}\ln(\alpha_2 - 1 + z^2) \tag{3.9}$$

for $T \geq T_c$. In particular, at T_c

$$W(\bar{\sigma}) \sim \frac{2}{\pi}\frac{z^2}{|z_2|}\ln|z|, \tag{3.10}$$

with

$$\bar{\sigma} = -\frac{4}{\pi}\frac{z}{|z_2|}\ln|z|. \tag{3.11}$$

For $\bar{\sigma} \sim 0$ this last equation may be solved approximately by iteration to give

$$z \sim -\tfrac{1}{4}\bar{\sigma}\pi|z_2|/\ln|\bar{\sigma}|, \tag{3.12}$$

which may be substituted in (3.10) to give

$$W(\bar{\sigma}) \sim \tfrac{1}{8}\pi|z_2|\bar{\sigma}^2/\ln|\bar{\sigma}|. \tag{3.13}$$

Therefore, for $\bar{\sigma}$ and ξ near zero, we use the approximation

$$\beta\bar{\sigma} + \mathfrak{F}(\xi) \sim W(\bar{\sigma}) + \tfrac{1}{2}\xi^2\mathfrak{F}''(\xi) \tag{3.14}$$

in the integral (1.6) to obtain, with $\bar{\mathcal{N}} = 2\mathcal{N}$,

$$p(\bar{\sigma}) \sim \mathcal{N}\frac{\beta}{2\pi}e^{-2\mathcal{N}W(\bar{\sigma})}\int_{-\epsilon}^{\epsilon} d\xi \exp\left[4\mathcal{N}(\beta^2/\pi|z_2|)\xi^2\ln|\xi|\right], \tag{3.15}$$

where $0 < \epsilon < 1$. For large $\mathcal{N}$,

$$\int_{-\epsilon}^{\epsilon} d\xi \exp(\mathcal{N}\xi^2\ln|\xi|) \sim \left(\frac{\pi}{\mathcal{N}\ln\mathcal{N}}\right)^{1/2}, \tag{3.16}$$

and so we find

$$p(\bar{\sigma}) \sim \left(\frac{|z_2|\mathcal{N}}{4\ln\mathcal{N}}\right)^{1/2}\exp\left[\tfrac{1}{4}\pi\mathcal{N}|z_2|\bar{\sigma}^2/\ln\bar{\sigma}\right], \tag{3.17}$$

which is easily seen to obey the normalization (1.11*b*) to leading order as $\mathcal{N} \to \infty$.

Now consider the bulk. Here we have not been able to compute $F(H)$ as a function of H and, in particular, we have not been able to compute $M(H)$. However, if we are willing to make a few assumptions, we may use the function $p(\bar{\sigma})$ to show that, if at T_c, as $H \to 0$,

$$M(H) \sim K \operatorname{sgn}(H)|H|^{1/\delta} \tag{3.18}$$

and as $M^2 + N^2 \to \infty$,

$$\langle \sigma_{0,0}\sigma_{M,N} \rangle \sim \frac{f(0, \theta)}{(M^2 + N^2)^{\eta/2}}, \tag{3.19}$$

then

$$\delta = \max [1, 4\eta^{-1} - 1]. \tag{3.20}$$

We derive (3.20) by calculating the second moment of $p(\bar{\sigma})$ at $T = T_c$ and $H = 0$ in two different ways. From (3.18),

$$F(H) \sim -K\delta(\delta + 1)^{-1}|H|^{1+1/\delta}. \tag{3.21}$$

Thus

$$\xi_0 \sim \operatorname{sgn}(\bar{\sigma})(K^{-1}|\bar{\sigma}|)^{\delta}, \tag{3.22}$$

and, with $\bar{\mathcal{N}} = 4\mathcal{M}\mathcal{N}$, we find from (1.6), (1.7), and (1.10) that

$$p(\bar{\sigma}) \sim \frac{1}{2}\left(\frac{\delta + 1}{K}\right)^{\delta/(\delta+1)} \frac{(\beta 4\mathcal{M}\mathcal{N})^{1/(\delta+1)}}{\Gamma[1/(\delta + 1)]} \exp\left(-\beta 4\mathcal{M}\mathcal{N} \frac{K^{-\delta}}{\delta + 1}|\bar{\sigma}|^{\delta+1}\right). \tag{3.23}$$

We therefore obtain, as $\mathcal{M} \to \infty$ and $\mathcal{N} \to \infty$,

$$\int_{-1}^{1} p(\bar{\sigma})\bar{\sigma}^2\, d\bar{\sigma} \sim \left[\frac{(\delta + 1)K^{\delta}}{4\beta\mathcal{M}\mathcal{N}}\right]^{2/(\delta+1)} \frac{\Gamma[3/(\delta + 1)]}{\Gamma[1/(\delta + 1)]}. \tag{3.24}$$

Alternatively, we may write, as $\mathcal{M} \to \infty$ and $\mathcal{N} \to \infty$,

$$\int_{-1}^{1} p(\bar{\sigma})\bar{\sigma}^2\, d\bar{\sigma} \sim \frac{1}{(4\mathcal{M}\mathcal{N})^2} \sum_{j=-\mathcal{M}+1}^{\mathcal{M}} \sum_{j'=-\mathcal{M}+1}^{\mathcal{M}} \sum_{k=-\mathcal{N}+1}^{\mathcal{N}} \sum_{k'=-\mathcal{N}+1}^{\mathcal{N}} \langle \sigma_{j,k}\sigma_{j',k'} \rangle. \tag{3.25}$$

Using the form (3.19) for $\langle \sigma_{j,k}\sigma_{j',k'} \rangle$ when the separation between the spins is large (we may neglect terms arising from short-range order because they contribute to a higher order in $(\mathcal{M}\mathcal{N})^{-1}$ than the terms we are retaining), we have, on the assumption $\eta \leq 2$, that, as $\mathcal{M} \to \infty$ and $\mathcal{N} \to \infty$,

$$\int_{-1}^{1} p(\bar{\sigma})\bar{\sigma}^2\, d\bar{\sigma} \sim \frac{C}{\mathcal{M}\mathcal{N}} \sum_{M=M_0}^{\mathcal{M}} \sum_{N=N_0}^{\mathcal{N}} \left(\frac{1}{M^2 + N^2}\right)^{\eta/2} \sim \frac{C'}{(\mathcal{M}\mathcal{N})^{\eta/2}}. \tag{3.26}$$

We equate (3.24) and (3.26) and see that if the $\mathcal{M}\mathcal{N}$ dependence of each side is to be the same we must have

$$-\frac{2}{\delta + 1} = -\frac{1}{2}\eta. \tag{3.27}$$

If $\eta > 2$, the sum in (3.25) converges and δ must be equal to 1. This proves (3.20).

We must now understand precisely what forms (3.18) and (3.19) mean for a lattice of $2\mathscr{M}$ rows and $2\mathscr{N}$ columns with $\mathscr{M}$ and $\mathscr{N}$ finite. Conventionally, T_c and critical exponents like δ and η are defined only in an infinite lattice. Indeed, for a finite lattice, we know that all thermodynamic functions must be analytic because the partition function is the sum of a finite number of terms. However, it is clear physically that (3.19) will have meaning for a finite lattice if we set $T = T_c$ of the bulk. If $r = (M^2 + N^2)^{1/2}$ is much larger than the distance between sites but much smaller than the smallest lattice dimension, then (3.19) must hold with the same η as the exponent in the limit $\mathscr{M},\mathscr{N} \to \infty$. If r, $\mathscr{M}$ and $\mathscr{N}$ go to ∞ proportionally, however, while we expect some form similar to (3.19) to hold, it is not necessarily the case that the η so defined will be the same as the η previously obtained. Even if the two η's are the same, there is every reason to suppose that the proportionality constant in (3.19) will now acquire an angular dependence which is determined by the shape of the lattice. A similar discussion applies to the exponent δ.

In spite of these ambiguities, let us make the very plausible assumption that the δ and η which appear in (3.20) are equal to the corresponding values for the infinite lattice. Using the known value $\eta = \frac{1}{4}$ for the two-dimensional Ising model, we obtain $\delta = 15$. Furthermore, we find from (3.23) that for the bulk of Onsager's lattice at $T = T_c$

$$p(\bar{\sigma}) \sim \text{const} \exp\left(-\text{const}\, \mathscr{M}\mathscr{N}|\bar{\sigma}|^{16}\right). \tag{3.28}$$

We may slightly generalize (3.20) to the case of a d-dimensional lattice in which the magnetic field does not interact with the entire lattice but only with a d_1-dimensional sublattice. We find in this case

$$\delta = \max\left[2d_1(\eta + d - 2)^{-1} - 1, 1\right], \tag{3.29}$$

where δ is defined by (3.18) and η by

$$\langle \sigma_0 \sigma_{\mathbf{r}} \rangle \sim r^{2-d-\eta}. \tag{3.30}$$

If we assume that this δ and η are the infinite lattice values, we find that for a magnetic field interacting with a row of spins in the interior of a two-dimensional Ising lattice the magnetization of the sites interacting with the field behaves as $\operatorname{sgn}(H)|H|^{1/7}$ at $T = T_c$ and H near zero. This is to be contrasted with the $-\mathfrak{H} \ln |\mathfrak{H}|$ behavior of the boundary magnetization found in (VI.5.37).

We may give an alternative derivation of (3.29) which is valid for an infinite lattice by considering the behavior of the correlation functions for small H at $T = T_c$. If at $T = T_c$ the correlation functions are integrable, M goes linearly to zero as H goes to zero and $\delta = 1$. We therefore exclude this case and assume that the correlation functions are not integrable at $T = T_c$ and $H = 0$. However, even at $T = T_c$, when $H \neq 0$ the correlation functions approach the limiting value of M^2 in an integrable fashion for sufficiently large separations. For values of the separation that are not so large, however, $\langle\sigma_0\sigma_{\mathbf{r}}\rangle$ is approximated by the nonintegrable $T = T_c$, $H = 0$ value. The distance r_0 which separates these two regions depends on H and may be defined in two separate ways. We can define the correlation length exponent κ by $H^{-\kappa} = r_0$ in such a way that the correlation function may be expanded as a function of $rH^\kappa =$ const as $r \to \infty$ and $H \to 0$ times a power of r alone. (For the case of the boundary correlation function $\kappa = 2$, see (VII.8.43).) By studying the divergence as $H \to 0$ of

$$\chi = KH^{-1+1/\delta} = \sum_{\mathbf{r}=0}^{\infty} (\langle\sigma_0\sigma_{\mathbf{r}}\rangle - M^2) \sim \sum_{\mathbf{r}=0}^{r_0} cr^{-(d-2+\eta)}, \tag{3.31}$$

where the sums are over the d_1-dimensional subspace whose spins interact with H, we find

$$\kappa = \frac{\delta - 1}{(d_1 - d - \eta + 2)\delta}. \tag{3.32}$$

Alternatively, we may also define $r_0' = H^{-\kappa'}$ as the value of the separation when the $T = T_c$, $H = 0$ correlation function equals the limiting value as $r \to \infty$ of the $T = T_c$, $H \neq 0$ correlation function. This gives

$$cH^{-\kappa'(d-2+\eta)} = K^2H^{2/\delta}, \tag{3.33}$$

so that

$$\kappa' = \frac{2}{\delta(d - 2 + \eta)}. \tag{3.34}$$

If we identify κ and κ' we recover (3.29). This derivation is somewhat superior to the previous one because it deals only with critical exponents of the infinite lattice. However, the assumption that $\kappa = \kappa'$ is not a rigorous statement. For the two-dimensional Ising model, if $d_1 = 2$, (3.32) gives $\kappa = 8/15$, whereas if $d_1 = 1$, $\kappa = 8/7$.

4. BOUNDARY HYSTERESIS: A REFINED INTERPRETATION

In Sec. 2 we calculated $P(\bar{\sigma})$ in the case where the number of rows $(2\mathcal{M})$ of the half plane was taken to infinity before the number of columns $(2\mathcal{N})$ was. In this case, we evaluated the leading approximation to $p(\bar{\sigma})$ and noted that we could use this $\mathfrak{H} = 0$ probability function to calculate the boundary spin probability for all $\mathfrak{H}$. For $|\mathfrak{H}|$ not too large, the probability function was seen to be bimodal and we interpreted the secondary maximum of the probability function as a metastable state. However, this secondary maximum disappeared when $\mathfrak{M}_1^s(\mathfrak{H}) = 0$, and for $|\mathfrak{H}|$ larger than this value it was unclear from these considerations whether the magnetization would follow $\mathfrak{M}_1(\mathfrak{H})$ or $\mathfrak{M}_1^c(\mathfrak{H})$. In order to resolve this question of how far the boundary magnetization will follow its analytic continuation and to study the effect of the order $\mathcal{M} \to \infty$ followed by $\mathcal{N} \to \infty$, we will compute $P(\bar{\sigma}; \mathcal{M}, \mathcal{N})$, the boundary spin probability function at $\mathfrak{H} = 0$ for finite $\mathcal{M}$ and $\mathcal{N}$. The function $P(\bar{\sigma}; \mathcal{M}, \mathcal{N})$ is still expressed in terms of the partition function by (1.3). From (VI.3.26) we have

$$\frac{Z^2_{\mathcal{M},\mathcal{N}}(\mathfrak{H})}{Z^2_{\mathcal{M},\mathcal{N}}(0)} = (\cosh \beta\mathfrak{H})^{4\mathcal{N}} \times \prod_{\theta} \frac{1 - i(z^2/z_2\mathfrak{c})v'/v + \alpha^{-4\mathcal{M}}(v'/v)^2[1 + i(z^2/z_2\mathfrak{c})v/v']}{1 + \alpha^{-4\mathcal{M}}(v'/v)^2}, \tag{4.1}$$

where the product is over $\theta = \pi(2n - 1)/2\mathcal{N}$, $1 \le n \le 2\mathcal{N}$, and the dependence of $Z(\mathfrak{H})$ on $\mathcal{M}$ and $\mathcal{N}$ has been made explicit by writing $Z(\mathfrak{H}) = Z_{\mathcal{M},\mathcal{N}}(\mathfrak{H})$. Using the Poisson summation formula

$$\sum_{n=1}^{2\mathcal{N}} \delta\left[\theta - \frac{\pi(2n - 1)}{2\mathcal{N}}\right] = \frac{\mathcal{N}}{\pi} \sum_{m=-\infty}^{\infty} (-1)^m e^{i\theta 2\mathcal{N}m} \tag{4.2}$$

we have

$$\frac{Z_{\mathcal{M},\mathcal{N}}(\mathfrak{H})}{Z_{\mathcal{M},\mathcal{N}}(0)} = (\cosh \beta\mathfrak{H})^{2\mathcal{N}} \times \exp\left\{\frac{\mathcal{N}}{2\pi}\int_{-\pi}^{\pi} d\theta \sum_{m=-\infty}^{\infty} (-1)^m e^{2\mathcal{N}mi\theta} \ln \left[\!\left[\frac{1}{1 + \alpha^{-4\mathcal{M}}(v'/v)^2} \times \left[1 - \frac{iz^2}{z_2\mathfrak{c}}\frac{v'}{v} + \frac{1}{\alpha^{4\mathcal{M}}}\left(\frac{v'}{v}\right)^2\left(1 + \frac{iz^2}{z_2\mathfrak{c}}\frac{v}{v'}\right)\right]\right]\!\right]\right\}. \tag{4.3}$$

We are interested in an approximation to $Z_{\mathcal{M},\mathcal{N}}(\mathfrak{H})/Z_{\mathcal{M},\mathcal{N}}(0)$ more accurate than that used in Sec. 2. To that end define

$$\mathfrak{F}(\mathfrak{H}; \mathcal{M}) = -\frac{1}{\beta}\left\{\cosh \beta\mathfrak{H} + \frac{1}{4\pi}\int_{-\pi}^{\pi} d\theta \ln \left[\!\left[\left[1 + \frac{1}{\alpha^{4\mathcal{M}}}\left(\frac{v'}{v}\right)^2\right]^{-1} \times \left[\left(1 - \frac{iz^2}{z_2\mathfrak{c}}\frac{v'}{v}\right) + \frac{1}{\alpha^{4\mathcal{M}}}\left(\frac{v'}{v}\right)^2\left(1 + \frac{iz^2}{z_2\mathfrak{c}}\frac{v}{v'}\right)\right]\right]\!\right]\right\} \tag{4.4}$$

and write

$$\frac{Z_{\mathcal{M},\mathcal{N}}(\mathfrak{H})}{Z_{\mathcal{M},\mathcal{N}}(0)} = \exp\left[-2\mathcal{N}\beta\mathfrak{F}(\mathfrak{H}; \mathcal{M})\right] \exp\left\{\frac{\mathcal{N}}{\pi}\int_{-\pi}^{\pi} d\theta \sum_{m=1}^{\infty} (-1)^m \times e^{2\mathcal{N}mi\theta} \ln \left[\!\left[\frac{1}{1 + \alpha^{-4\mathcal{M}}(v'/v)^2}\left[1 - \frac{iz^2}{z_2\mathfrak{c}}\frac{v'}{v} + \frac{1}{\alpha^{4\mathcal{M}}}\left(\frac{v'}{v}\right)^2 \times \left(1 + \frac{iz^2}{z_2\mathfrak{c}}\frac{v}{v'}\right)\right]\right]\!\right]\right\}. \tag{4.5}$$

To approximate the integral in (4.5) we must first locate the singularities of the integrand near the unit circle in the $e^{i\theta}$ plane. This integrand is singular when either

$$1 - \frac{iz^2}{z_2 \mathrm{c}} \frac{v'}{v} + \frac{1}{\alpha^{4\mathscr{M}}} \left(\frac{v'}{v}\right)^2 \left(1 + \frac{iz^2}{z_2 \mathrm{c}} \frac{v}{v'}\right) = 0 \tag{4.6a}$$

or

$$1 + \left(\frac{v'}{v}\right)^2 \frac{1}{\alpha^{4\mathscr{M}}} = 0. \tag{4.6b}$$

Define $r_{\mathscr{M}}(\mathfrak{H})$ to be that solution of (4.6*a*) which approaches r of Chapter VI when $\mathscr{M} \to \infty$. When $\ln \mathfrak{H}$ is too large, and $E_1 < 0$ or $E_1 > 0$ and $T > T_c$, (4.6*b*) has no solutions near $|e^{i\theta}| = 1$ so that to a high degree of accuracy (1.5) holds. Hence the only refinement we may need in our analysis is for $E_1 > 0$ and $T < T_c$. Here the only solutions to (4.6*a*) near $|e^{i\theta}| = 1$ are $r_{\mathscr{M}}(\mathfrak{H})$ and $r_{\mathscr{M}}(\mathfrak{H})^{-1}$. Similarly, the only values of $e^{i\theta}$ near $|e^{i\theta}| = 1$ when (4.6*b*) holds are $r_{\mathscr{M}}(0)$ and $r_{\mathscr{M}}(0)^{-1}$. When θ is near 0 and $T < T_c$, we find from (VI.3.20) that

$$\frac{v'}{v} \sim -\frac{z_2^2(1 + z_1)^2 - (1 - z_1)^2}{2z_2 z_1 \theta}. \tag{4.7}$$

Using (4.7) in (4.6*a*) we find that, for $r_{\mathscr{M}}$ near 1,

$$(r_{\mathscr{M}} - 1)^2 \sim \frac{z_2^2(1 + z_1)^2 - (1 - z_1)^2}{z_1 z_2^2} \left[z^2\left(1 - \frac{1}{\alpha(0)^{4\mathscr{M}}}\right) + \frac{1}{4} \frac{z_2^2(1 + z_1)^2 - (1 - z_1)^2}{z_1 \alpha(0)^{4\mathscr{M}}}\right], \tag{4.8}$$

so that if we define $\mathfrak{H}_0$ by $-i\mathfrak{H}_0 > 0$, $z_0 = \tanh \beta\mathfrak{H}_0$, and

$$z_0^2 = -\frac{z_2^2 \mathfrak{M}_1^2(0^+)}{\alpha(0)^{4\mathscr{M}}[1 - \alpha(0)^{-4\mathscr{M}}]}, \tag{4.9}$$

we have, for $\mathfrak{H}$ near $\mathfrak{H}_0$, by (VI.5.19)

$$r_{\mathscr{M}}(\mathfrak{H}) \sim 1 - 2\mathfrak{M}_1(0^+)[1 - \alpha(0)^{-4\mathscr{M}}]^{1/2}(z^2 - z_0^2)^{1/2}. \tag{4.10}$$

In terms of $r_{\mathscr{M}}(\mathfrak{H})$ and $r_{\mathscr{M}}(0)$ we find that

$$\begin{aligned}\int_{-\pi}^{\pi} d\theta e^{2\mathscr{N}mi\theta} \ln \left\{\frac{1}{1 + \alpha^{-4\mathscr{M}}(v'/v)^2} \left[1 - \frac{iz^2}{z_2 \mathrm{c}} \frac{v'}{v} + \frac{1}{\alpha^{4\mathscr{M}}} \left(\frac{v'}{v}\right)^2 \left(1 + \frac{iz^2}{z_2 \mathrm{c}} \frac{v}{v'}\right)\right]\right\} \\ = \int_{-\pi}^{\pi} d\theta e^{2\mathscr{N}mi\theta} \ln \left|\frac{e^{i\theta} - r_{\mathscr{M}}(\mathfrak{H})}{e^{i\theta} - r_{\mathscr{M}}(0)}\right|^2 + O(\alpha_2^{2\mathscr{N}}) \\ = -\frac{\pi}{\mathscr{N}m} [r_{\mathscr{M}}(\mathfrak{H})^{2\mathscr{N}m} - r_{\mathscr{M}}(0)^{2\mathscr{N}m}] + O(\alpha_2^{2\mathscr{N}}),\end{aligned} \tag{4.11}$$

and so, using

$$\sum_{m=1}^{\infty} (-1)^m \frac{1}{\mathscr{N} m} X^{2\mathscr{N} m} = -\frac{1}{\mathscr{N}} \ln(1 + X^{2\mathscr{N}}), \tag{4.12}$$

we obtain the improved approximation to $Z_{\mathscr{M},\mathscr{N}}(\mathfrak{H})/Z_{\mathscr{M},\mathscr{N}}(0)$:

$$\frac{Z_{\mathscr{M},\mathscr{N}}(\mathfrak{H})}{Z_{\mathscr{M},\mathscr{N}}(0)} = \frac{1 + r_{\mathscr{M}}(\mathfrak{H})^{2\mathscr{N}}}{1 + r_{\mathscr{M}}(0)^{2\mathscr{N}}} e^{-2\mathscr{N}\beta\mathfrak{F}(\mathfrak{H};\mathscr{M})}[1 + O(\alpha_2^{2\mathscr{N}})]. \tag{4.13}$$

We first verify that $Z_{\mathscr{M},\mathscr{N}}(\mathfrak{H})$ is an analytic function of $\mathfrak{H}$ (at least for $\mathfrak{H}$ near the imaginary axis). As seen from (4.10), the function $r_{\mathscr{M}}(\mathfrak{H})$ has square-root branch points at $\mathfrak{H} = i\pi n \pm \mathfrak{H}_0$, where n is an integer. Define the cut $\mathfrak{H}$-plane (Fig. 13.3) by joining these branch points pairwise

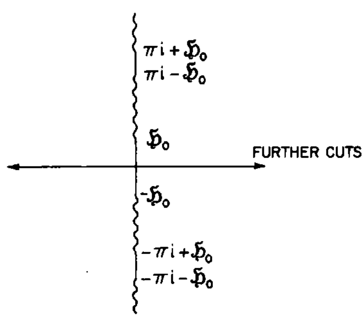


Fig. 13.3. The cut $\mathfrak{H}$-plane.

with cuts along the imaginary axis in such a way that no branch cut crosses the real axis. It is obvious from (4.10) that in the cut $\mathfrak{H}$-plane

$$r_{\mathscr{M}}(\mathfrak{H}) = r_{\mathscr{M}}(-\mathfrak{H}). \tag{4.14}$$

Furthermore, from (4.8) and (4.10) we may continue $r_{\mathscr{M}}(\mathfrak{H})$ through these branch cuts on the imaginary axis. This analytic continuation of $r_{\mathscr{M}}(\mathfrak{H})$ we call $r^c_{\mathscr{M}}(\mathfrak{H})$ and find

$$r_{\mathscr{M}}(\mathfrak{H}) = [r^c_{\mathscr{M}}(\mathfrak{H})]^{-1}. \tag{4.15}$$

The foregoing considerations may also be applied to $\mathfrak{F}(\mathfrak{H};\mathscr{M})$ to show that the branch points of $\mathfrak{F}(\mathfrak{H};\mathscr{M})$ on the imaginary axis are the same as the branch points of $r_{\mathscr{M}}(\mathfrak{H})$. From (4.4) it is clear that $\mathfrak{F}(\mathfrak{H};\mathscr{M})$ is real for real $\mathfrak{H}$ and for $\mathfrak{H}$ in the cut $\mathfrak{H}$-plane that obeys

$$\mathfrak{F}(\mathfrak{H};\mathscr{M}) = \mathfrak{F}(-\mathfrak{H};\mathscr{M}). \tag{4.16}$$

Furthermore, we may continue $\mathfrak{F}(\mathfrak{H};\mathscr{M})$ through the cuts of the $\mathfrak{H}$-plane on the imaginary axis. First consider $0 < |\mathfrak{H}| < |\mathfrak{H}_0|$. When we continue

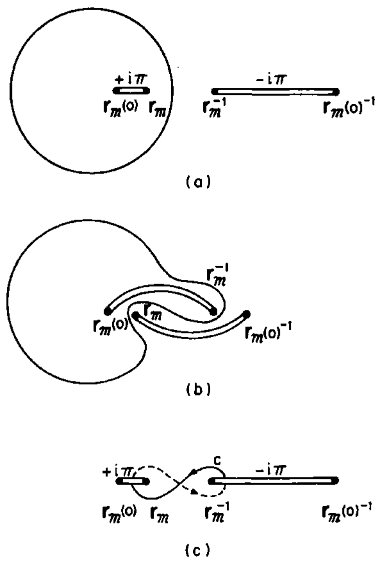


Fig. 13.4. Integration contour for (*a*) $\mathfrak{F}(\mathfrak{H};\mathscr{M})$, (*b*) $\mathfrak{F}^c(\mathfrak{H};\mathscr{M})$, and (*c*) $\mathfrak{F}^c(\mathfrak{H};\mathscr{M}) - \mathfrak{F}(\mathfrak{H};\mathscr{M})$ in the $e^{i\theta} = \zeta$ plane. Only cuts at $r_{\mathscr{M}}(\mathfrak{H})$ and $r_{\mathscr{M}}(0)$ are indicated. The definition of the imaginary part of the logarithm is shown.

$\mathfrak{H}$ around $\mathfrak{H}_0$, $r_{\mathscr{M}}(\mathfrak{H}) \to r^c_{\mathscr{M}}(\mathfrak{H}) = r^{-1}_{\mathscr{M}}(\mathfrak{H})$ and the contour of integration is deformed as in Fig. 13.4. Therefore, with $\zeta = e^{i\theta}$,

$$\begin{aligned}\mathfrak{F}^c(\mathfrak{H};\mathscr{M}) - \mathfrak{F}(\mathfrak{H};\mathscr{M}) &= -\frac{1}{4\pi i\beta}\int_c \frac{d\zeta}{\zeta}\ln\left\{\frac{1}{1+\alpha^{-4\mathscr{M}}(v'/v)^2}\left[\left(1-\frac{iz^2}{z_2\mathfrak{c}}\frac{v'}{v}\right)\right.\right.\\ &\qquad\left.\left.+\frac{1}{\alpha^{4\mathscr{M}}}\left(\frac{v'}{v}\right)^2\left(1+\frac{iz^2}{z_2\mathfrak{c}}\frac{v}{v'}\right)\right]\right\}\\ &= \frac{1}{2\beta}\int_{r_{\mathscr{M}}(\mathfrak{H})}^{r_{\mathscr{M}}(\mathfrak{H})^{-1}}\frac{d\zeta}{\zeta} = -\frac{1}{\beta}\ln r_{\mathscr{M}}(\mathfrak{H}).\end{aligned} \tag{4.17}$$

This result may be analytically continued to all $\mathfrak{H}$ and establishes that

$$\mathfrak{F}^c(\mathfrak{H};\mathscr{M}) - \mathfrak{F}(\mathfrak{H};\mathscr{M}) = -\frac{1}{\beta}\ln r_{\mathscr{M}}(\mathfrak{H}). \tag{4.18}$$

With the aid of (4.15) and (4.18) it is easily seen that, even though $\mathfrak{F}(\mathfrak{H};\mathscr{M})$ fails to be analytic at $\pm in\pi \pm \mathfrak{H}_0$, $Z_{\mathscr{M},\mathscr{N}}(\mathfrak{H})$ does not have any branch points on the imaginary axis.

We now use (4.13) to obtain an improved approximation of $P(\bar{\sigma};\mathscr{M},$

$\mathscr{N}$), the probability that, in a lattice of $2\mathscr{M}$ rows and $2\mathscr{N}$ columns with $\mathfrak{H} = 0$, the average boundary spin is $\bar{\sigma}$. Consider only the case $T < T_c$. Then using (4.13) we obtain

$$P(\bar{\sigma}; \mathscr{M}, \mathscr{N}) \sim \frac{\beta}{2\pi i} \int_{-i\pi/\beta}^{i\pi/\beta} d\xi \, \frac{1 + r_{\mathscr{M}}(\xi)^{2\mathscr{N}}}{1 + r_{\mathscr{M}}(0)^{2\mathscr{N}}} \exp\{-2\mathscr{N}\beta[\mathfrak{F}(\xi; \mathscr{M}) + \xi\bar{\sigma}]\}. \tag{4.19}$$

In writing this, we have omitted the terms of $O(\alpha_2^{2\mathscr{N}})$. Therefore, terms arising from (4.19) which are smaller than $O(\alpha_2^{2\mathscr{N}})$ must be discarded as meaningless. It is these $O(\alpha_2^{2\mathscr{N}})$ terms which at $T = T_c$ were discussed in Sec. 3. The integral is now to be evaluated by steepest descents, where, in contrast to the less accurate expression of Sec. 2, (4.19) has *two* points of steepest descent instead of one. The integrand is analytic on the imaginary axis, so we may deform the path to pass slightly to the right of the axis. Using (4.18) we may rewrite (4.19) as the sum of two integrals,

$$\begin{aligned} P(\bar{\sigma}; \mathscr{M}, \mathscr{N}) = \frac{\beta}{2\pi i} \int_{-i\pi/\beta}^{i\pi/\beta} d\xi \, \frac{1}{1 + r_{\mathscr{M}}(0)^{2\mathscr{N}}} \\ \times \{\exp[-2\mathscr{N}\beta(\mathfrak{F}(\xi; \mathscr{M}) + \xi\bar{\sigma})] \\ + \exp[-2\mathscr{N}\beta(\mathfrak{F}^c(\xi; \mathscr{M}) + \xi\bar{\sigma})]\}. \end{aligned} \tag{4.20}$$

When $|\bar{\sigma}| > \mathfrak{M}_1(0^+)$, the steepest-descents points are determined from

$$\bar{\sigma} = \mathfrak{M}_1(\xi_1; \mathscr{M}) = -\mathfrak{F}'(\xi_1; \mathscr{M}) \tag{4.21a}$$

and

$$\bar{\sigma} = \mathfrak{M}_1^c(\xi_2; \mathscr{M}) = -\mathfrak{F}^{c\prime}(\xi_2; \mathscr{M}). \tag{4.21b}$$

When $\mathfrak{H}$ is away from zero and $\mathscr{M}$ is large but finite, $\mathfrak{M}_1(\mathfrak{H}; \mathscr{M})$ and

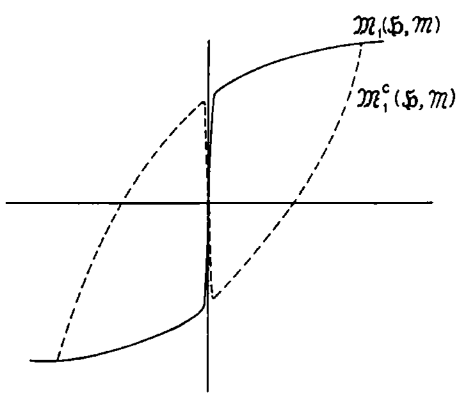


Fig. 13.5. Schematic plot of the functions $\mathfrak{M}_1(\mathfrak{H}; \mathscr{M})$ and $\mathfrak{M}_1^c(\mathfrak{H}; \mathscr{M})$.

$\mathfrak{M}_1^c(\mathfrak{H};\mathscr{M})$, as shown schematically in Fig. 13.5, are virtually identical with their $\mathscr{M}\to\infty$ limits. The function $\mathfrak{M}_1(\mathfrak{H};\mathscr{M})$ has been analyzed in detail in Sec. 5 of Chapter VI. Define the functions

$$W_1 = -\beta[\xi\bar{\sigma} + \mathfrak{F}(\xi_1;\mathscr{M})] \tag{4.22a}$$

and

$$W_2 = -\beta[\xi\bar{\sigma} + \mathfrak{F}^c(\xi_2;\mathscr{M})]. \tag{4.22b}$$

Then for $|\bar{\sigma}| > \mathfrak{M}_1(0^+)$,

$$P(\bar{\sigma};\mathscr{M},\mathscr{N}) \sim \frac{1}{1+r_{\mathscr{M}}(0)^{2\mathscr{N}}}\frac{1}{2}\left(\frac{\beta}{\pi\mathscr{N}}\right)^{1/2}\left[\frac{e^{2\mathscr{N}W_1}}{\chi(\xi_1)^{1/2}} + \frac{e^{2\mathscr{N}W_2}}{\chi^c(\xi_2)^{1/2}}\right], \tag{4.23}$$

where

$$\chi = \mathfrak{M}_1'(\xi;\mathscr{M}) \qquad \text{and} \qquad \chi^c = \mathfrak{M}_1^{c\prime}(\xi;\mathscr{M}) \tag{4.24}$$

and we have kept only the first term in the asymptotic expansion of each integral. When $|\bar{\sigma}|$ is larger than the value of $\mathfrak{M}_1$ where $\mathfrak{M}_1 = \mathfrak{M}_1^c$, then the second term of (4.23) is smaller than $O(\alpha_2^{\frac{3}{2}\mathscr{N}})$ and must be discarded. In (4.23), we may let $\mathscr{N}$ and $\mathscr{M}$ tend to infinity in any manner we please and still obtain the same answer up to a factor which is independent of $\bar{\sigma}$.

When $\bar{\sigma}$ is very close to $\mathfrak{M}_1(0^+)$, the steepest-descents point ξ_1 is comparable in magnitude to $\mathfrak{H}_0$ and the previous evaluation breaks down because higher-order terms in the asymptotic expansions may no longer be ignored. For $|\bar{\sigma}| < \mathfrak{M}_1(0^+)$, there is still, nominally, a steepest-descents point on the first sheet of $\mathfrak{F}$ but the rapid variation of $\mathfrak{F}$ near this point makes the point unimportant for an asymptotic expansion. In this region, we must deform the contour of integration of the first term of (4.20) through the imaginary-axis branch cuts to give an integral taken solely on the second sheet of $\mathfrak{F}$ plus an additional integral whose path is from $-\mathfrak{H}_0$ to $\mathfrak{H}_0$ once on each sheet (Fig. 13.6). We may evaluate the integral on the second sheet and the second integral of (4.20) by steepest descents, where now both ξ_1 and ξ_2 ($|\xi_1| < |\xi_2|$) satisfy (4.22b). As seen

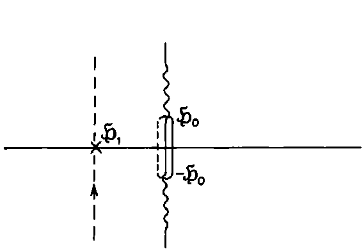


Fig. 13.6. Integration paths for $P(\bar{\sigma};\mathscr{M},\mathscr{N})$ when $|\bar{\sigma}| < \mathfrak{M}_1(0^+)$.

from Fig. 13.5, (4.22*b*) has three solutions for $|\bar{\sigma}| < \mathfrak{M}_1(0^+)$ but the one closest to $\xi = 0$ must be discarded. We thus obtain

$$P(\bar{\sigma}; \mathscr{M}, \mathscr{N}) = \frac{1}{1 + r_{\mathscr{M}}(0)^{2\mathscr{N}}} \frac{1}{2} \left(\frac{\beta}{\pi\mathscr{N}}\right)^{1/2} \left[\frac{e^{2\mathscr{N}W_1}}{\chi^c(\xi_1)^{1/2}} + \frac{e^{2\mathscr{N}W_2}}{\chi^c(\xi_2)^{1/2}}\right] + I_{\mathscr{M},\mathscr{N}}(\bar{\sigma}), \tag{4.25}$$

where

$$I_{\mathscr{M},\mathscr{N}}(\bar{\sigma}) = \frac{\beta}{2\pi} \int_{-\mathfrak{H}_0}^{\mathfrak{H}_0} d\xi \frac{1 - r_{\mathscr{M}}(\xi)^{2\mathscr{N}}}{1 + r_{\mathscr{M}}(0)^{2\mathscr{N}}} \exp\{-2\mathscr{N}\beta[\xi\bar{\sigma} + \mathfrak{F}(\xi; \mathscr{M})]\}. \tag{4.26}$$

Only $I_{\mathscr{M},\mathscr{N}}$ depends on the order in which the $\mathscr{M}$ and $\mathscr{N} \to \infty$ limits are taken.

To analyze (4.26), define

$$h = -i2\mathscr{N}\mathfrak{H}_0 = \mathscr{N}\alpha(0)^{-2\mathscr{M}}\{[z_2(1 + z_1)^2 - (1 - z_1)^2] \times z_1[1 - \alpha(0)^{-4\mathscr{M}}]\}^{1/2}. \tag{4.27}$$

In Sec. 2, we analyzed the case $\mathscr{M} \to \infty$ and then $\mathscr{N} \to \infty$, which corresponds to $h = 0$. For h not to tend to zero as $\mathscr{N}$ and $\mathscr{M} \to \infty$, $\mathscr{N}$ must be *exponentially* larger than $\mathscr{M}$. It is straightforward to approximate $I_{\mathscr{M},\mathscr{N}}$ when h is small. We use the fact that, because $|\xi| < |\mathfrak{H}_0| \sim 0$, we have $|r_{\mathscr{M}}(\xi)| < |r_{\mathscr{M}}(0)|$ and may approximate

$$\mathfrak{F}(\xi; \mathscr{M}) \sim \frac{1}{2\beta} \ln \frac{r_{\mathscr{M}}(\xi)}{r_{\mathscr{M}}(0)} + O(\xi^2) \tag{4.28}$$

to obtain

$$I_{\mathscr{M},\mathscr{N}}(\bar{\sigma}) \sim \frac{\beta}{2\pi i} \int_{-\mathfrak{H}_0}^{\mathfrak{H}_0} d\xi \frac{r_{\mathscr{M}}(\xi)^{-\mathscr{N}} - r_{\mathscr{M}}(\xi)^{\mathscr{N}}}{r_{\mathscr{M}}(0)^{-\mathscr{N}} + r_{\mathscr{M}}(0)^{\mathscr{N}}} e^{-2\mathscr{N}\beta\xi\bar{\sigma}}. \tag{4.29}$$

When $h \ll 1$ we may change variables to

$$\zeta = \xi/\mathfrak{H}_0 \tag{4.30}$$

and use (4.10) to obtain

$$\begin{aligned} I_{\mathscr{M},\mathscr{N}}(\bar{\sigma}) &\sim h\mathfrak{M}_1(0^+)[1 - \alpha(0)^{-4\mathscr{M}}]^{1/2} \frac{1}{2\pi} \int_{-1}^{1} d\zeta (1 - \zeta^2)^{1/2} e^{ih\bar{\sigma}\zeta} \\ &= \tfrac{1}{2}\mathfrak{M}_1(0^+)[1 - \alpha(0)^{-4\mathscr{M}}]^{1/2} \frac{1}{\bar{\sigma}} J_1(h\bar{\sigma}), \end{aligned} \tag{4.31}$$

where J_1 is the Bessel function of the first kind. The Bessel function may then be expanded in a power series, and we find

$$P(\bar{\sigma}; \mathscr{M}, \mathscr{N}) \sim \frac{1}{4} \left(\frac{\beta}{\pi\mathscr{N}}\right)^{1/2} \left[\frac{e^{2\mathscr{N}W_1}}{\chi^c(\xi_1)^{1/2}} + \frac{e^{2\mathscr{N}W_2}}{\chi^c(\xi_2)^{1/2}}\right] + \frac{1}{4} \mathfrak{M}_1(0^+)[1 - \alpha(0)^{-4\mathscr{M}}]^{1/2} h\left[1 - \frac{h^2\bar{\sigma}^2}{8} + O(h^4\bar{\sigma}^2)\right]\cdot \tag{4.32}$$

In this expression for $P(\bar{\sigma}; \mathscr{M}, \mathscr{N})$ there are two different sorts of $\bar{\sigma}$ dependance: (1) Gaussian tails of magnitude $e^{2\mathscr{N}W_1}$ and $e^{2\mathscr{N}W_2}$, and (2) a polynomial of magnitude $2\mathscr{N}\alpha(0)^{-2\mathscr{M}}$. For different ways of taking the thermodynamic limit, the range of $\bar{\sigma}$ in which one term dominates the other is different. In particular, if $\mathscr{M} = K\mathscr{N}$ and $\mathscr{N} \to \infty$, $P(\bar{\sigma}; \mathscr{M}, \mathscr{N})$ will be a constant for $|\bar{\sigma}| < \bar{\sigma}_0$, where $\bar{\sigma}_0$ is determined from

$$K \ln \alpha(0) + W_1(\bar{\sigma}_0) = 0. \tag{4.33}$$

In the opposite limit $h \to \infty$, it is convenient to define

$$h' = 2\mathscr{N}\alpha(0)^{-2\mathscr{M}} = 2\mathscr{N}[z_2(1 + z_1)/(1 - z_1)]^{-2\mathscr{M}}. \tag{4.34}$$

In this case $\mathscr{N}$ is so much larger than $\mathscr{M}$ that $r_{\mathscr{M}}(0)^{\mathscr{N}} \sim 0$ and, except for $\xi = \mathfrak{H}_0$, $r_{\mathscr{M}}(\xi)^{-\mathscr{N}} - r_{\mathscr{M}}(\xi)^{\mathscr{N}} \sim r_{\mathscr{M}}(\xi)^{-\mathscr{N}}$. We may therefore approximate $I_{\mathscr{M},\mathscr{N}}$ by

$$I_{\mathscr{M},\mathscr{N}}(\bar{\sigma}) \sim \frac{\beta}{2\pi i}\int_{-i\epsilon}^{i\epsilon} d\xi \frac{r_{\mathscr{M}}(0)^{\mathscr{N}}}{r_{\mathscr{M}}(\xi)^{\mathscr{N}}} \exp(-2\mathscr{N}\bar{\sigma}\beta\xi), \tag{4.35}$$

where ϵ is some small real number less than $|\mathfrak{H}_0|$. Finally, we approximate $r_{\mathscr{M}}(\mathfrak{H})$ by (4.10), and use (4.30) to obtain

$$I_{\mathscr{M},\mathscr{N}}(\bar{\sigma}) \sim \frac{\beta\mathfrak{H}_0}{2\pi i}\int_{-\epsilon'}^{\epsilon'} d\zeta[1 - \mathfrak{M}_1(0^+)\beta i\zeta^2\mathfrak{H}_0]^{-\mathscr{N}} \exp(-2\mathscr{N}\mathfrak{H}_0\bar{\sigma}\beta\zeta). \tag{4.36}$$

For $T < T_c$ and $h'/2\mathscr{N} \ll 1$, this expression may be approximated as

$$I_{\mathscr{M},\mathscr{N}}(\bar{\sigma}) \sim \frac{\beta\mathfrak{H}_0}{2\pi i}\int_{-\epsilon'}^{\epsilon'} d\zeta \exp[-\tfrac{1}{2}h'\mathfrak{M}_1(0^+)^2 z_2\zeta^2] \exp[-iz_2h'\mathfrak{M}_1(0^+)\bar{\sigma}\zeta], \tag{4.37}$$

from which we find that if $|\bar{\sigma}| < \mathfrak{M}_1(0^+)$

$$P(\bar{\sigma}; \mathscr{M}, \mathscr{N}) \sim \left(\frac{h'z_2}{2\pi}\right)^{1/2} \frac{1}{2\mathscr{N}} \exp\left(-\frac{1}{2}h'\bar{\sigma}^2 z_2\right) + \frac{1}{4}\left(\frac{\beta}{\pi\mathscr{N}}\right)^{1/2}$$
$$\times \{\chi^c(\xi_1)^{-1/2}e^{2\mathscr{N}W_1} + \chi^c(\xi_2)^{-1/2}e^{2\mathscr{N}W_2}\}. \tag{4.38}$$

The first term is a Gaussian centered about $\bar{\sigma} = 0$ of width $z_2h'^{-1/2}$ and area 1. This is to be expected because $h' \to \infty$ means that the number of columns is exponentially larger than the number of rows and the lattice for finite $\mathscr{M}$ and $\mathscr{N}$ looks extremely one-dimensional. There is clearly only one maximum in $P(\bar{\sigma}; \mathscr{M}, \mathscr{N})$ in this $h' \to \infty$ case. Therefore, a metastable state can surely *not* exist when $\mathscr{N} \to \infty$ and then $\mathscr{M} \to \infty$. There is a simple physical explanation for this. The factor

$$[z_2(1 + z_1)/(1 - z_1)]^{-2\mathscr{M}}$$

is the "boundary tension" free-energy contribution to the partition function found, in Sec. 4 of Chapter V, to arise when two regions of opposite magnetization have a boundary in common. This domain wall may occupy any of $2\mathscr{N}$ sites on the boundary. When h' is large, the gain in entropy that the lattice obtains by breaking up into domains outweighs the loss in energy, so the lattice breaks up into many small regions of opposite magnetization, which means there is no spontaneous magnetization.

For further interpretation of the meaning of the several pieces of $P(\bar{\sigma}; \mathscr{M}, \mathscr{N})$ we confine ourselves to the $\mathscr{M} \to \infty$, $h \to 0$ limit where (4.32) applies and the last term vanishes. As argued in Sec. 2, if we begin with a state in one of the two peaks of $P(\bar{\sigma})$ the system will surely stay in that state as long as the peak exists as a separate maximum. When $\mathfrak{M}_1^c(\mathfrak{H})$ is zero, however, we can no longer determine from looking at $P(\bar{\sigma}; \mathscr{M}, \mathscr{N})$ alone whether the magnetization will fall to $\mathfrak{M}_1(\mathfrak{H})$ or continue on $\mathfrak{M}_1^c(\mathfrak{H})$. To understand what happens, it is necessary to examine $\mathfrak{M}_J(\mathfrak{H})$, the magnetization in the Jth row.

We obtain a formula for $\mathfrak{M}_J(\mathfrak{H})$ from the formalism of Sec. 2 of Chapter VII. Note that

$$\sigma_{J,0} = \sigma_{1,0}(\sigma_{1,0}\sigma_{2,0})(\sigma_{2,0}\sigma_{3,0})\cdots(\sigma_{J-1,0}\sigma_{J,0}). \tag{4.39}$$

Define $Y^{(J)}$ to be

$$Y^{(J)} = \begin{array}{cc}
 & \begin{array}{cccccccc} 10 & 20 & \cdots & J0 & 00 & 10 & \cdots & J\text{–}10 \\ D & D & & D & U & U & & U \end{array} \\
\begin{array}{cc} 10 & D \\ 20 & D \\ \vdots & \\ J0 & D \\ 00 & U \\ 10 & U \\ \vdots & \\ J\text{–}10 & U \end{array} &
\begin{bmatrix}
0 & 0 & \cdots & 0 & -(z^{-1}-z) & 0 & \cdots & 0 \\
0 & 0 & \cdots & 0 & 0 & -(z_2^{-1}-z_2) & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & \cdots & 0 & 0 & 0 & \cdots & -(z_2^{-1}-z_2) \\
z^{-1}-z & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\
0 & z_2^{-1}-z_2 & \cdots & 0 & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & \cdots & z_2^{-1}-z_2 & 0 & 0 & \cdots & 0
\end{bmatrix}
\end{array}. \tag{4.40}$$

Calling $Q^{(J)}$ the submatrix of A^{-1} in the space in which $Y^{(J)}$ is defined, we have

$$\mathfrak{M}_J = \pm z z_2^{J-1} \operatorname{Pf}[Y^{(J)}] \operatorname{Pf}[Y^{(J)-1} + Q^{(J)}], \tag{4.41}$$

where the sign is chosen to make $\mathfrak{M}_J$ have the same sign as does $\mathfrak{H} z_2^{J-1}$. This is written explicitly as

$$\mathfrak{M}_J = \pm(1 - z^2)(1 - z_2^2)^{J-1}$$

$$\times \operatorname{Pf}\begin{bmatrix}
A^{-1}(1,0;1,0)_{DD} & A^{-1}(1,0;2,0)_{DD} & \cdots & A^{-1}(1,0;J,0)_{DD} & A^{-1}(1,0;0,0)_{DU} + (z^{-1}-z)^{-1} & A^{-1}(1,0;1,0)_{DU} & \cdots & A^{-1}(1,0;J-1,0)_{DU} \\
A^{-1}(2,0;1,0)_{DD} & A^{-1}(2,0;2,0)_{DD} & \cdots & A^{-1}(2,0;J,0)_{DD} & A^{-1}(2,0;0,0)_{DU} & A^{-1}(2,0;1,0)_{DU} + (z_2^{-1}-z_2)^{-1} & \cdots & A^{-1}(2,0;J-1,0)_{DU} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
A^{-1}(J,0;1,0)_{DD} & A^{-1}(J,0;2,0)_{DD} & \cdots & A^{-1}(J,0;J,0)_{DD} & A^{-1}(J,0;0,0)_{DU} & A^{-1}(J,0;1,0)_{DU} & \cdots & A^{-1}(J,0;J-1,0)_{DU} + (z_2^{-1}-z_2)^{-1} \\
A^{-1}(0,0;1,0)_{UD} - (z^{-1}-z)^{-1} & A^{-1}(0,0;2,0)_{UD} & \cdots & A^{-1}(0,0;J,0)_{UD} & A^{-1}(0,0;0,0)_{UU} & A^{-1}(0,0;1,0)_{UU} & \cdots & A^{-1}(0,0;J-1,0)_{UU} \\
A^{-1}(1,0;1,0)_{UD} & A^{-1}(1,0;2,0)_{UD} - (z_2^{-1}-z_2)^{-1} & \cdots & A^{-1}(1,0;J,0)_{UD} & A^{-1}(1,0;0,0)_{UU} & A^{-1}(1,0;1,0)_{UU} & \cdots & A^{-1}(1,0;J-1,0)_{UU} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
A^{-1}(J-1,0;1,0)_{UD} & A^{-1}(J-1,0;2,0)_{UD} & \cdots & A^{-1}(J-1,0;J,0)_{UD} - (z_2^{-1}-z_2)^{-1} & A^{-1}(J-1,0;0,0)_{UU} & A^{-1}(J-1,0;1,0)_{UU} & \cdots & A^{-1}(J-1,0;J-1,0)_{UU}
\end{bmatrix}. \tag{4.42}$$

We may simplify (4.42) if we note from (VII.3.16a), (VII.3.16b), (VII.3.16f), and (VII.3.16g) that, because the integrands are all odd functions of θ when $k = k'$,

$$A^{-1}(j, k; j', k)_{DD} = A^{-1}(j, k; j', k)_{UU} = 0. \tag{4.43}$$

Using this, the Pfaffian in (4.42) reduces to a determinant and we have $\mathfrak{M}_J = \pm(1 - z^2)(1 - z_2^2)^{J-1}$

$$\times \det\begin{bmatrix} A^{-1}(1,0;0,0)_{DU} + (z^{-1} - z)^{-1} & A^{-1}(1,0;1,0)_{DU} & \cdots & A^{-1}(1,0;J-1,0)_{DU} \\ A^{-1}(2,0;0,0)_{DU} & A^{-1}(2,0;1,0)_{DU} + (z_2^{-1} - z_2)^{-1} & \cdots & A^{-1}(2,0;J-1,0)_{DU} \\ \vdots & \vdots & \vdots & \vdots \\ A^{-1}(J,0;0,0)_{DU} & A^{-1}(J,0;1,0)_{DU} & \cdots & A^{-1}(J,0;J-1,0)_{DU} + (z_2^{-1} - z_2)^{-1} \end{bmatrix}. \tag{4.44}$$

The question of spontaneous magnetization and hysteresis may be dealt with just as in Chapter VI. We see from (VII.3.16) that as $\mathfrak{H} \to 0$ all of the matrix elements are continuous except those in the first column, which may be written

$$A^{-1}(j, 0; 0, 0)_{DU} = \frac{1}{2\pi} z z_1$$
$$\times \int_{-\pi}^{\pi} d\theta \frac{|1 + e^{i\theta}|^2 \alpha^{-j+1}}{z^2 z_1 |1 + e^{i\theta}|^2 - z_2^2(1 + z_1^2 + 2z_1 \cos\theta) + z_2(1 - z_1^2)\alpha}. \tag{4.45}$$

The singularities of the integrand of (4.45) are exactly the same as those of (VI.5.1). Therefore, the discussion of Sec. 5 of Chapter VI applies. In particular, if $T > T_c$, (4.45) will vanish as $\mathfrak{H} \to 0$; but if $T < T_c$ and $E_1 > 0$, (4.45) is discontinuous as $\mathfrak{H} \to 0$ and, following (VI.5.19), has the limit

$$\lim_{\mathfrak{H} \to 0^+} A^{-1}(j, 0; 0, 0)_{DU} = \frac{1}{2z_1^{1/2}|z_2|} [z_2^2(1 + z_1)^2 - (1 - z_1)^2]^{1/2} \alpha(1)^{-j+1}, \tag{4.46}$$

where

$$\alpha(1) = z_2 \frac{1 + z_1}{1 - z_1}. \tag{4.47}$$

Furthermore, the factor α^{-j+1} in the numerator of (4.45) does not affect the factorization of the denominator made for $j = 1$ in (VI.5.8). Therefore, these matrix elements, and hence $\mathfrak{M}_J$ itself, may be analytically continued through $\mathfrak{H} = 0$ just as $\mathfrak{M}_1$ was. More specifically,

$$\begin{aligned} A^{-1c}(j, 0; 0, 0)_{DU} - A^{-1}(j, 0; 0, 0)_{DU} &= (1 - z^2)^{-1}[\mathfrak{M}_1^c(\mathfrak{H}) - \mathfrak{M}_1(\mathfrak{H})]\alpha(r)^{-j+1} \\ &= (1 - z^2)^{-1}[\mathfrak{M}_1^c(\mathfrak{H}) - \mathfrak{M}_1(\mathfrak{H})][(1 + z_1)(z_2^2 - z^2)z_2^{-1} \\ &\quad \times (1 - z_1)^{-1}(1 - z^2)^{-1}]^{-j+1}. \end{aligned} \tag{4.48}$$

Therefore, for any J,

$$\begin{aligned} \mathfrak{M}_J^c(\mathfrak{H}) - \mathfrak{M}_J(\mathfrak{H}) &= \pm[\mathfrak{M}_1^c(\mathfrak{H}) - \mathfrak{M}_1(\mathfrak{H})](1 - z_2^2)^{J-1} \\ &\times \det\begin{bmatrix} 1 & A^{-1}(1, 0; 1, 0)_{DU} & \cdots & A^{-1}(1, 0; J-1, 0)_{DU} \\ \alpha(r)^{-1} & A^{-1}(2, 0; 1, 0)_{DU} + (z_2^{-1} - z_2)^{-1} & \cdots & A^{-1}(2, 0; J-1, 0)_{DU} \\ \vdots & \vdots & & \vdots \\ \alpha(r)^{-J+1} & A^{-1}(J, 0; 1, 0)_{DU} & \cdots & A^{-1}(J, 0; J-1, 0)_{DU} + (z_2^{-1} - z_2)^{-1} \end{bmatrix}. \end{aligned} \tag{4.49}$$

For our purpose, we will not evaluate either (4.44) or (4.49) explicitly. First of all, as an example, we compute the spontaneous magnetization in the second row. This is

$$\begin{aligned} \lim_{\mathfrak{H}\to 0^+} \mathfrak{M}_2 = \pm(1 - z_2^2) \lim_{\mathfrak{H}\to 0^+} \Bigg[& A^{-1}(1, 0; 0, 0)_{DU} \\ & \times \left(A^{-1}(2, 0; 1, 0)_{DU} + \frac{1}{1/z_2 - z_2}\right) \\ & - A^{-1}(2, 0; 0, 0)_{DU} A^{-1}(1, 0; 1, 0)_{DU}\Bigg]. \end{aligned} \tag{4.50}$$

Using (4.46) and (VII.3.16), we find

$$\begin{aligned} \mathfrak{M}_2(0^+) = \pm(1 - z_2^2)\frac{1}{2z_1^{1/2}|z_2|}[z_2^2(1 + z_1)^2 - (1 - z_1)^2]^{1/2} \\ \times \left[\frac{-z_2}{2\pi}\int_{-\pi}^{\pi} d\theta \frac{\mathfrak{D}_{2\mathcal{M}-1}\mathfrak{D}_1}{\mathfrak{C}_{2\mathcal{M}}} + \frac{1}{1/z_2 - z_2} \right. \\ \left. + \frac{1 - z_1}{z_2^2(1 + z_1)}\frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta \frac{1}{\alpha}\right], \end{aligned} \tag{4.51}$$

which reduces to

$$\mathfrak{M}_2(0^+) = \frac{1}{2z_1^{1/2}|z_2|}\,[z_2^2(1 + z_1)^2 - (1 - z_1)^2]^{1/2}$$

$$\times \left[\frac{1}{z_2} - \frac{z_1(1 - z_2^2)}{z_2^2(1 - z_1^2)}\,\frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta\,\frac{1}{\alpha}\,(e^{i\theta} - 1)(e^{-i\theta} - 1)\right]. \tag{4.52}$$

As $T \to T_c$, the bracket remains finite and nonzero, so the magnetization in the second row goes to zero as a square root, just as $\mathfrak{M}_1$ does. We conjecture that all $\mathfrak{M}_J$ go to zero as $(1 - T/T_c)^{1/2}$ when $T \to T_c^-$ for any now J. We furthermore conjecture that, for $E_2 > 0$, $\mathfrak{M}_J(\mathfrak{H})$ monotonically approaches the spontaneous magnetization of the bulk. This conjecture has been numerically studied[2] for $1 \le J \le 10$. The results of this study are in complete agreement with the behavior of $\mathfrak{M}_J(\mathfrak{H})$ indicated schematically in Fig. 13.7 for $T/T_c = 0.9$.

Our second observation is that, because the determinant in (4.49) is finite for all $\mathfrak{H}$, the value of $\mathfrak{H}_c$ such that $\mathfrak{M}_J^c(\mathfrak{H}_c) = \mathfrak{M}_J(\mathfrak{H}_c)$ is the same for all J. The bulk magnetization can take on only the values $\pm\mathfrak{M}_\infty$ (the bulk magnetization of Yang studied in Chapter X), so the bulk spin must flip discontinuously from $+$ to $-\mathfrak{M}_\infty$ at $\mathfrak{H} = \mathfrak{H}_c$ (see Fig. 13.7). Even though the magnetization in the first J rows may have passed beyond $\mathfrak{M}_J^c(\mathfrak{H}) = 0$, there are still an infinite number of rows in which the magnetization has not yet passed $\mathfrak{M}_J^c(\mathfrak{H}) = 0$. From this viewpoint, there is no reason to single out the passing of $\mathfrak{M}_J^c(\mathfrak{H})$ through zero or the disappearance of a secondary maximum in $P(\bar{\sigma})$ as the criteria for the *entire* system to fall from $\mathfrak{M}_J^c(\mathfrak{H})$ to $\mathfrak{M}_J(\mathfrak{H})$. The analytic continuation of $\mathfrak{M}_J(\mathfrak{H})$ will characterize the entire system as long as for each and every $\mathfrak{M}_J(\mathfrak{H})$ the analytic continuation is possible. For finite J, $\mathfrak{M}_J(\mathfrak{H})$ is continuable not only beyond $\mathfrak{H} = 0$ but even beyond $\mathfrak{H} = \pm\mathfrak{H}_c$. However, $\mathfrak{M}_\infty(\mathfrak{H})$ *cannot* be continued beyond $\pm\mathfrak{H}_c$ because, as we have seen, the bulk magnetization will be discontinuous at $\mathfrak{H} = \pm\mathfrak{H}_c$. Therefore for the system as a whole continuation past $\pm\mathfrak{H}_c$ is meaningless and in each row the transition from $\mathfrak{M}_J^c$ to $\mathfrak{M}_J$ occurs at the same value of $\mathfrak{H}$. Hence we conclude that $\mathfrak{M}_J$ and its analytic continuation behave as in Fig. 13.7(a) and that the loop shown in Fig. 13.2 is incorrect.

This discussion gives a natural interpretation to each of the first two terms of (4.23) and (4.32) taken *separately*. We are really observing a thermodynamic system which, for some values of $\mathfrak{H}$, has not one but two stable states. The fact that there are two distinct stable states is reflected in $P(\bar{\sigma})$ by the two terms and $P(\bar{\sigma})$ is really the sum of two

2. C. K. Lai, unpublished.

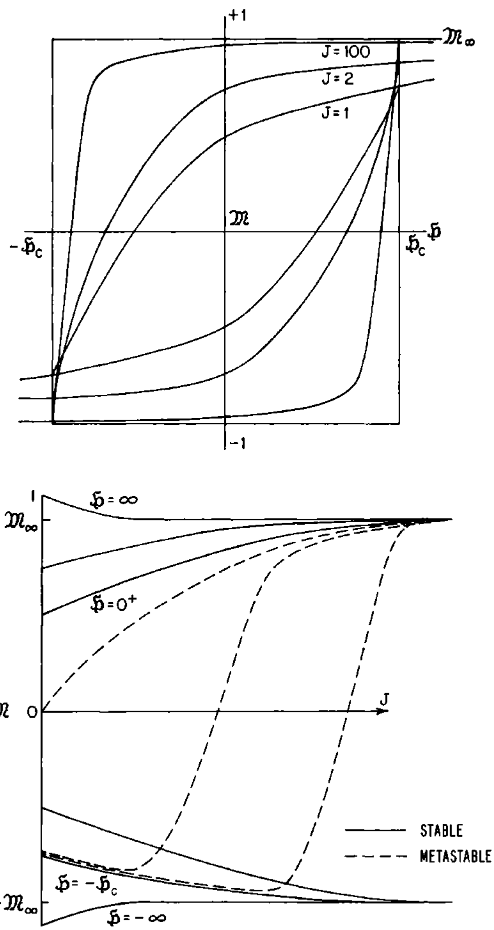


Fig. 13.7. Schematic behavior of $\mathfrak{M}_J(\mathfrak{H})$ for $E_1 = E_2$: (*a*) $\mathfrak{M}_J(\mathfrak{H})$ versus $\mathfrak{H}$ for various J; the analytic continuation of $\mathfrak{M}_J(\mathfrak{H})$ is shown for that range of $\mathfrak{H}$ such that $\mathfrak{M}_J(\mathfrak{H}) \geq \mathfrak{M}_J^s(\mathfrak{H})$; (*b*) $\mathfrak{M}_J(\mathfrak{H})$ versus J for various $\mathfrak{H}$; the metastable values between $\mathfrak{H} = 0^+$ and $-\mathfrak{H}_c$ are reached from positive values of $\mathfrak{H}$.

separate conditional probabilities: the probability that the average boundary spin is $\bar{\sigma}$ and the bulk spin is $+M$ and the probability that the average boundary spin is $\bar{\sigma}$ and the bulk spin is $-M$. Each of these probability functions is monomodal and previous discussions of secondary maxima fail to apply.

5. MISFIT BOND

We now turn to the question of the influence of boundary conditions on the boundary-spin probability functions and will see that when $T < T_c$ these boundary conditions can drastically alter $P(\bar{\sigma})$ for $-\mathfrak{M}(0^+) < \bar{\sigma} < \mathfrak{M}(0^+)$. We study this by looking at the same half-plane lattice previously considered but instead of imposing cyclic boundary conditions by joining the $\mathcal{N}$th and the $(-\mathcal{N}+1)$th columns by bonds of energy E_1 we join them by bonds of energy $-E_1$.

We will compute the boundary-spin probability function $P_{(1)}(\bar{\sigma})$ for this lattice from (1.3). For this purpose, we need an expression for the partition function $Z_{(1)}$. The evaluation of the partition function in the presence of a boundary magnetic field may be reduced, by exactly the same arguments as were used in Sec. 2 of Chapter VI, to the evaluation of an appropriate Pfaffian as

$$Z_{(1)} = \tfrac{1}{2}(2\cosh\beta E_1)^{4\mathcal{M}\mathcal{N}}(\cosh\beta E_2)^{2\mathcal{N}(2\mathcal{M}-1)}(\cosh\beta\mathfrak{H})^{2\mathcal{N}}\,\mathrm{Pf}\,A_{(1)}, \tag{5.1}$$

where $A_{(1)}$ is the matrix whose Pfaffian counts the lattice of Fig. 13.8(a). The elements of $A_{(1)}$ are exactly the same as those of A given in (VI.2.6) except that (VI.2.6d) is replaced by

$$A_{(1)}(0,\mathcal{N};0,-\mathcal{N}+1) = -A^T_{(1)}(0,-\mathcal{N}+1;0,\mathcal{N}) = -A_{(1)}(0,0;0,1) \tag{5.2}$$

and

$$A_{(1)}(j,\mathcal{N};j,-\mathcal{N}+1) = -A^T_{(1)}(j,-\mathcal{N}+1;j,\mathcal{N}) = A_{(1)}(j,0;j,1) \tag{5.3}$$

for $1 \le j \le 2\mathcal{M}$.

The matrix $A_{(1)}$ is neither cyclic nor nearly cyclic, so we cannot

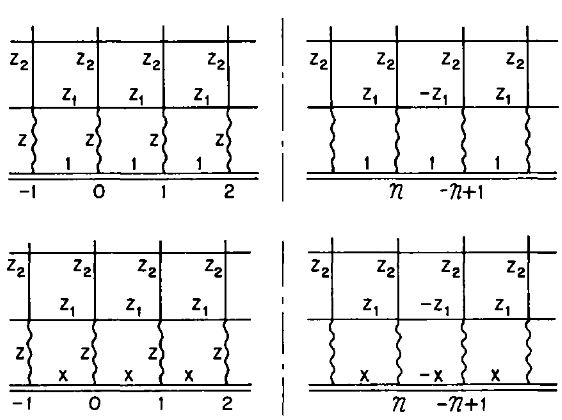


Fig. 13.8. (a) Misfit bond lattice; (b) comparison cyclic lattice.

immediately evaluate its Pfaffian. However, its Pfaffian may be evaluated by relating it to the Pfaffian of the cyclic matrix A_x which counts the weighted polygons drawn on the lattice of Fig. 13.8(b). The elements of A_x are the same as those of $A_{(1)}$ except for elements connecting sites in the zeroth row, where we have

$$A_x(0,k;0,k+1) = -A_x^T(0,k+1;0,k)$$
$$= \begin{array}{c|cccc} & R & L & U & D \\ \hline R & 0 & x & 0 & 0 \\ L & 0 & 0 & 0 & 0 \\ U & 0 & 0 & 0 & 0 \\ D & 0 & 0 & 0 & 0 \end{array} \tag{5.4}$$

for $-\mathcal{N}+1 \leq k \leq \mathcal{N}-1$ and

$$A_x(0,\mathcal{N};0,-\mathcal{N}+1) = -A_x^T(0,-\mathcal{N}+1;0,\mathcal{N}) = A_x(0,0;0,1). \tag{5.5}$$

When $x = 1$, $\operatorname{Pf} A_x = 0$ because for every diagram that can be drawn on the lattice of Fig. 13.8(b) there is a complementary diagram which differs from the original only in using (omitting) all the bonds in the zeroth row which are omitted (used) in the original. This complementary diagram has the same magnitude as the original one but opposite sign.

Consider all terms that may appear in the expansion of $\operatorname{Pf} A_{(1)}$, that correspond to diagrams drawn on Fig. 13.8(a), and that differ: (1) only in the two ways the sites in the zeroth row may be connected together, and (2) by translation. If one such diagram has l bonds in the zeroth row, the complementary diagram has $2\mathcal{N}-l$ bonds in the zeroth row. Let the value of such a diagram when it is in a position such that none of the l zero-row bonds are between $\mathcal{N}$ and $-\mathcal{N}+1$ be d. Then the sum of this class of diagrams is

$$2(2\mathcal{N}-l)d - 2ld = 4(\mathcal{N}-l)d. \tag{5.6}$$

Now consider the same diagrams drawn on the lattice of Fig. 13.8(b) which now contribute to $\operatorname{Pf} A_x$. The sum of this same class of diagrams is now

$$(2\mathcal{N}-l)(x^l - x^{2\mathcal{N}-l})d + l(x^l - x^{2\mathcal{N}-l})d = 2\mathcal{N}x^l(1 - x^{2(\mathcal{N}-l)})d. \tag{5.7}$$

If we sum (5.6) and (5.7) over all possible d we reconstitute the Pfaffians of $A_{(1)}$ and A_x respectively. From (5.7) we see that $\lim_{x\to 1} \operatorname{Pf} A_x = 0$ as expected but also that we have the identity

$$\left.\frac{\partial \operatorname{Pf} A_x}{\partial x}\right|_{x=1} = -\mathcal{N} \operatorname{Pf} A_{(1)}. \tag{5.8}$$

Therefore

$$\frac{\partial^2}{\partial x^2} \det A_x|_{x=1} = 2\mathcal{N}^2 \det A_{(1)}. \tag{5.9}$$

We may evaluate $\det A_x$ in a manner analogous to the evaluation of $\det A$ in Sec. 3 of Chapter VI. Since A_x is a cyclic matrix,

$$\det A_x = \prod_{\phi} \det B_x(\phi), \tag{5.10}$$

where the product is over

$$\phi = n\pi/\mathcal{N}, \tag{5.11}$$

$n = 0, 1, \ldots, 2\mathcal{N} - 1$, and $B_x(\phi)$ is the $4(2\mathcal{M} + 1) \times 4(2\mathcal{M} + 1)$ matrix defined as in (VI.3.3) with θ replaced by ϕ and B_{00} replaced by

$$B_{x0,0}(\phi) = \begin{bmatrix} 0 & 1 + xe^{i\phi} & -1 & -1 \\ -1 - xe^{-i\phi} & 0 & 1 & -1 \\ 1 & -1 & 0 & 1 \\ 1 & 1 & -1 & 0 \end{bmatrix}. \tag{5.12}$$

Defining

$$\mathfrak{c}_x = 2ix \sin \phi |1 + xe^{i\phi}|^{-2} \tag{5.13a}$$

and

$$\mathfrak{d}_x = (1 - x^2)|1 + xe^{i\phi}|^{-2} \tag{5.13b}$$

and following the procedure of Chapter VI, we find

$$\det A_x = \prod_{\phi} [|1 + xe^{i\phi}|^2 |1 + z_1 e^{i\phi}|^{4\mathcal{M}} \det \mathfrak{C}_x(\phi)], \tag{5.14}$$

where the elements of $\mathfrak{C}_x(\phi)$ are identical with those of $\mathfrak{C}(\theta)$ of (VI.3.8) except that

$$\mathfrak{C}_{x0,0}(\phi) = \begin{bmatrix} -\mathfrak{c}_x & \mathfrak{d}_x \\ -\mathfrak{d}_x & \mathfrak{c}_x \end{bmatrix}. \tag{5.15}$$

Evaluating $\det \mathfrak{C}_x(\phi)$ as in Chapter VI we obtain

$$\det A_x = \prod_{\phi} |1 - xe^{i\phi}|^2 |1 + z_1 e^{i\phi}|^{4\mathcal{M}} \lambda^{2\mathcal{M}}$$
$$\times \left[v^2 \left(1 - \frac{iz^2/z_2 \mathfrak{c}_x}{1 - \mathfrak{d}_x^2 \mathfrak{c}_x^{-2}} \frac{v'}{v} \right) + \alpha^{-4\mathcal{M}} v'^2 \left(1 + \frac{iz^2/z_2 \mathfrak{c}_x}{1 - \mathfrak{d}_x^2 \mathfrak{c}_x^{-2}} \frac{v}{v'} \right) \right]. \tag{5.16}$$

Since

$$\prod_{\phi} |1 - xe^{i\phi}|^2 = (1 - x^{2\mathcal{N}})^2, \tag{5.17}$$

we may use (5.16) and (5.9) to evaluate (5.1) as

$$Z_{(1)}^2 = (2\cosh\beta E_1)^{8\mathcal{M}\mathcal{N}}(\cosh\beta E_2)^{4\mathcal{N}(2\mathcal{M}-1)}(\cosh\beta\mathfrak{H})^{4\mathcal{N}} \times \prod_\phi |1 + z_1 e^{i\phi}|^{4\mathcal{M}}\lambda^{2\mathcal{M}} \lim_{x\to 1}\prod_\phi\left[v^2\left(1 - \frac{iz^2/z_2\mathfrak{c}_x}{1-\mathfrak{d}_x^2\mathfrak{c}_x^{-2}}\frac{v'}{v}\right) + \alpha^{-4\mathcal{M}}v'^2\left(1 + \frac{iz^2/z_2\mathfrak{c}_x}{1-\mathfrak{d}_x^2\mathfrak{c}_x^{-2}}\frac{v}{v'}\right)\right]. \tag{5.18}$$

The $\phi = 0$ term in this last product must be treated separately. For $T > T_c$ we have

$$Z_{(1)}^2 = (2\cosh\beta E_1)^{8\mathcal{M}\mathcal{N}}(\cosh\beta E_2)^{4\mathcal{N}(2\mathcal{M}-1)}(\cosh\beta\mathfrak{H})^{4\mathcal{N}} \times \prod_\phi |1 + z_1 e^{i\phi}|^{4\mathcal{M}}\lambda^{2\mathcal{M}} \prod_\phi{}'\left[v^2\left(1 - \frac{iz^2}{z_2\mathfrak{c}}\frac{v'}{v}\right) + \alpha^{-4\mathcal{M}}v'^2\left(1 + \frac{iz^2}{z_2\mathfrak{c}}\frac{v}{v'}\right)\right], \tag{5.19a}$$

and for $T < T_c$

$$Z_{(1)}^2 = (2\cosh\beta E_1)^{8\mathcal{M}\mathcal{N}}(\cosh\beta E_2)^{4\mathcal{N}(2\mathcal{M}-1)}(\cosh\beta\mathfrak{H})^{4\mathcal{N}}\alpha(0)^{-4\mathcal{M}} \times \prod_\phi |1 + z_1 e^{i\phi}|^{4\mathcal{M}}\lambda^{2\mathcal{M}} \prod_\phi{}'\left[v^2\left(1 - \frac{iz^2}{z_2\mathfrak{c}}\frac{v'}{v}\right) + \alpha^{-4\mathcal{M}}v'^2\left(1 + \frac{iz^2}{z_2\mathfrak{c}}\frac{v}{v'}\right)\right], \tag{5.19b}$$

where $\prod'_\phi$ means to take the product over all $\phi \neq 0$ satisfying (5.11) and we have used the facts that for $T > T_c$

$$v(0) = 1$$

and as $\phi \to 0$

$$v'(\phi) \sim 2z_1z_2\phi[z_2^2(1 + z_1)^2 - (1 - z_1)^2]^{-1}, \tag{5.20a}$$

and for $T < T_c$

$$v'(0) = 1$$

and as $\phi \to 0$

$$v(\phi) \sim -2z_1z_2\phi[z_2^2(1 + z_1)^2 - (1 - z_1)^2]^{-1}. \tag{5.20b}$$

To convert (5.19) into an integral we must reinstate the $\phi = 0$ term into the product and use the Poisson sum formula appropriate to the $2\mathcal{N}$ roots of 1,

$$\sum_{n=0}^{2\mathcal{N}-1}\delta\left(\phi - \frac{n\pi}{\mathcal{N}}\right) = \frac{\mathcal{N}}{\pi}\sum_{m=-\infty}^{\infty} e^{2\mathcal{N}mi\phi}. \tag{5.21}$$

The integrals are then exactly the same as those analyzed in Sec. 4 with the exception of the omission of $(-1)^m$. A completely analogous calculation therefore gives for $T > T_c$

$$\frac{Z_{(1)}(\mathfrak{H})}{Z_{(1)}(0)} = \frac{(\cosh \beta\mathfrak{H})^{2\mathcal{N}} \exp\{-2\mathcal{N}\beta\mathfrak{F}(\mathfrak{H};\mathcal{M})[1 + O(\alpha_2^{-2\mathcal{N}})]\}}{\{1 + 4z^2 z_1[1 - \alpha(0)^{-4\mathcal{M}}][(1 - z_1)^2 - z_2^2(1 + z_1)^2]\}^{1/2}} \tag{5.22a}$$

and for $T < T_c$,

$$\frac{Z_{(1)}(\mathfrak{H})}{Z_{(1)}(0)} = \frac{(\cosh \beta\mathfrak{H})^{2\mathcal{N}} \exp\{-2\mathcal{N}\beta\mathfrak{F}(\mathfrak{H};\mathcal{M})[1 + O(\alpha_2^{2\mathcal{N}})]\}}{\{1 + 4z^2 z_1[\alpha(0)^{4\mathcal{M}} - 1][z_2^2(1 + z_1)^2 - (1 - z_1)^2]^{-1}\}^{1/2}}$$
$$\times \frac{1 - r_{\mathcal{M}}(\mathfrak{H})^{2\mathcal{N}}}{1 - r_{\mathcal{M}}(0)^{2\mathcal{N}}}, \tag{5.22b}$$

where

$$Z_{(1)}^2(0) = (2\cosh \beta E_1)^{8\mathcal{M}\mathcal{N}}(\cosh \beta E_2)^{4\mathcal{N}(2\mathcal{M}-1)} \prod_{\phi} |1 + z_1 e^{i\phi}|^{4\mathcal{M}}$$
$$\times \lambda^{2\mathcal{M}} v^2[1 + \alpha^{-4\mathcal{M}}(v'/v)^2]. \tag{5.23}$$

Expression (5.22*a*) is exactly the same as the partition function above T_c when there is no misfit bond, with the exception of the denominator. This extra factor is easily interpreted as the decrease in free energy caused by the boundary magnetic field forcing spins on opposite sides of the misfit seam to point in the same direction. When $T \to T_c^+$, this factor becomes very small, on the order of $(2\mathcal{M})^{-1}$. This is because very near T_c the correlation length is very large and the boundary magnetic field is able to line spins up across the seam at depths into the bulk on the order of $2\mathcal{M}$.

To show that the misfit bonds have destroyed the bimodal character of $P(\bar{\sigma})$, we consider the $\mathcal{M} \to \infty$ limit of (5.22*b*) and obtain

$$\lim_{\mathcal{M}\to\infty} \frac{Z_{(1)}(\mathfrak{H})}{Z_{(1)}(0)} = \frac{1 - r(\mathfrak{H})^{2\mathcal{N}}}{4\mathcal{N}\mathfrak{M}_1(0^+)(z^2)^{1/2}} \exp[-2\mathcal{N}\beta\mathfrak{F}(\mathfrak{H})], \tag{5.24}$$

where $\mathfrak{F}(\mathfrak{H})$ and $(z^2)^{1/2}$ are analytic in the $\mathfrak{H}$-plane cut along the entire imaginary $\mathfrak{H}$-axis because we have let $\mathcal{M} \to \infty$. Similarly, the $\mathfrak{H}$-plane in which $r(\mathfrak{H})$ is analytic is cut along the imaginary axis. The second sheet of all of these functions may be obtained by continuing through this cut as we did in (4.15) and (4.18) for finite $\mathcal{M}$. If we use those expressions for $r^c(\mathfrak{H})$ and $\mathfrak{F}^c(\mathfrak{H})$ in (5.24), we find that, as expected, $Z_{(1)}(\mathfrak{H})$ does not have a branch cut on the imaginary axis.

We now use (5.24) in (1.3) to obtain

$$P_{(1)}(\bar{\sigma}) = \frac{\beta}{2\pi i}\int_{-i\pi/\beta}^{i\pi/\beta} d\xi\, \frac{1 - r(\mathfrak{H})^{2\mathcal{N}}}{4\mathcal{N}z\mathfrak{M}_1(0^+)}\, e^{-2\mathcal{N}\beta[\mathfrak{F}(\xi)+\bar{\sigma}\xi]}, \tag{5.25}$$

where the integration path has been deformed slightly to the right of the imaginary axis. We evaluate (5.25) by steepest descents, where as before the terms of $O(1)$ and $O(r(\mathfrak{H})^{2\mathcal{N}})$ have different steepest-descents points and must be evaluated separately. But once this separation is made, we see that each separate term has a pole at $\xi = 0$ so that when the steepest-descents point occurs for negative ξ we pick up an extra contribution from this pole. When $\bar{\sigma}$ is enough larger than $\mathfrak{M}_1(0^+)$ that the steepest-descents points are away from $\xi = 0$, we have

$$P_{(1)}(\bar{\sigma}) = \frac{1}{8\mathcal{N}\mathfrak{M}_1(0^+)}\left(\frac{\beta}{\mathcal{N}\pi}\right)^{1/2}\left[\coth\beta\xi_1\frac{e^{2\mathcal{N}w_1}}{\chi(\xi_1)^{1/2}} - \coth\beta\xi_2\frac{e^{2\mathcal{N}w_2}}{\chi^c(\xi_2)^{1/2}}\right], \tag{5.26}$$

with ξ_1 and ξ_2 given by (4.21). When $0 < |\bar{\sigma}| < \mathfrak{M}_1(0^+)$

$$P_{(1)}(\bar{\sigma}) = \frac{1}{2\mathcal{N}\mathfrak{M}_1(0^+)} + \frac{1}{8\mathcal{N}\mathfrak{M}_1(0^+)}\left(\frac{\beta}{\pi\mathcal{N}}\right)^{1/2}$$
$$\times\left[\coth\beta\xi_1\frac{e^{2\mathcal{N}w_1}}{\chi^c(\xi_1)^{1/2}} - \coth\beta\xi_2\frac{e^{2\mathcal{N}w_2}}{\chi^c(\xi_2)^{1/2}}\right]. \tag{5.27}$$

When $\mathcal{N} \gg 1$ this expression is dominated by a constant. This flatness of $P_{(1)}(\bar{\sigma})$ has an obvious physical interpretation. When $\mathfrak{H} = 0$, the $-E_1$ bonds force the lattice to break up into two domains of opposite spin. One wall between these domains must be the column of $-E_1$ bonds but the other wall may be anywhere. Therefore, the surface magnetization is uniformly distributed between $-\mathfrak{M}_1(0^+)$ and $\mathfrak{M}_1(0^+)$, depending on where the other domain wall may be. This physical picture applies to the bulk as well and we expect that the bulk probability functions as well as $P_{(1)}$ are flat between $-M$ and M. To prove this, one needs to consider the behavior of the correlation functions when the separation becomes large. For the boundary spin-spin correlation, it is straightforward to show from Chapter VII that for large k

$$\langle\sigma_{1,0}\sigma_{1,k}\rangle \to \mathfrak{M}_1^2(\mathcal{N} - |k|)/\mathcal{N} + O(\alpha_2^{|k|}). \tag{5.28}$$

For completeness, it remains only to evaluate (5.25) when $\bar{\sigma}$ is very close to $\mathfrak{M}_1(0^+)$. This is easily done in terms of the complementary error function and we obtain

$$P_{(1)}(\bar{\sigma}) \sim \frac{1}{2\mathcal{N}\mathfrak{M}_1(0^+)}\frac{1}{\pi^{1/2}}\,\mathrm{Erfc}\,\{[\bar{\sigma} - \mathfrak{M}_1(0^+)](\mathcal{N}\beta/\chi)^{1/2}\}. \tag{5.29}$$

CHAPTER XIV
An Ising Model with Random Impurities: Specific Heat

1. INTRODUCTION[1]

We now turn to a most interesting practical question raised at the end of Chapter II, namely, how can we generalize statistical mechanics to deal with the experimental situation in which we do not completely know the interaction energy of the system, owing to the presence of impurities? This type of statistical mechanics is not nearly as well developed as the familiar statistical mechanics presented in Chapter II. We will therefore not even give the pretense of generality but confine ourselves very closely to the Ising model. In this way we hope to provide a concrete guide for future studies of the properties of impure and amorphous materials.

As discussed in Chapter II, the term impurity refers not only to the presence of foreign material in a sample but to any physical property that makes lattice sites different from one another. One such property is a defect or vacancy in the lattice. Another is the presence in the sample of different isotopes; for example, nickel contains roughly 68 percent of Ni^{58}, 26 percent of Ni^{60}, 1 percent of Ni^{61}, 4 percent of Ni^{62}, and 1 percent of Ni^{64}. The distribution of these impurities is governed by spin-independent forces which have been neglected in our discussion. We can distinguish at least two different situations:

(1) As the temperature changes, the distribution of impurities may change; such a situation will occur, for example, near the melting point of a lattice.

(2) The distribution of impurities may be independent of temperature, at least on the time scale of laboratory measurements; such a situation

1. This chapter is based on the work of B. M. McCoy and T. T. Wu, *Phys. Rev.* **176**, 631 (1968), *Phy. Rev. Letters* **21**, 549 (1968).

will obtain when the temperature of a lattice is well below the melting temperature. Impurities of this sort are said to be "frozen in," and in this book we will consider "frozen in" impurities exclusively.

If these "frozen in" impurities distribute themselves through the system in a periodic fashion, then, though the symmetry of the lattice would be reduced, it would not be destroyed. With sufficient labor, such an ordered sort of impurity can be studied in the Ising model by means of the techniques we have presented. However, such an ordering of impurities does not usually take place. Therefore, if we want to study realistically the effects of impurities in magnetic systems, we have to allow the impurities to be distributed at random throughout the lattice. The regularity of the system now has been not merely reduced but totally destroyed. A phase transition is a cooperative phenomenon in which the entire system takes part. It is therefore not at all obvious that the translationally invariant Onsager lattice should possess a phase-transition behavior that is in any way related to such an impure system.

The most realistic way in which we could introduce impurities into the Ising model would be to replace some host spins, which interact with themselves with interaction energies E_1 and E_2, by impurity spins, which interact with the host spins with interaction energies E_1' and E_2' and with themselves with energies E_1'' and E_2''. Such a model has proved to be intractable. Therefore, we consider the following modification of Onsager's lattice, which may be studied analytically and still embodies the essential feature of destroying some of the translational symmetry of the system. We retain the features of Onsager's rectangular lattice to the extent that all horizontal interactions are the same and that the vertical interaction $E_2(j)$ between any site in the jth row and its nearest neighbor in the $(j + 1)$th row is the same no matter what column these sites are in. However, $E_2(j)$ is allowed to vary randomly from row to row. More specifically, we assume that, for $j \neq j'$, $E_2(j)$ and $E_2(j')$ are independent random variables with identical probability distributions $P(E_2)\, dE_2$.

Let us try to describe the model in greater detail. We are considering a collection of Ising lattices, each of which is specified by a particular set of interactions $\{E_2(j)\}$. We are interested in the thermodynamic limit where the size of these lattices becomes infinite. If, in the thermodynamic limit, the free energy of each lattice in our collection varied wildly from lattice to lattice our model would be useless. In that case the free energy of our random lattices would depend in detail on the arrangement of interactions. Fortunately, this is physically unreasonable and, indeed, will be seen in Sec. 2 not to be the case. In the thermodynamic limit the free energy per site of each lattice does approach, with probability 1, the same value. Therefore, with probability 1 the Curie temperatures of any two lattices from this collection are the same. Furthermore, we expect the spontaneous magnetization of any two lattices to be the same with probability 1, because the spontaneous magnetization, like the free energy, is an average property of the entire lattice. However, not all quantities of interest have distributions which are so sharply peaked. For example, the spin-spin correlation function of neighboring spins does depend in detail on the local value of the interaction energies. For such quantities one needs more than an average value to characterize the result of a measurement made at an arbitrary position in the impure lattice.

The complete investigation of all aspects of this random Ising model has not been made. In this chapter we begin the investigation by considering the free energy in the absence of a magnetic field.[2] In Sec. 2 we will formulate the mathematical problem to be solved and find a general formula for the critical temperature in terms of $P(E_2)$. In Sec. 3 we will derive several general properties of the integral equation found in Sec. 2. There is a great deal that can be said about the equations we derive because they depend on the arbitrary function $P(E_2)$. We wish to emphasize the physical consequences of random impurities. Therefore we specialize our treatment in Sec. 4 to a particular distribution $P(E_2)$ which has a narrow width (of order N^{-1})[3] that is particularly mathematically tractable. This distribution is in no way physically distinguished and our results are expected to be typical of a large class of narrow distributions. We show that, whereas the critical temperature is shifted by a temperature of the order of N^{-1}, the specific heat deviates appreciably (to order 1 as $N \to \infty$) from Onsager's specific heat only for $T - T_c \sim O(N^{-2})$. We furthermore find that at T_c the term of order 1 in the specific heat is not logarithmically divergent but is an infinitely differentiable function of T though it is not analytic. Finally we conclude in Sec. 5 with a discussion of several of the technical aspects of the calculation and of the relation of this computation to the experimental situation.

2. FORMULATION OF THE PROBLEM

We are interested in studying a particular class of rectangular two-dimensional Ising models with $\mathscr{M}$ rows and $2\mathscr{N}$ columns. We impose cyclic boundary conditions in the horizontal direction only. This class of systems is characterized by the interaction energies

$$\begin{aligned}\mathscr{E} = &-E_1 \sum_{j=1}^{\mathscr{M}} \sum_{k=-\mathscr{N}+1}^{\mathscr{N}} \sigma_{j,k}\sigma_{j,k+1} \\ &- \sum_{j=1}^{\mathscr{M}-1} E_2(j) \sum_{k=-\mathscr{N}+1}^{\mathscr{N}} \sigma_{j,k}\sigma_{j+1,k},\end{aligned} \tag{2.1}$$

2. The free energy of the one-dimensional random Ising model may be studied in the presence of a magnetic field. However, as this study says nothing about phase transitions, we will not discuss it here. For details see C. Fan and B. McCoy, *Phys. Rev.* **182**, 614 (1969).
3. This N is not to be confused with the N of the previous chapters.

where $\sigma_{j,k}$ is equal to $+1$ or -1, j and k label, respectively, the row and column of each lattice site, and $k = \mathcal{N} + 1$ is identified with $k = -\mathcal{N} + 1$. As far as thermodynamics is concerned we may restrict E_1 and E_2 to be positive without loss of generality. We are interested in the limit $\mathcal{N} \to \infty$ and $\mathcal{M} \to \infty$; only in this limit will a phase transition occur. We complete the characterization by requiring that $E_2(j)$ be independent random variables with the probability density function $P(E_2)$.

Call $Z_{\{E_2\}}$ the partition function for the system described by (2.1) where the collection of bounds $\{E_2(j)\}$ is chosen at random according to the probability density function $P(E_2)$. We are interested in F_r, the free energy per site of the system in the thermodynamic limit. Under the assumption that with probability 1 this limit exists, F_r is defined as

$$F_r = -\frac{1}{\beta} \lim_{\substack{\mathcal{M}\to\infty \\ \mathcal{N}\to\infty}} \frac{1}{2\mathcal{M}\mathcal{N}} \ln Z_{\{E_2\}}. \tag{2.2}$$

Our class of lattices shares with Onsager's lattice the property of translational invariance in the horizontal direction. Therefore the calculation of Sec. 3 of Chapter VI may be taken over word for word[4] to show that for any set of energies $E_2(j)$

$$\begin{aligned} Z^2_{\{E_2\}} &= (2\cosh\beta E_1)^{4\mathcal{M}\mathcal{N}} \prod_{j=1}^{\mathcal{M}-1} [\cosh\beta E_2(j)]^{4\mathcal{N}} \\ &\quad \times \prod_{\theta} |1 + z_1 e^{i\theta}|^{2\mathcal{M}} \det C_{\{E_2\}}(\theta), \end{aligned} \tag{2.3}$$

where $\prod_\theta$ is the product over

$$\theta = \pi(2n-1)/2\mathcal{N}, \qquad n = 1, 2, \ldots, 2\mathcal{N}, \tag{2.4}$$

$$z_1 = \tanh\beta E_1, \tag{2.5a}$$

$$z_2(j) = \tanh\beta E_2(j), \tag{2.5b}$$

and $\beta = 1/kT$. The $2\mathcal{M} \times 2\mathcal{M}$ matrix $C_{\{E_2\}}(\theta)$ is defined by

$$C_{j,j} = \begin{bmatrix} ia & b \\ -b & -ia \end{bmatrix}, \tag{2.6a}$$

$$C_{j,j+1} = -C^T_{j+1,j} = \begin{bmatrix} 0 & 0 \\ z_2(j) & 0 \end{bmatrix} \tag{2.6b}$$

(compare with (VI.3.9)) and all other matrix elements are zero. Here we use

$$a(\theta) = -2z_1 \sin\theta |1 + z_1 e^{i\theta}|^{-2}, \tag{2.7a}$$

$$b(\theta) = (1 - z_1^2)|1 + z_1 e^{i\theta}|^{-2}. \tag{2.7b}$$

4. The notation of Chapter VI has been slightly modified to make the reality properties of our equations manifest. In particular, $\mathfrak{a} = -ia$, $\mathfrak{D}_n = iD_n$, $\mathfrak{c} = -ic$, $\bar{\mathfrak{D}}_n = i\bar{D}_n$, while $\mathfrak{C}_n = C_n$ and $\mathfrak{b} = b$.

More explicitly, $C_{(E_2)}(\theta)$ may be written as

$$\begin{bmatrix} ia & b & & & & & & & \\ -b & -ia & z_2(1) & & & & & & \\ & -z_2(1) & ia & b & & & & & \\ & & -b & -ia & z_2(2) & & & & \\ & & & -z_2(2) & & & & & \\ & & & & \ddots & & & & \\ & & & & & & z_2(\mathcal{M}-1) & & \\ & & & & & -z_2(\mathcal{M}-1) & ia & b \\ & & & & & & -b & -ia \end{bmatrix}. \tag{2.8}$$

We may further follow the procedure of Chapter VI and define C_n to be the determinant of the $2n \times 2n$ random matrix of the form (2.8) and iD_n to be the corresponding $(2n-1) \times (2n-1)$ random determinant with the last row and column removed. Then $\det C_{(E_2)}(\theta) = C_{\mathcal{M}}(\theta)$ and we obtain the recursion relation for $n \geq 0$,

$$\begin{bmatrix} C_{n+1}(\theta) \\ D_{n+1}(\theta) \end{bmatrix} = \begin{bmatrix} a^2 + b^2 & a \\ a & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & z_2(n)^2 \end{bmatrix} \begin{bmatrix} C_n(\theta) \\ D_n(\theta) \end{bmatrix}, \tag{2.9}$$

together with the boundary condition

$$C_0(\theta) = 1, \qquad D_0(\theta) = 0, \tag{2.10}$$

where $z_2(0) = 0$ by definition.

Therefore the free energy F_r is given as

$$F_r = -\frac{1}{\beta}\Big[\ln(2\cosh\beta E_1) + \int_0^\infty dE_2 P(E_2) \ln\cosh\beta E_2 + \frac{1}{4\pi}\int_{-\pi}^{\pi} d\theta \ln|1 + z_1 e^{i\theta}|^2 + \frac{1}{4\pi}\int_{-\pi}^{\pi} d\theta \lim_{\mathcal{M}\to\infty} \mathcal{M}^{-1} \ln C_{\mathcal{M}}(\theta)\Big]. \tag{2.11}$$

The object $C_n(\theta)$ is the first component of the vector we obtain by applying n random matrices of the form

$$\begin{bmatrix} a^2 + b^2 & a\lambda \\ a & \lambda \end{bmatrix} \tag{2.12}$$

to the initial vector $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$. Here $\lambda \equiv z_2^2$ is a random variable with the normalized probability distribution function $\mu(\lambda)$ given by

$$\mu(\lambda)\, d\lambda = P(E_2)\, dE_2. \tag{2.13}$$

The general theory of such random matrix products, in particular the existence with probability 1 of the limit of the right-hand side of (2.11), has been presented in a rigorous manner by Furstenberg.[5]

We begin our evaluation of (2.11) by noting that

$$\lim_{\mathscr{M}\to\infty} \mathscr{M}^{-1} \ln C_{\mathscr{M}}(\theta) = \lim_{\mathscr{M}\to\infty} \mathscr{M}^{-1} \sum_{n=0}^{\mathscr{M}-1} \ln \frac{C_{n+1}}{C_n}. \tag{2.14}$$

By means of the recursion relation (2.9) this may be rewritten as

$$\lim_{\mathscr{M}\to\infty} \mathscr{M}^{-1} \sum_{n=0}^{\mathscr{M}-1} \ln \frac{C_{n+1}}{C_n} = \lim_{\mathscr{M}\to\infty} \mathscr{M}^{-1} \sum_{n=0}^{\mathscr{M}-1} \ln \left[a^2 + b^2 + a\lambda(n)\frac{D_n}{C_n}\right]. \tag{2.15}$$

This can be interpreted as an average over n. The only drawback is that, whereas the $\lambda(n)$ are independent random variables, the D_n/C_n are not at all independent. We now remark that, because the matrix (2.12) is real and acts on a two-dimensional vector space,

$$x_n = C_n/D_n \tag{2.16}$$

may be thought of as the tangent of the angle which the vector $\begin{bmatrix} C_n \\ D_n \end{bmatrix}$ makes with the D-axis. From (2.9) we find

$$x_{n+1} = \frac{(a^2 + b^2)x_n + a\lambda(n)}{ax_n + \lambda(n)}. \tag{2.17}$$

Because the space of angular dependence of these vectors is compact, as n becomes large the variable x_n will approach a limiting stationary distribution $\nu(x)$ that is independent of the initial vector.[5] This stationary distribution is characterized by the property that, if we apply a random matrix (2.12) to it and average the resulting distribution over $\mu(\lambda)$ of (2.13), $\nu(x)$ will transform into itself. Therefore $\nu(x)$ satisfies the equation

$$\nu(x) = \int_{-\infty}^{\infty} dx' \int_0^1 d\lambda \delta\left[x - \frac{(a^2 + b^2)x' + a\lambda}{ax' + \lambda}\right]\mu(\lambda)\nu(x'). \tag{2.18}$$

We may perform the λ integration to obtain

$$\nu(x) = \frac{b^2}{(x-a)^2} \int_{-\infty}^{\infty} dx' |x'| \mu\left(x' \frac{a^2 + b^2 - ax}{x - a}\right)\nu(x'). \tag{2.19}$$

The work of Furstenberg[5] guarantees that a solution to this equation exists and that if $\mu(\lambda)$ is not $\delta(\lambda - \bar{\lambda})$ this solution is unique.

Once we possess a stationary distribution $\nu(x)$ we may replace the average over n in (2.15) by an average over λ and over x. We thus arrive

5. H. Furstenberg, *Trans. Am. Math. Soc.* **108**, 377 (1963).

at the final result that with probability 1

$$\lim_{\mathcal{M}\to\infty} \mathcal{M}^{-1} \ln C_{\mathcal{M}}(\theta) = \int_{-\infty}^{\infty} dx\nu(x) \int_0^1 d\lambda\mu(\lambda) \ln (a^2 + b^2 + a\lambda/x). \tag{2.20}$$

An identical analysis may be carried out for the quantity $D_{\mathcal{M}}$ and we find that with probability 1

$$\lim_{\mathcal{M}\to\infty} \mathcal{M}^{-1} \ln D_{\mathcal{M}}(\theta) = \int_{-\infty}^{\infty} dx\nu(x) \int_0^1 d\lambda\mu(\lambda) \ln (\lambda + ax). \tag{2.21}$$

Since $C_{\mathcal{M}}$ and $D_{\mathcal{M}}$ are the components of the same vector, their average rate of growth must each be separately equal to the average rate of growth of the vector itself. Therefore the right-hand sides of (2.20) and (2.21) must be equal, so that

$$\int_{-\infty}^{\infty} dx\nu(x) \int_0^1 d\lambda\mu(\lambda) \ln (a^2 + b^2 + a\lambda/x)$$
$$= \int_{-\infty}^{\infty} dx\nu(x) \int_0^1 d\lambda\mu(\lambda) \ln (\lambda + ax). \tag{2.22}$$

To prove this directly, consider the difference d between the two sides of (2.22):

$$d = \int_{-\infty}^{\infty} dx\nu(x) \int_0^1 d\lambda\mu(\lambda) \ln \left(\frac{a^2 + b^2 + a\lambda/x}{\lambda + ax}\right). \tag{2.23}$$

This may be rewritten as

$$d = \int_{-\infty}^{\infty} dx\nu(x) \int_0^1 d\lambda\mu(\lambda) \ln \left(x \frac{a^2 + b^2 + a\lambda/x}{\lambda + ax}\right) - \int_{-\infty}^{\infty} dx\nu(x) \ln x. \tag{2.24}$$

In the first integral we replace the variable λ by

$$q = x \frac{a^2 + b^2 + a\lambda/x}{\lambda + ax} \tag{2.25}$$

to obtain

$$d = \int_{-\infty}^{\infty} dq \int_{-\infty}^{\infty} dx\mu\left(x \frac{a^2 + b^2 - qa}{q - a}\right) \frac{xb^2}{(q - a)^2} \nu(x) \ln q$$
$$- \int_{-\infty}^{\infty} dx\nu(x) \ln x. \tag{2.26}$$

We now use the integral equation (2.19) on the first term of (2.26) to find that, as expected, $d = 0$.

We may readily derive the expression for the critical temperature T_c in terms of $P(E_2)$ if we note that at $a = 0$ the matrix (2.12) is diagonal. The only possible stationary distributions of vectors are those with the vectors parallel to the C- or D-axis. In the first case the vectors are multiplied by $b^2(0)$ under the action of (2.12), so we find

$$\lim_{\theta\to 0}\lim_{\mathscr{M}\to\infty} \mathscr{M}^{-1}\ln C_{\mathscr{M}} = \ln b(0)^2, \tag{2.27}$$

and in the latter case the vectors are multiplied by λ, so that

$$\lim_{\theta\to 0}\lim_{\mathscr{M}\to\infty} \mathscr{M}^{-1}\ln D_{\mathscr{M}} = \int_0^1 d\lambda\mu(\lambda)\ln\lambda. \tag{2.28}$$

The free energy is related to the larger of these two expressions and the condition for $T = T_c$ is obtained by equating (2.27) and (2.28):

$$\begin{aligned} 0 &= \int_0^1 d\lambda\mu(\lambda)\ln\,[\lambda b(0)^{-2}] \\ &= \int_0^\infty dE_2P(E_2)\ln\left[z_2^2\left(\frac{1+z_1}{1-z_1}\right)^2\right] \end{aligned} \tag{2.29a}$$

or

$$2\beta E_1 + \int_0^\infty dE_2P(E_2)\ln z_2 = 0. \tag{2.29b}$$

If $P(E_2) = \delta(E_2 - E_2^0)$, then (2.29) reads

$$z_2^0\frac{1+z_1}{1-z_1} = 1, \tag{2.30}$$

which is the known result for $T = T_c$ in the ferromagnetic Onsager lattice. The correctness of this criterion for locating T_c will be seen more explicitly in Sec. 4, where we demonstrate for a specific $\mu(\lambda)$ that at the T_c given by (2.29) the free energy F_r is not an analytic function of the temperature.

We note that (2.29) has the property that T_c is zero if $P(E_2) = p\delta(E_2) + \cdots$, where $0 < p \le 1$. This is to be expected for our model. A delta function at $E_2 = 0$ means that in every random lattice there are, with probability 1, vertical bonds with zero strength a finite distance apart. But for our class of lattices the condition $E_2(j) = 0$ cuts the lattice into two separate pieces. Therefore the term $p\delta(E_2)$ causes the lattice, with probability 1, to be cut up into an infinite number of strips of finite width, and any two-dimensional Ising lattice that is not infinite in both dimensions has no critical temperature. However, we also note that if $\mu(\lambda)$ is bounded near $E_2 = 0$ and $E_1 > 0$, then T_c is greater than zero.

Finally we remark that the argument leading to (2.29a) does not depend on the fact that E_2 rather than E_1 is random. We therefore see by a similar argument that if E_1 and E_2 are random with the joint probability density $P(E_1, E_2)$ there is a ferromagnetic phase transition at T_c determined from

$$\int_0^\infty dE_1 \int_0^\infty dE_2 P(E_1, E_2) \ln \left(\frac{1}{z_2}\frac{1-z_1}{1+z_1}\right) = 0. \tag{2.31}$$

3. INTEGRAL EQUATION FOR $\nu(x)$

In this section we study several general properties of the integral equation (2.19). The limits of (2.19) have formally been written as $-\infty$ to $+\infty$, but over much of this range $\nu(x)$ vanishes identically. To see this, first consider the stationary distribution corresponding to the Onsager lattice where

$$\mu(\lambda) = \delta(\lambda - \bar{\lambda}). \tag{3.1}$$

The stationary angular distribution of vectors will clearly be a delta function at that value of x which is unchanged by the application of the matrix (2.12) with $\lambda = \bar{\lambda}$. From (2.17) we see that the values of x which satisfy this eigenvector equation obey

$$x_0(\bar{\lambda}) = \frac{(a^2 + b^2)x_0(\bar{\lambda}) + a\bar{\lambda}}{ax_0(\bar{\lambda}) + \bar{\lambda}}, \tag{3.2a}$$

which is also usefully expressed as

$$\bar{\lambda} = x_0(\bar{\lambda})\,\frac{a^2 + b^2 - ax_0(\bar{\lambda})}{x_0(\bar{\lambda}) - a}. \tag{3.2b}$$

There are two solutions to (3.2) because the matrix (2.12) has two eigenvalues. To obtain the correct free energy we must choose that solution which has the larger eigenvalue. It may easily be seen from (2.12) or from (2.20) and (2.21) that the correct solution of (3.2) is

$$x_0(\bar{\lambda}) = (1/2a)\{a^2 + b^2 - \bar{\lambda} + [(a^2 + b^2 - \bar{\lambda})^2 + 4\bar{\lambda}a^2]^{1/2}\}, \tag{3.3a}$$

with

$$x_0(\bar{\lambda})^{-1} = (1/2a\bar{\lambda})\{-(a^2 + b^2 - \bar{\lambda}) + [(a^2 + b^2 - \bar{\lambda})^2 + 4\bar{\lambda}a^2]^{1/2}\}. \tag{3.3b}$$

If we use (3.1) and (3.3) in (2.21) we find that the free energy for Onsager's lattice is

$$\begin{aligned} -\beta F_0 &= \ln(2\cosh\beta E_1 \cosh\beta E_2) \\ &\quad + \frac{1}{4\pi}\int_{-\pi}^{\pi} d\theta \ln [\tfrac{1}{2}|1 + z_1 e^{i\theta}|^2\{a^2 + b^2 + \bar{z}_2^2 \\ &\quad + [(a^2 + b^2 - \bar{z}_2^2)^2 + 4a^2\bar{z}_2^2]^{1/2}\}], \end{aligned} \tag{3.4}$$

which agrees with (V.3.6).

From (3.3) we see that the eigenvector of the matrix (2.12) with the larger eigenvalue always lies in the range

$$ax_0(1) < ax < ax_0(0) = a^2 + b^2. \tag{3.5}$$

Consider any vector not in this range. Pick any matrix of the form (2.12) with $\bar{\lambda}$ not equal to 0 or 1 such that the eigenvector with the smaller eigenvalue does not lie in the direction of this vector. If we apply this matrix to the vector sufficiently many times, the resultant vector will lie inside (3.5). But this is true not only if all the matrices correspond to $\bar{\lambda}$ but also if the matrices correspond to λ's lying in some neighborhood of $\bar{\lambda}$. Therefore there is a nonzero probability that after the application of (2.12) a finite number of times on a given vector the resultant vector will lie in the range (3.5). Furthermore, it is clear from (2.17) and (3.2) that if x_n satisfies (3.5) then x_{n+1} does also. Therefore we conclude that no

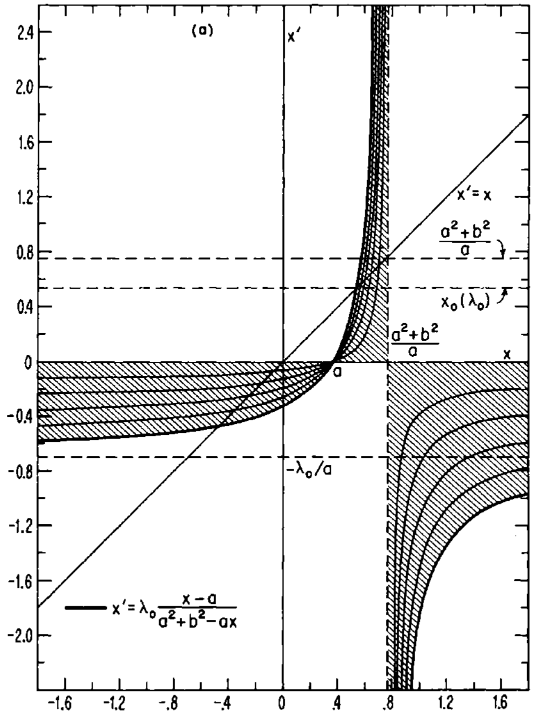


Fig. 14.1. (*a*) Contours along which the function $\mu[x'(a^2 + b^2 - ax)/(x - a)]$ is constant. The kernel of the integral equation for $\nu(x)$ is different from zero only in the shaded region.

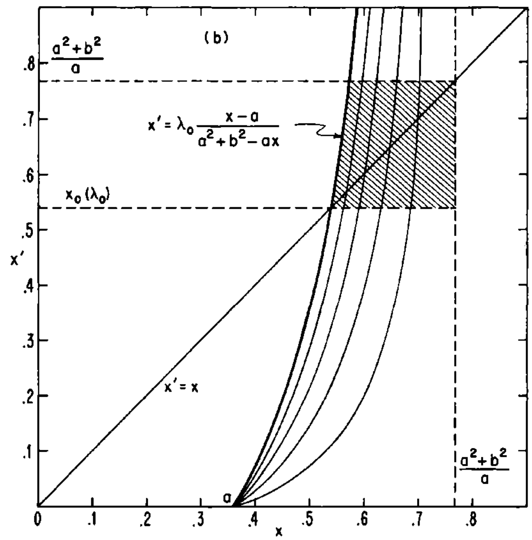


Fig. 14.1. (*b*) Enlargement of (*a*). The shaded region is the only region in which the kernel of the integral equation does not vanish and $\nu(x)$ and $\nu(x')$ are different from zero. In both figures we have, for definiteness, considered the case $x_0' = 0$.

distribution of vectors that does not vanish outside the range $ax_0(1) < ax < (a^2 + b^2)$ can be stationary.

In fact the same argument shows that, if

$$\mu(\lambda) \equiv 0 \quad \text{unless} \quad \lambda_0' \le \lambda \le \lambda_0, \tag{3.6}$$

then

$$\nu(x) \equiv 0 \quad \text{unless} \quad ax_0(\lambda_0) < ax < ax_0(\lambda_0'). \tag{3.7}$$

To see what restriction (3.7) puts on the limits of integration in (2.19), it is convenient to plot in Fig. 14.1, for $a > 0$, (1) the region in the x-x'-plane where the kernel of (2.19) is not zero; (2) the contours along which $\mu[x'(a^2 + b^2 - ax)/(x - a)]$ is constant; and (3) the region where $\nu(x)$ and $\nu(x')$ are different from zero. We then readily see that (2.19) may be more explicitly written (when $a > 0$) as

$$\nu(x) = \frac{b^2}{(x-a)^2} \int_{\max[x_0(\lambda_0), \lambda_0'\Phi(x)]}^{\min[\lambda_0\Phi(x), x_0(\lambda_0')]} dx' x' \nu(x') \mu\left(x' \frac{a^2 + b^2 - ax}{x - a}\right) \tag{3.8}$$

for $x_0(\lambda_0) < x < x_0(\lambda_0')$ and $\nu(x) \equiv 0$ otherwise, where

$$\Phi(x) = \frac{x - a}{a^2 + b^2 - ax}.$$

If $a < 0$, we clearly have

$$\nu(x, a) = \nu(-x, -a). \tag{3.9}$$

In the sequel we concentrate on the special case $\lambda_0' = 0$, where (3.8) specializes to

$$\nu(x) = \frac{b^2}{(x-a)^2}\int_{x_0(\lambda_0)}^{\min[\lambda_0\Phi(x),\,x_0(0)]} dx' x' \nu(x')\mu\left(x'\,\frac{a^2+b^2-ax}{x-a}\right), \tag{3.8a}$$

where $x_0(0) = (a^2 + b^2)/a$.

An important difference between the Onsager lattice and all random lattices may be seen from Fig. 14.1. If $\mu(\lambda) = \delta(\lambda - \bar{\lambda})$, then, as we have seen earlier, $\nu(x)$ is given by a delta function at that value of x that lies within the interval (3.5) where the curve $x' = \bar{\lambda}(x - a)/(a^2 + b^2 - ax)$ intersects the line $x = x'$. This intersection is at the point $x_0(\bar{\lambda})$ given by (3.3). There are three distinct cases:

(*a*) if $b(0)^2 > \bar{\lambda}(T > T_c)$ then as $\theta \to 0$

$$x_0(\bar{\lambda}) \sim [b(0)^2 - \bar{\lambda}]/a; \tag{3.10a}$$

(*b*) if $b(0)^2 < \bar{\lambda}(T < T_c)$ then as $\theta \to 0$

$$x_0(\bar{\lambda}) \sim \bar{\lambda}a/[\bar{\lambda} - b(0)^2]; \tag{3.10b}$$

(*c*) if $b(0)^2 = \bar{\lambda}(T = T_c)$ then as $\theta \to 0$

$$x_0(\bar{\lambda}) \to \pm\bar{\lambda}^{1/2}. \tag{3.10c}$$

We see from (3.10) that a delta-function distribution of λ leads to a delta-function stationary distribution. In the limit $\theta \to 0$, the delta-function stationary distribution remains at a finite value of x if $T = T_c$ but moves to zero (or infinity) if T is less than (or greater than) T_c.

Contrast this case with the case of a very narrow $\mu(\lambda)$. As long as a is sufficiently far away from zero a narrow $\mu(\lambda)$ must give rise to a correspondingly narrow $\nu(x)$ because the projection on the x-axis of the region of the $x = x'$ line where the kernel of (3.8) is appreciably different from zero is small. However, if θ gets close enough to zero and T is such that $\mu(\lambda)$ is different from zero in the region (however small) where $\lambda \sim b(0)^2$, then the above-mentioned projection on the x-axis becomes enormous. This dramatic broadening of $\nu(x)$ when $T \sim T_c$ and $\theta \sim 0$ will be exploited in the next section to obtain the dominant contribution to the specific heat for the particular narrow distribution

$$\mu(\lambda) = N\lambda_0^{-N}\lambda^{N-1} \tag{3.11}$$

for $0 \le \lambda \le \lambda_0 = \tanh^2 \beta E_2^0$. If λ is outside this range, $\mu(\lambda) = 0$. The foregoing discussion, however, shows that there is nothing particular about this form of $\mu(\lambda)$, and we expect that the physical properties which

(3.11) leads to will be qualitatively the same for a wide class of narrow distributions.

Before studying the power-law distribution (3.11) in detail, we find it convenient to perform some manipulations on (3.8*a*) which are useful for any $\mu(\lambda)$ such that $\mu(\lambda) = 0$ if $\lambda > \lambda_0$. We first note that it is possible to change variables so that the upper limit of (3.8*a*) is transformed from a curve and a straight line into two straight lines. To do this let

$$\eta = \frac{x_0(x - x_0)}{\lambda_0 + x_0 x}, \tag{3.12}$$

where $x_0 \equiv x_0(\lambda_0)$. We also introduce

$$B^2 = \frac{\lambda_0(x_0 - a)}{x_0(\lambda_0 + ax_0)} = \frac{a^2 + b^2 + \lambda_0 - [(a^2 + b^2 - \lambda_0)^2 + 4a^2\lambda_0]^{1/2}}{a^2 + b^2 + \lambda_0 + [(a^2 + b^2 - \lambda_0)^2 + 4a^2\lambda_0]^{1/2}}, \tag{3.13}$$

so that

$$0 \le \eta \le B^2 \le 1. \tag{3.14}$$

Define

$$\nu(x) = X(\eta)\frac{d\eta}{dx} = X(\eta)\frac{(1 - \eta)^2 x_0}{\lambda_0 + x_0^2}, \tag{3.15}$$

so that

$$\int_0^{B^2} X(\eta)\,d\eta = 1. \tag{3.16}$$

Then (3.8*a*) may be rewritten as

$$X(\eta) = \frac{\lambda_0 B^2(\lambda_0 + x_0^2)}{(B^2 x_0^2 + \lambda_0\eta)^2}\int_0^{\min[B^2, \eta B^{-2}]} d\eta' X(\eta')$$
$$\times \frac{\eta'\lambda_0 + x_0^2}{1 - \eta'}\,\mu\left(\frac{\eta'\lambda_0 + x_0^2}{1 - \eta'}\,\frac{B^2 - \eta}{\lambda_0^{-1}B^2 x_0^2 + \eta}\right). \tag{3.17}$$

This equation may be cast into a somewhat simpler form when $\eta \le B^4$ if we define

$$Y(\eta) = \int_0^{\eta} X(\eta')\,d\eta' \tag{3.18}$$

and integrate (3.17) over η to obtain

$$Y(\eta) = \lambda_0 B^2(\lambda_0 + x_0^2)\int_0^{\eta} d\eta_1 \int_0^{\eta_1 B^{-2}} d\eta' X(\eta')$$
$$\times \frac{\eta'\lambda_0 + x_0^2}{(1 - \eta')(B^2 x_0^2 + \lambda_0\eta_1)^2}\,\mu\left(\frac{\eta'\lambda_0 + x_0}{1 - \eta'}\,\frac{B^2 - \eta_1}{\lambda_0^{-1}B^2 x_0^2 + \eta_1}\right). \tag{3.19}$$

Furthermore make the change of variable from η_1 to ζ, defined by

$$\zeta = \frac{\eta'\lambda_0 + x_0^2}{1 - \eta'} \frac{B^2 - \eta_1}{\lambda_0^{-1}B^2x_0^2 + \eta_1}, \tag{3.20}$$

and interchange the order of integration to obtain

$$\begin{aligned} Y(\eta) &= \int_0^{\eta B^{-2}} d\eta' X(\eta') \int_{\zeta(\eta)}^1 d\zeta \mu(\zeta) \\ &= Y(\eta B^{-2}) - \int_0^{\eta B^{-2}} d\eta' X(\eta') \int_0^{\zeta(\eta)} d\zeta \mu(\zeta), \end{aligned} \tag{3.21}$$

where

$$\zeta(\eta) = \frac{\lambda_0\eta' + x_0^2}{1 - \eta'} \frac{B^2 - \eta}{\lambda_0^{-1}B^2x_0^2 + \eta}.$$

Using the definition of Y, we may rewrite this as

$$\int_\eta^{\eta B^{-2}} d\eta' X(\eta') = \int_0^{\eta B^{-2}} d\eta' X(\eta') \int_0^{\zeta(\eta)} d\zeta \mu(\zeta). \tag{3.22}$$

It remains only to write out the special case (3.11). We evaluate the ζ integral in (3.22) and obtain

$$\begin{aligned} \int_\eta^{\eta B^{-2}} d\eta' X(\eta') = \int_0^{\eta B^{-2}} d\eta' X(\eta') N^{-1}\left(\frac{\lambda_0\eta' + x_0^2}{1 - \eta'} \frac{B^2 - \eta}{\lambda_0^{-1}B^2x_0^2 + \eta}\right) \\ \times \mu\left(\frac{\lambda_0\eta' + x_0^2}{1 - \eta'} \frac{B^2 - \eta}{\lambda_0^{-1}B^2x_0^2 + \eta}\right). \end{aligned} \tag{3.23}$$

The right-hand side of this equation may be further simplified using the original integral equation (3.17) and we obtain

$$\int_\eta^{\eta B^{-2}} d\eta' X(\eta') = \frac{(B^2 - \eta)(B^2x_0^2 + \eta\lambda_0)}{NB^2(\lambda_0 + x_0^2)} X(\eta). \tag{3.24}$$

Finally, it is useful to make the exponential change of variable

$$\eta = e^{-\tau}, \tag{3.25}$$

where $-\ln B^2 < \tau < \infty$. Call

$$U(\tau) = \eta X(\eta) \tag{3.26}$$

so that

$$\int_{-\ln B^2}^{\infty} d\tau U(\tau) = 1. \tag{3.27}$$

Then we obtain

$$\int_\tau^{\tau + \ln B^2} d\tau' U(\tau') = -\frac{(B^2 - e^{-\tau})(B^2x_0^2 + \lambda_0 e^{-\tau})}{NB^2(\lambda_0 + x_0^2)} e^{\tau} U(\tau). \tag{3.28}$$

4. POWER-LAW DISTRIBUTION

In this section we determine the dominant contribution to the specific heat of the lattice characterized by the power-law distribution (3.11). We consider only the case of large N and ignore all contributions to the specific heat which vanish as $N \to \infty$. Then the discussion of Sec. 3 shows that when a is away from zero $\nu(x)$ is given by a narrow distribution which will differ but little from the $\nu(x)$ of an Onsager problem. We are not interested in these small deviations and concentrate our attention on the opposite extreme, when a is close to zero. From (2.29a) we find that $T = T_c$ if

$$\ln [b(0)^2\lambda_0^{-1}] = \ln B^2(0) = -N^{-1}. \tag{4.1}$$

When B^2 is close to this value and $a \sim 0$, the discussion of Sec. 3 shows that $\nu(x)$ is very broad. Therefore when x is of order 1, $\nu(x)$, and hence $U(\tau)$, may be treated as slowly varying. Furthermore, (4.1) shows that the region of integration of (3.28) is of the order of N^{-1}. Hence to leading order in N^{-1} we may expand

$$U(\tau') \sim U(\tau) + (\tau' - \tau)U'(\tau) \tag{4.2}$$

and carry out the integration in (3.28) to obtain the approximate differential equation

$$\tfrac{1}{2}(\ln B^2)^2 \frac{d}{d\tau} U(\tau) + U(\tau) \ln B^2 = \frac{-(B^2 - e^{-\tau})(B^2 x_0^2 e^{\tau} + \lambda_0)}{NB^2(\lambda_0 + x_0^2)} U(\tau). \tag{4.3}$$

This is readily solved and we find

$$U(\tau) = C_N(B^2, x_0) \exp \{s\tau - te^{-\tau} - ue^{\tau}\} \tag{4.4}$$

where, by (3.3),

$$\begin{aligned} s &= 2(\ln B^2)^{-2}[-\ln B^2 - N^{-1}(\lambda_0 x_0^{-1} - x_0)/(\lambda_0 x_0^{-1} + x_0)] \\ &= 2(\ln B^2)^{-2}\{-\ln B^2 + N^{-1}(a^2 + b^2 - \lambda_0) \\ &\quad \times [(a^2 + b^2 - \lambda_0)^2 + 4\lambda_0 a^2]^{-1/2}\}, \end{aligned} \tag{4.5a}$$

$$\begin{aligned} t &= 2(\ln B^2)^{-2} N^{-1} B^{-2} \lambda_0 x_0^{-1}(\lambda_0 x_0^{-1} + x_0)^{-1} \\ &= (\ln B^2)^{-2} N^{-1} B^{-2}\{1 - (a^2 + b^2 - \lambda_0) \\ &\quad \times [(a^2 + b^2 - \lambda_0)^2 + 4\lambda_0 a^2]^{-1/2}\}, \end{aligned} \tag{4.5b}$$

$$\begin{aligned} u &= 2(\ln B^2)^{-2} N^{-1} B^2 x_0(\lambda_0 x_0^{-1} + x_0)^{-1} \\ &= (\ln B^2)^{-2} N^{-1} B^2\{1 + (a^2 + b^2 - \lambda_0) \\ &\quad \times [(a^2 + b^2 - \lambda_0)^2 + 4\lambda_0 a^2]^{-1/2}\}, \end{aligned} \tag{4.5c}$$

and $C_N(B^2, x_0)$ is an appropriate normalization constant. Therefore when $T \sim T_c$ and $\theta \sim 0$ we obtain

$$X(\eta) \sim C_N(B^2, x_0^2)\eta^{-s-1}e^{-t\eta - u/\eta}. \tag{4.6}$$

This approximation to $X(\eta)$ forms the basis of all further considerations of this section.

To give insight into the structure of $X(\eta)$ we first remark that as $N \to \infty$ the power-law distribution (3.11) approaches $\delta(\lambda - \lambda_0)$. Therefore when $T \neq T_c$ and $\theta \neq 0$ we find that the exact $\nu(x)$ must approach $\delta(x - x_0)$ as $N \to \infty$, and hence $X(\eta)$ must approach $\delta(\eta)$. Our approximation to $X(\eta)$ was derived under the assumption that $T - T_c$ and θ were small and hence it is not obvious that (4.6) will approach $\delta(\eta)$ as $N \to \infty$. To see that this is in fact the case we note that the maximum of $\eta X(\eta)$ is reached at

$$\eta_m = (1/2t)[-s + (s^2 + 4tu)^{1/2}] \tag{4.7a}$$

and its width (in the sense of a steepest-descent integral) is

$$\begin{aligned} w_\eta &= \left[\frac{\partial^2}{\partial\eta^2}\left(s \ln \eta + t\eta + \frac{u}{\eta}\right)\right]^{-1/2}\Bigg|_{\eta=\eta_m} \\ &= \frac{\eta_m^{3/2}}{(2u - s\eta_m)^{1/2}}. \end{aligned} \tag{4.7b}$$

If $T \neq T_c$ and $\theta \neq 0$ are fixed and $N \to \infty$, $s = -2(\ln B^2)^{-1} + O(N^{-1})$, $t = O(N^{-1})$, and $u = O(N^{-1})$ so that $\eta_m = O(N^{-1})$ and $w_\eta = O(N^{-1})$. Therefore $X(\eta) \to \delta(\eta - \eta_m)$ in the sense that in evaluating the normalization integral of $X(\eta)$ we may replace $X(\eta)$ by $\delta(\eta - \eta_m)$.

We are interested in the contributions of order 1 to the specific heat when N is large. This is found by using our approximation for $X(\eta)$ in the integral (2.20), which in terms of η is

$$\lim_{\mathcal{M}\to\infty} \mathcal{M}^{-1} \ln C_{\mathcal{M}}(\theta) = \int_0^{B^2} d\eta X(\eta) \int_0^1 d\lambda \mu(\lambda) \ln\left[a^2 + b^2 + \frac{a\lambda(1 - \eta)}{\eta\lambda_0/x_0 + x_0}\right]. \tag{4.8}$$

Define $f(\eta)$ by

$$\begin{aligned} f(\eta) &= \ln\left[a^2 + b^2 + \frac{a\lambda(1 - \eta)}{n\lambda_0/x_0 + x_0}\right] \\ &= \ln\left\{a^2 + b^2 + 2a^2\lambda\left[(a^2 + b^2 - \lambda_0)\right.\right. \\ &\quad \left.\left. + \frac{1 + \eta}{1 - \eta}[(a^2 + b^2 - \lambda_0)^2 + 4\lambda_0 a^2]^{1/2}\right]^{-1}\right\}. \end{aligned} \tag{4.9}$$

When $T \neq T_c$ and $\theta \neq 0$ are fixed and $N \to \infty$, we see that if $\eta = O(N^{-1})$

$$f(\eta) = \ln[a^2 + b^2 + a\lambda/x_0] + O(N^{-1}).$$

Therefore our approximation $X(\eta)$ may be replaced by $\delta(\eta - \eta_m)$ for the purpose of obtaining the leading-order term of (4.8). This is the behavior expected of the exact $X(\eta)$ in this limit, so we conclude that approximation (4.6) may be used for *all* T and θ for the purpose of obtaining the leading-order term in the specific heat when $N \to \infty$.

In fact, for our limited purpose, $X(\eta)$ is well approximated by $\delta(\eta - \eta_m)$ not only when $T \neq T_c$ and $\theta \neq 0$ are fixed and $N \to \infty$ but also when a is of the order of $N^{-\epsilon}$ and $b(0)^2 - \lambda_0$ is of the order of $N^{-\gamma}$, where $0 < \epsilon < 1$ and $0 < \gamma < 1$. There are three cases to be considered: (*a*) $\gamma > \epsilon$; (*b*) $\gamma < \epsilon$ and $b(0)^2 - \lambda_0 < 0$; (*c*) $\gamma < \epsilon$ and $b(0)^2 - \lambda_0 > 0$. We find

(*a*) $\eta_m = O(N^{-1+\epsilon})$, $w_\eta = O(N^{-1+\epsilon/2})$, $f(\eta) = \ln b^2 + O(N^{-\epsilon})$;

(*b*) $\eta_m = O(N^{-1-2\epsilon+3\gamma})$, $w_\eta = O(N^{-1-2\epsilon+5\gamma/2})$,

$f(\eta) = \ln b^2 + O(N^{-\gamma})$;

(*c*) $\eta_m = O(N^{-1+\gamma})$, $w_\eta = O(N^{-1+\gamma/2})$, $f(\eta) = \ln b^2 + O(N^{-2\epsilon+\gamma})$.

Since the variations in $f(\eta)$ caused by deviations in η of the order of w_η vanish as $N \to \infty$, we conclude that in these cases for our purpose $X(\eta)$ may be replaced by $\delta(\eta - \eta_m)$.

Because of the fact that even if $T \sim T_c$ the contribution of $\nu(x) - \delta(x - x_m)$ to the specific heat is very small for $|a| \gg N^{-1}$, it is useful to consider the contributions of $\delta(x - x_m)$ and $\nu(x) - \delta(x - x_m)$ separately. It is easily seen that x_m obeys

$$x_m^2 a[1 + b^{-2}G] - x_m[a^2 + b^2 - \lambda_0 + G(1 + 2a^2b^{-2})] \\ -\lambda_0 a[1 - G(a^2 + b^2)\lambda_0^{-1}b^{-2}] = 0, \tag{4.10a}$$

where

$$G = -N^{-1}(\ln B^2)^{-1}[(a^2 + b^2 - \lambda_0)^2 + 4a^2\lambda_0]^{1/2}. \tag{4.10b}$$

If we use $\delta(x - x_m)$ for $\nu(x)$ in (2.20) we find, correct to order N^{-1},

$$\begin{aligned} -\beta\bar{F}_r &= \int_0^\infty dE_2 P(E_2) \ln(2\cosh\beta E_1 \cosh\beta E_2) \\ &\quad + \frac{1}{4\pi}\int_{-\pi}^{\pi} d\theta \int_{-\infty}^{\infty} dx\,\delta(x - x_m) \int_0^1 d\lambda\,\mu(\lambda) \\ &\quad \times \ln\{|1 + z_1 e^{i\theta}|^2(a^2 + b^2 + a\lambda/x)\} \\ &\sim \ln(2\cosh\beta E_1 \cosh\beta E_2^0) \\ &\quad + \frac{1}{4\pi}\int_{-\pi}^{\pi} d\theta \ln\left\{\frac{|1 + z_1 e^{i\theta}|^2}{2[1 - G(a^2 + b^2)/\lambda_0 b^2]}\right. \\ &\quad \times \left(a^2 + b^2 + \lambda_0 - \frac{G}{\lambda_0 b^2}[2(a^2 + b^2)^2 + \lambda_0(b^2 + 2a^2)]\right) \\ &\quad + \left[\!\!\left[\left[a^2 + b^2 - \lambda_0 + G\left(1 + \frac{2a^2}{b^2}\right)\right]^2\right.\right. \\ &\quad \left.\left.\left. + 4a^2\lambda_0\left(1 + \frac{G}{b^2}\right)\left(1 - G\frac{a^2 + b^2}{\lambda_0 b^2}\right)\right]\!\!\right]^{1/2}\right\}. \end{aligned} \tag{4.11}$$

By comparing $\bar{F}_r$ with the Onsager free energy F_0 of (3.4) we conclude that, to order N^{-1}, $\bar{F}_r$ is the same as F_0 except that the critical temperature has been shifted from $b(0)^2 - \lambda_0 = 0$ to

$$b(0)^{-2} - \lambda_0 = -G(0) = -[b(0)^2 - \lambda_0]N^{-1}[\ln b(0)^2\lambda_0^{-1}]^{-1}, \tag{4.12}$$

which is exactly the same equation for T_c as (4.1). Therefore over the range of T in which $\nu(x)$ is well approximated by $\delta(x - x_m)$, F_r is dominated by a term which has an apparent logarithmic divergence at T_c.

To study the behavior very near T_c we write

$$F_r - \bar{F}_r \sim -\frac{1}{\beta 4\pi}\int_{-\pi}^{\pi} d\theta \int_{-\infty}^{\infty} dx[\nu(x) - \delta(x - x_m)] \ln (a^2 + b^2 + a\lambda_0/x), \tag{4.13}$$

where the λ integral has been evaluated to $O(N^{-1})$. We consider only T close enough to T_c that $b^2 - \lambda_0 < 0$. The $\sim$ sign is to mean that both sides lead to the same specific heat to order 1 as $N \to \infty$. Furthermore we have seen that unless $a^2 + b^2 - \lambda_0 = O(N^{-1})$ we cannot have a contribution of order 1 to (4.13). Therefore $ax_0^{-1} = O(N^{-1})$ and, since $|x_0| < |x|$, we may expand the logarithm of (4.13) to obtain

$$\begin{aligned} F_r - \bar{F}_r &\sim -\frac{1}{\beta 4\pi}\int_{-\pi}^{\pi} d\theta \int_{-\infty}^{\infty} dx[\nu(x) - \delta(x - x_m)] \frac{a\lambda_0}{(a^2 + b^2)x} \\ &= -\frac{1}{\beta\pi}\int_{-\pi}^{\pi} d\theta \frac{a^2\lambda_0}{a^2 + b^2}\int_0^{B^2} d\eta[X(\eta) - \delta(\eta - \eta_m)] \\ &\quad \times \left\{a^2 + b^2 - \lambda_0 + \frac{1+\eta}{1-\eta}[(a^2 + b^2 - \lambda_0)^2 + 4a^2\lambda_0]^{1/2}\right\}^{-1}. \end{aligned} \tag{4.14}$$

To evaluate this approximately to order 1 we need to find the correct range of θ, η, and $T - T_c$. We have previously considered the case $a \gg N^{-1}$ and $|b^2 - \lambda_0| \gg N^{-1}$ and seen via a steepest-descent integration that the contribution is negligible. In a similar fashion we may show that the cases (1) a is of order N^{-1}, (2) $a = o(N^{-1})$ and $s = o(N)$ give only contributions of order N^{-1} to the specific heat. The only region that gives a contribution of order 1 to the specific heat as $N \to \infty$ is $a = O(N^{-2})$ and $T - T_c = O(N^{-2})$.

When $T - T_c = O(N^{-2})$ and $a = O(N^{-2})$, $X(\eta)$ and $\delta(\eta - \eta_m)$ do not cancel at all so that F_r and $\bar{F}_r$ must be evaluated separately. Because $\bar{c}^r = -T\bar{F}_r''(T)$ is to leading order in N the same as Onsager's specific heat, we may use (V.3.119) to find

$$\begin{aligned} \bar{c}^r = \frac{4k\beta_c^2}{\pi}\Bigg\{&\frac{z_{1c}z_{2c}^0}{(1 - z_{1c})^2(1 - z_{2c}^0)^2}[E_1(1 - z_{1c}) + E_2^0(1 - z_{2c}^0)]^2 \\ &\times \left[\!\left[\ln\frac{T_c}{|T - T_c|} - \ln\frac{1}{8}\beta_c[E_1(z_{1c} + z_{1c}^{-1}) + E_2^0(z_{2c}^0 + z_{2c}^{0\,-1})]\right]\!\right] \\ &- \left[E_1^2\frac{4z_{1c}^2 z_{2c}^{02}}{(1 - z_{2c}^0)^4}\,\mathrm{gd}\,2\beta_c E_1 + 2E_1E_2^0 \right. \\ &\left. + E_2^{02}\frac{4z_{1c}^2 z_{2c}^{02}}{(1 - z_{1c})^4}\,\mathrm{gd}\,2\beta_c E_2^0\right]\Bigg\}, \end{aligned} \tag{4.15}$$

where gd stands for the gudermannian [gd $x = \tan^{-1}\sinh x$], the subscript c means $T = T_c$, and $z_{2c}^0 = \tanh \beta_c E_2^0$.

We evaluate c^r by splitting the θ integration into two regions, one for $0 < \theta \leq O(N^{-2})$ and the other for $\theta \gg N^{-2}$. In the second region the integrand of (4.14) is small. Therefore to leading order the parts of c^r and $\bar{c}^r$ coming from angular integration over this second region are equal. It is easily seen that the large angles give a contribution to c^r that is constant. The point of separation between the two regions is not well defined but, as will shortly be verified, the precise choice of this cut off does not affect the temperature-dependent part of c^r but only the constant. Therefore we may evaluate the leading contribution to c^r as $N \to \infty$ when $T - T_c = O(N^{-2})$ up to a constant by integrating θ only up to $O(N^{-2})$. We then may determine the constant by the requirement that, when $T - T_c \gg N^{-2}$, $c^r \sim \bar{c}^r$, where $\bar{c}^r$ is given by (4.15).

To carry out this evaluation explicitly, we define

$$\phi = -\frac{8}{\lambda_0^{1/2}} \frac{z_1}{(1 + z_1)^2} N^2 \theta, \tag{4.16}$$

so that

$$a = \tfrac{1}{4} N^{-2} \lambda_0^{1/2} \phi + O(N^{-4}). \tag{4.17}$$

We further define δ by

$$\frac{1}{\lambda_0}\left(\frac{1 - z_1}{1 + z_1}\right)^2 - \exp(-N^{-1}) = \tfrac{1}{2} N^{-2} \delta. \tag{4.18}$$

As $N \to \infty$, δ is to be of order 1. Explicitly,

$$\delta = (T - T_c) N^2 4k\beta_c^2 \frac{1 + z_{2c}^0}{z_{2c}^0} \{[E_1(1 - z_{1c}) + E_2^0(1 - z_{2c}^0)] + O(N^{-1})\}. \tag{4.19}$$

We then have

$$\begin{aligned} c^r &= -T \frac{\partial^2 F_r}{\partial T^2} \\ &\sim -k\beta_c^3 16 \left(\frac{1 + z_{2c}^0}{z_{2c}^0}\right)^2 [E_1(1 - z_{1c}) + E_2^0(1 - z_{2c}^0)]^2 N^4 \frac{\partial^2 F_r}{\partial \delta^2}. \end{aligned} \tag{4.20}$$

Furthermore

$$a^2 + b^2 - \lambda_0 = -\lambda_0 N^{-1}[1 - (2N)^{-1}(\delta + 1)] + O(N^{-3}) \tag{4.21}$$

and

$$\ln B^2 = -N^{-1}[1 - (2N)^{-1}\delta] + O(N^{-3}). \tag{4.22}$$

We then find

$$s = -\delta + O(N^{-1}), \tag{4.23a}$$

$$t = 2N + O(1), \tag{4.23b}$$

$$u = (8N)^{-1}\phi^2 + O(N^{-2}). \tag{4.23c}$$

Therefore

$$c^r \sim -\frac{k\beta_c^2}{8\pi}\frac{(1+z_{1c})^2(1+z_{2c}^0)^2}{z_{1c}z_{2c}^0}[E_1(1-z_{1c})+E_2^0(1-z_{2c}^0)]^2N^{-1}$$
$$\times \frac{\partial^2}{\partial\delta^2}\int_0^{N^2} d\phi\phi^2\int_0^1 d\eta\eta^{\delta-1}$$
$$\times \exp(-2N\eta-\phi^2/8N\eta)C_N(\phi,\delta)\left(1-\frac{1+\eta}{1-\eta}\right)^{-1}+\bar{K}, \tag{4.24}$$

where the coefficient of N^2 is arbitrary and $\bar{K}$ is determined by the requirement that as $\delta\to\infty$, $c^r\to\bar{c}^r$.

The normalization constant $C_N(\phi,\delta)$ is determined from the requirement that

$$1 = C_N\int_0^1 d\eta\eta^{\delta-1}\exp(-2N\eta-\phi^2/8N\eta). \tag{4.25}$$

Letting $\xi = 4N\phi^{-1}\eta$ we have

$$C_N^{-1} = (4N)^{-1}\phi\int_0^{4N\phi^{-1}} d\xi(\xi\phi/4N)^{\delta-1}\exp[-\tfrac{1}{2}\phi(\xi+1/\xi)]. \tag{4.26}$$

The upper limit may be extended to ∞ and we find

$$C_N^{-1}\sim 2(\phi/4N)^\delta K_\delta(\phi), \tag{4.27}$$

where we note that $K_\delta(\phi)$, the modified Bessel function of the third kind of order δ, has the representation

$$K_\delta(\phi) = \frac{1}{2}\int_0^\infty d\xi\exp\left[-\frac{1}{2}\phi(\xi+1/\xi)\right]\xi^{-\delta-1}. \tag{4.28}$$

Similarly, we find

$$\int_0^1 d\eta\eta^{\delta-1}\exp(-2N\eta-\phi^2/8N\eta)\left(1-\frac{1+\eta}{1-\eta}\right)^{-1}\sim -(\phi/4N)^{\delta-1}K_{\delta-1}(\phi). \tag{4.29}$$

If we also note that $(1-z_{1c}^2)(1-z_{2c}^{02}) = 4|z_{1c}|\,|z_{2c}^0| + O(N^{-1})$, we have

$$c^r\sim\frac{4k\beta_c^2}{\pi}\frac{z_{1c}z_{2c}^0}{(1-z_{1c})^2(1-z_{2c}^0)^2}[E_1(1-z_{1c})+E_2^0(1-z_{2c}^0)]^2$$
$$\times\frac{\partial^2}{\partial\delta^2}\int_0^{N^2} d\phi\,\frac{\phi K_{\delta-1}(\phi)}{K_\delta(\phi)}+\bar{K}. \tag{4.30}$$

As $\phi\to\infty$,[6]

$$\frac{K_{\delta-1}(\phi)}{K_\delta(\phi)}\to 1-\phi^{-1}(\delta-\tfrac{1}{2})+\tfrac{1}{2}\phi^{-2}(\delta^2-\tfrac{1}{4})+O(\phi^{-3}), \tag{4.31}$$

6. A. Erdelyi, ed., *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), vol. 2, p. 85.

so there is a term in (4.30) that behaves as $\ln N^2$ (where we remember that the coefficient of N^2 is arbitrary). We explicitly extract this term to write

$$\frac{\partial^2}{\partial\delta^2}\int_0^{N^2} d\phi\,\frac{\phi K_{\delta-1}(\phi)}{K_\delta(\phi)}$$
$$= \int_0^\infty d\phi\left[\phi\,\frac{\partial^2}{\partial\delta^2}\frac{K_{\delta-1}(\phi)}{K_\delta(\phi)} - \frac{1}{\phi+1}\right] + \ln N^2 + O(N^{-1}) \tag{4.32}$$

which, from the recursion relation[7]

$$K_{\delta-1}(\phi) = -\frac{\delta}{\phi}K_\delta(\phi) - \frac{d}{d\phi}K_\delta(\phi), \tag{4.33}$$

may be reexpressed as

$$\int_0^\infty d\phi\left[\frac{\partial^2}{\partial\delta^2}\ln K_\delta(\phi) - \frac{1}{\phi+1}\right] + \ln N^2 - 1 + O(N^{-1})$$
$$= R(\delta) + \ln N^2 - 1 + O(N^{-1}), \tag{4.34}$$

which defines the function $R(\delta)$.

For convenience we absorb the -1 term of (4.34) into $\bar{K}$ of (4.30) by defining

$$K = \bar{K} - \frac{4k\beta_c^2}{\pi}\frac{z_{1c}z_{2c}^0}{(1-z_{1c})^2(1-z_{2c}^0)^2}\,[E_1(1-z_{1c}) + E_2^0(1-z_{2c}^0)]^2. \tag{4.35}$$

To determine K we must expand (4.34) as $\delta\to\infty$. We use the expansion[8]

$$K_\delta(\phi) \sim (\pi/2)^{1/2}\frac{1}{(\delta^2+\phi^2)^{1/4}}\exp\left[-(\delta^2+\phi^2)^{1/2} + \delta\sinh^{-1}\frac{\delta}{\phi}\right]$$
$$\times\left\{1 + \left[-\frac{1}{8} + \frac{5}{24(1+\phi^2/\delta^2)}\right]\frac{1}{(\delta^2+\phi^2)^{1/2}}\right\} \tag{4.36}$$

to find that as $\delta\to\infty$

$$\int_0^\infty d\phi\left[\frac{\partial^2}{\partial\delta^2}\ln K_\delta(\phi) - \frac{1}{\phi+1}\right] + \ln N^2$$
$$= \ln 2 + \ln N^2\delta^{-1} - \tfrac{1}{8}\delta^{-2} + O(\delta^{-3}). \tag{4.37}$$

Therefore we find, as $\delta\to\infty$,

$$c^r(\delta) \to -\frac{4k\beta_c^2}{\pi}\frac{z_{1c}z_{2c}^0}{(1-z_{1c})^2(1-z_{2c}^0)^2}\,[E_1(1-z_{1c}) + E_2^0(1-z_{2c}^0)]^2$$
$$\times \ln\left\{2k\beta_c^2|T-T_c|\left(\frac{1}{z_{2c}^0}+1\right)[E_1(1-z_{1c}) + E_2^0(1-z_{2c}^0)]\right\} + K. \tag{4.38}$$

7. Reference 6, vol. 2, p. 79.
8. Reference 6, vol. 2, p. 26.

Comparing this with (4.15) gives

$$K = -\frac{4k\beta_c^2}{\pi}\left\{\frac{z_{1c}z_{2c}^0}{(1-z_{1c})^2(1-z_{2c}^0)^2}[E_1(1-z_{1c}) + E_2^0(1-z_{2c}^0)]^2 \right.$$
$$\times \left[\!\!\left[-\ln 2\beta_c\left(\frac{1}{z_{2c}^0}+1\right)[E_1(1-z_{1c}) + E_2^0(1-z_{2c}^0)] \right.\right.$$
$$\left.\left. + \ln \tfrac{1}{8}\beta_c\left[E_1\left(z_{1c}+\frac{1}{z_{1c}}\right) + E_2^0\left(z_{2c}^0 + \frac{1}{z_{2c}^0}\right)\right]\right]\!\!\right]$$
$$+ E_1^2\frac{4z_{1c}^2z_{2c}^{02}}{(1-z_{2c}^0)^4}\,\mathrm{gd}\, 2\beta_c E_1 + 2E_1E_2^0$$
$$\left. + E_2^{02}\frac{4z_{1c}^2z_{2c}^{02}}{(1-z_{1c})^4}\,\mathrm{gd}\, 2\beta_c E_2^0\right\}$$
$$= -\frac{4k\beta_c^2}{\pi}\{\tfrac{1}{2}[E_1^2\sinh 2\beta_c E_2^0 + 2E_1E_2^0 + E_2^{02}\sinh 2\beta_c E_1]$$
$$\times [\![\ln \tfrac{1}{4}\beta_c(E_1\coth 2\beta_c E_1 + E_2^0\coth 2\beta_c E_2^0)$$
$$- \ln 2\beta_c[(1+\coth\beta_c E_2^0)[E_1(1-\tanh\beta_c E_1)$$
$$+ E_2^0(1-\tanh\beta_c E_2^0)]]]\!]$$
$$+ E_1^2\sinh^2 2\beta_c E_2^0\,\mathrm{gd}\, 2\beta_c E_1 + 2E_1E_2^0$$
$$+ E_2^{02}\sinh^2 2\beta_c E_1\,\mathrm{gd}\, 2\beta_c E_2^0\}. \tag{4.39}$$

We therefore have as our final result that, when $T - T_c = O(N^{-2})$,

$$c^r \sim \frac{2k\beta_c^2}{\pi}[E_1^2\sinh 2\beta_c E_2^0 + 2E_1E_2^0 + E_2^{02}\sinh 2\beta_c E_1]$$
$$\times\left\{\int_0^\infty d\phi\left[\frac{\partial^2}{\partial\delta^2}\ln K_\delta(\phi) - \frac{1}{\phi+1}\right] + \ln N^2\right\} + K, \tag{4.40}$$

where δ is defined by (4.19) and K by (4.39). We note in particular that c^r is an even function of δ.

The specific heat (4.40) has been calculated for the random lattice characterized by $\mu(\lambda)$ given by (3.11). The corresponding probability density $P(E_2)$ is

$$P(E_2) = 2N(\tanh E_2^0\beta)^{-2N}\beta(1-\tanh^2\beta E_2)(\tanh\beta E_2)^{2N-1} \tag{4.41}$$

for $0 \le E_2 \le E_2^0$. This probability clearly depends on temperature. The probabilities envisioned in the original statement of the model were to be temperature independent. Fortunately, because the only significant deviation of c^r from $\bar{c}^r$ occurs when $T - T_c = O(N^{-2})$, we see that in the temperature range where (4.40) is valid

$$P(E_2) = \beta_c(1-\tanh^2\beta_c E_2)2N(\tanh E_2^0\beta_c)^{-2N}(\tanh\beta_c E_2)^{2N-1}[1+O(N^{-1})]. \tag{4.42}$$

Therefore $P(E_2)$ as given by (4.42) differs, when $T - T_c = O(N^{-2})$, from a temperature-independent probability by a term of $O(N^{-1})$, which is negligible.

To justify calling the temperature given by the solution of (4.1) the critical temperature we must show that c^r as given by (4.40) is not analytic at $\delta = 0$. For this purpose we integrate the integral in (4.40) by parts once and consider

$$\int_0^\infty d\phi\left[\frac{\partial^2}{\partial\delta^2}\frac{\phi K_\delta'(\phi)}{K_\delta(\phi)} + \frac{1}{\phi + 1}\right]. \tag{4.43}$$

When $\delta \to 0$ the singular behavior of this function comes from the region near $\phi = 0$. Thus we may obtain the most singular behavior of (4.43) if we integrate only from 0 to some small upper limit ϵ and expand for ϕ and δ near zero:

$$K_\delta(\phi) \sim (1/2\delta)[(\phi/2)^{-\delta} - (\phi/2)^\delta]. \tag{4.44}$$

Therefore we study

$$\int_0^\epsilon d\phi\delta\,\frac{\phi^{-\delta} + \phi^\delta}{\phi^{-\delta} - \phi^\delta} = \int_0^\epsilon d\phi\,\frac{2\delta}{1 - \phi^{2\delta}} - \delta\epsilon. \tag{4.45}$$

Now if $\epsilon < 1$, $\int_0^\epsilon d\phi/\ln\phi$ exists so the analytic properties of (4.43) are the same as

$$I(\delta) = \int_0^1 d\phi\left[\delta(1 - \phi^\delta)^{-1} + \frac{1}{\ln\phi}\right]. \tag{4.46}$$

We have been able to replace ϵ by 1 in (4.44) because the integrand is regular at $\phi = 1$. It is easily seen that $I(\delta) - I(-\delta) = \delta$, so we need consider only $\delta > 0$. Then if we let

$$\phi = e^{-\xi/\delta} \tag{4.47}$$

we find[9]

$$I(\delta) = \int_0^\infty d\xi e^{-\xi/\delta}\left(\frac{1}{1 - e^{-\xi}} - \frac{1}{\xi}\right) = \ln\delta - \psi(\delta^{-1}), \tag{4.48}$$

where $\psi(z) = \Gamma'(z)/\Gamma(z)$. For small δ we may use the asymptotic expansion[10] for $\psi(\delta^{-1})$ to obtain the formal power series valid for both positive and negative δ:

$$I(\delta) = \tfrac{1}{2}\delta + \sum_{n=1}^\infty B_{2n}\frac{\delta^{2n}}{2n}. \tag{4.49}$$

Here B_{2n} are the Bernoulli numbers defined by (XI.4.39). Therefore the most singular part of c^r is an *infinitely differentiable* function of T even

9. Reference 6, vol. 1, p. 18.
10. Reference 6, vol. 1, p. 47.

at T_c. However, from (XI.4.39) we see that as $n \to \infty$

$$(-1)^{n-1}B_{2n} = O[(2n)!\,(2\pi)^{-2n}]. \tag{4.50}$$

Thus (4.49) diverges for all $\delta \neq 0$ so c^r is *not* an analytic function of T at $T = T_c$. It is therefore correct to call T_c as determined from (4.1) the critical temperature.

Finally, it is useful to supplement these analytic considerations with a numerical evaluation of c^r when $T - T_c = O(N^{-2})$. We present the results in Figs. 14.2 and 14.3.

5. DISCUSSION

The principal result of this chapter is to exhibit an Ising model with random impurities where, to order 1, the specific heat is an infinitely differentiable function of the temperature even at T_c. This smooth behavior of c^r is in beautiful qualitative agreement with precise measurements near the Curie (or Néal) temperature T_c which have been made, for example, on EuS, $NiRbMnF_3$, and dysprosium aluminum garnet.[11] In other ferromagnetic (and antiferromagnetic) materials, c appears to diverge at some temperature T_c if measurements are made for $|T - T_c| \gtrsim 10^{-3}$. However, if T is sufficiently close to T_c, the specific heats deviate drastically from a diverging function (or even a function with an infinite first derivative at T_c) and are observed to be quite smooth at T_c. Although there is yet no conclusive evidence that this "smoothing out" of the diverging specific heat is due to random impurities and not to long-range forces or finite volume effects, we feel justified in proposing that random impurities can be the origin of these effects. In fact, the specific heat computed in this chapter is of the form

$$c_1[R(\delta) + c_2 - \ln w^2], \tag{5.1}$$

where

$$\delta = -(1 - T/T_c)/w^2. \tag{5.2}$$

If we choose $c_1 = 4.13$ J/mole deg, $c_2 = -1.30$, and $w = 2.68 \times 10^{-2}$, we find (Fig. 14.4) that some of these experimental data are in beautiful quantitative agreement with (5.1).

On the other hand, this particular model of random impurities is obviously artificial. It is not realistic to assume that all vertical bonds $E_2(j)$ in a given row will be equal if we are allowing $E_2(j)$ to vary from row to row. A realistic model of random impurities should not have such

11. See B. J. C. van der Hoeven, D. T. Teaney and V. L. Moruzzi, *Phys. Rev. Letters* **20**, 719 (1968) for EuS, see D. Teaney, V. Moruzzi and B. Argyle, *J. Appl. Phys.* **37**, 1122 (1966) for $NiRbMnF_3$, and see B. Keen, D. Landau and W. Wolf, *J. Appl. Phys.* **38**, 967 (1967) for dysprosium aluminum garnet.

RANDOM ISING MODEL: SPECIFIC HEAT

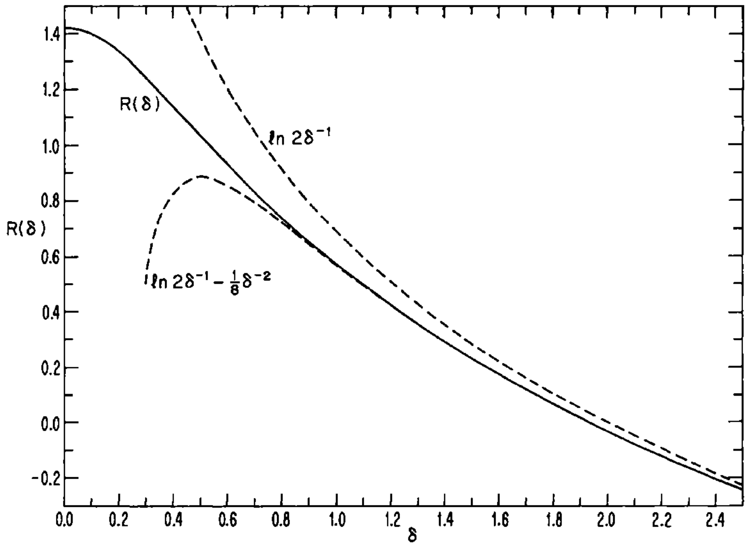


Fig. 14.2. The integral $R(\delta)$ as a function of δ.

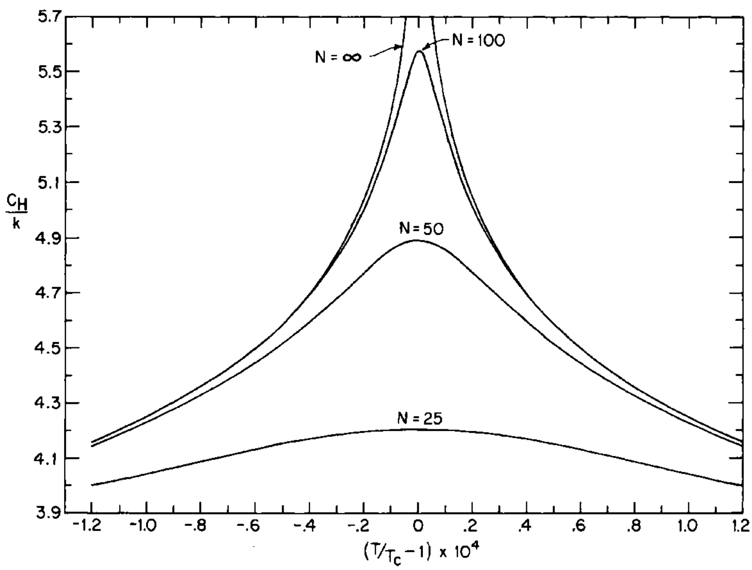


Fig. 14.3. Comparison of c of the pure Onsager lattice and c^r for several values of N for the case $E_1/k = E_2/k = 1$.

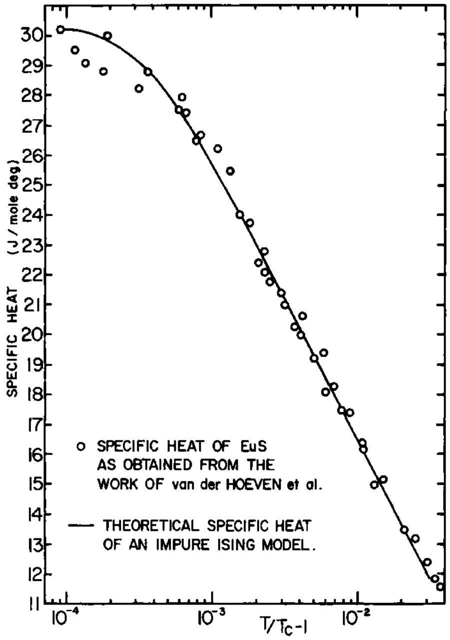


Fig. 14.4. Comparison of the impure Ising model specific heat with the observed specific heat of EuS for $T > T_c$.

a large amount of correlation between the random bonds. For this reason, we are extremely fortunate that the specific heat found in Sec. 4 is infinitely differentiable. If random impurities had increased the observed order of the phase transition to a higher but finite order, the question could very reasonably be asked whether relaxation of this very stringent correlation requirement would further increase the observed order. However, even the limited amount of randomness allowed in this model has made the dominant contribution to all derivatives of the specific heat continuous, so no further increase of the observed order is possible.

We are unable to ascertain which of the results of this chapter are qualitatively dependent on the very special sort of randomness allowed in our model. For example, we find that if the impurities have a narrow width of order N^{-1}, there is an effect of order 1 on the specific heat only when $|T - T_c| = O(N^{-2})$. We do not know whether this order of magnitude persists in general.

It must be emphasized that in this computation of the observed (order 1) specific heat we have in no way settled the question of the order of the phase transition. To answer this question, which admittedly is not very important physically, one must study the analytic behavior of all contributions to c^r. There are several reasons why this is not trivial. We mention two:

(1) The relation of the differential equation (4.3) to the integral equation (3.28) must be studied in detail. The naïve procedure of using more terms in the Taylor series expansion of $U(\tau)$ leaves one with a differential equation of order larger than 1 and the problem of determining the boundary conditions must be resolved.

(2) Formally, it is possible to write down an exact iterative solution to the integral equation (3.28). This iterative solution is analytic only in the segments $B^{2n} < \eta < B^{2(n-1)}$. The approximation employed in Sec. 4 approximates the analytic function which this segmented solution approaches when $n \to \infty$. This is the important region for the order-1 contributions to c^r, but in general the effects (if any) of the segmented nature of the exact solution are not understood.

CHAPTER XV

An Ising Model with Random Impurities: Boundary Effects

1. INTRODUCTION[1]

Ideally we would like to repeat for the impure Ising model of the last chapter all computations done for Onsager's lattice. Indeed, in this chapter we will parallel the development given Onsager's lattice in Chapters VI and VII by studying boundary effects. Also, it has been possible to study the nearest-neighbor spin-spin correlation functions of the bulk. Much further than this, however, it has proved impossible to go. The interesting quantities of the bulk which, for Onsager's lattice, were studied in Chapters X–XII remain to be computed for the impure lattice.[2]

Because of this lack of computations of bulk properties, the investigation of boundary effects assumes an importance much beyond that which it had in Onsager's lattice. In a sense which will be shortly made precise, the behaviors of the boundary magnetization and spin-spin correlation functions are lower bounds on the behavior of the corresponding bulk properties. This relation between boundary and bulk properties also exists for Onsager's lattice but was not exploited previously because all quantities involved may be studied precisely in their own right. For the impure lattice these bounds are all[2] that presently exist.

1. This chapter is based on the work of B. M. McCoy and T. T. Wu, *Phys. Rev.* **188**, 982 (1969), and B. M. McCoy, *Phys. Rev.* **188**, 1014 (1969).

2. It should be mentioned that there does exist one additional interesting qualitative result which has been proved directly for the bulk by R. B. Griffiths, *Phys. Rev. Letters* **23**, 17 (1969). He considers a random Ising model in which *each* individual interaction energy is an independent random variable E with the probability distribution function $P(E) = p\delta(E - \bar{E}) + (1 - p)\delta(E)$. For this model Griffiths shows that the bulk magnetization fails to be an analytic function of the field H at $H = 0$ for a range of temperatures above that at which spontaneous magnetization first appears.

RANDOM ISING MODEL: BOUNDARY EFFECTS

As in Chapters VI and VII, we consider a half-plane of Ising spins where the boundary row (called 1) is allowed to interact with a magnetic field $\mathfrak{H}$. We study the magnetization of this first row,

$$\mathfrak{M}_1(\mathfrak{H}) = \langle \sigma_{1,m} \rangle, \tag{1.1}$$

and the spin-spin correlation function between two spins in the first row,

$$\mathfrak{S}_{1,1}(m, \mathfrak{H}) = \langle \sigma_{1,0}\sigma_{1,m} \rangle. \tag{1.2}$$

The values of $\mathfrak{M}_1$ and $\mathfrak{S}_{1,1}$ are, in general, different for the different lattices in our collection even in the thermodynamic limit. This is in distinct contrast with the free energy and magnetization of the bulk, each of which approaches a value in the thermodynamic limit that is the same, with probability 1, for all lattices of our collection.[3]

Even though these boundary spin correlation functions are not probability 1 objects themselves, their average values provide lower bounds on certain probability 1 objects of the bulk. These bounds are obtained by using a theorem due to Griffiths which is proved in Appendix A.

Griffiths' Theorem. In any Ising model in which all interaction energies $E_1(j, k)$ and $E_2(j, k)$ are nonnegative and in which the magnetic fields $H_{j,k}$ that interact with the spins at sites (j, k) all have the same sign, the decrease (increase) of the strength of any $E_1(j, k)$, $E_2(j, k)$, or $|H_{j,k}|$ will not increase (decrease) the value of any spin correlation function such as $\langle \sigma_{j,k}\sigma_{j',k'} \rangle$ or $|\langle \sigma_{j,k} \rangle|$.

To establish the desired inequalities we remark that, if H is a magnetic field which interacts with all spins, the magnetization of any lattice in our collection may be written

$$M(H) = \lim_{\substack{\mathcal{M} \to \infty \\ \mathcal{N} \to \infty}} (4\mathcal{M}\mathcal{N})^{-1} \left\langle \sum_{j,k} \sigma_{j,k} \right\rangle_{\mathcal{M},\mathcal{N}}, \tag{1.3}$$

where

$$-\mathcal{M} + 1 \le j \le \mathcal{M}, \tag{1.4}$$

$$-\mathcal{N} + 1 \le k \le \mathcal{N}, \tag{1.5}$$

and we impose cyclic boundary conditions in the horizontal direction.

3. Several further remarks need to be made about $\langle \sigma_{l',m'}\sigma_{l,m} \rangle$ in the bulk. First of all, it depends on l', m', l, and m separately instead of on $l' - l$ and $m' - m$ alone. However, for most experimental applications our interest is not in $\langle \sigma_{l',m}\sigma_{l,m} \rangle$, but in the average of this over all l', m', l, and m with $l' - l$ and $m' - m$ held fixed. This average is clearly equivalent to an average over E_2. Furthermore, it is not possible to compute M^2 as $\lim_{l^2+m^2\to\infty} \langle \sigma_{0,0}\sigma_{l,m} \rangle$ since $\lim_{m\to\infty} \langle \sigma_{l,0}\sigma_{l,m} \rangle$ depends on l and $\lim_{l\to\infty} \langle \sigma_{0,m}\sigma_{l,m} \rangle$ does not exist. Instead, we have $M = \lim_{l^2+m^2\to\infty} \langle (\langle \sigma_{0,0}\sigma_{l,m} \rangle)^{1/2} \rangle_{E_2}$. These last statements may be illustrated by considering the lattice in which $E_2(j)$ is given by $E_2(4n + 1) = E_2(4n + 2) = E_2^{(0)}$ and $E_2(4n + 3) = E_2(4n + 4) = E_2^{(1)}$, where n takes on all integer values. See Appendix B of the paper by B. M. McCoy and T. T. Wu of reference 1.

Now $M(H)$, being an average of $\langle\sigma_{j,k}\rangle$ over the entire lattice, is a probability 1 object. Hence

$$M(H) = \langle\!\langle\sigma_{1,0}\rangle\!\rangle_{E_2}, \tag{1.6}$$

where the notation $\langle\ \rangle_{E_2}$ denotes an average over all lattices in the collection. Consider any lattice out of the collection of lattices specified by a set of energies $\{E_2(j)\}$ where j satisfies (1.4). The magnetic field $\mathfrak{H}$ interacts with the row $j = 1$ only. Therefore, Griffiths' theorem says that for any $\{E_2(j)\}$, if H is numerically equal to $\mathfrak{H}$,

$$M(\mathfrak{H}) \le M(H). \tag{1.7}$$

We are interested in the relation between $M(H)$ and

$$\mathfrak{M}_1(\mathfrak{H}) = \langle\sigma_{1,0}\rangle_{HP}, \tag{1.8}$$

where $\langle\ \rangle_{HP}$ means a thermal average in an Ising lattice where the rows j satisfy

$$1 \le j \le \mathscr{M}$$

instead of (1.4). If we replace all vertical bonds between the row $j = 0$ and $j = 1$ in the original lattice specified by (1.4) by zero, we may apply Griffiths' theorem again to find

$$\mathfrak{M}_1(\mathfrak{H}) \le M(H). \tag{1.9}$$

But this inequality holds for every collection of bonds $\{E_2\}$, so it holds for the average as well; so

$$\langle\mathfrak{M}_1(\mathfrak{H})\rangle_{E_2} \le M(H). \tag{1.10}$$

A similar argument applied to $S_m(H) = \langle\sigma_{0,0}\sigma_{0,m}\rangle_{\text{bulk}}$ establishes that

$$\langle\mathfrak{S}_{1,1}(m, \mathfrak{H})\rangle_{E_2} \le \langle S_m(H)\rangle_{E_2}. \tag{1.11}$$

These lower bounds may be used to draw conclusions about the critical behavior of the bulk properties if we know that both the bulk and the boundary spontaneous magnetizations vanish at the same temperature as T is increased from zero. We are not able to show this directly. However, we will see in Sec. 2 that the boundary spontaneous magnetization vanishes at the same temperature T_c at which the observable specific heat found in Chapter XIV fails to be analytic. Thus, if we could show that the bulk spontaneous magnetization vanishes at the temperature at which the observable specific heat fails to be analytic we would have

$$\langle\mathfrak{M}_1(0^+)\rangle_{E_2} = M(0^+) = 0 \qquad \text{for } T \ge T_c. \tag{1.12}$$

This identification of the temperature at which $M(0^+)$ vanishes with the temperature at which the specific heat fails to be analytic has been discussed in Sec. 4 of Chapter X. No general proof of the validity of this seemingly natural assumption exists, but neither has a counter example been found. Therefore, we will assume it to be true and find from (1.10) and (1.12) that

$$\left\langle \frac{\partial \mathfrak{M}_1(\mathfrak{H})}{\partial \mathfrak{H}}\bigg|_{\mathfrak{H}=0} \right\rangle_{E_2} \leq \frac{\partial M(H)}{\partial H}\bigg|_{H=0}. \tag{1.13}$$

To relate further the boundary to the bulk and to compare the pure with the impure Ising model, it is useful to introduce some notation. It is often assumed in the study of critical phenomena that near T_c the singularities in the magnetization and $S_m(H)$ may be parameterized in terms of "critical exponents" as

$$M(0^+) \sim \text{const}\,(T_c - T)^{\beta} \quad \text{as} \quad T \to T_c^-, \tag{1.14a}$$

$$\frac{\partial M(H)}{\partial H}\bigg|_{H=0} \sim \begin{cases} \text{const}\,(T_c - T)^{-\gamma'} & \text{if } T \to T_c^- \\ \text{const}\,(T - T_c)^{-\gamma} & \text{if } T \to T_c^+, \end{cases} \tag{1.14b}$$

$$M(H) \sim \text{sgn}\,(H)\,\text{const}\,|H|^{1/\delta} \qquad \text{if } T = T_c, \tag{1.14c}$$

and if in addition m is large,

$$\langle S_m(0)\rangle_{E_2} \sim \begin{cases} \text{const}\, m^{-\eta} & \text{if } T = T_c & (1.14d) \\ M^2(0^+) + \text{const}\, m^{-a}e^{-m/\xi} & \text{if } T \neq T_c. & (1.14e) \end{cases}$$

In (1.14e) ξ depends on T and a may be different for T above and below T_c. If we define a similar set of "critical exponents" for $\langle \mathfrak{M}_1(\mathfrak{H})\rangle_{E_2}$ and $\langle \mathfrak{S}_{1,1}(m, \mathfrak{H})\rangle_{E_2}$ and use (1.13), we find

$$\beta_{\text{bulk}} \leq \beta_{\text{boundary}}, \tag{1.15a}$$

$$\gamma_{\text{bulk}} \geq \gamma_{\text{boundary}}, \tag{1.15b}$$

$$\delta_{\text{bulk}} \geq \delta_{\text{boundary}}, \tag{1.15c}$$

$$\eta_{\text{bulk}} \leq \eta_{\text{boundary}}, \tag{1.15d}$$

and, if $T > T_c$,

$$\xi_{\text{bulk}} \leq \xi_{\text{boundary}}. \tag{1.15e}$$

The results of our calculations of bulk properties of Onsager's lattice are all of this "critical exponent" form. For the boundary, on the other hand, it would superficially appear as if the susceptibility, which diverges as $-\ln|T - T_c|$, and the $T = T_c$ magnetization, which behaves as $-\mathfrak{H}\ln|\mathfrak{H}|$, are not of the form (1.14). This deviation is, however, not serious, since we can use the relation

$$\lim_{\gamma\to 0}\left(\frac{1}{\gamma}|T - T_c|^{-\gamma} - \frac{1}{\gamma}\right) = -\ln|T - T_c| \tag{1.16}$$

to interpret the logarithmic divergence of the boundary susceptibility as equivalent to $\gamma_{\text{boundary}} = 0$. Similarly, the behavior $-\mathfrak{H}\ln|\mathfrak{H}|$ is readily interpreted as $\delta_{\text{boundary}} = 1$. With these two remarks it is now easily seen that (1.15) holds for Onsager's lattice.

The most interesting aspect of the impure Ising model with [see (XIV.3.11)]

$$\mu(\lambda) = \begin{cases} N\lambda_0^{-N}\lambda^{N-1} & 0 \leq \lambda \leq \lambda_0 \\ 0 & \text{otherwise} \end{cases} \tag{1.17}$$

is that an interpretation of the "critical exponent" forms with finite critical exponents will *not* describe most of our results. In Sec. 2 we study $\langle \mathfrak{M}_1(\mathfrak{H}) \rangle_{E_2}$ when $T - T_c = O(N^{-2})$ and $\mathfrak{H} = O(N^{-1})$. We find in (2.40) that as $T \to T_c^-$

$$\langle \mathfrak{M}_1(0^+) \rangle_{E_2} \sim C_{\mathfrak{M}} N(T_c - T), \tag{1.18}$$

where

$$C_{\mathfrak{M}} = (2\pi)^{1/2} k\beta_c^2 \left(1 + \frac{1}{z_{2c}^0}\right) \frac{1}{z_{1c}^{1/2}} (1 + z_{1c})[E_1(1 - z_{1c}) + E_2^0(1 - z_{2c}^0)], \tag{1.19}$$

and the subscript c means $T = T_c$. This is in conformity with (1.14a). However, we also find that $\mathfrak{M}_1(\mathfrak{H})$ is not an analytic function of $\mathfrak{H}$ at $\mathfrak{H} = 0$ when $T - T_c = O(N^{-2})$. Most striking is the fact [see (2.55) and (2.68)] that there is a temperature range about T_c where

$$\left\langle \frac{\partial \mathfrak{M}_1(\mathfrak{H})}{\partial \mathfrak{H}} \bigg|_{\mathfrak{H}=0} \right\rangle_{E_2}$$

does not exist because when δ, which is proportional to $N^2(T - T_c)$, is neither zero nor an integer plus $\frac{1}{2}$,

$$\langle \mathfrak{M}_1(\mathfrak{H}) \rangle_{E_2} \sim \langle \mathfrak{M}_1(0^+) \rangle_{E_2} + C(\delta) N^{-1} (\beta_c \mathfrak{H} N)^{2|\delta|} + O(\mathfrak{H}^{4|\delta|}) + O(\mathfrak{H}) \tag{1.20}$$

for $\mathfrak{H} > 0$. Here

$$C(\delta) = 2^{3(\delta - 1/2)} \left(\frac{z_{1c}^{1/2}}{1 + z_{1c}}\right)^{2\delta - 1} \frac{1}{(z_{2c}^0)^{2\delta}} \frac{\pi^{1/2}}{\Gamma(\delta)} \csc \pi(\tfrac{1}{2} - \delta) \quad \text{if } T > T_c \tag{1.21a}$$

and

$$C(\delta) = 2^{-3\delta - 3/2} \left(\frac{z_{1c}^{1/2}}{1 + z_{1c}}\right)^{-2\delta - 1} (z_{2c}^0)^{2\delta} \frac{\Gamma(\frac{1}{2} - 2\delta)\Gamma(1 + \delta)}{\Gamma(-\delta)(1 - \delta)} \csc \pi(\tfrac{1}{2} + \delta) \quad \text{if } T < T_c. \tag{1.21b}$$

When $T < T_c$ we need the additional restriction that $|\delta|$ is not an integer. For the values of δ at which $C(\delta)$ is zero or infinity the form (1.20) breaks down. These exceptional values are studied also in Sec. 2. In particular, when $T = T_c$ ($\delta = 0$), (2.76) shows that

$$\langle \mathfrak{M}_1(\mathfrak{H}) \rangle_{E_2} \sim -\text{sgn}(\mathfrak{H}) 2^{-5/2} z_{1c}^{-1/2} (1 + z_{1c}) \pi^{1/2} N^{-1} [\ln N\beta_c |\mathfrak{H}|]^{-1}. \tag{1.22}$$

Therefore the "critical exponent" forms (1.14*b*) and (1.14*c*) do not at all describe the behavior of $\langle \mathfrak{M}_1(\mathfrak{H}) \rangle_{E_2}$. Hence (1.15) implies that for our random Ising model γ_{bulk} and δ_{bulk} do not exist.

It is not surprising that forms (1.14*b*) and (1.14*c*) are violated in our model because they are abstracted from calculations on Onsager's lattice in which the only relevant length scale is the coherence length ξ defined by (1.14*e*). In some sense our random lattice possesses two length scales, the coherence length ξ^0 of the pure Onsager lattice, which is known to be proportional to $|T - T_c|^{-1}$, and some sort of length associated with the impurities. Because the specific heat computed in Chapter XIV deviates appreciably from its Onsager value only when $T - T_c = O(N^{-2})$, we expect that this impurity length scale has the order of magnitude N^2.

In Sec. 3 we try to make these concepts more precise by studying $\langle \mathfrak{S}_{1,1}(m, \mathfrak{H}) \rangle_{E_2}$ when $m = O(N^2)$, $T - T_c = O(N^{-2})$, and $\mathfrak{H} = O(N^{-1})$. When $1 \ll m \ll N^2$ this average correlation function approaches its Onsager value. However, when $m \gg N^2$ and $T = T_c$, (3.44) shows that

$$\langle \mathfrak{S}_{1,1}(m, 0) \rangle_{E_2}|_{\delta=0} \sim \tfrac{1}{16} z_{1c}^{-1}(1 + z_{1c})^2 N^{-2}(\ln N^{-2}m)^{-1}. \tag{1.23}$$

Furthermore, (3.38) shows that, if the scaled temperature δ is of order 1 and $m \gg N^2$,

$$\langle \mathfrak{S}_{1,1}(m, 0) \rangle_{E_2} \sim \tfrac{1}{16} z_{1c}^{-1}(1 + z_{1c})^2 N^{-2}[\max(-\delta, 0) + D(\delta)(N^2/m)^{2|\delta|}], \tag{1.24}$$

where

$$D(\delta) = \frac{4\Gamma(2|\delta|)}{[\Gamma(|\delta|)]^2[\frac{1}{4}(z_{2c}^0/z_{1c})(1 + z_{1c})^2]^{2|\delta|}}. \tag{1.25}$$

Therefore, the "critical exponent" forms (1.14*d*) and (1.14*e*) fail to describe the behavior of $\langle \mathfrak{S}_{1,1}(m, 0) \rangle_{E_2}$ near T_c and (1.15) implies that η_{bulk} and ξ_{bulk} for $T > T_c$ and $T - T_c = O(N^{-2})$ do not exist.

Finally, it must be noted not only that the average values of the boundary spin correlation functions are of interest, but also that the probability distribution of these functions gives us additional insight into the microscopic details of the random Ising model. As presented in the references of footnote 1 the computation of this distribution is at the same time too complicated and too tentative to warrant inclusion in this book. We content ourselves with the remark that, when $\mu(\lambda)$ is given by (1.17), $\mathfrak{P}(\mathfrak{M}_1)$, the probability that $\mathfrak{M}_1$ takes on a certain value in the range $d\mathfrak{M}_1$, when $\mathfrak{M}_1(0^+) = O(N^{-1})$ is, in leading order, given by

$$\mathfrak{P}(\mathfrak{M}_1) \sim 2^{5/2} \frac{z_{1c}^{1/2}}{1 + z_{1c}} N e^{-\mathfrak{m}^2} \frac{\mathfrak{m}^{2|\delta|-1}}{\Gamma(|\delta|)}, \tag{1.26}$$

where

$$\mathfrak{m} = 2^{3/2} \frac{z_{1c}^{1/2}}{1 + z_{1c}} N \mathfrak{M}_1(0^+). \tag{1.27}$$

2. AVERAGE BOUNDARY MAGNETIZATION

In Sec. 4 of Chapter VII we found that in Onsager's lattice

$$\mathfrak{M}_1(\mathfrak{H}) = z + (1 - z^2)A^{-1}(1, 0; 0, 0)_{DU}, \tag{2.1}$$

where

$$A^{-1}(1, 0; 0, 0)_{DU} = \frac{1}{2\pi}\int_0^{2\pi} d\theta [B^{-1}(\theta)]_{1D,0U}. \tag{2.2}$$

However, the same derivation applies word for word for the random Ising model. Therefore we conclude that (2.2) holds, where the required inverse matrix elements of $B(\theta)$ are computed as

$$[B^{-1}]_{jl,j'l'} = \text{cofactor } C_{j'l',jl}/\det C, \tag{2.3}$$

where

$$l = U, D, \qquad l' = U, D$$

and

$$C(\theta) = \begin{array}{cc}
 & \begin{array}{cccccccccc} 0 & 0 & 1 & 1 & 2 & 2 & & \mathscr{M}-1 & \mathscr{M} & \mathscr{M} \\ D & U & D & U & D & U & \cdots & U & D & U \end{array} \\
\begin{array}{c} 0\ D \\ 0\ U \\ 1\ D \\ 1\ U \\ 2\ D \\ 2\ U \\ \vdots \\ \mathscr{M}-1\ U \\ \mathscr{M}\ D \\ \mathscr{M}\ U \end{array} &
\left[\begin{array}{cccccccccc}
ic & 0 & & & & & & & & \\
0 & -ic & z & & & & & & & \\
 & -z & ia & b & & & & & & \\
 & & -b & -ia & z_2(1) & & & & & \\
 & & & -z_2(1) & ia & b & & & & \\
 & & & & -b & -ia & & & & \\
 & & & & & & \ddots & & & \\
 & & & & & & & ia & z_2(\mathscr{M}-1) & \\
 & & & & & & & -z_2(\mathscr{M}-1) & ia & b \\
 & & & & & & & & -b & -ia
\end{array}\right]
\end{array}. \tag{2.4}$$

Here

$$c(\theta) = -2\sin\theta |1 + e^{i\theta}|^{-2} \tag{2.5}$$

and we recall that $z = \tanh \beta\mathfrak{H}$ and that a and b are defined by (XIV.2.7).

Define $C(j, j')$ to be the $2(j' - j) \times 2(j' - j)$ determinant of the matrix obtained from $C(\theta)$ by omitting all rows and columns of index less than j or greater than j'. Furthermore, define $i\bar{D}(j, j')$ as the $[2(j' - j) - 1] \times [2(j' - j) - 1]$ determinant of the matrix obtained from the matrix defining $C(j, j')$ by omitting the first (that is, the jD) row and column. Similarly $iD(j, j')$ is the $[2(j' - j) - 1] \times [2(j' - j) - 1]$

determinant obtained by omitting from the matrix defining $C(j,j')$ the last (that is, the $j'U$) row and column. In terms of these definitions we find

$$\det C = -c[-cC(1,\mathcal{M}) + z^2\bar{D}(1,\mathcal{M})]. \tag{2.6}$$

Similarly, we evaluate

$$\text{cofactor } C_{0U,1D} = c\bar{D}(1,\mathcal{M}). \tag{2.7}$$

to find

$$[B^{-1}]_{1D,0U} = z\bar{D}(1,\mathcal{M})[z^2\bar{D}(1,\mathcal{M}) - cC(1,\mathcal{M})]^{-1}. \tag{2.8}$$

Define the ratio

$$\frac{C(j,j')}{\bar{D}(j,j')} = -\bar{x}(j,j'). \tag{2.9}$$

Then we may write

$$[B^{-1}]_{1D,0U} = \frac{z}{z^2 + c\bar{x}(1,\mathcal{M})}. \tag{2.10}$$

The existence of the thermodynamic limit is equivalent to the existence of $\lim_{\mathcal{M}\to\infty} \bar{x}(1,\mathcal{M})$. This limit will, in general, be different for different lattices in our collection. Furthermore, $C(j,\mathcal{M})$ and $\bar{D}(j,\mathcal{M})$ obey the recursion relation

$$\begin{bmatrix} C(j-1,\mathcal{M}) \\ -\bar{D}(j-1,\mathcal{M}) \end{bmatrix} = \begin{bmatrix} a^2+b^2 & a \\ a & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & z_2^2(j-1) \end{bmatrix} \begin{bmatrix} C(j,\mathcal{M}) \\ -\bar{D}(j,\mathcal{M}) \end{bmatrix}. \tag{2.11}$$

From this we see that $\lim_{j\to\infty} \bar{x}(j,\mathcal{M})$ will not exist. However, we saw in Sec. 2 of Chapter XIV that the work of Furstenberg may be applied to the recursion relation (2.11) to show that, for $\mathcal{M}$ fixed and $\mathcal{M} - j \to \infty$,

$$\bar{x}(j,\mathcal{M}) \to \bar{x}, \tag{2.12}$$

where $\bar{x}$ is a random variable with the distribution function

$$\bar{\nu}(\bar{x}) = \nu(x). \tag{2.13}$$

Here $\nu(x)$ is the distribution function studied in the last chapter which satisfies (XIV.2.18). Therefore, we compute the average of $\mathfrak{M}_1(\mathfrak{H})$ over all sets of energies E_2 in the thermodynamic limit as

$$\langle \mathfrak{M}_1(\mathfrak{H})\rangle_{E_2} = z + (1 - z^2)z\frac{1}{2\pi}\int_0^{2\pi} d\theta \int_{-\infty}^{\infty} dx\, \frac{\nu(x)}{z^2 + cx}. \tag{2.14}$$

In this chapter we will confine our attention to the distribution function (1.17) studied in Chapter XIV. We know from (XIV.4.1) that T_c is located from

$$\ln\left(\frac{1}{z_{2c}^0}\frac{1 - z_{1c}}{1 + z_{1c}}\right) = -\tfrac{1}{2}N^{-1}. \tag{2.15}$$

Throughout this chapter we will make comparisons between quantities computed for the random lattice and for the corresponding Onsager lattice with the same E_1 and T_c. For this Onsager lattice $E_2 = \bar{E}_2$, where $\bar{z}_{2c}^{-1}(1 - z_{1c})/(1 + z_{1c}) = 1$. When N is large, usually the difference between $\bar{E}_2$ and E_2^0 is important only in locating T_c, so that to leading order in N^{-1} we will often be able to replace $\bar{E}_2$ by E_2^0. Quantities computed in this lattice will be denoted by a superscript 0.

We will confine our attention to the temperature region considered in Chapter XIV, where

$$\delta = (T - T_c)N^2 4k\beta_c^2(1 + 1/z_{2c}^0)[E_1(1 - z_{1c}) + E_2^0(1 - z_{2c}^0)] \tag{2.16}$$

is of order 1. In addition, it is easily seen from the expression for $\nu(x)$, (XIV.4.4), that, unless $z = O(N^{-1})$, (2.14) will not be sensibly different from its value for the Onsager lattice.

We therefore define

$$\bar{z} = \frac{zN}{\lambda_0^{1/2}} \frac{4z_{1c}^{1/2}}{1 + z_{1c}}, \tag{2.17}$$

and recall the definition of ϕ from (XIV.4.16),

$$\phi = -\frac{8}{\lambda_0^{1/2}} \frac{z_{1c}}{(1 + z_{1c})^2} N^2\theta. \tag{2.18a}$$

Then

$$c = \tfrac{1}{16}\lambda_0^{1/2} \frac{(1 + z_{1c})^2}{z_{1c}} N^{-2}\phi + O(N^{-3}). \tag{2.18b}$$

When ϕ and δ are of order 1 we find from Sec. 4 of Chapter XIV that

$$x = \lambda_0^{1/2}e^{-q} + O(N^{-1}) \tag{2.19}$$

and

$$\nu(x)\frac{dx}{dq} = \hat{U}(q) = \frac{1}{2K_\delta(\phi)} \exp\left[-\delta q - \frac{\phi}{2}(e^q + e^{-q})\right]. \tag{2.20}$$

We may now follow the procedure of Chapter XIV and divide the θ integration in (2.20) into two regions: one region where θ is of the order N^{-2} and a second where $|\theta|$ is much greater than N^{-2}. The contribution from this second region is (at least to leading order in N) a constant independent of δ and $\bar{z}$. We find

$$\langle\mathfrak{M}_1(\mathfrak{H})\rangle_{E_2} = \frac{1}{2}\frac{1 + z_{1c}}{z_{1c}^{1/2}}\frac{1}{\pi}N^{-1}\bar{z} \times \left[\int_0^{N^2} d\phi \int_{-\infty}^{\infty} dq \frac{\hat{U}(q)}{\bar{z}^2 + \phi e^{-q}} + \text{const} + O(N^{-1})\right]. \tag{2.21}$$

We may replace the upper limit of the ϕ integration by ∞ if we use the fact [which is easily seen from (2.20)] that

$$\lim_{\phi\to\infty} \hat{U}(q) = \delta(q) \tag{2.22}$$

to find for large ϕ

$$\int_{-\infty}^{\infty} dq \frac{\hat{U}(q)}{\bar{z}^2 + \phi e^{-q}} \sim \phi^{-1}. \tag{2.23}$$

Therefore

$$\begin{aligned}\langle \mathfrak{M}_1(\mathfrak{H})\rangle_{E_2} = \frac{1}{2}\frac{1 + z_{1c}}{z_{1c}^{1/2}}\frac{1}{\pi}N^{-1}\bar{z} \\ \times \Bigg[\int_0^{\infty} d\phi\left(\int_{-\infty}^{\infty} dq \frac{\hat{U}(q)}{\bar{z}^2 + \phi e^{-q}} - \frac{1}{\phi + 1}\right) \\ + \ln N^2 + \text{const} + O(N^{-1})\Bigg].\end{aligned} \tag{2.24}$$

The constant in (2.24) may be determined by demanding that the $\delta \to \pm\infty$ limits of $\langle \mathfrak{M}_1(\mathfrak{H})\rangle_{E_2}$ agree with the $T \sim T_c$ behavior of $\mathfrak{M}_1^0(\mathfrak{H})$ that may be obtained from Sec. 5 of Chapter VI. For the purpose of this book we will not need this constant and will not compute it. However, it is not without interest to study the manner in which (2.24) approaches its Onsager limit. For example, consider the case $T = T_c$ and $\bar{z} \to \infty$. We write

$$\begin{aligned}\int_0^{\infty} d\phi\left(\int_{-\infty}^{\infty} dq \frac{\hat{U}(q)}{\bar{z}^2 + \phi e^{-q}} - \frac{1}{\phi + 1}\right) \\ \sim \int_0^{\infty} d\phi\Bigg\{\int_{-\infty}^{\infty} dq \frac{\hat{U}(q)}{\bar{z}^2 + \phi}\Bigg[1 - \phi(e^{-q} - 1)\frac{1}{\bar{z}^2 + \phi} \\ + \phi^2(e^{-q} - 1)^2\frac{1}{(\bar{z}^2 + \phi)^2}\Bigg] - \frac{1}{\phi + 1}\Bigg\}.\end{aligned} \tag{2.25}$$

We cannot neglect ϕ in comparison with $\bar{z}^2$ in any of these terms. When ϕ is large we may use the asymptotic expansion of $K_\delta(\phi)$ given by (XIV.4.36) to find

$$\int_{-\infty}^{\infty} dq\hat{U}(q)e^{-q} = \frac{K_1(\phi)}{K_0(\phi)} = -\frac{d}{d\phi}\ln K_0(\phi) \sim 1 + \tfrac{1}{2}\phi^{-1} - \tfrac{1}{8}\phi^{-2} \tag{2.26}$$

and

$$\int_{-\infty}^{\infty} dq\hat{U}(q)(e^{-q} - 1)^2 = \frac{K_0(\phi) - 2K_1(\phi) + K_2(\phi)}{K_0(\phi)} \sim \phi^{-1}(1 + \tfrac{5}{4}\phi^{-1}). \tag{2.27}$$

Using these approximations we find that (2.25) is approximately given by

$$-\ln \bar{z}^2 - \frac{1}{8}\int_0^\infty d\phi \frac{1}{(\bar{z}^2+\phi)^2(\phi+1)} + O(\bar{z}^{-4})$$
$$= -\ln \bar{z}^2 - \tfrac{1}{8}\bar{z}^{-4}\ln \bar{z}^2 + O(\bar{z}^{-4}). \tag{2.28}$$

Consequently, for $T = T_c$ as $\bar{z} \to \infty$,

$$\langle \mathfrak{M}_1(\mathfrak{H})\rangle_{E_2} \sim \frac{1}{2}\frac{1+z_{1c}}{z_{1c}^{1/2}}\frac{1}{\pi} N^{-1}\bar{z}$$
$$\times [-2\ln(\bar{z}N^{-1}) + \text{const} - \tfrac{1}{8}\bar{z}^{-4}\ln \bar{z}^2 + O(\bar{z}^{-4})]$$
$$\sim -\frac{4}{\pi}\frac{1}{z_{2c}^0} z \ln z, \tag{2.29}$$

which agrees with (VI.5.37).

We proceed to analyze (2.24) in several stages. First we will determine the spontaneous magnetization and then will study the behavior when $\bar{z} \sim 0$ for $\delta > 0$, $\delta < 0$, and $\delta = 0$.

(*A*) Spontaneous Magnetization

The average boundary spontaneous magnetization is defined to be

$$\langle \mathfrak{M}_1(0^+)\rangle_{E_2} = \lim_{\mathfrak{H}\to 0^+} \langle \mathfrak{M}_1(\mathfrak{H})\rangle_{E_2}. \tag{2.30}$$

Clearly the contributions to (2.24) from values of ϕ greater than some small positive number ϵ will vanish as $\bar{z} \to 0$. Then if we let

$$q = q' - \ln \phi/2 \tag{2.31}$$

and

$$\phi = 2^{1/2}|\bar{z}|\alpha, \tag{2.32}$$

we find

$$\lim_{\mathfrak{H}\to 0^+} \langle \mathfrak{M}_1(\mathfrak{H})\rangle_{E_2} = \frac{1}{2^{1/2}}\frac{1+z_{1c}}{z_{1c}^{1/2}}\frac{1}{\pi} N^{-1}$$
$$\times \lim_{\bar{z}\to 0^+}\int_0^{\epsilon/\bar{z}\sqrt{2}} d\alpha \frac{1}{2K_\delta(2^{1/2}\bar{z}\alpha)}\int_{-\infty}^{\infty} dq' \left(\frac{1}{2^{1/2}}\bar{z}\alpha\right)^\delta$$
$$\times \exp(-\delta q' - e^{q'} - \tfrac{1}{2}\bar{z}^2\alpha^2 e^{-q'})\frac{1}{1+\alpha^2 e^{-q'}}. \tag{2.33}$$

In the $\bar{z} \to 0^+$ limit we may omit the term proportional to $\bar{z}^2$ in the exponential. We may also expand for small ϕ,

$$2K_\delta(\phi) \sim \Gamma(|\delta|)(\tfrac{1}{2}\phi)^{-|\delta|}, \tag{2.34}$$

and replace the upper limit of α integration by infinity. If $\delta > 0$, (2.33) surely is zero. If $\delta < 0$,

$$\langle\mathfrak{M}_1(0^+)\rangle_{E_2} = \frac{1}{2^{1/2}}\frac{1+z_{1c}}{z_{1c}^{1/2}}\frac{1}{\pi}N^{-1}\frac{1}{\Gamma(|\delta|)} \times \int_0^\infty d\alpha \int_{-\infty}^\infty dq' \exp(-\delta q' - e^{q'})\frac{1}{1+\alpha^2 e^{-q'}}, \tag{2.35}$$

from which, if we interchange the orders of integration and let

$$\alpha = e^{q'/2}\alpha', \tag{2.36}$$

we obtain

$$\langle\mathfrak{M}_1(0^+)\rangle_{E_2} = \frac{1}{2^{3/2}}\frac{1+z_{1c}}{z_{1c}^{1/2}}N^{-1}\frac{\Gamma(\frac{1}{2}+|\delta|)}{\Gamma(|\delta|)}. \tag{2.37}$$

When $\delta \to -\infty$, (2.37) is approximated as

$$\begin{aligned}\langle\mathfrak{M}_1(0^+)\rangle_{E_2} &= \frac{1}{2^{3/2}}\frac{1+z_{1c}}{z_{1c}^{1/2}}N^{-1}|\delta|^{1/2}[1 - \tfrac{1}{8}|\delta|^{-1} + O(\delta^{-2})] \\ &\sim \frac{1+z_{1c}}{z_{1c}^{1/2}}\Big\{(T_c - T)\tfrac{1}{2}\beta_c^2 k(1+z_{2c}^0)\frac{1}{z_{2c}^0} \\ &\qquad \times [E_1(1-z_{1c}) + E_2^0(1-z_{2c}^0)]\Big\}^{1/2}. \end{aligned}\tag{2.38}$$

This last expression is seen to agree with the $T \sim T_c$ behavior of $\mathfrak{M}_1^0(0^+)$ as given by (VI.5.35) if we note that near T_c

$$\begin{aligned}\alpha_2 &\sim 1 + (T - T_c)k\beta_c^2\left[E_1\frac{1-z_{1c}^2}{z_{1c}} + 2E_2^0\right] \\ &\sim 1 + (T-T_c)k\beta_c^2\frac{1}{2}\frac{(1+z_{1c})^2}{z_{1c}}(1+z_{2c}^0) \\ &\qquad \times [E_1(1-z_{1c}) + E_2^0(1-z_{2c}^0)]. \end{aligned}\tag{2.39}$$

When $\delta \to 0$,

$$\langle\mathfrak{M}_1(0^+)\rangle_{E_2} \sim \frac{\pi^{1/2}}{2^{3/2}}\frac{1+z_{1c}}{z_{1c}^{1/2}}N^{-1}|\delta|. \tag{2.40}$$

Therefore, the average boundary spontaneous magnetization vanishes linearly as $T \to T_c^-$, as opposed to the square root of the Onsager case. Finally, for the case $E_1 = E_2^0$ we compare (2.37) with $\mathfrak{M}_1^0(0^+)$ by plotting them in Fig. 15.1 for the same values of N and δ considered in Fig. 14.3.

(B) $\bar{z}$ *Near Zero,* $\delta > 0$

Consider first the restriction

$$n - \tfrac{1}{2} < \delta < n + \tfrac{1}{2}, \tag{2.41}$$

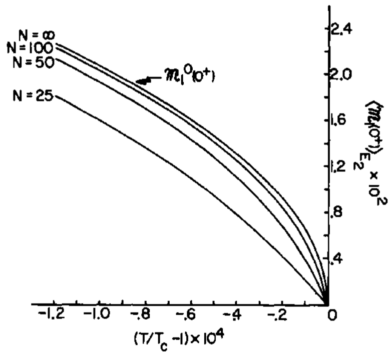


Fig. 15.1. Comparisons of $\mathfrak{M}_1^0(0^+)$ and $\langle \mathfrak{M}_1(0^+)\rangle_{E_2}$ for several values of N for the case $E_1 = E_2^0$.

where n is a nonnegative integer, and write

$$\frac{1}{\bar{z}^2 + \phi e^{-q}} = \phi^{-1}e^q \sum_{k=0}^{n-1} (-\bar{z}^2\phi^{-1}e^q)^k + \frac{(-\bar{z}^2\phi^{-1}e^q)^n}{\bar{z}^2 + \phi e^{-q}}, \tag{2.42}$$

where the first summation is to be omitted if $n = 0$. We introduce this expression in (2.24) and write

$$\langle \mathfrak{M}_1(\mathfrak{H})\rangle_{E_2} \sim \frac{1}{2} \frac{1 + z_{1c}}{z_{1c}^{1/2}} \frac{1}{\pi} N^{-1} \left(\sum_{k=0}^{n-1} I_k + I_n^{(1)} + \text{const}\, \bar{z} + \bar{z} \ln N^2\right), \tag{2.43}$$

where

$$\begin{aligned} I_k &= (-1)^k \bar{z}^{2k+1} \int_0^\infty d\phi \biggl(\frac{1}{2K_\delta(\phi)} \phi^{-k-1} \\ &\qquad \times \int_{-\infty}^{\infty} dq \exp\left[(k + 1 - \delta)q - \frac{\phi}{2}(e^q + e^{-q})\right] - (\phi + 1)^{-1}\delta_{k,0}\biggr) \\ &= (-1)^k \bar{z}^{2k+1} \int_0^\infty d\phi \left[\phi^{-k-1} \frac{K_{1+k-\delta}(\phi)}{K_\delta(\phi)} - (\phi + 1)^{-1}\delta_{k,0}\right] \end{aligned} \tag{2.44}$$

for $k < n$ and

$$\begin{aligned} I_n^{(1)} &= (-1)^n \bar{z}^{2n+1} \int_0^\infty d\phi \frac{1}{2K_\delta(\phi)} \phi^{-n} \\ &\qquad \times \int_{-\infty}^{\infty} dq \exp\left[(n - \delta)q - \frac{\phi}{2}(e^q + e^{-q})\right] \frac{1}{\bar{z}^2 + \phi e^{-q}}. \end{aligned} \tag{2.45}$$

Because of the restriction (2.41) the integrals in (2.44) and (2.45) converge. We will see shortly that for δ fixed and greater than $\frac{1}{2}$, $I_n^{(1)} = O(\bar{z})$ as $\bar{z} \to 0$. However, when $\delta \to n - \frac{1}{2}$, I_{n-1} will tend to infinity. More specifically, if (2.41) holds and $\delta \sim n - \frac{1}{2}$, we may study the singular part of I_{n-1} by using approximation (2.34) to write

$$I_{n-1} = (-1)^{n+1}\bar{z}^{2n-1}\frac{\Gamma(\delta - n)}{\Gamma(\delta)}\frac{1}{2^n}\int_0^{\epsilon} d\phi(\tfrac{1}{2}\phi)^{2(\delta-n)} + O(1)$$

$$= (-1)^{n+1}\bar{z}^{2n-1}\pi^{1/2}\frac{1}{\Gamma(n-\frac{1}{2})}\frac{1}{2^n}\frac{1}{\delta - n + \frac{1}{2}} + O(1), \tag{2.46}$$

where $O(1)$ means finite as $\delta \to n - \frac{1}{2}$.

If $\delta > \frac{1}{2}$ we may use (2.43) to write the average boundary zero field susceptibility as

$$\left\langle \frac{\partial \mathfrak{M}_1(\mathfrak{H})}{\partial \mathfrak{H}}\bigg|_{\mathfrak{H}=0}\right\rangle_{E_2} = 2\beta_c \frac{1}{z_{2c}^0}\frac{1}{\pi}\left\{\int_0^\infty d\phi\left[\phi^{-1}\frac{K_{1-\delta}(\phi)}{K_\delta(\phi)} - (\phi + 1)^{-1}\right]\right.$$
$$\left. + \ln N^2 + \text{const} + O(N^{-1})\right\}. \tag{2.47}$$

When $\delta \to \infty$ we may use the relation

$$K_{\delta-1}(\phi) = -\delta\phi^{-1}K_\delta(\phi) - \frac{\partial K_\delta(\phi)}{\partial \phi} \tag{2.48}$$

and the asymptotic expansion (XIV.4.36)

$$K_\delta(\phi) \sim (\tfrac{1}{2}\pi)^{1/2}(\delta^2 + \phi^2)^{-1/4}\exp\left[-(\delta^2 + \phi^2)^{1/2} + \delta\sinh^{-1}(\delta/\phi)\right] \tag{2.49}$$

to find

$$\left\langle \frac{\partial \mathfrak{M}_1(\mathfrak{H})}{\partial \mathfrak{H}}\bigg|_{\mathfrak{H}=0}\right\rangle_{E_2}$$
$$\sim 2\beta_c \frac{1}{z_{2c}^0}\frac{1}{\pi}\left(-\ln N^{-2}\delta + \ln 2 - 1 + \text{const} + \delta^{-1}\frac{\pi}{4}\right)$$
$$= -2\beta_c\frac{1}{z_{2c}^0}\frac{1}{\pi}\ln(T - T_c) + O(1), \tag{2.50}$$

which is seen to agree with $\partial \mathfrak{M}_1^0(\mathfrak{H})/\partial\mathfrak{H}|_{\mathfrak{H}=0}$ given by (VI.5.38). However, from (2.46) we find that as $\delta \to \frac{1}{2}^+$

$$\left\langle \frac{\partial \mathfrak{M}_1(\mathfrak{H})}{\partial \mathfrak{H}}\bigg|_{\mathfrak{H}=0}\right\rangle_{E_2} = 4\beta_c\frac{1}{z_{2c}^0}\frac{1}{\delta - \frac{1}{2}} + O(1). \tag{2.51}$$

Therefore the average boundary susceptibility at zero field diverges at a temperature *above* T_c. This is completely different from the zero-field susceptibilities of either the bulk or the boundary of Onsager's lattice, which are known to be finite for all temperatures $T \neq T_c$.

When $\bar{z}$ is small we may study $I_n^{(1)}$ exactly as we studied the spontaneous magnetization. The contributions from values of ϕ greater than ϵ are $O(\bar{z}^{2n+1})$. When $\phi \sim 0$ we use (2.31), (2.32), (2.34), and (2.36) to find

$$I_n^{(1)} = \operatorname{sgn} z\,(-1)^n\left(\frac{|\bar{z}|}{2^{1/2}}\right)^{2\delta}2^{1/2}\frac{1}{\Gamma(\delta)}\int_{-\infty}^{\infty}dq'\exp(\tfrac{1}{2}q' - e^{q'})$$
$$\times\int_0^{\epsilon|\bar{z}|^{-1}\exp(-q'/2)}d\alpha'\frac{\alpha'^{2(\delta-n)}}{1+\alpha'^2} + O(\bar{z}^{2n+1}) + O(|\bar{z}|^{4\delta}). \tag{2.52}$$

The α' integral, for fixed ϵ and small $\bar{z}$, is approximately

$$\int_0^{\epsilon|\bar{z}|^{-1}\exp(-q'/2)} d\alpha' \frac{\alpha'^{2(\delta-n)}}{1+\alpha'^2}$$

$$= \frac{1}{2}\left\{\pi \csc \pi\left(\frac{1}{2} + n - \delta\right) + |\bar{z}|^{-2\delta+2n+1}\left[\frac{1}{\delta - n - \frac{1}{2}} + O(1)\right]\right\}, \quad (2.53)$$

where $O(1)$ is a term that does not diverge as $\delta \to n + \frac{1}{2}$. Therefore,

$$I_n^{(1)} = (-1)^n \operatorname{sgn}(\bar{z}) \frac{|\bar{z}|^{2\delta}}{2^{\delta+1/2}} \frac{1}{\Gamma(\delta)} \pi^{3/2} \csc \pi(\tfrac{1}{2} + n - \delta)$$
$$+ (-1)^n \bar{z}^{2n+1}\left[\pi^{1/2} \frac{1}{\Gamma(n+\frac{1}{2})} \frac{2^{-n-1}}{\delta - n - \frac{1}{2}} + O(1)\right]$$
$$+ O(\bar{z}^{4\delta}) + O(\bar{z}^{2(\delta+1)}). \quad (2.54)$$

This contribution to $\langle\mathfrak{M}_1(\mathfrak{H})\rangle_{E_2}$ clearly fails to be analytic at $\mathfrak{H} = 0$ since the nth derivative does not exist. Indeed, if $0 < \delta < \frac{1}{2}$, $\langle\mathfrak{M}_1(\mathfrak{H})\rangle_{E_2}$ is not differentiable at all at $\mathfrak{H} = 0$ so the zero-field susceptibility will not exist.

It remains to lift the restriction (2.41) by allowing δ to be half an odd integer. We first explicitly exhibit $\langle\mathfrak{M}_1(\mathfrak{H})\rangle_{E_2}$ when (2.41) holds as

$$\langle\mathfrak{M}_1(\mathfrak{H})\rangle_{E_2} = \frac{1}{2}\frac{1+z_{1c}}{z_{1c}^{1/2}}\frac{1}{\pi}N^{-1}$$
$$\times\left\{\sum_{k=0}^{n-2} I_k + (-1)^{n-1}\bar{z}^{2n-1}\left[\frac{\pi^{1/2}}{\Gamma(n-\frac{1}{2})}\frac{1}{2^n(\delta-n+\frac{1}{2})} + O(1)\right]\right.$$
$$+ \operatorname{sgn}(\bar{z})|\bar{z}|^{2\delta}2^{-\delta-1/2}\frac{\pi^{3/2}}{\Gamma(\delta)}\csc\pi(\tfrac{1}{2}-\delta) + (-1)^n\bar{z}^{2n+1}$$
$$\times\left[\frac{\pi^{1/2}}{\Gamma(n+\frac{1}{2})}\frac{1}{2^{n+1}(\delta-n-\frac{1}{2})} + O(1)\right]$$
$$\left. + O(\bar{z}^{4\delta}) + O(\bar{z}^{2\delta+2}) + \ln N^2 + \text{const}\right\}. \quad (2.55)$$

In this form we may now let $\delta \to n' - \frac{1}{2}$ from either above or below and find

$$\lim_{\delta\to n'-1/2}\langle\mathfrak{M}_1(\mathfrak{H})\rangle_{E_2} = \frac{1}{2}\frac{1+z_{1c}}{z_{1c}^{1/2}}\frac{1}{\pi}N^{-1}$$
$$\times\left\{\sum_{k=0}^{n'-2} I_k + (-1)^{n'}\frac{\pi^{1/2}}{2^{n'-1}\Gamma(n'-\frac{1}{2})}\right.$$
$$\left.\times \operatorname{sgn}(\bar{z})\bar{z}^{2n'-1}\ln|\bar{z}| + O(\bar{z}^{2n'-1}) + \ln N^2 + \text{const}\right\}. \quad (2.56)$$

Therefore, for all positive δ (at least that are $O(1)$ as $N \to \infty$) $\langle \mathfrak{M}_1(\mathfrak{H}) \rangle_{E_2}$ is not an analytic function of $\mathfrak{H}$ at $\mathfrak{H} = 0$.

(*C*) $\bar{z}$ Near Zero, $\delta < 0$

The analysis of $\langle \mathfrak{M}_1(\mathfrak{H}) \rangle_{E_2}$ when $\delta < 0$ is only slightly more complicated than the case $\delta > 0$ just treated. When $\delta < 0$ we may use the results of subsection (*A*) to write

$$\begin{aligned}
&\langle \mathfrak{M}_1(\mathfrak{H}) \rangle_{E_2} \\
&\quad = \operatorname{sgn}(\bar{z}) \langle \mathfrak{M}_1(0^+) \rangle_{E_2} + \frac{1}{2} \frac{1 + z_{1c}}{z_{1c}^{1/2}} \frac{1}{\pi} N^{-1} \bar{z} \\
&\qquad \times \left\{ \int_0^\infty d\phi \left[\int_{-\infty}^\infty dq \left(\frac{1}{2K_\delta(\phi)} \exp\left[-\delta q - \frac{\phi}{2}(e^q + e^{-q}) \right] \right. \right. \right. \\
&\qquad\qquad \left. \left. - \frac{1}{\Gamma(|\delta|)} (\tfrac{1}{2}\phi)^{|\delta|} \exp\left(-\delta q - \frac{\phi}{2} e^q \right) \right) \frac{1}{\bar{z}^2 + \phi e^{-q}} - \frac{1}{\phi + 1} \right] \\
&\qquad\qquad \left. + \ln N^2 + \text{const} + O(N^{-1}) \right\}.
\end{aligned} \tag{2.57}$$

When $\delta < -\frac{1}{2}$ the second term is $O(\bar{z})$ as $\bar{z} \to 0$; therefore,

$$\begin{aligned}
&\left\langle \frac{\partial \mathfrak{M}_1(\mathfrak{H})}{\partial \mathfrak{H}} \bigg|_{\mathfrak{H}=0} \right\rangle_{E_2} \\
&\quad = 2\beta_c \frac{1}{z_{2c}^0} \frac{1}{\pi} \left\{ \int_0^\infty d\phi \left[\phi^{-1} \int_{-\infty}^\infty dq e^q \left(\frac{1}{2K_\delta(\phi)} \exp\left[-\delta q - \frac{\phi}{2}(e^q + e^{-q}) \right] \right. \right. \right. \\
&\qquad\qquad \left. \left. - \frac{1}{\Gamma(|\delta|)} (\tfrac{1}{2}\phi)^{|\delta|} \exp\left[-\delta q - \frac{\phi}{2} e^q \right] \right) - \frac{1}{\phi + 1} \right] \\
&\qquad\qquad \left. + \ln N^2 + \text{const} + O(N^{-1}) \right\} \\
&\quad = 2\beta_c \frac{1}{z_{2c}^0} \frac{1}{\pi} \left\{ \int_0^\infty d\phi \left[\phi^{-1} \left(\frac{K_{|\delta|+1}(\phi)}{K_{|\delta|}(\phi)} - 2\phi^{-1}|\delta| \right) - \frac{1}{\phi + 1} \right] \right. \\
&\qquad\qquad \left. + \ln N^2 + \text{const} + O(N^{-1}) \right\},
\end{aligned} \tag{2.58}$$

which, if we use the recursion relation[4]

$$K_{|\delta|+1}(\phi) = K_{1-|\delta|}(\phi) + 2|\delta|\phi^{-1}K_{|\delta|}(\phi), \tag{2.59}$$

4. A. Erdelyi, ed., *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), vol. 2, p. 79.

becomes

$$\left\langle \frac{\partial \mathfrak{M}_1(\mathfrak{H})}{\partial \mathfrak{H}}\bigg|_{\mathfrak{H}=0} \right\rangle_{E_2} = 2\beta_c \frac{1}{z_{2c}^0} \frac{1}{\pi} \left\{ \int_0^\infty d\phi \left[\frac{1}{\phi} \frac{K_{1-|\delta|}(\phi)}{K_{|\delta|}(\phi)} - \frac{1}{\phi + 1} \right] + \ln N^2 + \text{const} + O(N^{-1}) \right\}, \tag{2.47'}$$

which is exactly the same as (2.47) except that δ is replaced by $|\delta|$. Thus

$$\left\langle \frac{\partial \mathfrak{M}_1(\mathfrak{H}; \delta)}{\partial \mathfrak{H}}\bigg|_{\mathfrak{H}=0} \right\rangle_{E_2} = \left\langle \frac{\partial \mathfrak{M}_1(\mathfrak{H}; -\delta)}{\partial \mathfrak{H}}\bigg|_{\mathfrak{H}=0} \right\rangle_{E_2}, \tag{2.60}$$

and the zero-field susceptibility diverges as a simple pole when $\delta \to -\frac{1}{2}^-$ as well as when $\delta \to +\frac{1}{2}^+$.

We may also use the procedures of subsection (B) to show that, in addition to a Taylor series in $|\bar{z}|$, $\langle \mathfrak{M}_1(\mathfrak{H}) \rangle_{E_2}$ contains terms proportional to $|\bar{z}|^{|2\delta|}$. Values of $\phi > \epsilon$ contribute only to the odd terms in this series. Any divergences in these terms as $\delta \to -n' + \frac{1}{2}$ and any other terms come from the region $0 < \phi < \epsilon$. Consider first the case

$$n - \tfrac{1}{2} < |\delta| < n + \tfrac{1}{2}, \tag{2.61}$$

$$\delta \neq -n, \tag{2.62}$$

where n is a nonnegative integer. When $\phi \sim 0$ we use the complete expansion[5]

$$2K_{|\delta|}(\phi) = \frac{\pi}{\sin |\delta|\pi} \left\{ \sum_{k=0}^{\infty} \frac{(\frac{1}{2}\phi)^{2k-|\delta|}}{k!\,\Gamma(k + 1 - |\delta|)} - \sum_{k=0}^{\infty} \frac{(\frac{1}{2}\phi)^{2k+|\delta|}}{k!\,\Gamma(k + 1 + |\delta|)} \right\} \tag{2.63}$$

to find

$$\frac{1}{2K_{|\delta|}(\phi)} = \frac{(\frac{1}{2}\phi)^{|\delta|}}{\Gamma(|\delta|)} \times \left\{ \sum_{k=0}^{\infty} A_k (\tfrac{1}{2}\phi)^{2k} + (\tfrac{1}{2}\phi)^{2|\delta|} \frac{\Gamma(1 - |\delta|)}{\Gamma(1 + |\delta|)} \sum_{k=0}^{\infty} B_k \phi^{2k} + O(\phi^{4|\delta|}) \right\}, \tag{2.64}$$

where the only properties of A_k and B_k we need are

$$A_0 = B_0 = 1 \tag{2.65}$$

and, as $\delta \to -n$,

$$A_k = O(1) \qquad \text{for } 0 \leq k \leq n - 1, \tag{2.66}$$

$$A_n = \frac{-\Gamma(1 - |\delta|)}{n!\,\Gamma(n + 1 - |\delta|)}. \tag{2.67}$$

5. Reference 4, vol. 2, p. 5.

Using these approximations we find

$$\begin{aligned}
\langle \mathfrak{M}_1(\mathfrak{H})\rangle_{E_2} &= \operatorname{sgn}(\bar{z})\langle \mathfrak{M}_1(0^+)\rangle_{E_2} + \operatorname{sgn}(\bar{z}) \sum_{k=1}^{2n-2} M^{(k)}|z|^k \\
&\quad + \operatorname{sgn}(\bar{z}) \frac{1}{2} \frac{1+z_{1c}}{z_{1c}^{1/2}} \frac{1}{\pi} N^{-1} \\
&\quad \times \left\{ \frac{2^{\delta-1/2}}{|\bar{z}|^{2\delta}} \pi \csc \pi(\tfrac{1}{2}+\delta) \frac{\Gamma(\frac{1}{2}-2\delta)\Gamma(1+\delta)}{\Gamma(1-\delta)\Gamma(-\delta)} \right. \\
&\quad + |\bar{z}|^{2n-1} \left(\frac{(-1)^n}{2^n(\delta+n-\frac{1}{2})} \frac{\Gamma(2n-\frac{1}{2})\Gamma(\frac{3}{2}-n)}{\Gamma(n+\frac{1}{2})\Gamma(n-\frac{1}{2})} + O(1) \right) \\
&\quad + \bar{z}^{2n} \left(2^{-n-1/2}\pi \frac{\Gamma(\frac{1}{2}+2n)}{n![(n-1)!]^2(\delta+n)} \right) \\
&\quad + |\bar{z}|^{2n+1} \left(\frac{(-1)^{n+1}}{2^{n+1}(\delta+n+\frac{1}{2})} \frac{\Gamma(2n+\frac{3}{2})\Gamma(\frac{1}{2}-n)}{\Gamma(n+\frac{3}{2})\Gamma(n+\frac{1}{2})} + O(1) \right) \\
&\quad \left. + O(\bar{z}^{-2\delta+2}) + O(\bar{z}^{-4\delta}) \right\},
\end{aligned} \tag{2.68}$$

where the coefficients $M^{(k)}$ with $k \le 2(n-1)$ are analytic in δ for $|\delta| \le n + \frac{1}{2}$. Note that the coefficient of $\bar{z}^{2n}$ has a pole at $\delta = -n$ and the coefficient of $\bar{z}^{2n-1}$ has a pole at $\delta = -n + \frac{1}{2}$. We may now lift the restriction (2.62) by letting $\delta \to -n$ to obtain

$$\begin{aligned}
\lim_{\delta \to -n} \langle \mathfrak{M}_1(\mathfrak{H})\rangle_{E_2} &= \operatorname{sgn}(\bar{z})\langle \mathfrak{M}_1(0^+)\rangle_{E_2} + \operatorname{sgn}(\bar{z}) \sum_{k=1}^{2n-1} M^{(k)}|\bar{z}|^k \\
&\quad + \operatorname{sgn}(\bar{z}) \frac{1}{2} \frac{1+z_{1c}}{z_{1c}^{1/2}} \frac{1}{\pi} N^{-1}|\bar{z}|^{2n} \\
&\quad \times \left\{ 2^{-n-1/2}\pi \frac{\Gamma(\frac{1}{2}+2n)}{n!\,[(n-1)!]^2} \ln \bar{z}^2 + O(1) \right\} \\
&\quad + O(\bar{z}^{2n+1}),
\end{aligned} \tag{2.69}$$

and we may lift restriction (2.61) by letting $\delta \to -n' + \frac{1}{2}$ to obtain

$$\begin{aligned}
\lim_{\delta \to -n'+1/2} \langle \mathfrak{M}_1(\mathfrak{H})\rangle_{E_2} &= \operatorname{sgn}(\bar{z})\langle \mathfrak{M}_1(0^+)\rangle_{E_2} + \operatorname{sgn}(\bar{z}) \sum_{k=1}^{2n'-2} M^{(k)}|\bar{z}|^k \\
&\quad + \operatorname{sgn}(\bar{z}) \frac{1}{2} \frac{1+z_{1c}}{z_{1c}^{1/2}} \frac{1}{\pi} N^{-1}|\bar{z}|^{2n'-1} \\
&\quad \times \left\{ \frac{(-1)^{n'}}{2^{n'}} \frac{\Gamma(2n'-\frac{1}{2})\Gamma(\frac{3}{2}-n')}{\Gamma(n'+\frac{1}{2})\Gamma(n'-\frac{1}{2})} \ln \bar{z}^2 + O(1) \right\}.
\end{aligned} \tag{2.70}$$

Therefore, not only does $\langle \mathfrak{M}_1(\mathfrak{H})\rangle_{E_2}$ fail to be analytic at $\mathfrak{H} = 0$ because of the presence of terms proportional to $\operatorname{sgn}(\bar{z})|\bar{z}|^{2k}$ but $\lim_{\mathfrak{H}\to 0^+} (\partial^n/\partial\mathfrak{H}^n)$

$\langle\mathfrak{M}_1(\mathfrak{H})\rangle_{E_2}$ does not exist if $n \geq |\delta| + \frac{1}{2}$. In particular, the zero-field susceptibility does not exist if $-\frac{1}{2} \leq \delta \leq 0$.

(*D*) $\bar{z}$ Near Zero, $\delta = 0$

It remains to study the case $\delta = 0$. The previous approximations fail in this case because neglected terms of order $O(\bar{z}^{4|\delta|})$ become important. From (2.24) we have

$$\langle\mathfrak{M}_1(\mathfrak{H})\rangle_{E_2}|_{\delta=0} = \frac{1}{2}\frac{1+z_{1c}}{z_{1c}^{1/2}}\frac{1}{\pi}N^{-1}\bar{z}\Bigg\{\int_0^{\infty} d\phi\Bigg[\int_{-\infty}^{\infty} dq\,\frac{1}{2K_0(\phi)} \times \exp\left(-\frac{\phi}{2}(e^q + e^{-q})\right)\frac{1}{\bar{z}^2 + \phi e^{-q}} - \frac{1}{\phi+1}\Bigg] + \ln N^2 + \text{const} + O(N^{-1})\Bigg\}. \tag{2.71}$$

As before, values of $\phi > \epsilon$ contribute only to a Taylor series in odd powers of $\bar{z}$. When $\phi \sim 0$ we approximate[6]

$$K_0(\phi) \sim -\left[\ln\frac{\phi}{2} + \gamma\right] + o(1) = -[\ln(\phi A 2^{-1/2}) + o(1)], \tag{2.72}$$

where $\gamma \sim 0.577216$ is Euler's constant and

$$A = 2^{-1/2}e^{\gamma}. \tag{2.73}$$

Then using (2.31) and (2.32) we may approximate

$$\langle\mathfrak{M}_1(\mathfrak{H})\rangle_{E_2}|_{\delta=0} \sim -\operatorname{sgn}(\bar{z})2^{-3/2}\frac{1+z_{1c}}{z_{1c}^{1/2}}\frac{1}{\pi}N^{-1}\int_0^{\epsilon/|\bar{z}|} d\alpha\,\frac{1}{\ln|\bar{z}|\alpha A} \times \int_{-\infty}^{\infty} dq'\,\frac{\exp(-e^{q'})}{1+\alpha^2 e^{-q'}}. \tag{2.74}$$

Because $\epsilon \ll 1$ we may expand

$$\frac{1}{\ln|\bar{z}|\alpha A} \sim \frac{1}{\ln|\bar{z}|A}\left(1 - \frac{\ln\alpha}{\ln|\bar{z}|A} + \cdots\right). \tag{2.75}$$

Then we may obtain the leading terms in the approximation by interchanging orders of integration and replacing the upper limit of the α integration by ∞, to obtain

$$\langle\mathfrak{M}_1(\mathfrak{H})\rangle_{E_2}|_{\delta=0} \sim -\operatorname{sgn}(\bar{z})2^{-5/2}\frac{1+z_{1c}}{z_{1c}^{1/2}}\pi^{1/2}N^{-1}\frac{1}{\ln|\bar{z}|A} \times \left[1 - \frac{1}{2\ln|\bar{z}|A}\psi(\tfrac{1}{2}) + \cdots\right], \tag{2.76}$$

6. Reference 4, vol. 2, p. 9.

where[7]

$$\psi(\tfrac{1}{2}) = \Gamma'(\tfrac{1}{2})/\Gamma(\tfrac{1}{2}) = -\gamma - 2\ln 2. \tag{2.77}$$

Clearly (2.76) vanishes more slowly than any fractional power of $\mathfrak{H}$ as $\mathfrak{H} \to 0$ and is therefore not of the form (1.14*c*) which is parameterized by the "critical exponent" δ.

3. AVERAGE SPIN-SPIN CORRELATION FUNCTIONS

There are, of course, many distinct spin-spin correlation functions for two spins near the boundary of our half-plane of Ising spins, and we will confine our interest to the special case when both spins are in the boundary row 1. We then use the formalism of Chapter VII and find that for any lattice in our collection

$$\begin{aligned}\mathfrak{S}_{1,1}(m, \mathfrak{H}) = (1 - z^2)\{&[A^{-1}(1, 0; 0, 0)_{DU} + (z^{-1} - z)^{-1}]^2 \\ &- [A^{-1}(1, m; 0, 0)_{DU}]^2 \\ &- A^{-1}(1, 0; 1, m)_{DD}A^{-1}(0, 0; 0, m)_{UU}\},\end{aligned} \tag{3.1}$$

where, from Sec. 2 with $\bar{x}(j,j'; \theta) = \bar{x}(j,j')$,

$$\begin{aligned}A^{-1}(1, m; 0, 0)_{DU} &= \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{im\theta}[B^{-1}(\theta)]_{1D,0U} \\ &= \frac{1}{2\pi} z \int_0^{2\pi} d\theta \frac{e^{im\theta}}{z^2 + c\bar{x}(1, \mathscr{M}; \theta)},\end{aligned} \tag{3.2a}$$

and, using an argument similar to that of Sec. 2,

$$A^{-1}(1, 0; 1, m)_{DD} = \frac{1}{2\pi i}\int_0^{2\pi} d\theta \frac{e^{-im\theta}}{\bar{x}(1, \mathscr{M}; \theta) + z^2/c}, \tag{3.2b}$$

and
$$A^{-1}(0, 0; 0, m)_{UU} = -\frac{1}{2\pi i}\int_0^{2\pi} d\theta \frac{e^{-im\theta}}{c + z^2/\bar{x}(1, \mathscr{M}; \theta)}. \tag{3.2c}$$

The first term in (3.1) is recognized as $\mathfrak{M}_1(\mathfrak{H})^2$.

We are interested only in the $\mathfrak{H} \to 0$ limit of (3.1). In discussing $\mathfrak{S}_{1,1}(m, \mathfrak{H})$ it is immaterial whether we let $\mathscr{M} \to \infty$ before or after $\mathfrak{H} \to 0$. For convenience, let $\mathfrak{H} \to 0$ first.[8] Then it is easily seen that, for $0 \le \theta \le 2\pi$, $\bar{x}(1, \mathscr{M}; \theta) \ne 0$. Therefore, the first two terms in (3.1) vanish as $\mathfrak{H} \to 0$. Furthermore, if $m \ne 0$,

$$\lim_{\mathfrak{H}\to 0} A^{-1}(0, 0; 0, m)_{UU} = -1, \tag{3.3}$$

7. Reference 4, vol. 1, p. 19.
8. The opposite order is explicitly considered by B. M. McCoy, *Phys. Rev.* **188**, 1014 (1969).

so we conclude that for any collection of energies $\{E_2\}$

$$\mathfrak{S}_{1,1}(m, 0) = A^{-1}(1, 0; 1, m)_{DD} = \frac{1}{2\pi i}\int_0^{2\pi} d\theta \frac{e^{-im\theta}}{\bar{x}(1, \mathscr{M}; \theta)}. \tag{3.4}$$

This is to be averaged over $\{E_2\}$ in the $\mathscr{M} \to \infty$ limit and we find

$$\langle \mathfrak{S}_{1,1}(m, 0)\rangle_{E_2} = \frac{1}{2\pi i}\int_0^{2\pi} d\theta e^{-im\theta}\int_{-\infty}^{\infty} dx \frac{\nu(x)}{x}. \tag{3.5}$$

To study the leading term of (3.5) when $\delta = O(1)$, we make the substitutions (2.16), (2.18), and (2.19). We also define

$$\bar{m} = \tfrac{1}{8}\lambda_0^{1/2}\frac{(1 + z_{1c})^2}{z_{1c}} N^{-2}m. \tag{3.6}$$

As before, we consider the contributions to the θ integral from $0 < \theta < N^{-2}$ and $\theta > N^{-2}$ separately. The contribution from $\theta > N^{-2}$ is, to lowest order in N, independent of δ and depends only on m. Therefore, we have

$$\begin{aligned}\langle \mathfrak{S}_{1,1}(m, 0)\rangle_{E_2} = {} & \frac{1}{8}\frac{(1 + z_{1c})^2}{z_{1c}}\frac{1}{\pi} N^{-2}\int_0^{N^2} d\phi \int_{-\infty}^{\infty} dq\hat{U}(q)e^{q} \sin \bar{m}\phi \\ & + f(m) + O(N^{-2}),\end{aligned} \tag{3.7}$$

where $f(m)$ is the contribution to $A^{-1}(1, 0; 1, m)_{DD}$ from $\phi > N^{-2}$.

The N^2 dependence of the integral in (3.7) is made explicit by using (2.22) to find for large ϕ that

$$\int_{-\infty}^{\infty} dq\hat{U}(q)e^{q} \sim 1. \tag{3.8}$$

Therefore if we add and subtract 1 in the ϕ integral we may extend the upper limit of integration to infinity and obtain

$$\begin{aligned}\langle \mathfrak{S}_{1,1}(m, 0)\rangle_{E_2} = {} & \frac{1}{8}\frac{(1 + z_{1c})^2}{z_{1c}}\frac{1}{\pi} N^{-2}\int_0^{\infty} d\phi \sin \bar{m}\phi \int_{-\infty}^{\infty} dq\hat{U}(q)(e^{q} - 1) \\ & + \bar{f}(m) + O(N^{-2}),\end{aligned} \tag{3.9}$$

where

$$\bar{f}(m) = f(m) - \frac{1}{z_{2c}^0 m}\left\{\cos\left[\tfrac{1}{8}z_{2c}^0 \frac{(1 + z_{1c})^2}{z_{1c}} m\right] - 1\right\}. \tag{3.10}$$

The function $\bar{f}(m)$ may be made explicit by exploiting the fact that it is independent of δ. Therefore, $\bar{f}(m)$ may be computed by considering $|\delta| \sim N^2$ and requiring that the term in $\langle \mathfrak{S}_{1,1}(m, 0)\rangle_{E_2}$ which is independent of N agree either with the leading term of the $T \to T_c$ limit of expansions (VII.5.29) or (VII.6.11) of $\mathfrak{S}_{1,1}^0(m, 0)$, which are valid for $m|T - T_c| \gg 1$, or with the leading term of the $t \to \infty$ ($t' \to \infty$) behavior of $\mathfrak{S}^0_{1,1}(m, 0)$ given by expansions (VII.8.41) or (VII.8.42), which are valid for $m|T - T_c| = O(1)$. We do not expect to be able to reproduce more than the first term that depends on m of the expansion because the approximation (3.9) neglects all terms of order $O(N^{-2})$.

We carry this out by substituting $\hat{U}(q)$ from (2.20) in (3.9) and using (2.48) to find

$$\langle \mathfrak{S}_{1,1}(m, 0)\rangle_{E_2} = -\frac{1}{8}\frac{(1 + z_{1c})^2}{z_{1c}}\frac{1}{\pi}N^{-2} \times \int_0^\infty d\phi \sin \bar{m}\phi\left(\frac{\delta}{\phi} + 1 + \frac{d \ln K_\delta(\phi)}{d\phi}\right) + \bar{f}(m) + O(N^{-2}). \tag{3.11}$$

When $|\delta| \to \infty$ we use the asymptotic expansion (2.49) and obtain

$$\langle \mathfrak{S}_{1,1}(m, 0)\rangle_{E_2} \sim \frac{1}{8}\frac{(1 + z_{1c})^2}{z_{1c}}\frac{1}{\pi}N^{-2}\int_0^\infty d\phi \sin \bar{m}\phi \times \left[-\frac{\delta}{\phi} + \frac{(\phi^2 + \delta^2)^{1/2}}{\phi} - 1 + \frac{1}{2}\frac{\phi}{\delta^2 + \phi^2}\right] + \bar{f}(m). \tag{3.12}$$

Since

$$\begin{aligned}
\int_0^\infty d\phi \sin \bar{m}\phi&\left[\frac{(\phi^2 + \delta^2)^{1/2}}{\phi} - 1\right] \\
&= \frac{1}{2i}\int_{-\infty}^\infty d\phi e^{i\bar{m}\phi}\left\{\left[\frac{(\phi^2 + \delta^2)^{1/2} - |\delta|}{\phi}\right] - 1\right\} + \frac{\pi}{2}|\delta| \\
&= \frac{\pi}{2}|\delta| + |\delta|\int_1^\infty d\xi e^{-\bar{m}|\delta|\xi}\frac{(\xi^2 - 1)^{1/2}}{\xi} \\
&= \frac{\pi}{2}|\delta| + |\delta|\int_{\bar{m}|\delta|}^\infty d\xi' \frac{K_1(\xi')}{\xi'}
\end{aligned} \tag{3.13}$$

and

$$\int_0^\infty d\phi \frac{\phi}{\phi^2 + \delta^2}\sin \bar{m}\phi = \frac{\pi}{2}e^{-\bar{m}|\delta|}, \tag{3.14}$$

we explicitly find

$$\langle \mathfrak{S}_{1,1}(m, 0)\rangle_{E_2} \xrightarrow[|\delta| \to \infty]{} \frac{1}{8}\frac{(1 + z_{1c})^2}{z_{1c}}\frac{1}{\pi}N^{-2} \times \left\{-\frac{\pi}{2}(\delta - |\delta|) + |\delta|\int_{\bar{m}|\delta|}^\infty d\xi \frac{K_1(\xi)}{\xi} + \frac{\pi}{4}e^{-\bar{m}|\delta|}\right\} + \bar{f}(m). \tag{3.15}$$

The first two terms in this expansion do not depend on N when $|\delta| \sim N^2$, and they agree with the leading term of (VII.8.40) when $T > T_c$ and with the first two terms of (VII.8.40) when $T < T_c$. Therefore we conclude that

$$\bar{f}(m) = 0. \tag{3.16}$$

To analyze further $\langle \mathfrak{S}_{1,1}(m, 0)\rangle_{E_2}$ it is useful to rewrite (3.11). First note that, since

$$K_{|\delta|}(\phi) \sim \text{const}\ \phi^{-|\delta|} \quad \text{for} \quad \phi \sim 0, \tag{3.17}$$

we have

$$\begin{aligned}\int_0^\infty d\phi \sin \bar{m}\phi\left[\frac{d \ln K_{|\delta|}(\phi)}{d\phi} + 1\right] &\\ = -\frac{\pi}{2}|\delta| + \frac{1}{2i}\int_0^\infty & d\phi e^{i\bar{m}\phi}\left[\frac{d}{d\phi}\ln \phi^{|\delta|}K_{|\delta|}(\phi) + 1\right]\\ -\frac{1}{2i}\int_0^\infty & d\phi e^{-i\bar{m}\phi}\left[\frac{d}{d\phi}\ln \phi^{|\delta|}K_{|\delta|}(\phi) + 1\right].\end{aligned} \tag{3.18}$$

In the first (second) integral, we may deform the contour of integration to the positive (negative) imaginary ϕ-axis. Then we may use the relation[9]

$$(e^{\pm \pi i/2}\xi)^{|\delta|}K_{|\delta|}(e^{\pm \pi i/2}\xi) = \tfrac{1}{2}\xi^{|\delta|}\pi[-Y_{|\delta|}(\xi) \mp iJ_{|\delta|}(\xi)], \tag{3.19}$$

where $J_{|\delta|}(\xi)$ and $Y_{|\delta|}(\xi)$ are the Bessel functions of the first and second kind which are defined as

$$J_\delta(\phi) = \sum_{l=0}^{\infty} \frac{(-1)^l(\phi/2)^{2l+\delta}}{l!\,\Gamma(l + \delta + 1)} \tag{3.20}$$

and

$$Y_\delta(\phi) = [J_\delta(\phi)\cos \delta\pi - J_{-\delta}(\phi)]/\sin \delta\pi. \tag{3.21}$$

Thus we obtain the desired result

$$\begin{aligned}&\langle \mathfrak{S}_{1,1}(m, 0)\rangle_{E_2}\\ &\quad = \frac{1}{8}\frac{(1 + z_{1c})^2}{z_{1c}}\frac{1}{\pi}N^{-2}\\ &\quad\times\left\{\frac{\pi}{2}[-\delta + |\delta|] + \frac{2}{\pi}\int_0^\infty d\xi \frac{e^{-\bar{m}\xi}}{\xi}\frac{1}{Y_{|\delta|}^2(\xi) + J_{|\delta|}^2(\xi)}\right\} + o(N^{-2}).\end{aligned} \tag{3.22}$$

In this form, it is clear that

$$\begin{aligned}\lim_{m\to\infty}\langle \mathfrak{S}_{1,1}(m, 0)\rangle_{E_2} &= \begin{cases}\dfrac{1}{8}\dfrac{(1 + z_{1c})^2}{z_{1c}}N^{-2}|\delta| & T < T_c\\ 0 & T > T_c\end{cases}\\ &= [\mathfrak{M}_1^0(0^+)]^2,\end{aligned} \tag{3.23}$$

9. Reference 4, vol. 2, p. 6.

where the last equation may be obtained from (2.38). This is exactly the value that is obtained in the Onsager lattice. This contrasts strongly with the value of $\langle \mathfrak{M}_1(\mathfrak{H})\rangle_{E_2}$ obtained in Sec. 2 and is a vivid demonstration of the fact that $\mathfrak{M}_1(\mathfrak{H})$ is not a probability 1 object.

In general, $\langle \mathfrak{S}_{1,1}(m, 0)\rangle_{E_2}$ cannot be expressed in terms of tabulated functions. When $|\delta| = \frac{1}{2}$ or $\frac{3}{2}$, however, more simplification is possible.

(i) $|\delta| = \frac{1}{2}$

In this case

$$J^2_{1/2}(\xi) + Y^2_{1/2}(\xi) = 2/\pi\xi \tag{3.24}$$

and we find

$$\langle \mathfrak{S}_{1,1}(m, 0)\rangle_{E_2} = \frac{1}{8}\frac{(1 + z_{1c})^2}{z_{1c}}\frac{1}{\pi}N^{-2}\left\{\frac{\pi}{2}[-\delta + \tfrac{1}{2}] + \frac{1}{\bar{m}}\right\} + o(N^{-2}). \tag{3.25}$$

This is precisely equal to the leading term of the $T = T_c$, $\mathfrak{H} = 0$ expansion of $\mathfrak{S}^0_{1,1}(m, 0)$ for large m given by (VII.8.42). Furthermore, this approaches its $\bar{m} \to \infty$ limit as $1/\bar{m}$. But since $T \neq T_c$, this slow algebraic approach to the $\bar{m} \to \infty$ limit contrasts dramatically with the exponential approach to the $\bar{m} \to \infty$ limit exhibited by $\mathfrak{S}^0_{1,1}(m, 0)$, and assumed by the "critical exponent" description of correlation functions discussed in the introduction.

(ii) $|\delta| = \frac{3}{2}$

In this case

$$J^2_{3/2}(\xi) + Y^2_{3/2}(\xi) = (2/\pi\xi)(1 + 1/\xi^2) \tag{3.26}$$

and we find

$$\begin{aligned}\langle \mathfrak{S}_{1,1}(m, 0)\rangle_{E_2} &= \frac{1}{8}\frac{(1 + z_{1c})^2}{z_{1c}}\frac{1}{\pi}N^{-2} \\ &\times \left\{\frac{\pi}{2}[-\delta + \tfrac{3}{2}] + \frac{1}{\bar{m}} - \int_0^\infty d\alpha\, \frac{1}{\alpha + 1}\sin \bar{m}\alpha\right\} + o(N^{-2}).\end{aligned} \tag{3.27}$$

Let $\alpha'/\bar{m} = \alpha + 1$ and find

$$\begin{aligned}\langle \mathfrak{S}_{1,1}(m, 0)\rangle_{E_2} &= \frac{1}{8}\frac{(1 + z_{1c})^2}{z_{1c}}\frac{1}{\pi}N^{-2} \\ &\times \left[\frac{\pi}{2}(-\delta + \tfrac{3}{2}) + \frac{1}{\bar{m}} - \sin \bar{m}\,\mathrm{Ci}\,\bar{m} + \cos \bar{m}\,\mathrm{si}\,\bar{m}\right] + o(N^{-2}),\end{aligned} \tag{3.28}$$

where Ci $\overline{m}$ and si $\overline{m}$ are the sine and cosine integrals defined by (VII.8.50) and (VII.8.51). When $\overline{m}$ is small we may use the expansion[10] of Ci $\overline{m}$ and si $\overline{m}$ to write

$$\langle \mathfrak{S}_{1,1}(m,0)\rangle_{E_2} = \frac{1}{8}\frac{(1+z_{1c})^2}{z_{1c}}\frac{1}{\pi}N^{-2}\Bigg\{\frac{\pi}{2}(-\delta+\tfrac{3}{2})+\frac{1}{\overline{m}} - \sin\overline{m}\left[\gamma+\ln\overline{m}+\sum_{n=1}^{\infty}\frac{(-1)^n\overline{m}^{2n}}{(2n)!\,2n}\right] - \cos\overline{m}\left[\frac{\pi}{2}-\sum_{n=1}^{\infty}\frac{(-1)^n\overline{m}^{2n+1}}{(2n+1)!\,(2n+1)}\right]\Bigg\} + o(N^{-2}). \tag{3.29}$$

This is clearly not *equal* to the leading term of the $T = T_c$, $\mathfrak{H} = 0$ expansion of $\mathfrak{S}^0_{1,1}(m,0)$ given in Chapter VII, but it *approaches* it as $\overline{m} \to 0$. When $\overline{m}$ is large, we have the asymptotic expansion

$$\langle \mathfrak{S}_{1,1}(m,0)\rangle_{E_2} \sim \frac{1}{8}\frac{(1+z_{1c})^2}{z_{1c}}\frac{1}{\pi}N^{-2} \times\left\{\frac{\pi}{2}(-\delta+\tfrac{3}{2})-\sum_{n=1}^{\infty}(-1)^n(2n)!\,\overline{m}^{-2n-1}\right\}. \tag{3.30}$$

Again we see that the approach to the $\overline{m} \to \infty$ limit is algebraic rather than exponential.

With the orientation provided by these two special cases, we turn to the general case and study the most interesting limiting cases of (3.22): (*a*) δ fixed, $\overline{m} \to 0$; (*b*) $\delta \neq 0$ fixed, $\overline{m} \to \infty$; and (*c*) $\delta = 0$, $\overline{m} \to \infty$.

(*a*) δ fixed, $\overline{m} \to 0$

In this case, we expect to make contact with Chapter VII. In particular, we expect that when $\overline{m} \sim N^{-2}$ the term independent of N should agree with the $T = T_c$, $m \to \infty$ behavior of $\mathfrak{S}^0_{1,1}(m,0)$ given in (VII. 8.42). We have previously seen in the special cases $|\delta| = \frac{1}{2}$ and $|\delta| = \frac{3}{2}$ that this is the case but that in the case of $|\delta| = \frac{3}{2}$ the approach to this limit is somewhat complicated by the presence of terms involving $\ln \overline{m}$.

To study this limit in the general case, we note[11] that for large ξ

$$J^2_{|\delta|}(\xi) + Y^2_{|\delta|}(\xi) \sim \frac{2}{\pi\xi}\sum_{k=0}^{\infty}[1\cdot 3\cdots(2k-1)]\frac{\Gamma(\frac{1}{2}+|\delta|+k)}{\Gamma(\frac{1}{2}+|\delta|-k)}\frac{1}{2^k\xi^{2k}} \sim \frac{2}{\pi\xi}[1+\tfrac{1}{8}(4\delta^2-1)/\xi^2+\cdots], \tag{3.31}$$

10. Reference 4, vol. 2, p. 146.
11. See, for example, G. N. Watson, *A Treatise on the Theory of Bessel Functions* (Cambridge University Press, Cambridge, England, 1945) p. 449.

where for our limited purpose we retain only the first two terms. We then write

$$\int_0^\infty d\xi e^{-\bar{m}\xi} \frac{2}{\pi\xi} \frac{1}{Y_{|\delta|}^2(\xi) + J_{|\delta|}^2(\xi)}$$
$$= \int_0^\infty d\xi e^{-\bar{m}\xi}\left[\frac{2}{\pi\xi} \frac{1}{Y_{|\delta|}^2(\xi) + J_{|\delta|}^2(\xi)} - 1 + \frac{1}{8}\frac{4\delta^2 - 1}{1 + \xi^2}\right]$$
$$+ \int_0^\infty d\xi e^{-\bar{m}\xi}\left(1 - \frac{1}{8}\frac{4\delta^2 - 1}{1 + \xi^2}\right). \tag{3.32}$$

In the first integral, we write

$$e^{-\bar{m}\xi} = 1 - \bar{m}\xi + \tfrac{1}{2}\bar{m}^2\xi^2 + (e^{-\bar{m}\xi} - 1 + \bar{m}\xi - \tfrac{1}{2}\bar{m}^2\xi^2). \tag{3.33}$$

The last integral is of the same form as was studied in the special case $|\delta| = \frac{3}{2}$. Thus

$$\int_0^\infty d\xi e^{-\bar{m}\xi} \frac{2}{\pi\xi} \frac{1}{Y_{|\delta|}^2(\xi) + J_{|\delta|}^2(\xi)}$$
$$= A_0(\delta) + \bar{m}A_1(\delta) + \tfrac{1}{2}\bar{m}^2 A_2(\delta) + o(\bar{m}^2) + \bar{m}^{-1}$$
$$- \tfrac{1}{8}(4\delta^2 - 1)[\sin\bar{m}\,\mathrm{Ci}\,\bar{m} - \cos\bar{m}\,\mathrm{si}\,\bar{m}], \tag{3.34}$$

where

$$A_j(\delta) = \int_0^\infty d\xi\xi^j\left[\frac{2}{\pi\xi}\frac{1}{Y_{|\delta|}^2(\xi) + J_{|\delta|}^2(\xi)} - 1 + \frac{1}{8}\frac{4\delta^2 - 1}{1 + \xi^2}\right], \qquad j = 0, 1, 2. \tag{3.35}$$

We may use the expansions of Ci and si and obtain

$$\langle \mathfrak{S}_{1,1}(m, 0)\rangle_{E_2} \xrightarrow[\bar{m}\to 0]{} \frac{1}{8}\frac{(1 + z_{1c})^2}{z_{1c}}\frac{1}{\pi}N^{-2}\left\{\frac{\pi}{2}(-\delta + |\delta|) + \frac{1}{\bar{m}} + A_0(\delta)\right.$$
$$- \frac{\pi}{10}(4\delta^2 - 1) - \tfrac{1}{8}(4\delta^2 - 1)\bar{m}\ln\bar{m}$$
$$+ \bar{m}[A_1(\delta) - \tfrac{1}{8}(4\delta^2 - 1)(\gamma + \tfrac{1}{18})]$$
$$\left. + \bar{m}^2\tfrac{1}{2}A_2(\delta) + O(\bar{m}^2)\right\}. \tag{3.36}$$

As expected, when $\bar{m} \sim N^{-2}$ the term independent of N agrees with (VII.8.42).

(*b*) $\bar{m} \to \infty$, $\delta \neq 0$

The most unusual feature of (3.22) is its asymptotic behavior as $\bar{m} \to \infty$. We have already seen in the special cases $|\delta| = \frac{1}{2}$ and $|\delta| = \frac{3}{2}$ that this behavior is algebraic rather than exponential and is therefore not of the form assumed by the "critical exponent" parameterization. To see that this behavior holds for general values of δ we approximate for small ξ and $|\delta| \neq 1$,

$$\frac{1}{Y_{|\delta|}^2(\xi) + J_{|\delta|}^2(\xi)} = \frac{\pi^2}{[\Gamma(|\delta|)]^2}\left(\frac{\xi}{2}\right)^{2|\delta|}\left[1 + 2\left(\frac{\xi}{2}\right)^2 \frac{1}{1-|\delta|} + 2\left(\frac{\xi}{2}\right)^{2|\delta|} \times \cos|\delta|\pi \frac{\Gamma(-|\delta|+1)}{\Gamma(|\delta|+1)} + O(\xi^{4|\delta|}) + O(\xi^{2|\delta|+2})\right] \tag{3.37}$$

and thus find that (3.22) asymptotically becomes

$$\begin{aligned}\langle \mathfrak{S}_{1,1}(m,0)\rangle_{E_2} \xrightarrow[\bar{m}\to\infty]{} & \frac{1}{8}\frac{(1+z_{1c})^2}{z_{1c}} N^{-2}\left\{\frac{1}{2}[-\delta + |\delta|] + \frac{2}{[\Gamma(|\delta|)]^2}\right.\\ & \times\left[(2\bar{m})^{-2|\delta|}\Gamma(2|\delta|) + 2(2\bar{m})^{-2|\delta|-2}\Gamma(2|\delta|+2)\right.\\ & \times \frac{1}{1-|\delta|} + 2(2\bar{m})^{-4|\delta|}\cos|\delta|\pi\frac{\Gamma(1-|\delta|)\Gamma(4|\delta|)}{\Gamma(1+|\delta|)}\\ & \left.\left. + O(\bar{m}^{-6|\delta|}) + O(\bar{m}^{-4|\delta|-2})\right]\right\}.\end{aligned} \tag{3.38}$$

When $|\delta| = \frac{1}{2}$ or $\frac{3}{2}$ the terms in $1/\bar{m}$ that are explicitly given here agree with the preceding results. We may study the case $|\delta| = 1$ by letting $|\delta| \to 1$ in (3.38) and find

$$\begin{aligned}\langle \mathfrak{S}_{1,1}(m,0)\rangle_{E_2}\big|_{|\delta|=1} \xrightarrow[\bar{m}\to\infty]{} & \frac{1}{8}\frac{(1+z_{1c})^2}{z_{1c}} N^{-2}\left\{\frac{1}{2}[-\delta + |\delta|]\right.\\ & \left. + \tfrac{1}{2}\bar{m}^{-2} + \tfrac{1}{2}\bar{m}^{-4}[-3\ln 2\bar{m} + 4] + o(\bar{m}^{-4})\right\}.\end{aligned} \tag{3.39}$$

When $0 < |\delta| \leq \frac{1}{2}$, the leading term in (3.38) is still correct, but the neglected terms of order $O(\bar{m}^{-6|\delta|})$ are now larger than the retained terms of order $O(\bar{m}^{-4|\delta|})$ and thus these higher terms are no longer meaningful. Indeed, when $|\delta| \to 0$, (3.38) loses its validity altogether.

(*c*) $\bar{m} \to \infty$, $\delta = 0$

The final limiting case of $\langle \mathfrak{S}_{1,1}(m,0)\rangle_{E_2}$ to be considered is $\bar{m} \to \infty$ and $T = T_c$. This is the one temperature at which the "critical exponent" description allows a spin-spin correlation function to approach its limiting value in a power-law fashion as parameterized by (1.14*d*). In the bulk of the two-dimensional Ising model, $\eta = \frac{1}{4}$, whereas on the boundary $\eta = 1$. However, we have just seen that, if $|\delta|$ is made sufficiently small, in our random model, even if $T \neq T_c$, $\langle \mathfrak{S}_{1,1}(m,0)\rangle_{E_2}$ may be made to approach its $m \to \infty$ value in a power-law fashion with a power as close to zero as we please. Therefore, it is expected that at T_c $\langle \mathfrak{S}_{1,1}(m, 0)\rangle_{E_2}$ will not be of the form (1.14d). To see that this is indeed so, we approximate[12] for small ξ,

$$\frac{1}{Y_0^2(\xi) + J_0^2(\xi)} \sim \left[\frac{4}{\pi^2}\left(\ln \frac{\xi}{A'}\right)^2 + 1\right]^{-1}$$
$$\sim \tfrac{1}{4}\pi^2\left(\ln\frac{\xi}{A'}\right)^{-2}\left[1 - \tfrac{1}{4}\pi^2\left(\ln\frac{\xi}{A'}\right)^{-2} + \cdots\right], \tag{3.40}$$

where

$$A' = 2e^{-\gamma+1}. \tag{3.41}$$

Therefore,

$$\langle \mathfrak{S}_{1,1}(m, 0)\rangle_{E_2}|_{\delta=0} \sim \frac{1}{16}\frac{(1 + z_{1c})^2}{z_{1c}} N^{-2} \int_0^\infty d\xi e^{-\bar{m}\xi} \frac{1}{\xi}\left(\ln\frac{\xi}{A'}\right)^{-2}$$
$$\times \left[1 - \tfrac{1}{4}\pi^2\left(\ln\frac{\xi}{A'}\right)^{-2}\right]$$
$$= -\bar{m}\frac{1}{16}\frac{(1 + z_{1c})^2}{z_{1c}} N^{-2} \int_0^\infty d\xi e^{-\bar{m}\xi}\left[\left(\ln\frac{\xi}{A'}\right)^{-1}\right.$$
$$\left. - \tfrac{1}{12}\pi^2\left(\ln\frac{\xi}{A'}\right)^{-3}\right], \tag{3.42}$$

where to obtain the last expression we have integrated by parts. We now may let $x = \bar{m}\xi$ and expand the logarithms as

$$\frac{1}{\ln x/\bar{m}A'} \sim \frac{1}{-\ln \bar{m}A'}\left[1 + \frac{\ln x}{\ln \bar{m}A'} + \left(\frac{\ln x}{\ln \bar{m}A'}\right)^2 + \cdots\right], \tag{3.43}$$

to obtain the desired result,

$$\langle \mathfrak{S}_{1,1}(m, 0)\rangle_{E_2}|_{\delta=0} \sim \frac{1}{16}\frac{(1 + z_{1c})^2}{z_{1c}} N^{-2}\frac{1}{\ln A'\bar{m}}$$
$$\times \left\{1 - \frac{\gamma}{\ln A'\bar{m}} + \left(\gamma^2 - \frac{\pi^2}{12}\right)\frac{1}{(\ln A'\bar{m})^2}\right\}. \tag{3.44}$$

12. Reference 4, vol. 2, pp. 6, 7.

CHAPTER XVI
Epilogue

We have now concluded our tour of the map of the Ising model that was presented in Fig. 0.1 of the Preface. In the course of this trip we have examined each facet of the subject in fine and complete detail. The trip being completed, we can now sit back and have a relaxed overview of the entire expedition.

In the Preface we stated three goals of this book. We feel that the second and third of these goals have been met. Furthermore, throughout the text we have, at appropriate places, given as precise a formulation as we are able of unsolved problems to which we believe future attention should be directed. But in and of itself, this does not quite meet the first and most important goal of this book, because without further comment these problems remain buried in the text where only the most dedicated of readers will find them. The first goal is attained only if the current status and future problems of the two-dimensional Ising model are made easily accessible to all. Accordingly, we have listed in Tables 2–5 our opinions about what problems exist and where progress should be sought. Of course, it must be recognized that, though a description of an accomplished fact can be made objective, prognostications of future research must necessarily be subjective. Therefore, we freely admit that by their very existence these tables incorporate our own biased point of view.

The first and most important bias embodied in these tables is that there are four of them. This represents our belief that the Ising model comprises at least four submodels: (1) Onsager's lattice at $H = 0$, (2) the boundary of Onsager's lattice which interacts with the magnetic field $\mathfrak{H}$, (3) the random lattice of Chapter XIV at $H = 0$, and (4) the boundary of this random lattice with the magnetic field $\mathfrak{H}$. Within these four categories we denote our opinions as follows:

TABLE 2. Onsager's lattice with $H = 0$.

Property	Prospect of doing future research	Reference to known results
Specific heat	0	(V.2.24)
Spontaneous magnetization	0	(X.4.9)
Behavior of spin-spin correlation functions for widely separated spins:		(XI.2.43, 2.46, 3.24, 3.27)
(1) T away from T_c	0	(XII.3.50, 4.39)
(2) $T = T_c$	1	(XI.4.43, 7.2)
(3) T near T_c	1	XII, Sec. 5
Magnetic susceptibility	1	XII, Sec. 5
Magnetization for $T = T_c$, $H \sim 0$	2	XIII, Sec. 3

TABLE 3. Boundary of Onsager's lattice interacting with the field $\mathfrak{H}$.

Property	Prospect of doing future research	Reference to known results
Specific heat	0	VI, Sec. 4
On the boundary row:		
(1) magnetization	0	(VI.5.1)
(2) spin-spin correlation functions	0	VII
Relation of magnetization and spin-spin correlation functions of rows at finite distance from boundary to their bulk values	2	XIII, Sec. 4

TABLE 4. The random Ising lattice with $H = 0$.

Property	Prospect of doing future research	Reference to known results
Specific heat	1	(XIV.4.40)
Spontaneous magnetization	1	XV, Sec. 1
Behavior of average spin-spin correlation functions for widely separated spins	1	XV, Sec. 1
Magnetic susceptibility	2	XV, Sec. 1
Magnetization for $T = T_c$, $H \sim 0$	2	XV, Sec. 1
Probability distribution for spin correlation functions	3	

TABLE 5. The boundary of the random Ising lattice interacting with the field $\mathfrak{H}$.

Property	Prospect of doing future research	Reference to known results
Specific heat	3	
On the boundary row:		
(1) average magnetization	1	(XV.2.24)
(2) average spin-spin correlation functions	1	XV, Sec. 3
(3) probability distribution for boundary magnetization and spin-spin correlation functions	1	(XV.1.26)
Relation of average magnetization and spin-spin correlation functions of rows at finite distance from boundary to their bulk values	3	

0 = Everything is known; there is nothing more to be done.[1]

1 = Something is known; progress can certainly be made.

2 = Something is known; progress may be hoped for.

3 = Little or nothing is known; we do not see how progress can be made.

In all cases where something is known about a topic, we have listed the appropriate chapter, section, and, when possible, equation number where this information may be found. For example, in connection with Table 2, the results concerning the asymptotic expansion of $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ for $T \neq T_c$ are given by Eqs. (2.43), (2.46), (3.24), and (3.27) of Chapter XI and Eqs. (3.50) and (4.39) of Chapter XII. These constitute a complete set of results since they cover all possible values of M/N and all $T \neq T_c$. Therefore the prospect of doing further research is 0. On the other hand,

1. It must be recognized that, while the entire development in this book rests on the use of Pfaffians, the two-dimensional Ising model does not *have* to be solved this way. Indeed, the original approach of Onsager does not involve Pfaffians at all. By the phrase "nothing more to be done" we mean that there is no quantity whose analytic expression is unknown. Without a doubt the known results can be obtained by many different methods, but we feel that such an investigation, which merely reproduces known results, is pointless. To be of value, such a reproduction must either represent true simplification or result in new physical insights. In all cases which are marked by a "0" we do not believe that alternative derivations will give either new insights or true simplification.

in the case $T = T_c$, the results for the asymptotic expansion of $\langle\sigma_{0,0}\sigma_{M,N}\rangle$, given by Eqs. (4.43) and (7.2) of Chapter XI, cover only the three special cases $M = 0$, $N = 0$, and $M = N$. Thus complete information is not known, and we rate its prospect for future research as 1.

We also wish to draw the reader's attention to two detailed discussions of unsolved problems in this book. The first of these discussions is in Sec. 5 of Chapter XII. There we are concerned with some conjectures about the asymptotic behavior of $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ at the critical temperature T_c. Furthermore, in that section we make precise the meaning of the phrase "T near T_c" and show how the asymptotic expansion for T near T_c is related to the behavior of the magnetic susceptibility near T_c.

The second discussion is to be found in Sec. 5 of Chapter XIV. There we point out in detail the many technical assumptions in our treatment of random impurities. Of these restricting assumptions we wish to re-emphasize that our model of random impurities does not allow all bonds to be independent random variables. It would be most interesting to relax this restriction and to study a fully random model. Unfortunately, we do not have the slightest idea how this can be done.

In addition to these comments on the tables, several further remarks need to be made about what we have not listed.

As mentioned in the Introduction, we have confined ourselves, with one exception in Chapter VIII, to the square lattice. Such a restriction is not necessary and, as the example of the triangular lattice in Chapter VIII shows, the consideration of other solvable lattices is at times useful. On the other hand, it is our opinion that the most interesting feature of the other nearest-neighbor two-dimensional Ising lattices is the fact that they are uninteresting. The investigation of the specific heat and spontaneous magnetization of these lattices shows that, though T_c varies from lattice to lattice, the behavior of all these lattices near T_c is qualitatively the same. In all cases the specific heat diverges as $\ln |T - T_c|$ and the bulk spontaneous magnetization vanishes as $(T_c - T)^{1/8}$. Accordingly, we feel that a complete study of these lattices is a waste of time. There is no point in reproducing all the computations done on the square lattice for the triangular, hexagonal, Kagome, and other lattices unless the computation reveals some physical phenomenon not already exhibited by the square lattice.

Conspicuously missing from the tables of future problems are:

(1) the calculation of the free energy of the two-dimensional Ising model when $H \neq 0$, and

(2) the calculation of the free energy of the three-dimensional Ising model.

This omission is intentional. These two problems are both extremely difficult. Indeed, they have existed for a quarter of a century and absolutely no progress has been made.[2] Of course there is no denying that it would be nice to have them solved exactly. However, we contend that it is an impediment rather than an incentive to progress to focus on these two problems. Instead one must critically determine what information one really wants from their solutions.

For the first problem, we feel that there are only two physically significant questions to ask. First, for $T < T_c$ it is important to obtain the analytic properties at $H = 0$ of $M(H)$, the magnetization as a function of the applied magnetic field, and to determine whether or not $M(H)$ can be analytically continued beyond $H = 0$. If $M(H)$ can be so continued, a second physical question related to hysteresis may be asked, namely, how far beyond $H = 0$ can the analytic continuation be carried out.[3] It may not be impossible to answer the first question without having an explicit closed form for $M(H)$. However, to answer the second question such a closed form appears indispensable.

Our interest in the three-dimensional Ising model is even more circumscribed. The importance of the two-dimensional model is due to the physical insight into phase transitions it provides. Unless the information contained in an exact solution to the three-dimensional model provides us with additional insight, this solution, while mathematically satisfying and exquisite, will be physically useless.

With this discussion of problems to be solved, as given in Tables 2–5, we have fulfilled our original goals as far as we are able. How well we have actually attained these goals can only be judged by the reader. We should be most pleased if our book can in any way contribute to its own obsolescence by stimulating progress in this field.

2. By no progress, we mean no progress toward an explicit solution. However, a few inequalities have been proved. In particular, beyond the very general property that $\partial M/\partial H > 0$ for all H, it has been shown by R. B. Griffiths, C. A. Hurst, and S. Sherman that $\partial^2 M/\partial H^2 \leq 0$ for $H > 0$.

3. For the solution of these problems in the simpler case where the magnetic field is applied to the boundary row only, see Chapter VI, in particular Sec. 5(C).

APPENDIX A

We collect in this appendix several theorems concerning certain combinations of thermal averages of products of σ's. These results are set aside in an appendix because they are of a more general character than most of the other results in this book. In particular, the results of this appendix are just as valid for three as for two dimensions. For this reason, it is useful to change the notation and label a lattice site not by the double indices j and k, but just by a single index. Furthermore, the restriction to nearest-neighbor interactions made at the very beginning of the text will not be made in this appendix. Also, the magnetic interaction of a spin with an external magnetic field will be allowed to vary from spin to spin. Therefore, we consider the interaction energy

$$\mathscr{E} = -\sum_{j<k} E_{j,k}\sigma_j\sigma_k - \sum_j H_j\sigma_j, \tag{A.1}$$

where the sum over j and k is over all sites of the lattice. In this appendix, N will denote the total number of lattice sites, and N will always be kept finite.

In terms of these notations, we will prove several results which have been noted in the text. In particular, we will show that if all $E_{j,k} \geq 0$ and all nonvanishing H_j are of the same sign, then

$$\langle\sigma_j\sigma_k\sigma_l\sigma_m\rangle_N - \langle\sigma_j\sigma_k\rangle_N\langle\sigma_l\sigma_m\rangle_N \geq 0, \tag{A.2}$$

where $\langle\ \rangle_N$ indicates a thermal average in the lattice of N sites. An immediate consequence of this inequality is that

$$\frac{\partial\langle\sigma_j\sigma_k\rangle_N}{\partial E_{l,m}} = \frac{1}{Z}\,[\langle\sigma_j\sigma_k\sigma_l\sigma_m\rangle_N - \langle\sigma_j\sigma_k\rangle_N\langle\sigma_l\sigma_m\rangle_N] \geq 0. \tag{A.3}$$

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We also show that

$$\operatorname{sgn} H_j \frac{\partial \langle \sigma_j \sigma_k \rangle_N}{\partial H_j} \geq 0, \tag{A.4}$$

$$\operatorname{sgn} H_j \frac{\partial \langle \sigma_j \rangle_N}{\partial E_l} \geq 0, \tag{A.5}$$

and

$$\frac{\partial \langle \sigma_j \rangle_N}{\partial H_l} \geq 0. \tag{A.6}$$

These are the results referred to in the text as Griffiths' theorem.[1]

To prove these results, we first establish several elementary properties of spin correlation functions. Consider first the case $H_j = 0$. Then it is clear from symmetry considerations that

$$\langle \sigma_j \rangle_N = 0. \tag{A.7}$$

More generally, the average of any product of an odd number of σ's vanishes. In addition we may establish

Theorem 1. If $H_j = 0$ and all $E_{j,k} \geq 0$, then the average of an even number of σ's is nonnegative.

Proof. It is convenient to note that the addition of a constant $\mathscr{E}_0$ to the right-hand side of (A.1) affects the partition function only by multiplying it by $e^{-\beta \mathscr{E}_0}$. Such an extra factor in the partition function adds a temperature-independent constant to the Helmholtz free energy but does not affect the average of any product of σ's. Therefore, instead of considering $\mathscr{E}$ we will, for convenience, consider $\mathscr{E}'$, defined by

$$\mathscr{E}' = -\sum_{\substack{j,k \\ j<k}} E_{j,k}(\sigma_j \sigma_k - 1). \tag{A.8}$$

By definition, the partition function Z_N' of $\mathscr{E}'$ with N sites is positive. To prove Theorem 1, consider first the special case $\langle \sigma_j \sigma_k \rangle_N$. If $N = 2$, then

$$Z_N' \langle \sigma_j \sigma_k \rangle_N = 2[1 - e^{-2\beta E_{j,k}}] \geq 0. \tag{A.9}$$

To extend this result to a general value of N we proceed by induction. We assume that

$$\langle \sigma_j \sigma_k \rangle_N \geq 0 \tag{A.10}$$

1. The inequalities (A.3) and (A.5) were first derived for $H = 0$ by R. B. Griffiths, *J. Math. Phys.* **8**, 478 (1967). In particular, (A.2) is derived in this paper and, because it is the second theorem of the paper, it is sometimes called Griffiths' second inequality. The generalization of (A.4) and (A.6) to $H \neq 0$ and the derivation of (A.4) and (A.6) are given in a companion paper by R. B. Griffiths, *J. Math. Phys.* **8**, 484 (1967).

for all j and k in every system of N spins. We then must prove that this guarantees that

$$\langle\sigma_j\sigma_k\rangle_{N+1} \geq 0 \tag{A.11}$$

for all j and k in every system of $N + 1$ spins which may be formed by adding a new spin to the old lattice. Denote the added spin by σ_l. There are two cases to consider: (1) $l = j$ or $l = k$, and (2) $l \neq j$ and $l \neq k$. We consider the second case first. For convenience define

$$X_{m,m'} = e^{-\beta E_{m,m'}}. \tag{A.12}$$

Clearly $X_{m,m'}$ is a monotonically decreasing function of $E_{m,m'}$ which satisfies

$$X_{m,m'} = 1 \quad \text{if} \quad E_{m,m'} = 0 \tag{A.13}$$

and

$$X_{m,m'} = 0 \quad \text{if} \quad E_{m,m'} = \infty. \tag{A.14}$$

We connect σ_l to the system of N spins in several stages. First consider σ_l connected to only one other site, say σ_m. Clearly $Z'_{N+1}\langle\sigma_j\sigma_k\rangle_{N+1}$ is a linear function of $X_{l,m}$. Therefore, because of (A.13) and (A.14), it suffices to prove that

$$Z'_{N+1}\langle\sigma_j\sigma_k\rangle_{N+1} \geq 0 \tag{A.15}$$

for $X_{l,m} = 1$ and $X_{l,m} = 0$. If $X_{l,m} = 1$, the spin σ_l does not interact at all with the other spins and $\langle\sigma_j\sigma_k\rangle_{N+1}$ has the value $\langle\sigma_j\sigma_k\rangle_N$ which, by hypothesis, satisfies (A.10). On the other hand, if $X_{l,m} = 0$, then $E_{l,m} = \infty$. This infinite-strength interaction forces σ_l to have always the same value as σ_m. Therefore, in this case as well, $\langle\sigma_j\sigma_k\rangle_{N+1}$ has the value $\langle\sigma_j\sigma_k\rangle_N$. Accordingly we conclude that if σ_l is connected to the N spin lattice by one bond then (A.11) holds.

The same procedure allows us to prove that (A.11) holds when σ_l interacts with two spins. Let the second bond be to $\sigma_{m'}$. If $X_{l,m'} = 1$, then $E_{l,m'} = 0$. This is the case just considered. Furthermore, if $X_{l,m'} = 0$, then $E_{l,m'} = \infty$ and σ_l and $\sigma_{m'}$ must have the same value. Thus the system of $N + 1$ spins reduces to a new system of N spins and by hypothesis (A.10) holds for this new system. Therefore, using the linearity of $Z'_{N+1}\langle\sigma_j\sigma_k\rangle_{N+1}$ as a function of $X_{l,m'}$, we conclude that (A.11) holds when σ_l is connected to the rest of the spins by two bonds. This procedure may clearly be continued until σ_l is connected to all other spins of the system by bonds of arbitrary strength. Hence, we conclude that if the added spin σ_l is such that $l \neq k$ and $l \neq j$ then (A.11) holds.

To complete the proof for $\langle\sigma_j\sigma_k\rangle_{N+1}$ we must consider case 1, where the added spin σ_l is identical with one of the spins, say σ_j, whose average is being computed. But the proof that in this case (A.10) implies (A.11) is exactly similar to the proof just given. Therefore we conclude generally that the validity of (A.10) implies the validity of (A.11). But we have already seen in (A.9) that the conditions of the theorem insure that (A.10) holds for $N = 2$. Thus it follows by induction that (A.10) holds for all N.

To complete the proof of Theorem 1 we must show that this same procedure can be carried through for any product of an even number of σ's. It is clear that the proof that the validity of (A.10) implies the validity of (A.11) may be carried out no matter how many σ's are in the product. But, furthermore, we may also use this procedure to show that a product containing $2n$ spins must be positive in a lattice of $N = 2n$ spins. Therefore we conclude that Theorem 1 holds.

We next consider the more general case where either $H_j \geq 0$ or $H_j \leq 0$ for all j. In this case the average of an odd number of σ's does not have to vanish and Theorem 1 generalizes to

Theorem 2. If $E_{j,k} \geq 0$ and $H_j \geq 0$ or $H_j \leq 0$ then the thermal average of any even number of σ's is positive and the thermal average of any odd number of σ's has the same sign as do the nonvanishing H_j.

Proof. The proof is entirely similar to the proof of Theorem 1 with two exceptions. First we note that when $X_{l,m} = 0$ the spins σ_l and σ_m have the same value and act as if they are one spin which interacts with the magnetic field $H_l + H_m$. This field is nonnegative (nonpositive) because H_l and H_m are each separately nonnegative (nonpositive). Secondly, we note that when all $X_{m,m'} = 1$, functions involving an even number of σ's, like $Z'_N\langle\sigma_j\sigma_k\rangle_N$, are not zero but instead have a value, like

$$Z'_N\langle\sigma_j\sigma_k\rangle_N = (e^{\beta H_j} - e^{-\beta H_j})(e^{\beta H_k} - e^{-\beta H_k}), \tag{A.16}$$

which is positive if either $H_j \geq 0$ or $H_j \leq 0$. Similarly, when $X_{m,m'} = 1$, a function involving an odd number of σ's will have the same sign as the nonzero values of H_j. With these modifications, the proof of Theorem 1 applies and will be omitted.

We now turn to Griffiths' theorem. To give a concise proof[2] of this theorem we introduce some further notation. Let A, B, and C denote a configuration of the set of N spins. The spin variables σ_j are functions of the configuration. We make this apparent by writing $\sigma_j(A)$.

The utility of these notations is that it allows us to introduce the concept of the product AB of configuration A with configuration B, by making the definition that

$$\sigma_j(AB) = \sigma_j(A)\sigma_j(B). \tag{A.17}$$

2. The proof of Griffiths' theorem we give is that of J. Ginibre, *Phys. Rev. Letters* **23**, 828 (1969).

APPENDIX A

It is also convenient to let R and S stand for collections of sites and to write

$$\sigma_R = \prod_{r \in R} \sigma_r. \tag{A.18}$$

Define the product RS to be the collection of those sites which are either in R or in S but not in both. Then it is clear that since $\sigma_j^2 = 1$ we must have

$$\sigma_R \sigma_S = \sigma_{RS}. \tag{A.19}$$

We may now prove

Theorem 3. If $E_{j,k} \geq 0$ for all j and k, and if either $H_j \geq 0$ or $H_j \leq 0$ for all j, then, if the number of spins in the product σ_{RS} is even,

$$\langle \sigma_{RS} \rangle_N - \langle \sigma_R \rangle_N \langle \sigma_S \rangle_N \geq 0, \tag{A.20}$$

whereas if the number of spins in the product σ_{RS} is odd and there is some $H_j \neq 0$,

$$\operatorname{sgn}(H_j)[\langle \sigma_{RS} \rangle_N - \langle \sigma_R \rangle_N \langle \sigma_S \rangle_N] \geq 0. \tag{A.21}$$

Proof. By definition we have

$$\begin{aligned}
Z_N^2&[\langle \sigma_{RS} \rangle_N - \langle \sigma_R \rangle_N \langle \sigma_S \rangle_N] \\
&= Z_N \sum_A \sigma_{RS}(A) \exp[-\beta \mathscr{E}(A)] \\
&\quad - \left\{ \sum_A \sigma_R(A) \exp[-\beta \mathscr{E}(A)] \right\} \left\{ \sum_A \sigma_S(A) \exp[-\beta \mathscr{E}(A)] \right\} \\
&= \sum_A \sum_B [\sigma_{RS}(A) - \sigma_R(A)\sigma_S(B)] \exp[-\beta \mathscr{E}(A) - \beta \mathscr{E}(B)],
\end{aligned} \tag{A.22}$$

where $\sum_A$ indicates a summation over all possible configurations which A may assume and the dependence of the interaction energy $\mathscr{E}$ on the configuration A is made explicit. Let $C = AB$. Then we may use (A.17) and (A.19) to write

$$\sigma_R(A)\sigma_S(B) = \sigma_S(C)\sigma_{RS}(A) \tag{A.23}$$

and

$$\begin{aligned}
-&\mathscr{E}(A) - \mathscr{E}(B) \\
&= \sum_{j,k} E_{j,k}\sigma_j(A)\sigma_k(A) + \sum_j H_j \sigma_j(A) + \sum_{j,k} E_{j,k}\sigma_j(B)\sigma_k(B) + \sum_j H_j \sigma_j(B) \\
&= \sum_{j,k} E_{j,k}[1 + \sigma_j(C)\sigma_k(C)]\sigma_j(A)\sigma_k(A) + \sum_j H_j[1 + \sigma_j(C)]\sigma_j(A).
\end{aligned} \tag{A.24}$$

Using these identities, we convert the double summation over A and B to a summation over A and C to obtain

$$Z_N^2[\langle\sigma_{RS}\rangle_N - \langle\sigma_R\rangle_N\langle\sigma_S\rangle_N]$$

$$= \sum_C [1 - \sigma_S(C)]\left\{\sum_A \sigma_{RS}(A) \exp\left(\beta\right.\right.$$

$$\left.\left.\times \left[\sum_{j,k} E_{j,k}[1 + \sigma_j(C)\sigma_k(C)]\sigma_j(A)\sigma_k(A) + \sum_j H_j[1 + \sigma_j(C)]\sigma_j(A)\right]\right)\right\}. \quad \text{(A.25)}$$

The factor $1 - \sigma_S(C)$ is surely never negative for any C. Furthermore, for fixed C, the quantity in the last bracket is, up to a positive normalization factor, the thermal average of the spin product σ_{RS} for some new Ising lattice with the interaction energy

$$-\sum_{j,k} E_{j,k}[1 + \sigma_j(C)\sigma_k(C)]\sigma_j\sigma_k - \sum_j H_j[1 + \sigma_j(C)]\sigma_j. \quad \text{(A.26)}$$

But from the hypotheses that, for all j and k, $E_{j,k} \geq 0$ and that for all j either $H_j \geq 0$ or $H_j \leq 0$ it follows that, for all C and all j and k,

$$E_{j,k}[1 + \sigma_j(C)\sigma_k(C)] \geq 0 \quad \text{(A.27)}$$

and that for all C and all j either

$$H_j[1 + \sigma_j(C)] \geq 0$$

or

$$H_j[1 + \sigma_j(C)] \leq 0. \quad \text{(A.28)}$$

Therefore, we may apply Theorem 2 to conclude that if the number of spins in σ_{RS} is even then this last bracket is positive, whereas if the number of spins in σ_{RS} is odd and there is some j for which $H_j \neq 0$ then the sign of this last bracket is the same as that of H_j. Hence, Theorem 3 follows.

The inequalities (A.3)–(A.6) follow immediately from Theorem 3. Therefore, we have established Griffiths' theorem, as used in Sec. 1 of Chapter XV.

APPENDIX B

Although the constant $\bar{A}$ defined by (XI.4.28) cannot be expressed as a finite combination of familiar transcendental constants like π, e, γ, or $\zeta(n)$, it can be shown that

$$A = e^{1/4} 2^{1/12} C_G^{-3}, \tag{B.1}$$

where C_G is Glaisher's constant,[1] defined by

$$\ln C_G = \tfrac{1}{12} + \lim_{N\to\infty} \left[\sum_{n=1}^{N-1} n \ln n - \tfrac{1}{2}(N^2 - N + \tfrac{1}{6}) \ln N + \tfrac{1}{4}N^2 \right], \tag{B.2}$$

and is known to be given approximately by

$$C_G \sim 1.282427130. \tag{B.3}$$

However, since Glaisher's constant surely is not well known we present here a direct method of obtaining the value of $\bar{A}$ quoted in (XI.4.29). We do this by expressing $\bar{A}$ as a rapidly converging infinite series involving transcendental constants whose values are tabulated and readily available.

In the defining expression (XI.4.28) replace $\ln(1 - 1/4l^2)$ by its power-series expansion and interchange the order of summation to find

$$\bar{A} = -\sum_{n=2}^{\infty} \frac{1}{4^n n} \zeta(2n - 1), \tag{B.4}$$

where the Riemann zeta function $\zeta(s)$ is defined as

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}. \tag{B.5}$$

1. J. W. L. Glaisher, *Messenger of Math.* **24**, 1 (1894).

As $s \to \infty$, $\zeta(s) \to 1$, so it is useful to rewrite (B.4) as

$$\bar{A} = -\sum_{n=2}^{\infty} \frac{1}{4^n n} [\zeta(2n-1) - 1] + \tfrac{1}{4} + \ln(1 - \tfrac{1}{4}). \tag{B.6}$$

The values of $\zeta(2n - 1)$, though not known exactly, have been obtained with great accuracy.[2] The first few of these zeta functions are:

$$\begin{aligned} \zeta(3) &\sim 1.202{,}056{,}903, \\ \zeta(5) &\sim 1.036{,}927{,}755, \\ \zeta(7) &\sim 1.008{,}349{,}277, \\ \zeta(9) &\sim 1.002{,}008{,}393, \\ \zeta(11) &\sim 1.000{,}494{,}189, \\ \zeta(13) &\sim 1.000{,}122{,}713. \end{aligned} \tag{B.7}$$

Using these values in (B.6) we immediately obtain (XI.4.29).

2. For example, the values of $\zeta(n)$ up to $n = 42$ are tabulated in M. Abramowitz and I. A. Stegun, eds., *Handbook of Mathematical Functions* (Dover, New York, 1965), p. 811.

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[Numerals in parentheses refer to equations.]

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