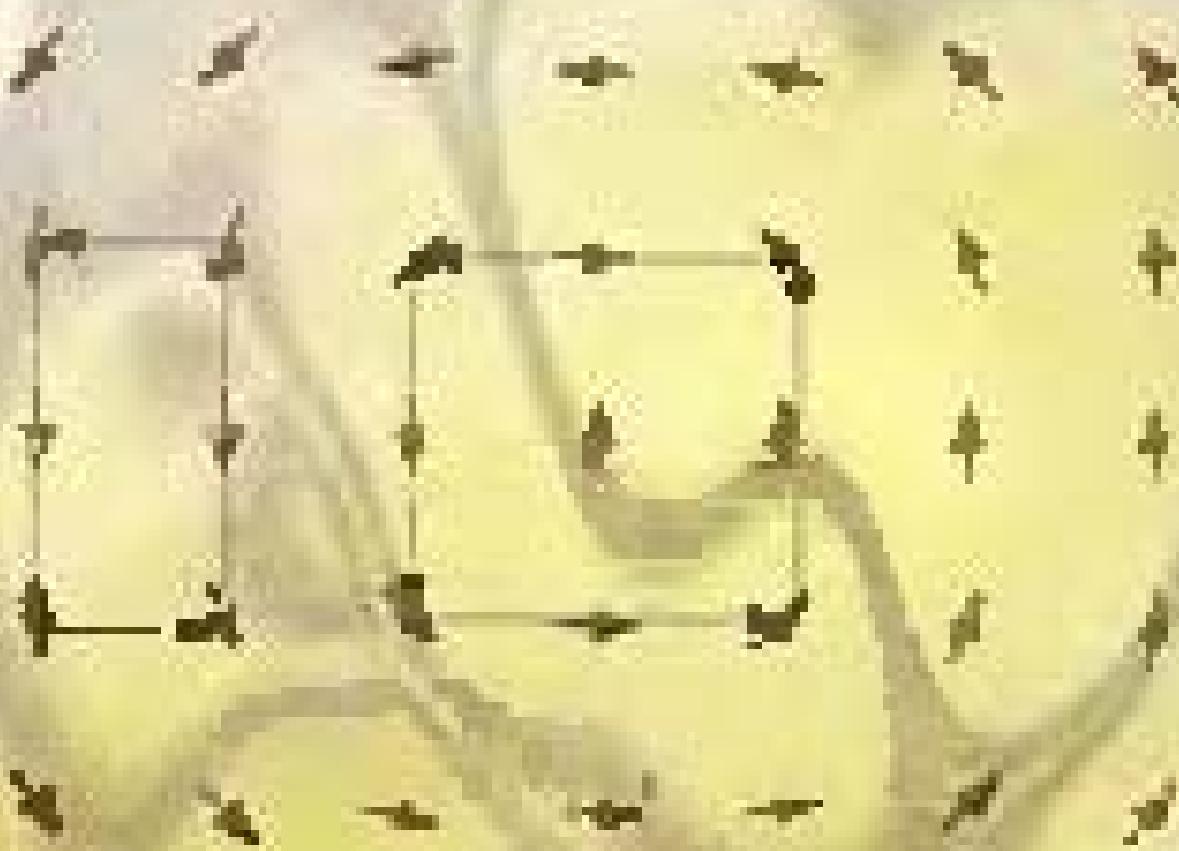


STATISTICAL PHYSICS

Statics, Dynamics and Renormalization



Leo P Kadanoff

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Introduction

A traditional physics education includes material in thermodynamics, kinetic theory, statistical mechanics, and hydrodynamics, each in its separate course or portion of a course. Other, weakly related, courses describe quantum mechanics, condensed matter physics, atomic and particle physics, and perhaps plasma physics, differential equations, hydrodynamics, etc.

In the meantime, there has been an explosion and a reorganization in the intensity and variety of research in what one might call ‘physical dynamics’. Some workers are developing dynamical systems theory and looking at effectively low-dimensional systems. The low-dimensional problems have a myriad of applications to fundamental understanding of chaos, to medical diagnostics, to understanding market dynamics. Others are looking at fascinating properties of condensed matter systems, as for example the nature of glasses, cascade processes in low temperature systems, fluid turbulence, the fracture of materials, and earthquake or avalanche dynamics. In each case, the dynamical processes involved are analyzed with statistical tools with the analysis and the dynamics being the joint subject of the research. Similar subjects and similar methods are studied far from the boundaries of conventional condensed matter physics. Studies of star counts should be aimed at an understanding of the time-development which produced the stars and its manifestation in the statistics of counts. Particle theory develops its methodologies in parallel to those of condensed matter physics, so that the study of phase transition, of interface motion and of crumpling is the joint domain of both groups of scholars. In one example, renormalization ideas have been jointly developed by both groups. Thus I argue that we must think anew about how to present the material in the parts of physics which involve the fundamentals of dynamics and its statistical analysis. In fact, despite the straw man erected by my opening words about the traditional physics curriculum this rethinking has gone on almost everywhere good physics is taught. These notes are intended to be my contribution of the continuing process of modification of our teaching. They are intended to be a partially coherent whole, accessible to someone with some training in undergraduate physics, with some knowledge of the associated mathematics, together with an ample intelligence and curiosity. (Translation: I think the material is hard; I hope it will be rewarding.) I have included much more material than should be covered in a one quarter statistical mechanics course. In fact, there is probably more material than can be covered in two quarters. However, with an appropriate selection, some dynamics and some statistical mechanics could be covered within one quarter. The course includes some topics which are properly parts

of kinetic theory courses, a little which might belong to thermodynamics, some dynamics of the solid state, a few special topics in hydrodynamics, and a little applied mathematics. Because of my own special interests, there is also a large slug of renormalization group material, presented in its ‘real-space’ version. On the other hand, to keep the presentation relatively brief, the book leaves out many interesting topics which the reader and I might have wished to see included.

Whenever appropriate, it uses the results of experiments and computer simulations. The subject is presented from the perspective of a theorist. The exercises are, as usual, also set from the theoretical perspective. (We do not know much about how to train people for the experimental part of the art. What we do know is apparently better conveyed in face to face contacts than in the lecture mode reflected in this volume.) Many exercises ask for computer generated numerical results. It is assumed as a matter of course that each student has access to a computer and can use it effectively.

The material presented here was tried out in two courses I taught several different times at Chicago. One of these is a graduate level survey of statistical physics; the other a rather personal perspective on critical behavior. Thus, this book defines a progression starting at the book-learning part of graduate education and ending in the midst of topics at the research level. To supplement the research-level side the book includes some research papers. Several of these are classics in the field, including a suite of a half dozen works on self-organized criticality and complexity, a pair on diffusion limited aggregation, some papers on correlations near critical points, a few of the basic sources in the development of the real-space renormalization group, and also papers on magnetic behavior in a plain geometry. In addition to genuine classics, I have included a few of my own papers. Although their status as classics is somewhat suspect (since I am not the best judge of my own work) they do serve to illustrate and amplify some of the topics treated here.

The reader will see defects in presentation, in wording, in the figures, and in the use of L^AT_EX. All the defects are mine. I got a considerable amount of help in squeezing out the defects from Christophe Josserand, Alexi Tkachenko, Vachtang Putkaradze, Konstantin Gavrilov, and Roman Grigoriev.

As a graduate student I learned statistical physics from my Professors, Paul Martin and Roy Glauber. Afterward I learned from colleagues and from the students and postdocs. I have had the excellent fortune of working with a wide group of people who all care and cared deeply about science. We all share the view that statistical theory can form a small-but interesting-part of an informed view of nature.

As science turns to more and more complex systems, it might be that a statistical approach will become a crucial input to the next generation of scientific issues.

Bibliographic Note

This is a personal view of statistical physics. Some of the material covered comes from my own work. My papers are partially collected in a the volume with the title: From Order to Chaos: Essays Critical, Chaotic, and Otherwise — published by World Scientific.

The second edition will be published early in 1999. Throughout this book, I refer to the second edition with the abbreviation *LPK: Essays*. I also make much use of Cyril Domb's excellent book 'The Critical Point. A historical introduction to the modern theory of critical phenomena'. (Taylor and Francis, London, 1996). This is referred to as 'Domb, The critical point:'. Another very important source is the Domb, Green, Lebowitz multivolume work 'Phase transitions and Critical Phenomena' (Academic Press, London, New York (1971-...)). I shall describe this as *DGL*:. A few reprints are included in the present volume. They are indicated by *REPRINT*.

Part I

Fundamentals of Statistical Physics

Chapter 1

The Lectures — A Survey

Statistical Physics describes the result of the laws of classical and quantum mechanics when applied to richly complex situations. The complexity both permits and demands the use of probabilistic methods to describe what is happening. Naturally, the subject has a rich and complex logical structure. It is partially grounded in experiment and partially in a deep analysis of the consequences of the laws of mechanics. It contains some wonderfully general ideas: e.g. entropy, the Boltzmann distribution, concepts of relation to equilibrium, the idea of renormalization, but also some very specific mathematical structures: Gaussian models,¹ Boltzmann equations,² Langevin equations,³ various ensembles, etc. In addition, statistical physics is built upon deep and often exact analysis of interesting physical models from the Ehrenfest ‘wind tree’ model,⁴ to Onsager’s⁵ solution of the Ising⁶ model, to the development of fractals,⁷ as they appear for example in Diffusion Limited Aggregation.⁸

1.1 The Journey: Many Different Approaches

Statistical physics is connected to the remainder of physics by a multitude of experimental studies, theoretical arguments, empirical experience, and traditional usage. Once we get

¹See Chapter 3.

²I am disappointed that I could not include Boltzmann equations in this volume. One can find the classical approach in, for example, the book by Chapman and Cowling. S. Chapman and T. G. Cowling, ‘Mathematical Theory of Non-Uniform Gases’, Cambridge University Press, (1939).

³See Chapters 5 and 6.

⁴P. and T. Ehrenfest, ‘The Conceptual Foundations of the Statistical Approach to Mechanics’ (Cornell University Press, Ithaca, 1959).

⁵All of Onsager’s publications can be found in the volume *The Collected Work of Lars Onsager* (with commentary)’ (ed. P. C. Hemmer, H. Holden and S. Kjelstrup Ratkje, World Scientific, Singapore (1996)). The specific section on the Ising model starts at page 167.

⁶Named after E. Ising a physicist who investigated what happens when these spins are placed in a one-dimensional chain. See Hemmer, *et al.*, loc. cit. page 169.

⁷Benoit B. Mandelbrot, ‘The Fractal Geometry of Nature’ W. H. Freeman and Company, New York (1983).

⁸Thomas Witten and Leonard Sander, Phys. Rev. Lett. 47, 1400 (1981).

into the any aspect of the subject, we can travel outward to reach the entire, rich structure. One can start from several different entry ports.

We shall choose one of the traditional entry ways and begin, in the first section of the notes, to discuss *Statistical Mechanics*. This subject describes the long-time behavior of mechanical systems which have a dynamics specified in terms of Hamiltonian Mechanics. Almost all such systems, even those which are quite richly complex, given sufficient time in isolation will develop a relatively simple probabilistic behavior. Thus, Statistical Mechanics describes the behavior of systems, usually ones containing many particles, which are isolated long enough so that they can fall into equilibrium. Our concern in the next chapter will be to describe the canonical formalism of statistical mechanics and in particular to develop the simplest case, the one in which the system contains many weakly interacting particles.

In the next chapter (Chapter 3) we turn our attention to one of the most-used examples of statistical mechanics, the Gaussian system. Almost any idea in statistical physics can be studied by applying that idea to a Gaussian problem. Usually the problems so considered are solvable. Another set of solvable problems are ones in which interacting particles are arrayed on a one-dimensional lattice. In Chapter 4, these problems are solved by methods involving transfer matrices. These one-dimensional problems are interesting both for the own purposes, and also because they provide a direct connection between statistical physics and quantum mechanics. We construct the solution of the one-dimensional Ising model as a prototypical example. Then we turn to higher dimensional examples in order to provide a link from statistical mechanics to field theory and particle physics.

Of course, starting from equilibrium statistical mechanics begs many very interesting questions. How long need we wait to attain equilibrium? Why do we say that all systems reach the same equilibrium independent of their dynamics? Is this independence really true? How much can we say about the relaxation to equilibrium? How general is the mode of equilibration? To begin to treat these questions one must have a dynamical perspective. The next major section then discusses how equilibrium arises from dynamics. The first chapter of the section (Chapter 5) describes a prototypical dynamical problem: a random walk on a lattice. The next chapter (Chapter 6) considers the dynamics of Brownian motion, i.e. a heavy particle moving through a gas of lighter ones. Random collisions perturb the momentum of the heavy particle and eventually produce an equilibrium dynamics. This part concludes with a discussion of the close relation between the fluctuations within a system and the response of the same system to an external disturbance.

We then return to equilibrium behavior. We describe the relation between statistical mechanics and thermodynamics. Then the equilibrium analysis is extended to the grand canonical ensemble to treat some of the highly degenerate quantum systems within statistical mechanics. The discussion concludes with degenerate fermi systems and of phase transitions to a bose condensed state.

The next major section is a consideration of phase transitions and of critical phenomena. In recent decades, these problems have occupied a central position in statistical physics, while having rich implications for quantum field theory as well. The first chapter of the section develops an overview of the study of phase transitions. The next chapter treats

the mean field theory approach to critical phenomena. This theory captures (but only in part) what goes on in a phase transition. We argue for the mean field theory's incompleteness and its incorrectness for behavior very near the critical point. In the next chapter, we give a replacement phenomenological theory: the scaling/universality theory of critical phenomena.

Renormalization concepts provide a justification for the phenomenological theory. These are first introduced in one-dimensional examples and then described as a general approach. Two-dimensional Gaussian models are then used to give a specific example of the phenomenological theory. Two-dimensional examples are developed in more detail through 'real-space' renormalization techniques. The lectures end with some two 'advanced' topics: Duality (Chapter 16) and The Planar Model (Chapter 17).

1.2 The Main Sights

As we move along in the first part of our trip, we shall see some major sights. These are the great formulation ideas of statistical physics. Each of these provides a different way into the subject. As an introduction, I shall list of few of those here and now:

Operational Definition of Quantum Statistical Mechanics

Statistical mechanics is concerned with calculating the averages of certain operators, X . If $\langle \alpha | X | \alpha \rangle$ is the average of X in the quantum state $|\alpha\rangle$ then the average of X in a situation of statistical equilibrium is given by the Gibbs⁹ average

$$\langle X \rangle = \sum_{\alpha} \langle \alpha | X | \alpha \rangle \rho(\alpha), \quad (1.1)$$

where $\rho(\alpha)$ is the probability of observing the system in the state $|\alpha\rangle$ and is given by

$$\rho(\alpha) = \frac{\exp(-\beta E_{\alpha})}{Z(\beta)} \quad (1.2)$$

with β being proportional to the inverse temperature and $Z(\beta)$ being a normalizing factor called the partition function. Since the total probability of everything must sum up to unity, we must have that

$$Z(\beta) = \sum_{\alpha} \exp(-\beta E_{\alpha}). \quad (1.3)$$

Equations (1.1)–(1.3) together embody all of statistical mechanics appropriate for a system described by the usual quantum theory. But they look terribly naked. Where do

⁹Named after J. Williard Gibbs, the great American theorist, who first suggested the exponential form for the probability.

they come from? Can one derive them from something simpler and more fundamental? Is statistical mechanics a consequence of classical mechanics and/or of quantum mechanics? Why does the energy play a special role? Should there not be some kind of symmetry between energy and momentum? Does this approach always work?! Does it apply, for example, to superfluids or superconductors?

Another, parallel, approach begins by using classical, instead of quantum, concepts. In this situation one imagines N particles, each described by a d -component momentum \mathbf{p}_j and a vector coordinate \mathbf{q}_j , with $j = 1, 2, \dots, N$. Instead of summing over quantum states one integrates over a volume element in phase space:

$$d\Gamma_N = \frac{1}{W_N} \prod_{j=1}^N d\mathbf{p}_j d\mathbf{q}_j. \quad (1.4)$$

The W_N is a function of N picked to make an integral over the phase space as close as possible to the quantum sum over states. The energy in Eqs. (1.1)–(1.3) is the eigenvalue of the Hamiltonian. To go from quantum mechanics to classical mechanics one replaces the eigenvalue by the Hamiltonian function $H(p, q)$. Hence, in the classical mechanics description, these basic equations become:

Operational Definition of Classical Statistical Mechanics

The average of any function, X , of the p 's and q 's is

$$\langle X \rangle = \int d\Gamma_N \rho(p, q) X(p, q), \quad (1.5)$$

where $\rho(p, q)$ is the probability of observing the system at the point p, q in phase space. This probability is given by

$$\rho(p, q) = \frac{\exp(W(p, q))}{Z(\beta)}. \quad (1.6)$$

Here $W(p, q)$ determines the weight of the configuration with Hamiltonian coordinates p and q . This W is given in terms of the classical Hamiltonian $H(p, q)$ by

$$W(p, q) = -\beta H(p, q). \quad (1.7)$$

We shall, from time to time, call W the ‘action’, in correspondence to the time integral of the Lagrangian in mechanics. Equation (1.7) describes the Gibbs distribution, which forms the basis of statistical mechanics. If the Hamiltonian includes only a few particles this probability is called a Boltzmann distribution.

Once again, we demand that the total probability for all possible occurrences be unity, and see that this demand requires that the partition function $Z(\beta)$ has the value

$$Z(\beta) = \int d\Gamma_N \exp(-\beta H(p, q)). \quad (1.8)$$

Note that the normalizing factor, W_N , as defined in Eq. (1.4), does not affect any probability or average, but just changes the value for the auxiliary quantity, $Z(\beta)$.

This classical approach has all the difficulties, previously mentioned, of the quantum theory in addition to some difficulties of its own: What is the relation between classical and quantum statistical mechanics, as defined here. Is there an appropriate classical limit of the quantum theory? Can the classical theory describe all macroscopic systems? Again, what about superconductivity?

Free Energy Formulation

From the last two formulations, it looks as if the partition function plays a central role in statistical theory. Indeed it does. In fact, we can start from the partition function itself, and develop a connection with statistical mechanics through what is called statistical thermodynamics. We recall that thermodynamics defines a quantity called the free energy, $F(\beta, \{H\})$. That is to say that the free energy depends upon the inverse temperature, β , and upon the Hamiltonian function H . Statistical thermodynamics then considers the consequence of the statement that there is such a thing as an entropy which can be used to discuss changes in, for example, the energy, the particle number, and in some parameter λ contained in the Hamiltonian. The connection with the statistical mechanics described above is made by saying that the partition function is related to the free energy via the relation:

$$Z(\beta) = \exp[-\beta F(\beta, \lambda)]. \quad (1.9)$$

Here, λ is a parameter in the Hamiltonian. The classical situation is one in which each particle is held in a box of volume Ω , and then Ω is the parameter.

From the definitions (1.8) and (1.9) the change in the partition function is given by:

$$d \ln Z = -d[\beta F(\beta, \lambda)] = -\langle H \rangle d\beta - \beta \left\langle \frac{\partial H}{\partial \lambda} \right\rangle d\lambda. \quad (1.10)$$

In addition the free energy may be used to define the entropy S via:

$$F = \langle H \rangle - \frac{S}{k} \quad (1.11)$$

with k being the Boltzmann constant.¹⁰ Here, as we shall see, the entropy $\exp(S/k)$ is the typical number of quantum states available to the system.

¹⁰For clarity sometimes we shall write this constant as k_B .

The free-energy approach gives yet another useful starting point for statistical mechanics. It seems dry at first, but at last it will give a wide variety of useful results. In fact Lev Landau used it as a way of developing the entire theory.¹¹

Einstein took a different point of view yet.¹² He focused upon a very simple system: a so-called Brownian particle. A Brownian particle is a small piece of matter, perhaps a grain of pollen or dust, which is immersed in a fluid. These particles are observed, under the microscope, to dance around in an apparently irregular pattern. They can be described as moving under the influence of three kinds of forces: a regular force which might perhaps be described by a Hamiltonian containing a kinetic energy and a prescribed potential energy

$$H(\mathbf{p}, \mathbf{r}) = \frac{\mathbf{p}^2}{2m} + U(\mathbf{r}), \quad (1.12)$$

a random force which shows up as a series of apparently random forces $\eta(t)$ acting upon our piece of matter, and finally a frictional force which acts to slow down a particle in motion. Since the frictional force and the random force are both consequences of the fluid molecules' motion, one should expect that they might be related to one another. Following this line of thought, one describes the motion of the particle by using the:

Random Force (Langevin) Formulation

Let the particle move as a free particle under the influence of a random force $\eta(t)$.

The particle is described in the usual way by the two Hamiltonian equations of motion

$$\frac{d\mathbf{r}}{dt} = \frac{\mathbf{p}}{m}, \quad (1.13)$$

$$\frac{d\mathbf{p}}{dt} = -\nabla U + \eta - \frac{\mathbf{p}}{\tau}. \quad (1.14)$$

Here, τ is a relaxation time which describes the net effect of the frictional force in slowing down the particle in motion.

Equations (1.13) and (1.14) provide a very compact description of the particle in motion. It would, however, be nice to be able to obtain these equations from a more fundamental view of the fluid in motion. Then one could answer obvious questions, as for example, "What is the law of probabilities for the η ?" or "How are the random force, η , and the relaxation time, τ , related to one another?"

There is yet another formulation of this very same problem which eliminates the random force and instead describes the motion of one particle in a probabilistic fashion. The probability is defined by saying that

$$\rho(\mathbf{p}, \mathbf{r}, t)d\mathbf{p} d\mathbf{r} \quad (1.15)$$

¹¹L. Landau and E. M. Lifshitz, Statistical Physics, Pergamon, London (1958)

¹²R. Fürth, Investigation on the Brownian Motion (A. D. Cowper Trans.) Methuen, London, 1926.

is the probability for finding the particle within the volume element of size $d\mathbf{p} d\mathbf{r}$ in the phase space for the particle. Naturally, since the particle must be somewhere, the integral over the entire phase space of these bits of probability adds up to unity

$$\int \rho(\mathbf{p}, \mathbf{r}, t) d\mathbf{p} d\mathbf{r} = 1. \quad (1.16)$$

Using an argument which we shall develop in detail later, one can find an equation obeyed by the probability. In this formulation, we then have the

Probability Formulation: The Fokker–Planck Equation

This equation describes the rate of change of the probability in time. It has the form:

$$\begin{aligned} \frac{\partial}{\partial t} \rho(\mathbf{p}, \mathbf{r}, t) = & - \left(\frac{\mathbf{p}}{m} \right) \cdot \nabla \rho(\mathbf{p}, \mathbf{r}, t) - (-\nabla U) \cdot \nabla_{\mathbf{p}} \rho(\mathbf{p}, \mathbf{r}, t) \\ & + \nabla_{\mathbf{p}} \cdot \frac{\mathbf{p} \rho(\mathbf{p}, \mathbf{r}, t)}{\tau} + \nabla_{\mathbf{p}} \cdot [\nabla_{\mathbf{p}} \rho(\mathbf{p}, \mathbf{r}, t)] \frac{m}{\beta \tau}. \end{aligned} \quad (1.17)$$

Each term on the right hand side has a very direct physical significance. The first term describes how ρ changes because particles move from place to place. It is first proportional to their velocity \mathbf{p}/m . Then the time derivative occurs because there is a different likelihood of finding particles at different places. (Otherwise their motion would not change ρ .) The derivative is then proportional to a spatial gradient of ρ . The next two terms are proportional to gradients in momentum and represent the fact that the particle's momentum changes because of the force proportional to the gradient of the potential U (second term) and to the frictional damping of the momentum (third term). The last term represents a kind of diffusion in momentum produced by the random jiggling of molecular collision. Notice that the inverse temperature, β , enters into that term.

It is far from clear how and why one could argue that the Langevin and the Fokker Planck formulations describe the same basic physics. Nonetheless they do.

1.3 Is the Trip Worthwhile?

Our job in the next group of lectures is to see and understand the ideas which stand behind statistical physics and to try to grasp the full grandeur of the subject. We can expect this to be hard work.

But, if you are to share in this journey, you should be convinced that the trip will be worthwhile. Why should one study statistical physics? Let me list reasons: First of all, it is in itself a beautiful subject. It is wonderful to see and understand how all the different formulations and approaches discussed above are really one and the same. And as we shall see, there is an charming elegance in the structure of this subject. In addition, of course,

statistical physics is important as a tool in other branches of science and mathematics. Subjects as diverse as chemical reaction rates, the structure of black holes, the behavior of stock prices, the motion of vortices in superconductors, the average properties of a ball bouncing for a long time in some enclosure, the properties of turbulent fluid flows, and field theories of particle behavior are all studied with the aid of tools which are part of statistical mechanics. Another reason for learning statistical mechanics is that it is a subject of up-to-date research interest. All the subjects just mentioned are, to a large extent, not really understood. Current research is focused upon building our knowledge of these and other related topics. The research will call upon tools from all parts of the sciences, but especially and particularly from statistical mechanics.

Let me conclude this survey with a few words about methodology. From the descriptions given above, you might conclude that statistical mechanics is a theoretical subject in which the primary tools are the pencil and a piece of paper and some deep mathematical knowledge. In that sense, the outline given up to now is misleading. The world of many particle systems, which is the primary focus of statistical theory, is so diverse and rich that nobody could guess the richness that it contains using just pure thought or pure theory. Without experiment, superconductivity would probably remain undiscovered to this day. Once seen, the theorists could think about what had been observed and, in the end, explain much of what the experimentalists had discovered. But, experiment had to come first to expose the main phenomena. Consequently, any research study of statistical phenomena must be heavily based in experimental knowledge.

Experiment and theory form the two main traditional branches of physics study. In recent years, they have been joined by yet another method of learning about nature: computer simulation. Almost every scientist working in the area must learn how to use the computer effectively. There are two main purposes of computer use: Exploration and Checking. In both uses one programs a computer to find the solution to a set of equations which simulate something that goes on in nature. In exploration one is looking into uncharted territory hoping to find something new and unexpected. One's mind is open; one's computer program is set to output a wide variety of data which might reveal something new. The other mode is checking. One thinks one knows what is going on. One designs a program very carefully to verify or disprove one's conjecture. The answer that comes out should be simple and unambiguous: 'Yes' or 'No'. We shall try to use computer in both modes in this set of lectures.

Chapter 2

One Particle and Many

2.1 Formulation

This section is intended as a brief and selected overview of equilibrium statistical mechanics. For many readers it will indeed be a review. Nonetheless it will contain some examples and some discussion which will be crucial for what will happen further on.

There will be one single thread which will run through this discussion. We shall wish to ask about how statistical mechanics works out when the system contains many uncoupled or weakly coupled particles. In this case, as we shall see, we can in essence study the statistical system *one particle at a time*. In contrast, when many elements are coupled together, the problem must usually be solved all at once.¹ Since statistical systems are very large ‘all at once’ is very hard. For this reason, we shall spend some effort developing simplified model problems. Sometimes, we shall often have to resort to approximate methods of solution and sometimes we shall limit ourselves to obtaining the qualitative properties of solutions.

The discussion of how one particle behavior is related to many particle behavior will give us an excuse to review the entire subject and to set the notation that we shall use throughout.

We start from the canonical formulation of quantum statistical mechanics defined by Eqs. (1.1) through (1.3). We use the quantum view instead of the classical one since the very simplest examples can be found in the quantum case. And also the basic quantum formulation is both simple and elegant. Here we shall state the equations of this formulation in a slightly more general form than used in Chapter 1.

In matrix theory, and hence quantum mechanics, a diagonal sum over states is called a *trace*. That is, one defines a trace of any quantum mechanical operator X as:

$$\text{Trace } X = \sum_{\alpha} \langle \alpha | X | \alpha \rangle \quad (2.1)$$

¹Sometimes one can employ theoretical devices which effectively convert a many-degree-of-freedom problem into a one-particle problem. The methods for doing this are often somewhat sophisticated and interesting. Two such methods, describing respectively system arrayed on a line and so-called Gaussian systems are described in the next two chapters.

for any complete sum over states and any operator X . We shall often have to distinguish between traces which contain many particles and those containing only a few particles or degrees of freedom. The former will be written as ‘Trace’, note the cap, and the latter as ‘trace’. When we wish to describe something slightly more general including either ‘Trace’ or ‘trace’ or perhaps a slightly different kind of sum, we shall write Tr . The basic formulation then of quantum statistical mechanics is (see Eq. (1.1)) that the average of any operator X is

$$\langle X \rangle = \text{Tr}(\rho X), \quad (2.2)$$

where the statistical weight, ρ , is a quantum operator which can be expressed in terms of the Hamiltonian operator, H as

$$\rho = \frac{\exp(-\beta H)}{Z(\beta)} \quad (2.3)$$

and the probability distribution will be properly normalized when the partition function has the value

$$Z(\beta) = \text{Tr} \exp(-\beta H). \quad (2.4)$$

Sometimes we shall wish to distinguish between a partition function for a big system, which we shall call Z , and that for a small system which will be denoted by z .

2.2 The Ising Model

(Named after E. Ising, a physicist who investigated what happens when spins are placed on a one-dimensional chain.)

The kind of calculation we have just performed can be applied to many different situations. Imagine a single spin (perhaps belonging to an electron) localized at a point in space. The spin is sitting in a magnetic field which points in the z direction. The only interaction it feels is its coupling to the external magnetic field. With these assumptions, the spin is described by a Hamiltonian

$$H(\sigma_z) = -\mu B \sigma_z, \quad (2.5)$$

where B is the magnetic field and σ_z has only two possible values: ± 1 . There are then two possible situations and the probability of the two are described by $\rho(\sigma_z)$, where each outcome has a probability proportional to $\exp(\beta \mu B \sigma_z)$. Specifically, with this Hamiltonian,

$$\begin{aligned} \rho(1) &= z^{-1} \exp(h), \\ \rho(-1) &= z^{-1} \exp(-h), \end{aligned} \quad (2.6)$$

where h is an abbreviation for the dimensionless combination

$$h = \beta \mu B \quad (2.7)$$

and z is an overall constant which ensured the proper normalization of the probabilities:

$$1 = \rho(1) + \rho(-1). \quad (2.8)$$

In this way, we find that, following Eq. (1.3),

$$z = \exp(h) + \exp(-h) = 2 \cosh h. \quad (2.9)$$

The approach we have followed here shows that the dimensionless combination h determines the behavior of the spin. If temperature is high or the field is weak so that h is small, but positive, then the probability that the spin points along B is only slightly larger than that it points in the opposite direction. Conversely if B is large or the temperature is low, so that in consequence h is quite large, then it is exponentially more likely that the spin will point with the field rather than opposite to it. We say that the field has saturated the spin.

Now we can calculate the relevant averages which characterize the system. First, the average value of the spin, which is evaluated from (2.2) as

$$\langle \sigma_z \rangle = \rho(1) - \rho(-1) = z^{-1}[\exp(h) - \exp(-h)] = \tanh h. \quad (2.10)$$

This result can be interpreted by saying that for small h the average σ_z is quite small indeed while for large h the result saturates at a value close to one. The magnetization is defined to be $M = \mu\sigma_z$ so that the average M is $\mu \tanh h$. The magnetic susceptibility is defined to be the derivative of M with respect to B at fixed temperature and thus has the value

$$\chi = \frac{\partial \langle M \rangle}{\partial B} = \frac{\mu^2 \beta}{\cosh^2 h}. \quad (2.11)$$

In fact, this approach does correctly describe the behavior of a single isolated spin of an electron or nucleus in a solid. (The requirement is that there be no nearby spins to interact with it and the spin-dependent relativistic effects be small enough to be neglected.) This simple example shows how one can rather easily apply statistical mechanics to real situations in which there is some relatively simple subsystem weakly coupled to its environment.

2.3 *N* Independent Particles — Quantum Description

The statistical mechanics treatment of one quantum particle is easy. To deal with N non-interacting particles or N non-interacting excitations is equally easy, so long as the system is sufficiently dilute so that we do not have to worry about the Bose or the Fermi nature of the quantum particles or excitations.

If we have N independent quantum objects, then the Hamiltonian can be split into N terms in the form:

$$H = \sum_{j=1}^N H_j, \quad (2.12)$$

Here H_j is the Hamiltonian for the j th object, which for simplicity we shall call a particle. We assume that these particles are distinguishable, one from the other. Perhaps they are spins fixed to different positions in some solid's lattice. Since each one is fixed to a different position, they are not identical and we do not have to worry about quantum statistics. Each H_j has its own eigenvalues, $H'_j = \epsilon_{\alpha(j)}$, where $\alpha(j)$ is a label for the eigenvalue for the j th particle. The total energy is

$$E = \sum_{j=1}^N \epsilon_{\alpha(j)}. \quad (2.13)$$

In this case, we can evaluate the partition function. Since the different pieces of the Hamiltonian are independent of one another, the entire trace defining the partition function can be written as a product of traces over the individual particles:

$$Z(\beta) = \text{Trace } \exp(-\beta H) = \text{Trace} \prod_{j=1}^N \exp(-\beta H_j) = \prod_{j=1}^N \text{trace}_j \exp(-\beta H_j).$$

Each individual term is the trace of the individual subsystem, which we have decided to call $z(\beta)$:

$$z(\beta) = \text{trace}_j \exp(-\beta H_j). \quad (2.14)$$

All the z 's for all the different particles are the same because all the different particles share the very same probability distribution. Now, put all our results together and find that for N non-interacting subsystems:

$$Z(\beta) = [z(\beta)]^N \quad N \text{ distinguishable particles}. \quad (2.15a)$$

If the particles are identical (but the density is so low that there is no multiple occupation of any quantum state) then the formula (2.15a) is replaced by the statement:

$$Z(\beta) = \frac{[z(\beta)]^N}{N!} \quad N \text{ indistinguishable particles}. \quad (2.15b)$$

If the particles are truly indistinguishable, then putting the first particle into the single-particle state α and the second particle into the single-particle state ν is precisely the same situation as putting the first particle into ν and the second into α . Interchanging identical particles is no change at all. In the limit of low particle densities, the probability that any single-particle state is occupied is quite small. In this situation, we say we have a *non-degenerate* system the only effect of this indistinguishability is to introduce an extra counting factor which is the number of different ways N particles can be thrown into N different bins. There are N different ways of placing the first particle, $N - 1$ ways of placing the second, and so forth so that the total number of possible different placements is

$$N! = N \times (N - 1) \times (N - 2) \times \cdots \times 3 \times 2 \times 1. \quad (2.16)$$

Expressions (2.15a) and (2.15b) differ by this counting factor.

Equations (2.15a) and (2.15b) are quite a general result. They say, in essence, that if the system is made up of a sum of independent pieces so that the Hamiltonian is a sum of separate terms each representing a different part of the system, then the partition function for the entire system is the product of the individual partition functions for the pieces. Thus, knowing the behavior of the independent subsystems, we can predict the behavior of the entire system.

Furthermore, from Eq. (2.14) we see that the partition function for each of the pieces has exactly the same form, as the partition function for the entire system. (Compare Eq. (2.14) with Eq. (2.4)). In both cases the partition function is a trace of $\exp(-\beta H)$. When we see an algebraic structure like this trace of an exponential emerge in different contexts, we say that the result is *form invariant*. Here the form invariance is a requirement for an acceptable theory. Why? Because every system can be considered to be a piece of some larger system. If the basic formulation of the theory is to be correct, it must equally well apply to system and subsystem. It is comforting to recognize that the formulation of statistic mechanics given by Eqs. (2.2)–(2.4) has this necessary property.

2.4 Averages From Derivatives

The two different cases described by Eqs. (2.14) do differ, by one having an extra factor of $N!$ In the classical limit, it should not matter if the particles are or are not identical. Thus we might expect that this extra factor is quite irrelevant for most purposes. To see this we should ask: How can one calculate interesting things from the partition function? The basic answer is that one gets the physically interesting quantities by calculating derivatives of thermodynamic functions. One such function is the free energy, F defined by:

$$-\beta F = \ln Z(\beta). \quad (2.17)$$

An additive constant in the log of the partition function (e.g. $\log N!$) represents a count of the number of ways of getting a particular configuration. More easily observed quantities are all defined as derivatives of the free energy. Since one is differentiating logarithms of partition functions, these constant factors in Z just drop away. For example, consider the derivative of expression (2.17) with respect to β . From the definition of the partition function we find:

$$\frac{\partial}{\partial \beta} \ln Z = \frac{\partial}{\partial \beta} \ln \text{Tr } \exp(-\beta H) = -\text{Tr } H \frac{\exp(-\beta H)}{Z}.$$

Here the derivatives are taken with N and all the other parameters in the Hamiltonian held fixed. In this way, we see,

$$\frac{\partial}{\partial \beta} \ln Z = -\langle H \rangle = -E(\beta).$$

The expectation value of the Hamiltonian is called the average energy of the system and is denoted by E . In the usual thermodynamic analysis, the partition function depends upon

the volume of the system, Ω , the number of particles in it, N , and the inverse temperature β . Thus, from the partition function one can calculate the average energy as it depends upon those variables as:

$$E(\beta, N, \Omega) = \langle H \rangle = -\frac{d}{d\beta} \ln Z(\beta, N, \Omega). \quad (2.18)$$

Apply Eq. (2.18) to a situation like the one in Eq. (2.14) in which the system contains N non-interacting similar (and perhaps identical) subsystems. Notice how the $N!$ cancels out and we find:

$$E(\beta, N, \Omega) = \langle H \rangle = -\frac{d}{d\beta} \ln Z(\beta, N, \Omega) = -N \frac{d}{d\beta} \ln z(\beta) = N \langle H_j \rangle.$$

Thus, just as one might expect the average energy of the entire system is the sum of the energies of the constituent subsystems.

One can derive additional expressions for physical quantities by taking higher order derivatives of Z with respect to β . The result is:

$$\langle H^p \rangle = \frac{1}{Z(\beta)} \left(-\frac{d}{d\beta} \right)^p Z(\beta). \quad (2.19)$$

Here too any multiplicative constant in Z cancels out. One particularly interesting quantity is the squared fluctuations in the energy

$$\langle (H - \langle H \rangle)^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2 = \left(\frac{d}{d\beta} \right)^2 \ln Z(\beta) = -\frac{\partial}{\partial \beta} E(\beta, N, \Omega). \quad (2.20)$$

Equation (2.20) is an important result. On the left hand side one has the mean squared fluctuations in energy. The fluctuation is, of course, a statistical quantity in that it refers not to averages, but to deviations from the mean. On the right hand side one has a derivative with respect to β of the average energy. Since β is $1/kT$, (2.20) can be expressed as

$$\langle (H - \langle H \rangle)^2 \rangle = kT^2 \frac{\partial}{\partial T} E(\beta, N, \Omega) = kT^2 C_V. \quad (2.21)$$

The right hand side of Eq. (2.21) is proportional to the heat capacity, C_V , calculated as the amount of heat you must add to a system to raise its temperature by one degree if you perform the operation while holding the number of particles and the volume fixed.² Thus the energy fluctuations are related to a very familiar thermodynamic quantity.

The interested reader might now ask, what fluctuations? If one holds a bottle of water in ones hand one knows that the energy of the water has a very well defined value. So what is Eq. (2.21) doing talking about the fluctuations? The answer is simple. A statistical mechanical system does have fluctuations in the energy and essentially all measurable

²In classical thermodynamics, one often assumes that the particle number is being held constant. As an example, C_V is a derivative at fixed volume, V , and particle number, N .

quantities. However, as the system gets larger and larger the size of the fluctuations divided by the corresponding averages gets smaller and smaller. (In symbols, typical values of $(H - \langle H \rangle)/\langle H \rangle$ become small roughly in proportion to $N^{-1/2}$.) To make this statement more quantitative and concrete we should turn to the actual evaluation of partition functions in specific situations. Thus, we should go back and do partition function integrals and sums to see what is actually happening.

2.5 *N* Independent Particles in a Box

The formula for the energy explicitly involves the volume of the box in which the particles are confined. We know from our understanding of thermodynamics and mechanics that changing the volume changes the energy by an amount proportional to the pressure. We want to have the simplest problem in which we can see this working. This will be the partition function of a particle which moves freely, feeling no forces, within a box of side L and volume $\Omega = L^3$. From that we can get N particles in a box by using Eq. (2.14). Then, after a bit we shall be able to derive $P\Omega = N\beta^{-1}$ ($PV = NkT$ in the usual language.).

We do the quantum case first. To write the quantum partition function one needs to know and use the energy eigenfunction in a box. Let us have a Hamiltonian which is simply the kinetic energy for a single particle:

$$H = \frac{p_x^2 + p_y^2 + p_z^2}{2m}.$$

Imagine further that our quantum system has a wave function which obeys periodic boundary conditions

$$\psi(x, y, z) = \psi(x + L, y, z) = \psi(x, y + L, z) = \psi(x, y, z + L),$$

where L is the length of the side of the box. Now, if the particles have no forces acting on them, the usual form for the kinetic energy holds except that the momentum is quantized in the form:

$$\mathbf{p} = \frac{h(\nu_x, \nu_y, \nu_z)}{L},$$

where h is Planck's constant and the three ν 's are each integers. Thus, Eq. (2.14) becomes the statement

$$z(\beta) = \left[\sum_{\nu=-\infty}^{\infty} \exp\left(-\frac{\beta h^2 \nu^2}{2mL^2}\right) \right]^3. \quad (2.22)$$

In almost all situations, the temperature is sufficiently high and the size, L , is sufficiently large so that many many terms contribute to this sum over states.³ Whenever one has a

³The cases in which this is not true are particularly interesting. If one has nano-structures, objects of a typical size 10^{-9} meters, embedded in a solid, or if one is at temperatures well below one degree Kelvin, one can indeed have situations in which only a few states contribute to the statistical sum. These kinds of situations are subjects of 'hot' current research.

sum of the form:

$$S = \sum_{\nu=-\infty}^{\infty} F(\nu) \quad (2.23a)$$

and F is a slowly varying function of ν , one can-to an excellent approximation-replace the sum by an integral. (After all, integrals are really defined as the limit of such sums.) Thus, expression (2.23a) can be replaced by

$$S \rightarrow \int_{-\infty}^{\infty} dn F(n). \quad (2.23b)$$

In particular, then, expression (2.22) becomes

$$z(\beta) = \left[\int_{-\infty}^{\infty} dn \exp\left(-\frac{\beta h^2 n^2}{2mL^2}\right) \right]^3.$$

Let us go back to physical variables, replacing the integral over the ‘quantum number’, n , by an integral over the corresponding momentum $p = h\nu/L$. One then finds the one-particle partition function as

$$z(\beta) = \frac{\Omega}{h^3} \left[\int dp \exp\left(-\frac{\beta p^2}{2m}\right) \right]^3 = \frac{1}{h^3} \int_{\Omega} dr \int dp \exp\left(-\frac{\beta p^2}{2m}\right). \quad (2.24)$$

Here we have reexpressed the result in terms of an integral over phase space (the momentum, p , and the position, r) in order to compare it with the classical result.

In our definition, Eq. (1.4), of the classical statistical sum, the integral over phase space is divided by a weighting factor, $W(N)$. This factor is inserted to make the classical and quantum cases look similar. In Eq. (2.24) this similarity is achieved when we pick

$$W(1) = h^d, \quad (2.25)$$

with d being the dimension of space. Thus the quantum sums over states directly translates into a classical limit, in which one integrates over phase space if one picks the right multiplying factor in which each single-particle quantum state occupies a volume in phase space equal to h^d .

As previously, the many particle result is given as proportional to the one particle partition function raised to the N th power. That is, for both the quantum and the classical situations, where there are no forces except those produced by the walls of the box:

$$Z(\beta, N, \Omega) = \frac{[z(\beta, \Omega)]^N}{N!}. \quad (2.26)$$

In symbols then, in the classical limit, sums over energy levels can be replaced by phase space integrals according to:

$$\sum_{\alpha} \rightarrow \left(\frac{1}{N!} \right) \prod_{j=1}^N d\gamma_j \quad \text{with} \quad d\gamma_j = \frac{dp_j dq_j}{h^3}. \quad (2.27)$$

The result (2.26) may then be written as

$$Z(\beta, N, \Omega) = \frac{[\Omega J^3/h^3]^N}{N!}, \quad (2.28)$$

where J is the momentum space integral:

$$J = \int_{-\infty}^{\infty} dp \exp\left(\frac{-\beta p^2}{2m}\right) = J_0 \sqrt{m/\beta}. \quad (2.29)$$

The second equality is obtained by making a change of variables which converts p into dimensionless form. (We shall hardly need the value of the dimensionless integral, J_0 , in what follows. However the value is $J_0 = \sqrt{2\pi}$).

Our final result is that the partition function of a group of non-interacting particles is:

$$Z(\beta, N, \Omega) = \frac{[\Omega(mkT)^{3/2} J_0^3/h^3]^N}{N!}. \quad (2.30)$$

The average energy is the derivative of the logarithm of the partition function with respect to $\beta = (kT)^{-1}$. In doing the derivative, see the derivation of Eq. (2.19), we are supposed to keep the Hamiltonian fixed.

As indicated in Eq. (2.18) the average energy is given by

$$E = \langle H \rangle = -\frac{\partial}{\partial \beta} \ln Z(\beta, N, \Omega) \Big|_{\Omega, N}.$$

Then Eq. (2.30) gives us the familiar result

$$E = 3N \frac{kT}{2}. \quad (2.31)$$

This is, of course, a particular case of the law of equipartition of energy which says that in a situation in which classical mechanics applies and the Hamiltonian contains terms quadratic in the coordinates and/or momenta, one has an energy $kT/2$ for each such quadratic term. Each particle has three such terms for the three components of momentum, there are N particles, hence (2.31). In contrast a function like $U(r)$ which moves from a small value to a large one quite suddenly contributes no temperature dependent terms to the average energy. Thermodynamics defines the pressure in terms of the free energy,

$$F(\beta, N, \Omega) = -[\ln Z(\beta, N, \Omega)]kT, \quad (2.32)$$

by computing the work done by the system as it expands by an amount $d\Omega$. On one hand, this work is $pd\Omega$ where p is the pressure. This work is taken away from the free energy. Thus the work is $-d\Omega$ times the partial derivative of F with respect to Ω at fixed N and T , with the minus sign reflecting that the work done is taken away from the free energy. The pressure then is given by the formula

$$p(\beta, N, \Omega) = \frac{\partial}{\partial \Omega} kT \ln Z(\beta, N, \Omega) \Big|_{\beta, N}. \quad (2.33)$$

From (2.28) we get the dilute gas result

$$p(\beta, N, \Omega) = \frac{N}{\Omega} kT. \quad (2.34)$$

We shall return to the calculation of thermodynamic quantities several times. The relation between thermodynamics and statistical mechanics will be described more fully in Chapter 8.

2.6 Fluctuations Big and Small

There is one very important difference between a many particle system and one containing just a few particles. In the few particle case, each statistical variable we can construct tends to vary by a relatively large amount. That is to say that the fluctuations tend to be about as big as the average of the quantity. Thus, for this kind of situation one must think about the statistical fluctuations. In contrast, when the system is large one can construct some statistical quantities (for example the total energy) which are summed over many degrees of freedom. These variables tend to have very small fluctuations about their average. For this reason, it is quite sensible to characterize a large system by giving an instantaneous value of a quantity like the energy. From the energy and a few other numbers (e.g. N and Ω) one can find all the thermodynamic properties of the system. In contrast, knowing the energy of a single molecule at one instant does not help us one bit in finding its temperature.

One can use the partition function to calculate all kinds of properties of the energy, including its fluctuations.

Go back to Eq. (2.19) which expresses the average of various powers of the energy in terms of derivatives of the partition function. Recall in particular that the average energy and its fluctuations are respectively given by:

$$E = \langle H \rangle = -\frac{\partial}{\partial \beta} \ln Z(\beta, N, \Omega), \quad (2.35)$$

$$\langle (H - \langle H \rangle)^2 \rangle = \frac{\partial^2}{\partial \beta^2} \ln Z(\beta, N, \Omega). \quad (2.36)$$

The derivatives are taken at constant N and V . As we have seen if there are M quadratic degrees of freedom, then the partition function is proportional to $\beta^{-M/2}$. In that case, the average energy is $E = MkT/2$ while the mean squared fluctuation is

$$\langle (H - \langle H \rangle)^2 \rangle = \frac{1}{2} M(kT)^2 \quad (2.37)$$

for independent quadratic degrees of freedom in classical statistical mechanics at a temperature T .

There is a quite general result hidden here. We have come up with the (rather obvious) conclusion that if H is the sum of M independent pieces then its average is M times the

average of each piece. There being $3N$ quadratic terms in a kinetic energy in classical statistical mechanics, H , the average of the kinetic energy is $3NkT/2$. Quantities, like $\langle H \rangle$, which grow in proportion to the number of pieces, are called *extensive*. The opposite word, *intensive*, is applied to those quantities which do not change as the system just becomes larger without any change in its internal character. Thus the temperature or the average energy per particle are intensive quantities, while the total energy is extensive. It is also quite instructive to look at the fluctuations in the energy. Notice that the squared fluctuations are an extensive quantity. In fact, there is a contribution $(kT)^2/2$ to this fluctuation for every quadratic term in the Hamiltonian. The magnitude of the squared fluctuations is proportional to M and hence can be very large for large systems. However, for large M , the relative sizes of the fluctuations are very small indeed. The root mean squared (or RMS) fluctuation is:

$$\text{RMS}(H) = \sqrt{\langle (H - \langle H \rangle)^2 \rangle}, \quad (2.38)$$

while the relative size of the fluctuations is

$$\frac{\text{RMS}(H)}{H} = \sqrt{2M^{-1/2}}. \quad (2.39)$$

As the number of degrees of freedom become large, the relative fluctuations become very small indeed. This is a particular example of a much more general result:

In a system with large numbers of particles, N , the relative size of fluctuations in extensive quantities is very small in comparison to their mean. The mean increases in proportion to N ; the RMS fluctuations only increase as $N^{1/2}$. In large systems, therefore, extensive quantities will fluctuate little about their mean values.

For many purposes, we can replace these variables by the mean values.

2.7 The Problems of Statistical Physics

We have now finished the main part of our review of statistical mechanics. We begin to look ahead.

Part of our work to come is the description of the kinds of problems which arise in statistical physics. We should ask what are the exciting problems in the subject, including those exceptionally interesting problems which we might hope to see solved soon- and also those problems, perhaps recently solved, which might lead to something exciting in the near future.

But, before we get to this fun stuff, we have to do a little more work. Instead of describing problems by their potential intellectual importance, we should give a technical description of them. We have already distinguished between the quantum and the classical formulations of statistical physics. The difference between these formulations can give

important differences in calculation. For example, imagine a problem in which there are many independent particles, each with a one-particle Hamiltonian $H_j(p, r) = p^2/2m + U(r)$. In classical mechanics the statistical behavior of this problem can be obtained from doing an integral over phase space. The probabilities for momentum and position of each particle is very simple. Any average of a position or a momentum may be computed by doing an integral. On the other hand, in quantum theory p and r do not commute. However, in a quantum problem, if $U(r)$ is in any way complex, with more structure than the simplified potential which we used to hold particles in a box, then the calculations of the statistical properties are quite hard indeed. An eigenvalue problem must be solved in order to find the energy levels and wave functions, and then a sum over eigenstates must be carried out. This much harder first step is necessary to make any beginning of progress in even the simplest quantum models of an atom, molecule, or solid.

Nonetheless, each problem in which the Hamiltonian is a sum of independent terms referring to the different particles is quite simple. It can be solved one particle at a time.

In contrast, when there is an interaction among the particles things are both harder and more interesting. The usual model problem (which also represents rather accurately the behavior of monatomic molecules) involves a two-body interaction, $V(r)$ and a Hamiltonian:

$$H = \sum_{j=1}^N \left(\frac{p_j^2}{2m} + U(\mathbf{r}_j) \right) + \sum_{j < k=1}^N \sum_{j=k+1}^N V(\mathbf{r}_j - \mathbf{r}_k). \quad (2.40)$$

In classical situations, calculating the probability distributions for the momenta is an easy task, because we can do it by considering one particle at a time. In contrast, the calculation of the correlations of positions among the particles is tough and interesting, because we must look at all the particles at once. In quantum situations, all degrees of freedom are coupled and the entire problem is tough.

Of course, any Hamiltonian gives a description of the dynamics as well as of the statistical mechanics in the form:

$$\begin{aligned} \frac{d\mathbf{r}_j}{dt} &= \frac{\partial H}{\partial p_j}, \\ \frac{dp_j}{dt} &= -\frac{\partial H}{\partial \mathbf{r}_j}. \end{aligned} \quad (2.41)$$

These dynamical equations are far more complex than the statistical mechanical ones, and we may expect their solutions to be more subtle than anything in statistical mechanics.

What interesting things can happen in the situations described above? First and foremost, as we vary the temperature, the system can change into one or another of several interesting thermodynamic states called phases. Familiar phases include gases, and liquids, and solids-less familiar ones include liquid crystals and glasses. Some of these phases are shown in Fig. 2.1.

One reason that phase transitions are so interesting is that they can change the symmetry of the thermodynamic state of the system. For a proper definition of the thermodynamic

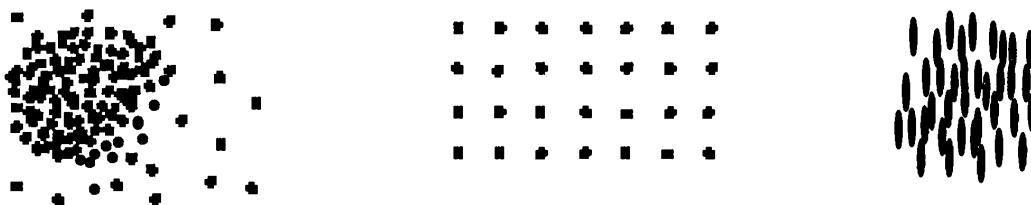


Fig. 2.1. Some Phases of Matter. In the left hand panel, a gas is shown in contact with a liquid. Such a contact among two fluids can break the translational symmetry which is shown within each of the two individual phases. In this case, a drop of liquid is surrounded by a less dense gas. At lower temperatures, see the center panel, the system tends to fall into a crystalline state. In the right hand panel, we see yet another environment called a liquid crystal. Here the molecules are lined up, but there is no crystalline symmetry. This will tend to occur when the molecules are elongated.

state see the book by D. Ruelle.⁴ For example, systems which interact via a two-body potential of the form $V(\mathbf{r} - \mathbf{r}')$ and U being zero, have translational invariance. If we change the origin of the spatial coordinate system, the entire system will still look the same. Every part of the system is exactly like every other part. Gases maintain this translational invariance. In making the transition from a gas to a liquid or a solid, the translational invariance of the entire system can be lost. If a liquid in one part of the system is sitting in contact with a gas in other part, the system is no longer the same everywhere. In a solid, there is a regular lattice which defines the position of the particles. Lattice points are different from other points, so that all points are not equivalent. One of the very interesting questions of physics is how symmetries which are present in the basic formulation of the problem might be lost in the way that formation is realized in nature. Statistical physics provides a wealth of concrete examples in which we can see into enough to start understand this mystery. That is one of the good points of studying the relation between problems in condensed matter physics and statistical theory: The condensed matter provides a bridge to an accessible real world, while the statistical physics provides a deep framework for the study of fundamental properties of that world.

If a liquid is cooled rapidly enough, it does not fall into a crystalline state, but instead into a glassy configuration in which the time development gets extremely slow. The glassy state is a bit of a mystery. It has quite remarkable properties. For example ordinary window glass has a characteristic internal oscillation time of about 10^{-12} seconds but can move only a little in the course of centuries at room temperature. This relaxation time for motion then has a value of order 10^{10} seconds at room temperature. How can any system develop two time constants which differ by so much? Hardly anything is understood about these glassy states, and much exciting research remains to be performed.

So far in this section we have talked about ordinary spatial degrees of freedom. However, for many purposes it is simpler and more instructive to separate spatial degrees of freedom from internal degrees. To do this one generally imagines a material which has internal structure produced by degrees of freedom which sit on the sites of a regular lattice. For

⁴D. Ruelle, *Statistical Physics: Rigorous Results* (Imperial College Press & World Scientific, 1999).

example one can imagine a lattice with lattice sites of the form

$$\mathbf{R} = a(n_1, n_2, \dots, n_\mu, \dots, n_d) \quad (2.42)$$

where d is the lattice dimension. One can then further imagine a variable, named $q_{\mathbf{R}}$, sitting on each of these lattice sites. Each degree of freedom takes on some prescribed values. For example in the Ising case, $q_{\mathbf{R}}$ is written as $\sigma_{\mathbf{R}}$ and each $\sigma_{\mathbf{R}}$ takes on the values ± 1 . Thus we define the basic trace operation at the site \mathbf{R} to be

$$\text{trace}_{\sigma_{\mathbf{R}}} = \sum_{\sigma_{\mathbf{R}}=-1}^1. \quad (2.43)$$

Alternatively $q_{\mathbf{R}}$ might be a Gaussian variable and the trace might be simply an integral over all real values of $q_{\mathbf{R}}$. A problem with a more complex internal symmetry might be one in which $q_{\mathbf{R}}$ has the nature of an angle so that each lattice site would contain an angular variable and the statistical sum at each site would be an integration of an angle which would go from zero to 2π . Each of these variables permits an investigation of some kind of basic internal symmetry and a discussion of how the internal symmetry at each site is reflected in the equilibrium or the time dependent statistical behavior. Thus all kinds of symmetries can be described within the context of a classical statistical mechanics. The simplest Hamiltonian for this kind of system would be of the form

$$H = \sum_{\mathbf{R}} u(q_{\mathbf{R}}) + \sum_{\langle \mathbf{R}, \mathbf{R}' \rangle} v(q_{\mathbf{R}}, q_{\mathbf{R}'}) . \quad (2.44)$$

Here the first sum covers all lattice sites, while the notation $\langle \mathbf{R}, \mathbf{R}' \rangle$ is intended to show that the second sum covers all pairs of nearest neighbors on the lattice. This Hamiltonian is particularly suitable for studying the effect of spins placed on atoms in a regular crystal. Thus the effect of internal degrees of freedom can be studied without taking into account the effects of the additional statistical variables representing the positions of the atoms.

Very often we shall not use the form (2.44) but instead write down an expression for

$$\mathcal{W}[q] = -\beta H[q] \quad (2.45)$$

as

$$\mathcal{W}[q] = \sum_{\mathbf{R}} U(q_{\mathbf{R}}) + \sum_{\langle \mathbf{R}, \mathbf{R}' \rangle} V(q_{\mathbf{R}}, q_{\mathbf{R}'}) . \quad (2.46)$$

The reason for using the notation \mathcal{W} is twofold. First, the statistical weight is directly a function of \mathcal{W} . Second, later on we shall have two different quantities which we can call a Hamiltonian and we shall wish to use the symbol \mathcal{W} , which is unambiguously the logarithm of the classical weight instead of using H , which might be ambiguous. The statistical weight function, \mathcal{W} is called an *action*.⁵

⁵Our ‘action’ is closely related to the time integral of a Lagrangian which is called an *action* in both classical and quantum mechanics.

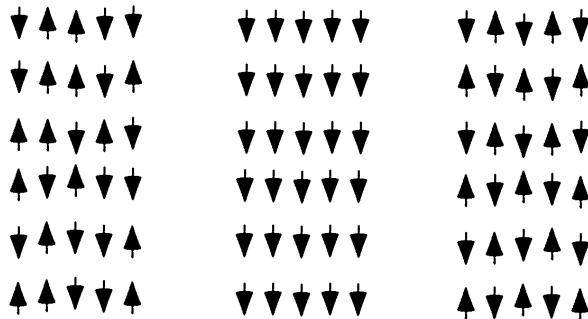


Fig. 2.2. Magnetic Phases of Matter. The magnetic materials are composed of spins on a lattice. Each spin can either point ‘up’ or ‘down’. In the paramagnet, see the left-hand panel, the spins point every which way. In the ferromagnet, center panel, they tend to point in the same direction. In the antiferromagnet, right-hand panel, neighboring spins tend to point in opposite directions.

One example might be the nearest neighbor Ising model in which q is σ and $-\beta H$ is

$$W[\sigma] = \sum_{\mathbf{R}} h\sigma_{\mathbf{R}} + \sum_{\langle \mathbf{R}, \mathbf{R}' \rangle} K\sigma_{\mathbf{R}}\sigma_{\mathbf{R}'} , \quad (2.47)$$

where h is the dimensionless magnetic field and K is called the coupling strength.

Equation (2.47) describes a situation in which the variables $q_{\mathbf{R}}$ are just spins sitting at different lattice sites. These interacting spins can give rise to several different magnetic states. (See Fig. 2.2) In one case, in which K is greater than zero, the interaction tends to make all spins point in the same direction. At low temperatures we have alignment of spins called ferromagnetism. With the opposite sign of the interaction we might perhaps get antiferromagnetism, with two sublattices, with opposite directions of the spins. Of course, it is possible to have a state in which the spins point in random directions. This situation is called paramagnetism. By studying these different situations, we learn about how the system can break its internal symmetries.

Homework

Problem 2.1 (Magnetization). This homework assignment asks that you redo the calculation we did above for a slightly more complicated case. Let j_z be a statistical variable which takes on the values $-1, 0$ and 1 . Let each single-particle Hamiltonian be

$$H = -\mu B_z j_z$$

- (a) Calculate the value of the average magnetization $\mu\langle j_z \rangle$. Plot this as a function of magnetic field.
- (b) For a one gauss field, what is the value of $h = \beta\mu B$ for an electron? At room temperature is the magnetization close to fully saturated?

- (c) If we have a system with 16 noninteracting spins, σ_z which take on the values ± 1 , and if the product $\beta\mu B$ has the value 0.1, what is the probability that the total spin

$$S_z = \sum_{j=1}^{16} \sigma_z^j$$

will take on the values $-16, 16, 0$?

Problem 2.2 (Evaluate the Integral for J_0). The integral defined by Eq. (2.28) is to be evaluated both numerically and analytically.

- (a) First derive the integral which defines J_0
- (b) Next calculate this integral numerically
- (c) To get the analytic result, use a trick: Write J_0^2 in the form of an two-dimensional integral

$$J_0^2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dy \exp\left(-\frac{x^2 + y^2}{2}\right).$$

Then convert the result to polar coordinates and evaluate.

- (d) Compare this analytical result to your direct numerical result for J_0 .

Problem 2.3 (Electric Polarization). Imagine that a certain molecule is sitting in a three-dimensional simple cubic lattice. In the lattice environment it has an electric dipole moment which can take six different values depending on how the molecule lines up with the lattice. The possible values of the dipole moment, \mathbf{q} , are given by $\mathbf{q}/q_0 = (1, 0, 0)$ or $(-1, 0, 0)$ or $(0, 1, 0)$ or $(0, -1, 0)$ or $(0, 0, 1)$ or $(0, 0, -1)$. If there were no electric field present, these six values would have precisely equal probabilities. However, an electric field, E , produces an extra dipole energy $\mathbf{q} \cdot \mathbf{E}$. Calculate the average dipole moment $\langle \mathbf{q} \rangle$ for a single such molecule at temperature T in a electric field \mathbf{E} .

Problem 2.4 (More Ising Spins). Consider two spins coupled together:

$$-\beta H = h(\sigma_1 + \sigma_2) + K\sigma_1\sigma_2,$$

where σ_1 and σ_2 commute and each independently takes on the values ± 1 .

- (a) What are the eigenvalues of this Hamiltonian? What are the degeneracies of the states?
- (b) Find the partition function, and the averages of $(\sigma_1 + \sigma_2)$ and $\sigma_1\sigma_2$.
- (c) How can these averages be computed in terms of derivatives of $\ln Z$?

Problem 2.5 (A Quantum Example). W. Pauli formulated the description of a spin 1/2 particle in terms of three matrices, which have become known as the Pauli spin matrices. These matrices are

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

One thinks of $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ as a vector with x , y , and z components. Imagine a system with two particles of spin 1/2. This system can be described in terms of two such vectors labeled σ_1 and σ_2 describing perhaps spins on different atoms. The different spins commute. Let these two spins be coupled together in the Hamiltonian

$$-\beta H = h(\sigma_{z1} + \sigma_{z2}) + K\sigma_1 \cdot \sigma_2.$$

Here the dot in $\sigma_1 \cdot \sigma_2$, represents the standard dot product of two vectors.

- (a) What are the eigenvalues of this Hamiltonian? What are the degeneracies of the states?
- (b) Find the partition function, and the averages of $\sigma_{z1} + \sigma_{z2}$ and $(\sigma_1 \cdot \sigma_2)$.
- (c) How can these averages be computed in terms of derivatives of $\ln Z$?

Chapter 3

Gaussian Distributions

3.1 Introduction

The simplest and most symmetrical problem in statistical mechanics uses a variable, like the classical momentum, which runs over all values in the interval between minus infinity and infinity. In this chapter, we use the symbol X for such a variable and $X_j(j = 1, 2, \dots, N)$ for N such variables. We might expect that such a variable has so much symmetry that it has the potential for producing situations which are both particularly tractable and also particularly robust. By robust one means that the basic problems or their solutions remain unchanged under a wide class of transformations. We start here by considering the probabilistic behavior with one Gaussian variable, X , and move on to the consideration of many such variables.

In one sense the discussion of this chapter is a natural outgrowth of the last one. There we were interested in the comparison between the structure of problems of the statistical mechanics of one particle and the ones with many non-interacting particles. With Gaussian variables, if the probability distribution is proportional to the exponential of a quadratic form in X (or the X_j 's) then the problem may once more be solved exactly as if it were a problem of non-interacting systems.

3.2 One Variable

A Gaussian probability distribution for a single random variable X is one in which the probability of finding X to lie between x and $x + dx$ has the form¹:

$$\frac{\exp[-\beta(x - \langle X \rangle)^2/2]}{\sqrt{2\pi/\beta}} dx. \quad (3.1)$$

This distribution contains two parameters, $\langle X \rangle$, which measures the center, or mean of the distribution and β , which measures its squared width. This squared width is called the

¹The word Gaussian is also used to describe an integral in which the integrand is the exponential of a quadratic form, i.e. $\int_{-\infty}^{\infty} dx \exp(-ax^2 + bx + c)$.

variance. As we have already seen, β is the inverse of the variance in the distribution, so that

$$\beta^{-1} = \langle (X - \langle X \rangle)^2 \rangle. \quad (3.2)$$

Any probability distribution in one variable, x , which varies over the entire real line and which is of the form of an exponential of a function quadratic in x

$$\rho \sim \exp(-ax^2 + bx + c)$$

may be cast into the structure shown on the right hand side of Eq. (3.1). (See Problem (3.1).)

Our work in describing statistical mechanics has relied quite heavily upon understanding the behavior of exponential functions of the basic variables. We continue along this track by analyzing the so-called *generating function*, $\langle \exp(iqX) \rangle$, with i being the square root of -1 and q being real. In this context, a generating function is the name for an average which is used to generate (i.e. *compute*) other averages. For the Gaussian case, our generating function is the integral

$$\langle \exp(iqX) \rangle = \int_{-\infty}^{\infty} dx \frac{\exp(-\beta(x - \langle X \rangle)^2/2)}{\sqrt{2\pi/\beta}} \exp(iqx)$$

which is easily evaluated to get the result:

For any Gaussian probability distribution with variance β^{-1} , the average of an exponential takes the form

$$\langle \exp(iqX) \rangle = \exp\left(iq\langle X \rangle - \frac{q^2}{2\beta}\right). \quad (3.3)$$

Conversely, if some variable, X , has a probability distribution for which

$$\langle \exp(iqX) \rangle = \exp\left[iqa - \frac{q^2}{2\beta}\right] \quad (3.4)$$

for all values of q , then the probability distribution for X must be Gaussian and a and β respectively have the interpretation of the mean and the inverse variance of the Gaussian.

These two statements look like very special results. Why should they be interesting or important?

One reason is that the Gaussian distribution exhibits a remarkable tenacity or stability, or what we call a peculiar robustness. Imagine that the variable X is of the form $X = aY + b$ where a and b are constants and Y is a Gaussian variable. Equation (3.3) then has the consequence that X is also a Gaussian random variable. Thus a linear function of a Gaussian random variable is also a Gaussian random variable. Next consider an X of the form

$$X = aY + bZ, \quad (3.5a)$$

where a and b are constants and Y and Z are independent Gaussian random variables. By independent it is meant that the fluctuations in the two variables are uncorrelated or *independent*. The mathematical definition of independence use the joint probability $\rho(z, y)dz dy$. This expression gives the probability for finding Z between z and $z + dz$ and, at the same time, finding Y between y and $y + dy$. Independence is that statement that the joint probability distribution $\rho(z, y)$ is a product of the individual probability distributions for Z and Y .

Thus it follows at once from Eq. (3.3) and the meaning of the word independent that X is also a Gaussian random variable. If you add up many independent Gaussian variables you end up with a new Gaussian variable. Thus, if

$$X = \sum_{j=1}^N a_j Y_j, \quad (3.5b)$$

where the a_j are constants and the Y_j are independent Gaussian random variables then the resulting X is certainly a Gaussian random variable. Consequently, a sum of very many Gaussian physical effects (represented say by the Y 's) is a net Gaussian effect.

3.3 Many Gaussian Variables

To describe the effect of many Gaussian Variables, we generalize Eqs. (3.5a) and (3.5b): $X_1, X_2, \dots, X_j, \dots, X_N$ are said to be a set of *Gaussian variables* if the expectation value of an exponential formed from a linear combination of these variables is an exponential of a quadratic form in the coefficients. The words are a mouthful, the equation is simple. For any vector \mathbf{q} with components $q_j (j = 1, 2, \dots, N)$ we have

$$\left\langle \exp \left(i \sum_{j=1}^N q_j X_j \right) \right\rangle = \exp \left(i \sum_{j=1}^N q_j \langle X_j \rangle - \sum_{j,k=1}^N q_j G_{jk} \frac{q_k}{2} \right). \quad (3.6)$$

Thus, the quadratic form defines this many-variable Gaussian.² Naturally, we shall usually write Eq. (3.6) in matrix-vector notation as

$$\langle \exp(i\mathbf{q} \cdot \mathbf{X}) \rangle = \exp \left(i\mathbf{q} \cdot \langle \mathbf{X} \rangle - \mathbf{q} \cdot \mathbf{G} \cdot \frac{\mathbf{q}}{2} \right). \quad (3.7)$$

Of course $\langle \mathbf{X} \rangle$ means the average of the vector \mathbf{X} and \mathbf{G} is related to a variance or correlation matrix for these variables. In fact, a second order power series expansion (in \mathbf{q}) of Eq. (3.7) implies:

$$\langle (X_j - \langle X_j \rangle)(X_k - \langle X_k \rangle) \rangle = G_{jk}. \quad (3.8)$$

²Analytic continuation enables us to extend this results to complex values of the q 's.

For the definition (3.6) to make sense, we require that G be a positive definite symmetric matrix.³ Often, G is called a green function.

What probability distribution could give rise to averages of the form (3.6)? The reader will not be surprised to hear that the defining probability distribution must be an exponential of a quadratic form. Specifically, I ask you to prove in a homework exercise that if

$$\rho(x_1, x_2, \dots, x_N) dx_1 dx_2 \cdots x_N$$

is defined to be the probability that X_1 have a value between x_1 and $x_1 + dx_1$ while X_2 has a value between x_2 and $x_2 + dx_2, \dots$ then from (3.6) it follows that:

$$\rho(x_1, x_2, \dots, x_N) = (2\pi)^{-N/2} (\det C)^{1/2} e^{-[(x - \langle X \rangle)C(x - \langle X \rangle)]/2} \quad (3.9)$$

Here C is a symmetric matrix which is the inverse of G , namely

$$\sum_{m=1}^N C_{jm} G_{mk} = \sum_{m=1}^N G_{jm} C_{mk} = \delta_{jk} \quad (3.10)$$

or in matrix form

$$CG = GC = 1. \quad (3.11)$$

The determinant of C has a value which is the product of all the eigenvalues of C .

The key results in obtaining the solution (3.10) are Eqs. (3.6) and (3.9). That solution makes the many-variable Gaussian case look just like the one-variable case. Imagine doing a change of variables from the X 's to the appropriate linear combination of X 's which serves to diagonalize the matrix C . Then G is simultaneously diagonalized. After this replacement the probability density is an exponential of a sum of terms, each one quadratic in one of the X -variables. Then, Eq. (3.6) gives the total probability as a product of probabilities for the individual linear combinations. Thereby the entire problem is reduced to a combination of subproblems for the individual and non-correlated linear combinations.

We have defined Gaussian correlations by using a generating function approach — and G appears in the solution for the generating function. Conversely, Eq. (3.9) shows that the matrix inverse of G , called C , appears in the basic problem definition. Thus to go from problem to solution, one need only invert a matrix.

³ Any anti-symmetric part of G will contribute nothing to the right hand side of Eq. (3.7). Hence we do not lose any generality by demanding that G is a symmetric matrix. Any symmetric real matrix is Hermitian. One can describe it by listing its eigenvalues, all of which must be real. If they are all positive then the matrix is said to be positive definite. However, if one eigenvalue is negative, then one can set up a Y as a linear combination of X_j corresponding to the eigen direction. A negative eigenvalue of G corresponds to a negative value of $\langle (Y - \langle Y \rangle)^2 \rangle$. This negativity is quite impossible for real Y . Consequently, only positive eigenvalues are possible in a formulation based upon Eq. (3.8).

An alternate formulation is possible, based upon Gaussian integrals. In that case the positivity is a condition for the convergence of the integrals.

3.4 Lattice Green Function

Suppose we have a lattice with lattice sites \mathbf{r}_n , and one variable, X_n , for each site, then we can define a particularly simple and important problem by giving the coefficient matrix

$$C_{n,m} = \begin{cases} 1 & \text{if } \mathbf{r}_n = \mathbf{r}_m \\ -K & \text{if } \mathbf{r}_n \text{ and } \mathbf{r}_m \text{ are nearest neighbors.} \end{cases} \quad (3.12)$$

In this problem definition the on-site interaction serves to normalize the Gaussian variables while the coupling K serves to define the strength of the interaction between different lattice sites. As we shall see this simple and exactly solvable problem is in fact closely related to several different situations involving phase transitions. The Gaussian problem itself undergoes a kind of phase transition at a point at which one of the eigenvalues of C approaches zero. When that happens, the correlation matrix G goes to infinity, and very large correlations tend to develop in the system. Some thermodynamic derivatives for the system become very large, and the system shows every sign of doing something interesting. We shall explore this interesting behavior in considerable detail below.

In the case defined by Eq. (3.12), and in many other situations describing a problem with a high degree of symmetry,⁴ one can relate the matrix and its inverse by using some sort of Fourier transform. In such situations, one can often obtain a full solution for the inverse.

For example if the lattice sites are set to be integers on a simple cubic lattice in dimension d , with a nearest neighbor separation, a :

$$\mathbf{r}_n = a(n_1, n_2, \dots, n_\mu, \dots, n_d), \quad (3.13)$$

then the natural representation of the C 's and G 's is as integrals over wave vector, each component going from $-\pi/a$ to π/a . Thus

$$C_{n,m} = \left(\frac{a}{2\pi}\right)^d \int_{-\pi/a}^{\pi/a} dq_1 \cdots \int_{-\pi/a}^{\pi/a} dq_\mu \cdots \int_{-\pi/a}^{\pi/a} dq_d C(\mathbf{q}) \exp[i\mathbf{q} \cdot (\mathbf{r}_n - \mathbf{r}_m)], \quad (3.14a)$$

$$G_{n,m} = \left(\frac{a}{2\pi}\right)^d \int_{-\pi/a}^{\pi/a} dq_1 \cdots \int_{-\pi/a}^{\pi/a} dq_\mu \cdots \int_{-\pi/a}^{\pi/a} dq_d G(\mathbf{q}) \exp[i\mathbf{q} \cdot (\mathbf{r}_n - \mathbf{r}_m)]. \quad (3.14b)$$

We say that \mathbf{q} 's which lie within the range of integration in expression (3.14a) lie in the first Brillouin zone. We then write this same multiple integral in an abbreviated notation as, for example,

$$G_{n,m} = \left(\frac{a}{2\pi}\right)^s \int_{-\pi/a}^{\pi/a} d^d \mathbf{q} G(\mathbf{q}) \exp[i\mathbf{q} \cdot (\mathbf{r}_n - \mathbf{r}_m)]. \quad (3.15)$$

⁴Here, of course, the symmetry is an invariance under spatial translations.

Note that the variables of integration must sit in the right zone. In view of the defining properties of Fourier transforms we have

$$\left(\frac{a}{2\pi}\right)^d \int_{-\pi/a}^{\pi/a} d^d \mathbf{q} \exp[i\mathbf{q} \cdot \mathbf{r}_n] = \delta_{\mathbf{r}_n, \mathbf{0}}, \quad (3.16a)$$

whenever \mathbf{r}_n is a difference between two lattice vectors. The inverse transform is derived from the relation

$$\sum_n \exp[i\mathbf{q} \cdot \mathbf{r}_n] = \delta(\mathbf{q}) \left(\frac{a}{2\pi}\right)^{-d}, \quad (3.16b)$$

whenever \mathbf{q} is in the first Brillouin zone. Here, $\delta(\mathbf{q})$ is a abbreviation for the product of delta functions

$$\delta(\mathbf{q}) = \prod_{\mu=1}^d \delta(q_\mu). \quad (3.17)$$

It is easy to calculate G . Working from Eqs. (3.12), (3.16a) and (3.16b)), we find that the Gaussian probability is defined by the nearest neighbor interaction which has the Fourier transform

$$C(\mathbf{q}) = 1 - 2K \sum_{\mu=1}^d \cos(q_\mu a). \quad (3.18)$$

As a consequence of Eq. (3.10) the Green function, $G(q)$ has a Fourier transform which obeys $C(\mathbf{q})G(\mathbf{q}) = 1$, so that

$$G(\mathbf{q}) = \frac{1}{1 - 2K \sum_{\mu=1}^d \cos(q_\mu a)}. \quad (3.19)$$

Thus the final result is the coordinate space expression

$$G_{n,m} = \left(\frac{a}{2\pi}\right)^d \int_{-\pi/q}^{\pi/a} d^d \mathbf{q} \frac{\exp[i\mathbf{q} \cdot (\mathbf{r}_n - \mathbf{r}_m)]}{1 - 2K \sum_{\mu=1}^d \cos(q_\mu a)}. \quad (3.20)$$

The quantities $G_{n,m}$ and $C_{n,m}$ can be considered to be matrices in some big space labeled by all the possible values of n . The transformation to Fourier variables \mathbf{q} is essentially a diagonalization of these matrices to a situation in which the diagonal element is labeled by \mathbf{q} and the diagonal elements are respectively $G(\mathbf{q})$ and $C(\mathbf{q})$. We require that these diagonal elements be positive in order that the whole calculation make any sense whatsoever. If K is positive, the most dangerous place is $\mathbf{q} = \mathbf{0}$. For this value of \mathbf{q} we have the minimum value of C , namely

$$C(0) = 1 - 2Kd. \quad (3.21)$$

Thus we might expect a kind of change in behavior as K approaches $1/(2d)$ from below. We shall investigate this point in considerable detail in several of the chapters below.

3.5 Gaussian Random Functions

In some of our later work, we shall need a simple generalization of the set of Gaussian random variables $\{X_j\}$. This generalization, $X(t)$ which is a random function of one parameter, t , defined in direct analogy to Eq. (3.6). We usually think of t as defining time and of $X(t)$ as a random process which goes on through time. Basically our definition says that any linear superposition of the $X(t)$ is a Gaussian random variable of the usual kind. This assumption leads us to define the Gaussian nature of $X(t)$ by using a generalization of Eq. (3.6). Specifically, define,

$$Q = \int_{-\infty}^{\infty} dt q(t) X(t), \quad (3.22)$$

using any ordinary function of time, $q(t)$. Then define the average of an exponential of Q by the statement

$$\left\langle \exp \left(i \int dt q(t) X(t) \right) \right\rangle = \exp \left[i \int dt q(t) \langle X(t) \rangle - \int ds dt q(s) G(s, t) q(t)/2 \right]. \quad (3.23a)$$

In this definition, $\langle X(t) \rangle$ is the average of the random function while the Green function G is the correlation function for $\delta X(t) = X(t) - \langle X(t) \rangle$ defined by

$$\langle \delta X(t) \delta X(s) \rangle = G(s, t). \quad (3.23b)$$

All this just generalizes Eq. (3.6) and what follows from the case of a set of random variables, X_j , parameterized by the discrete index j to a set $X(t)$ parameterized by a continuous variable t .

3.6 Central Limit Theorem

It is important that we have simple solutions for Gaussian problems. But we should also know how Gaussian behaviors can arise in the first place. The latter is explained by what is called the central limit theorem: I shall not state this theorem in its full generality here, but merely give one special case of it. Imagine that we had a set of Y_j 's, which are independent but identically distributed random variables, each with a finite variance. These might arise for example, as the kinetic energies of a group of essentially identical particles. The mathematical statistician calls such a set of variable *iid*, which means identically and independently distributed. Now form an X as in Eq. (3.5b). Imagine that all the a_j 's were equal to one another. Let N be very large. Then, according to the central limit theorem $\delta X = X - \langle X \rangle$ has a behavior in which all averages of powers of δX are correctly represented by a Gaussian distribution. In rough words,

Whenever some effect represented by the random variable, X , may be represented as the sum of many independent small effects, then the predominant behavior of X is Gaussian. Even more roughly: very complex multi-component causations produce Gaussian outcomes.

Thus, in the absence of other information, when behaviors are complex, one tends to assume Gaussian behavior. This assumption guides the analysis of error in experiments in the physical sciences and the analysis of most of the fluctuations observed in the biological or social sciences.

There is a sense in which this central limit theorem is true, and another sense in which it is false.⁵ Under the conditions stated, whenever the probability distribution function $\rho(x)$ is large it is correctly described by a Gaussian distribution. However, there are very unlikely large-deviation events in which $|(X - \langle X \rangle)|$ is much larger than the square root of the variance. This occurrence is very unlikely. So it may not be very serious that the Gaussian distribution usually miss-estimates these unlikely events. In particular, it is often true that very large deviations occur with a higher probability than the Gaussian distribution would predict.

3.7 Distribution of Energies

We carry through a specific calculation in which we shall see both the central limit theorem and also the non-Gaussian behavior of unlikely events. First let us set up the problem. Imagine that we have a total energy composed of a sum of very many Gaussian components. Thus we might have

$$H = \sum_{j=1}^N \frac{p_j^2}{2m}, \quad (3.24)$$

where the p_j 's are Gaussian variables, each with variance $m\beta^{-1}$. Physically, our problem is one in which an energy, H is composed of a sum of many quadratic kinetic energy terms. (Note that we cannot directly apply Eq. (3.4) since H is not a sum of Gaussian variables but their *squares*. Thus H is not a Gaussian random variable.).

In the remainder of this section, we shall set $m = 1$, since carrying around many factors of the mass is not very instructive.

We wish to calculate the probability, $\rho(E)$ that the value of H is E . To start off, imagine that you wished to calculate the probability that the value of H were less than E . The probability in question is $\langle \eta(E - H) \rangle$ where η is called the Heaviside function and is defined by

$$\eta(E - H) = \begin{cases} 1 & \text{for } E > H, \\ 0 & \text{otherwise.} \end{cases} \quad (3.25)$$

The derivative of the Heaviside function with respect to E is $\delta(H - E)$. In addition, the derivative of the probability that H were less than E is proportional to the probability that

⁵All theorems are true of course. Under the stated conditions for the theorem the results follow. However that does not mean that the inferences we draw are necessarily correct. Not all distributions can even be approximately described as Gaussian.

H is exactly E . In this way we reach the conclusion⁶

Whenever H is a random variable which has a continuum of possible values then whenever the probability function is sufficiently smooth, the probability that H will take on a value between E and $E + dE$ is $\rho(E)dE$ where the probability density $\rho(E)$ is given by

$$\rho(E, N) = \langle \delta(H - E) \rangle. \quad (3.26)$$

The N in Eq. (3.26) is a reminder that we have N quadratic terms in the Hamiltonian so that the specific probability distribution for the N p -values is:

$$\rho(p_1, p_2, \dots, p_N) = \frac{\exp\left(-\sum_{j=1}^N \beta p_j^2/2\right)}{Z(\beta)}. \quad (3.27a)$$

Because each p_j is statistically independent of each other momentum, the partition function has a product form

$$Z(\beta) = z(\beta)^N \quad (3.27b)$$

(see Eq. (2.14)). We have already calculated the partition function for a single quadratic degree of freedom. The result is

$$z(\beta) = \int dp e^{-\beta p^2/2} = \sqrt{\frac{2\pi}{\beta}}. \quad (3.27c)$$

Thus we can use Eq. (3.26) to calculate the probability of observing an energy E as

$$\rho(E, N) = \frac{1}{z^N} \int dp_1 dp_2 \cdots dp_N e^{-\beta E} \delta(H - E) \quad (3.28)$$

To do the integral effectively, think of the N momenta as one long momentum vector $\mathbf{p} = (p_1, p_2, \dots, p_N)$, so that the Hamiltonian is just proportional to square of the vector, $H = p^2/2$, and the integral in (3.28) can be written as an N -dimensional integral as:

$$dp_1 dp_2 \cdots dp_N = d^N \mathbf{p} = d\Omega_N p^{N-1} dp.$$

In the last form of writing the N -dimensional integral is expressed as an $N - 1$ dimensional angular integral, $d\Omega_N$, times a radial integration element $p^{N-1} dp$. (The latter form is required to give the entire integral the right dimensions.)

We can now write the probability as:

$$\rho(E, N) = \frac{1}{z^N} \int d\Omega_N \int p^{N-1} dp e^{-\beta E} \delta\left(\frac{p^2}{2} - E\right).$$

⁶In a system with quantized energy levels $\delta(H - E)$ takes on the values infinity and zero depending upon whether or not E is an energy level. Since the energy levels tend to be very close to one another, one can average over a small range of E . After the average, the function $\rho(E, N)$ will tend to be quite smooth.

The first integral gives the ‘solid’ angle of an N -dimensional sphere; the second is a simple delta function integral. The net result is that the probability of observing an energy E for a system of N particles known to have a temperature β^{-1} is

$$\rho(E, N) = \frac{1}{[z(\beta)]^N} \Omega_N (2E)^{(N-2)/2} e^{-\beta E}. \quad (3.29)$$

We check this formula by demanding that the integral over all E of the result (3.29) be unity. Thus, we find

$$1 = \frac{1}{(2\pi)^{N/2}} \Omega_N \int_0^\infty dE \beta (2\beta E)^{(N-2)/2} e^{-\beta E}.$$

We thus get an expression for the solid angle of an N -dimensional sphere,

$$\Omega_N = 2(\pi)^{N/2} \frac{1}{\int_0^\infty dE (E)^{(N-2)/2} e^{-\beta E}}.$$

The integral is the well-known definition of the gamma function, which is also expressed in terms of the factorial function:

$$\Gamma(n) = \int_0^\infty dx x^{n-1} e^{-x} = (n+1)!.$$

Thus our final result for the solid angle is

$$\Omega_N = \frac{2(\pi)^{N/2}}{\Gamma(N/2)}. \quad (3.30)$$

Thus, Eq. (3.29) gives

$$\rho(E, N) = \frac{1}{E\Gamma(N/2)} (\beta E)^{N/2} e^{-\beta E}. \quad (3.31)$$

3.8 Large Deviations

We are finally in a position to begin talking about the behavior of large deviations. In Fig. 3.1 we plot the probability of observing an energy value E in a system of N quadratic degrees of freedom. We have drawn this out for the first few even values of N . In general the logarithm of probability is of the form.

$$\left(\frac{N}{2} \ln \beta E \right) - \beta E. \quad (3.32)$$

The first term in Eq. (3.32) is like an entropy term since it describes the amount of phase space which is available at a given value of E . This term strongly increases with E . The second term describes an energy factor which demands that the probability fall off quite strongly for large E . These two terms together describe a situation in which phase space

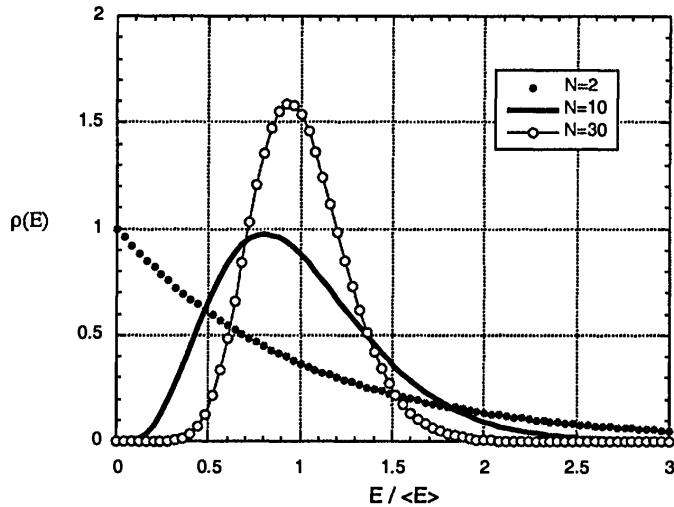


Fig. 3.1. Probability distributions for the energy for three different values of N .

increases with E while the energy term, $-\beta E$, which gives an even more rapidly decreasing probability.

The average value of E is defined by taking the integral of the probability of Eq. (3.31) time E . As we know from the consideration of many Gaussian variables the average energy is given by $N/(2\beta)$. A brief calculation shows that this is also the energy at which the right hand side of (3.32) reaches its peak. So as N gets larger, the average energy grows with N . The peak also has a variance, i.e. $\langle (E - \langle E \rangle)^2 \rangle$. This variance is dimensionally like an energy squared. If it grew as fast as $\langle E \rangle^2$, it would grow proportionally to N^2 . But in our discussion of intensive and extensive quantities, we said that the variance was extensive. Therefore, it must grow as N . As N increases, the peak in the distribution gets bigger and bigger. The width of the distribution only grows as $N^{1/2}$, so that the ratio of width to average gets smaller and smaller. The decrease of this relative width has as its consequence that the energy distribution gets sharper and sharper.

Next we ask about whether a Gaussian distribution does represent the behavior of the extreme values in this situation.

But before we go to work, we should ask about why that question is interesting. One answer is that the distribution of extreme events is of considerable practical and theoretic interest. For example, if we have a usual breeding population of 100 members of a species in which births are 90% female, it would be interesting to know what are the odds that one can produce a generation of all females. If you have a company which has reserves which fluctuate, how often will the reserves go negative? If you have a dam which holds back most of the floods, how often will you get a flood so much bigger than the usual to burst the dam? How often will a natural fluctuation in the weather produce a temperature of 120 degrees Fahrenheit in Chicago? If you have a group of atoms in contact with their environment, how often will a fluctuation cool them enough so that they will effectively freeze? In one model, glasses move so slowly because there are large clumps of material in correlated motion. This model might then be used to calculate the extremely small probability that the glass will

produce a clump of a given size. All interesting questions! All involve calculations of large deviations from some ‘normal’ behavior.

So now turn back to the distribution function given in Eq. (3.31). For large N we expect that probabilities can get very large so we take the natural logarithm of the probability. We know that the mean energy is $E = N\beta^{-1}/2$ so we use as our independent variable the ratio of energy to mean energy defined as

$$R = \frac{2\beta E}{N}. \quad (3.33)$$

Then Eq. (3.31) can be written as

$$\ln[\rho(E, N + 2)\beta^{-1}] = \frac{N}{2} \ln \frac{RN}{2} - \ln \frac{N}{2}! - \frac{NR}{2}.$$

To get a simple result for the entire expression, we should simplify the factorial. For large values of its argument one can get an excellent approximation for $M!$ using the Sterling approximation

$$\ln M! = M \ln M - M + \ln \sqrt{\frac{M}{2\pi}} + \dots \quad (3.34)$$

Each term is much smaller than the previous. If we include the first two we include all effects of order $N \ln N$ or N in the logarithm of the probability and the expression turns into the simple statement.

$$\ln[\rho(E, N + 2)\beta^{-1}] \cong \frac{N}{2}(1 - R + \ln R). \quad (3.35)$$

Notice that this expression has many simple features. It reaches a maximum at $R = 1$. Thus, the most probable value of the energy is its mean value. Near this point, we have an expansion of the form

$$\ln[\rho(E, N + 2)\beta^{-1}] = -\frac{N(R-1)^2}{4} + \frac{N(R-1)^3}{6} + \dots \quad (3.36)$$

The first term is the Gaussian approximation to the probability and the second is a non-Gaussian correction. For large N , the likely events all have $|(R-1)|$ of the order of or less than $N^{-1/2}$. Thus the deviation from the mean is usually small. In that case, the correction term in Eq. (3.36) is of order $N^{-1/2}$ compared with the first term. However, if we look for a sufficiently unlikely event, for example one in which $|(R-1)|$ is of order unity, then the non-Gaussian behavior can substantially modify the probability. In these circumstances the non-Gaussian term multiplies the probability by a factor of order of some power of $\exp N$. For large N that is a large factor.

Nonetheless in this example, the Gaussian approximation is really quite good. In Eq. (3.36) for large N the first term can get to be an extraordinarily large negative number before the second one counts for anything. For example, for a million degrees of freedom

($N = 10^6$) if we want to see an effect with a likelihood of e^{-100} we would then choose an energy only 2 per cent above the most likely energy, i.e. $R = 1.02$. Then the next correction provided by the second term would be an order one effect changing the 100 in the exponent to something like 99. We could hardly hope to see a change like that.

In contrast, the Gaussian approximation turns out to be quite poor in many situations involving fluid flow. For example one can study the behavior of a contaminant carried around by the motion of some fluid. If the fluid motion is chaotic, the contaminant gets spread in a very uneven fashion around the system. To see the unevenness one measures the probability $P(\Delta\rho, r)$ that two points in the fluid separated by a distance r will have a difference in density $P(\Delta\rho)$. This probability density is given empirically by an exponential distribution

$$P(\Delta\rho) = \frac{1}{2\sigma} e^{-|\Delta\rho|/\sigma}, \quad (3.37)$$

where σ is the standard deviation of $\Delta\rho$. Contrast this with usual Gaussian form

$$P(\Delta\rho) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(\Delta\rho)^2}{2\sigma^2}\right], \quad (3.38)$$

which has been the usual guess in statistical problems since the time of Galton.⁷ Chaotic and turbulent systems often show exponential behaviors, like (3.37). Improbable (very bad!!) events are much more likely with the exponential form than with the Gaussian form (3.38). For example, an event with $\Delta\rho = 6\sigma$ has a chance of 10^{-9} of occurring in the Gaussian case, while with the exponential the chance is 0.0025. The Gaussian estimate is clearly quite dangerously wrong in this situation.

3.9 On Almost Gaussian Integrals

We have already seen how statistical mechanics gives us very highly peaked probability distributions. Often this is a result of the same kind of phenomenon which we saw in the probability distribution for the energy: The probability includes one factor (often an energy factor) which is dying off very rapidly while another factor (often a number of states or an entropy factor) grows quite vividly. When the growth rate equals the decay rate, the probability reaches a quite sharp maximum.

The simplest integrals of this type have the structure

$$Y(N) = \int_a^b dx \exp(N\Gamma(x)), \quad (3.39)$$

where N is a number which goes to infinity and $\Gamma(x)$ is a smooth function which reaches a maximum at a single point x_0 within the interior of the range of integration. Take this

⁷Sir Francis Galton (1822–1911) pioneered the use of statistics in the social sciences.

simplest case and let $a < x_0 < b$. Now expand about x_0 . The expansion is one in which the linear term in $x - x_0$ must vanish because x_0 is an extremal, and thus takes the form

$$\Gamma(x) \cong \Gamma(x_0) + \frac{1}{2}\Gamma''(x_0)(x - x_0)^2 + \dots . \quad (3.40)$$

Here, we need $\Gamma''(x_0)$ to be negative so that we have a maximum in the integrand. Assuming that this is so, we substitute (3.40) into (3.39) and extend the range of integration in x to $[-\infty, \infty]$. The integral is easily performed to give the result:

$$Y = \sqrt{\frac{2\pi}{-\Gamma''(x_0)}} \exp[N\Gamma(x_0)] . \quad (3.41)$$

This method of integration is called the method of steepest descent or saddle-point integration. These names describe what one does when the vanishing slope appears someplace off the real axis in the complex plane. Notice that the leading N -dependence occurs in the exponent. The multiplicative factor of $1/\sqrt{N}$ is a relatively small correction.

3.10 Three Versions of Gaussian Problems

Social scientists, economists, and students of finance make very considerable use of Gaussian variables. In fact, there are at least three different ways that Gaussians are used in physics and other statistical applications.

(1) The first is the obvious situation in which the physical variables, X_j , have a Gaussian distribution. Then, in this case, averages of the X 's are given by formulas like

$$\langle (X_j - \langle X_j \rangle)(X_k - \langle X_k \rangle) \rangle = G_{jk} \quad (3.42)$$

and its higher order analog

$$\begin{aligned} & \langle (X_j - \langle X_j \rangle)(X_k - \langle X_k \rangle)(X_m - \langle X_m \rangle)(X_n - \langle X_n \rangle) \rangle \\ &= G_{jk}G_{mn} + G_{jm}G_{kn} + G_{jn}G_{km} . \end{aligned} \quad (3.43)$$

In this situation, we say the X 's are *normally distributed*.

(2) Another very common situation is one in which the basic variables, which we now call Z_j , are each the exponential of a linear combination of Gaussian variables, i.e.

$$\ln Z_j = \sum_k a_{j,k} X_k . \quad (3.44)$$

Here the a 's form a matrix of coefficients. In this case, we say that the Z 's have a log-normal distribution. Using Eq. (3.6) we can then form the average of Z_j as

$$\langle Z_j \rangle = \exp \left(\langle Y_j \rangle + \frac{1}{2} \langle (Y_j - \langle Y_j \rangle)^2 \rangle \right) , \quad (3.45)$$

where Y_j is an abbreviation for the composite Gaussian variable defined by the right hand side of Eq. (3.44). In this case, we say that the Z 's are log-normally distributed.

(3) In physics we also use complex exponentials of Gaussian variables, as for example,

$$\Phi = e^{i\theta}. \quad (3.46)$$

Since expression (3.46) is invariant under the change $\theta \rightarrow (\theta + 2\pi)$, the variable θ may be thought of as an angle. The Gaussian structure then gives the average of Φ in a form which is very much the same as in the log normal case, except for a crucial sign difference. Equation (3.6) implies:

$$\langle \Phi \rangle = \exp \left(i\langle \theta \rangle - \frac{1}{2} \langle (\theta - \langle \theta \rangle)^2 \rangle \right). \quad (3.47)$$

We shall refer to a variable like θ as a phase variable.

We shall, at various times, use all three of these kinds of variables of Gaussian theory.

Homework

Problem 3.1 (Generating Function). Equation (3.3) is followed by the line ‘Conversely if (3.3) is true, the distribution of X must be Gaussian, with variance β^{-1} ’. Prove this statement.

Problem 3.2 (Two Gaussian Variables). Consider a Hamiltonian involving two Gaussian variables, X and Y . Start from the statement that the average formed by these two variables is of the form

$$\langle \exp(aX + bY) \rangle = \exp[a^2 + b^2 - ab]$$

for any a and b . What is the probability distribution for X alone, for Y alone, for X and Y together?

Problem 3.3 (Breeding). If we have a usual breeding population of 100 members of a species in which births are 90% female, it would be interesting to know what are the odds that one can produce a generation of all females. What are they?

Problem 3.4 (Sterling Approximation). Statistical physics makes considerable use of an approximation for the factorial function called the Sterling approximation. See Eq. (3.34) An alternative form is that for large N :

$$N! \cong N^N e^{-N} \sqrt{2\pi N}.$$

- (a) Make a table for $N = 1, 2, \dots, 10$ to see how good this approximation is and to figure out the relative sizes of the successive terms.

- (b) There is a simple integral formula for $N!$, namely,

$$N! = \int_0^\infty dx x^N e^{-x}.$$

One can derive this formula by using

$$\frac{d}{dx} e^{-x} = -e^{-x}$$

and integrating by parts N times. Show how this derivation works.

- (c) Evaluate this integral by the saddle point method and in this way derive the Sterling approximation.

Problem 3.5 (Entropy of Dilute Gas). Consider a dilute gas of N identical atoms of energy E confined in a box of volume Ω . Let N be much larger than one.

- (a) Calculate the entropy of this gas.
- (b) Try to explain this answer using the classical limit of quantum mechanics and trying to estimate the volume in phase space occupied by such a gas.

Problem 3.6 (Higher Order Correlations). Derive Eq. (3.43). If X is a Gaussian variable with average $\langle X \rangle$ and variance β , what is the value of $\langle X^p \rangle$ for $p = 3, 4, 5$ and 6 ?

Chapter 4

Quantum Mechanics and Lattices

This chapter is concerned with the remarkable fact that there is an intimate link between quantum theory and statistical mechanics. Many problems in d -dimensional statistical mechanics with nearest neighbor interactions can be converted into quantum mechanics problems in $d - 1$ dimensions of space and one dimension of time. The quantum theory arises here in a Feynman path integral formulation.¹ Statistical mechanics problems on a one-dimensional lattice are equivalent to problems in ordinary quantum mechanics. One can thus solve many problems in one-dimensional statistical mechanics calculating partition functions, averages, and correlation functions in terms of their quantum analogs: ground states energies, quantum averages, and quantum time-dependent correlation functions. In higher dimensions, the corresponding quantum problem has its degrees of freedom sitting on the sites of a lattice. By an appropriate adjustment of coupling constants, one can construct a limiting case in which important correlations among the quantum variables extend over ranges of very many lattice constants. In this situation, the effect of the lattice can drop away, leaving us with a continuum problem, which is nothing more or less than a quantum field theory. Thus there is an intimate link between statistical mechanics and particle physics.

Just below, we start by reviewing the notation and concepts of quantum physics. We then look at the simplest example of this relationship between statistical physics and quantum physics by studying an Ising model and a Gaussian model, each with nearest neighbor interactions in one dimension. Then we go on to set up an Ising problem in two dimensions, and obtain some properties of its solutions. But instead of talking, let us start.

4.1 All of Quantum Mechanics in One Brief Section

To do quantum mechanics, one starts with a complete set of states $|q\rangle$ and $\langle p|$ which have the ortho-normality property $\langle q|q'\rangle = \delta_{q,q'}$ and a completeness relation

¹B. Hatfield, *Quantum Field Theory of Point Particles and Strings* (Addison-Wesley (1992)) Chapters 12, 13, 14.

$$\sum_q |q)(q| = 1 \quad (4.1)$$

and a trace operation

$$\text{trace } \mathcal{P} = \sum_q (q|\mathcal{P}|q). \quad (4.2)$$

If there is a continuum of states these relations must be modified, by having an integral replace the sum and a delta function replace the delta symbol. If we have a Hamiltonian \mathcal{H} , then the time dependence of the operator, \mathcal{P} , is

$$\mathcal{P}(t) = e^{i\mathcal{H}t} \mathcal{P} e^{-i\mathcal{H}t} \quad (4.3)$$

in units in which \hbar is equal to one. (In this chapter, we shall stick with these units.) Here $\mathcal{P}(0) = \mathcal{P}$ stands for the operator in the Schrödinger representation. Note then that the time translation operator is $\mathcal{T}(t) = \exp(i\mathcal{H}t)$. Thus the partition function is

$$Z(\beta) = \text{trace } \mathcal{T}(i\beta) = \sum_{\alpha} e^{-\beta\epsilon_{\alpha}}, \quad (4.4)$$

while the statistical average of any quantum operator \mathcal{Q} is

$$\langle \mathcal{Q} \rangle = \frac{\text{trace } \mathcal{T}(i\beta)\mathcal{Q}}{Z(\beta)}. \quad (4.5)$$

If you have two operators evaluated at different times, say $\mathcal{Q}(s)$ and $\mathcal{P}(t)$, then the average of the product of these is:

$$\langle \mathcal{Q}(s)\mathcal{P}(t) \rangle = \frac{\text{trace}[\mathcal{T}(i\beta)\mathcal{Q}(s)\mathcal{P}(t)]}{Z(\beta)}. \quad (4.6)$$

One final piece of information is that if β , the inverse temperature, goes to infinity then all the sums are dominated by the state of lowest energy. Then, $Z(\beta)$ is given in terms of the ground state energy, ϵ_0 , as $Z(\beta) = \exp(-\beta\epsilon_0)$ while the averages in Eqs. (4.5) and (4.6) are no longer statistical averages, but just expectation values in the ground state.

4.2 From $d = 1$ Models to Quantum Mechanics

We have already described situations in which there is a lattice and each site on the lattice is described by a variable $q_{\mathbf{R}}$. Now, we consider instead a situation in which the Ising variables appear on a line with coordinates $x_j = x_0 + ja$. Here j is an integer and a , which sets the scale of length, is called the *lattice constant*. Consider a statistical weight which has the same structure as in Eq. (2.46), but now specialized to the case of a one-dimensional system. (Recall that \mathcal{W} is $-\beta$ times a classical Hamiltonian. We wish to reserve the symbol, \mathcal{H} , for the quantum Hamiltonian and so we denote the logarithm of the weight in the classical

problem by the symbol \mathcal{W} . We call \mathcal{W} the *action*.) We have, as before, two terms in \mathcal{W} , an on site term $U(q)$ and a term coupling two nearest neighbor sites $V(q, q')$ so that:

$$\mathcal{W}[q] = \sum_{j=1}^N U(q_j) + \sum_{j=1}^N V(q_j, q_{j+1}). \quad (4.7)$$

For simplicity, we place the variables on a ring with N sites so that we have periodic boundary conditions

$$q_{j+N} = q_j, \quad (4.8)$$

then we can rearrange the sum (4.7) to the form

$$\mathcal{W}[q] = \sum_{j=1}^N w(q_j, q_{j+1}), \quad \text{where } w(q, p) = \frac{U(q) + U(p)}{2} + V(q, p). \quad (4.9)$$

The partition function sum defined by the statistical weight function (4.9) is

$$Z = \text{trace}_{q_1} \text{trace}_{q_2} \cdots \text{trace}_{q_N} \prod_{j=1}^N e^{w(q_j, q_{j+1})}. \quad (4.10)$$

The statistical mechanical interpretation of this expression is quite simple. The variable q_j describes the fluctuating statistical quantities which sit on site j . The total weighting function $\mathcal{W}[q]$ is a sum of individual weighting functions. The partition function sum is a sum over all such variables times a weighting function, $\exp(w(q_j, q_{j+1}))$. This factor determines the weight in the statistical sum coming from the bond connecting the j th and $(j + 1)$ th lattice sites. Equation (4.10) can also be converted into something with a very familiar ring of quantum mechanics. Note that if there are m values of q_j then $\exp(w(q_j, q_{j+1}))$ has the form of a $m \times m$ matrix. Now comes the trick. Write this as a matrix, in particular define the matrix or quantum operator \mathcal{T} by

$$(q|\mathcal{T}|p) = e^{w(q,p)}. \quad (4.11)$$

Here \mathcal{T} is called the *transfer matrix* because it transfers us from one site to the next. Note that Eq. (4.10) has the structure of many matrix multiplications, in particular

$$\begin{aligned} Z &= \text{trace}_{q_N} [\text{trace}_{q_1} (q_N|\mathcal{T}|q_1) \text{trace}_{q_2} \cdot (q_1|\mathcal{T}|q_2) \cdots \text{trace}_{q_{N-1}} (q_{N-2}|\mathcal{T}|q_{N-1}) (q_{N-1}|\mathcal{T}|q_N)] \\ &= \text{trace}_{q_N} (q_N|\mathcal{T}^N|q_N) = \text{trace } \mathcal{T}^N. \end{aligned} \quad (4.12)$$

We recognize the last expression as the usual trace of \mathcal{T}^N so that we have evaluated a statistical mechanical sum over N q -variables with nearest neighbor links as

$$Z = \text{trace } \mathcal{T}^N. \quad (4.13)$$

This remarkable but simple result gives the outcome of a one-dimensional classical statistical mechanics problem as equivalent to the outcome of a quantum mechanics problem. If the transfer matrix has all-positive eigenvalues, we can use the transfer matrix to define a quantum mechanical Hamiltonian, \mathcal{H} , by writing²

$$\mathcal{T} = e^{-\mathcal{H}}. \quad (4.14)$$

Thus, Eq. (4.13) then gives the partition function for a linear chain problem in terms of the partition function for an ordinary quantum Hamiltonian (defined as an $m \times m$ matrix) as

$$Z = \text{trace } e^{-N\mathcal{H}} = \sum_{\alpha} e^{-N\epsilon_{\alpha}} \quad (\text{general}). \quad (4.15)$$

Here the number of sites, N , serves as some sort of formal analog of the inverse temperature. When the sum is written in terms of a sum over eigenvalues of \mathcal{H} , we further see that in the limit of N going to infinity the sum is dominated by the ground state energy ϵ_0 , so that in this limit

$$Z = e^{-N\epsilon_0} \quad (N \rightarrow \infty) \quad (4.16)$$

Note that we have used the symbol, \mathcal{H} , normally connected with a Hamiltonian to describe space translation. Somewhere in the back of our minds sits a view in which space and time are not so different. (Think of relativity.) We shall interpret translations along our lattice as being analogous to translations in time. Almost analogous. Our lattice translation operator has no imaginary number, i , sitting in it. From (4.14) it is simply $\exp(-\mathcal{H})$, with \mathcal{H} real and Hermitian. So our space translations are really analogous to translations in a pure imaginary time.

4.3 An Example: The Linear Ising Chain

We calculate the partition function in the simplest case of this kind. Take an Ising model with spins σ_j at sites $j = 1, 2, \dots, N$. Take the magnetic field to be zero and arrange the couplings so that immediately neighboring sites j and $(j + 1)$ have a coupling K . The statistical weight for two neighboring sites having spin-values σ and σ' is then defined to be

$$e^{w(\sigma, \sigma')} = e^{K\sigma\sigma'} = (\sigma | \mathcal{T} | \sigma'). \quad (4.17)$$

Here σ and σ' each independently take on the values ± 1 . Equation (4.17) defines a two by two matrix. We can write any two by two matrix in question in terms of the usual Pauli spin matrices, specifically,

$$\mathbf{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (4.18)$$

²We can usually make the transfer matrix real and symmetric. It is Hermitian and thus has real eigenvalues. However, the eigenvalues need not be positive. If they are negative, then the Hamiltonian defined from the transfer matrix is complex. However, the matrix, \mathcal{T}^2 , is also Hermitian and has positive eigenvalues. Thus it can always be used to define a Hermitian Hamiltonian, $\mathcal{H} = -(\ln \mathcal{T}^2)/2$.

In going up and back between the notation of Eqs. (4.17) and (4.18) we have to think a little. In (4.17), we interpret σ and σ' as eigenvalues of the matrix τ_3 . Any two by two matrix, M can be written in terms of the eigenstates corresponding to these eigenvalues:

$$M = \begin{pmatrix} (-1|M| - 1) & (-1|M|1) \\ (1|M| - 1) & (1|M|1) \end{pmatrix}.$$

For example, Eq. (4.18) says that τ_3 is diagonal in the σ representation, and has diagonal elements equal to σ . It is, in fact, the quantum operator corresponding to the classical concept of a spin which takes on the values σ .

Notice that the matrix τ_3 has a matrix element $(\sigma|\tau_3|\sigma')$ which is, according to (4.18), equal to zero unless σ is equal to σ' , and equal to σ when this is true. Convert these words into an equation and find that the matrix elements in question are given by $(\sigma + \sigma')/2$. In the same way one can write all the matrices (4.18) in a more algebraic notation as

$$\begin{aligned} (\sigma|1|\sigma') &= \frac{1 + \sigma\sigma'}{2}, & (\sigma|\tau_1|\sigma') &= \frac{1 - \sigma\sigma'}{2}, \\ (\sigma|\tau_2|\sigma') &= i\frac{\sigma - \sigma'}{2}, & (\sigma|\tau_3|\sigma') &= \frac{\sigma + \sigma'}{2}. \end{aligned} \quad (4.19a)$$

An alternative and sometimes useful form for these Pauli matrices is

$$\begin{aligned} (\sigma|1|\sigma') &= \delta_{\sigma,\sigma'}, & (\sigma|\tau_1|\sigma') &= \delta_{\sigma,-\sigma'}, \\ (\sigma|\tau_2|\sigma') &= i\sigma\delta_{\sigma,-\sigma'}, & (\sigma|\tau_3|\sigma') &= \sigma\delta_{\sigma,\sigma'}. \end{aligned} \quad (4.19b)$$

In this problem, these matrices have a very direct physical meaning. The matrix τ_3 is diagonal in the σ -representation and represents the spin. Conversely, τ_1 has only off-diagonal elements. It is an operator whose effect is to change the σ -value.

Now we are in a position to write down the transfer matrix, \mathcal{T} . According to Eq. (4.17) the matrix element of \mathcal{T} is equal to e^K when $\sigma = \sigma'$ and equal to e^{-K} otherwise. In symbols,

$$(\sigma|\mathcal{T}|\sigma') = \frac{1 + \sigma\sigma'}{2}e^K + \frac{1 - \sigma\sigma'}{2}e^{-K}. \quad (4.20)$$

We can write this in pure matrix terms by using Eqs. (4.19) and (4.20) to obtain:

$$\mathcal{T} = e^K \mathbf{1} + e^{-K} \tau_1. \quad (4.21)$$

Alternatively we can write this interaction in exponential form by taking $\mathcal{T} = \exp(-\mathcal{H})$ and then writing this Hamiltonian in terms of the Pauli matrices as

$$-\mathcal{H} = \tilde{K}_0 \mathbf{1} + \tilde{K} \tau_1. \quad (4.22)$$

Here, \tilde{K} is the quantum version of the coupling caused by the interaction K while \tilde{K}_0 is just a constant term in the Hamiltonian. We can evaluate these new ‘couplings’ by taking

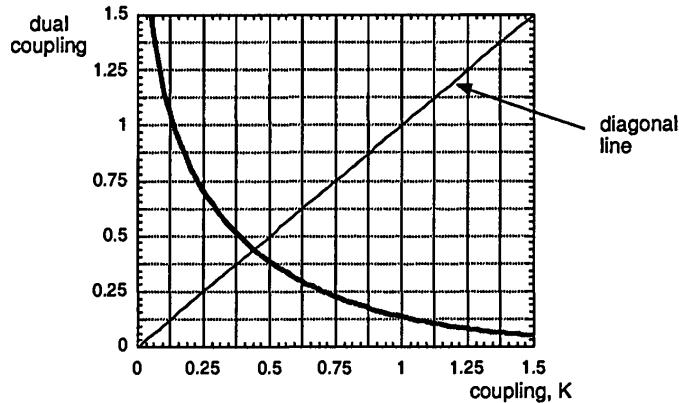


Fig. 4.1. Relationship between K and its dual, \tilde{K} . The dual coupling is plotted with the heavy line. Notice how this duality relation is symmetrical about the diagonal line.

the logarithm of (4.21) and comparing its value to (4.22). The result is

$$2\tilde{K}_0 = \ln \frac{\sinh 2K}{2}, \quad (4.23a)$$

$$\tilde{K} = -\frac{\ln \tanh K}{2}. \quad (4.23b)$$

We shall have a considerable use for these expressions later on. Figure 4.1 shows the relationship between K and \tilde{K} . If K is small \tilde{K} is large and vice versa. In fact the curve which shows the relationship between the two looks unchanged if it is turned on its side. That shows a special symmetry between the function that takes K into \tilde{K} and the inverse function which takes \tilde{K} into K .³ We can write the relationship between \tilde{K} and K in the particularly symmetrical form:

$$(\sinh 2\tilde{K}) \sinh 2K = 1. \quad (4.24a)$$

Call the function that takes K to \tilde{K} , by the name D , so that

$$\tilde{K} = D(K) = -\frac{\ln \tanh K}{2}. \quad (4.24b)$$

Then, according to (4.24a) it is equally true that $K = D(\tilde{K})$ and also that $D(D(K)) = K$. Thus D is a function which is its own inverse. We express the relationship between \tilde{K} and K by saying that \tilde{K} is the dual of K . Of course, it is equally true that K is the dual of \tilde{K} .

At this point, we can evaluate the partition function, and anything else, about the linear chain Ising model. To find the partition function go back to Eq. (4.13) and see:

$$Z = \text{trace}(e^K \mathbf{1} + e^{-K} \tau_1)^N.$$

³Given a function of one variable, $A(x)$, where x covers the range from minus infinity to infinity. If the function A always has a positive derivative then we can uniquely define an inverse function $B(x)$, which obeys $A(B(x)) = B(A(x)) = x$ for all x .

But the trace is a sum over eigenvalues and the eigenvalues of τ_1 are plus or minus one. Thus, the answer is:

$$Z = (2 \cosh K)^N + (2 \sinh K)^N. \quad (4.25)$$

If N is very large, the first term is much larger than the second and thus in this limit of large system size:

$$-\beta F = \ln Z = N \ln(2 \cosh K). \quad (4.26)$$

4.4 One-Dimensional Gaussian Model

One can go through exactly the same kind of analysis for the one-dimension Gaussian model. In this model the weight function depends upon a set of variables q_j , each of which runs from minus infinity to infinity. We pick exactly the same form of interaction as we used in the last chapter, now specialized to the one-dimensional case:

$$Z = \text{Tr}_{\{q\}} \prod_{j=1}^N \exp(w(q_j, q_{j+1})), \quad (4.27)$$

where the bond weight function takes the form

$$w(q, q') = -\frac{1}{4}(q^2 + q'^2) + Kqq' \quad (4.28)$$

and each q is a variable which runs from minus infinity to infinity. Therefore the Tr in Eq. (4.27) is an integral of N q -variables each of which runs from minus infinity to infinity. Alternatively, one can think of $\exp(w(q, p))$ as a kind of matrix element of a transfer matrix \mathcal{T} , described in terms of a Hamiltonian as

$$e^{w(q,p)} = (q|\mathcal{T}|p) = (q|e^{-\mathcal{H}}|p). \quad (4.29)$$

We now need to know about the eigenvalues and eigenstates of the operator \mathcal{T} .

We have already set up calculations like this as eigenvalue calculations. One way of thinking about the eigenvalue is to imagine that the sum over all the q 's from one up to $j - 1$ gives as a result the function $\Psi(q_j)$. Then, the next step is to calculate the next integral and get the next function of a q as $\Psi'(q_{j+1})$ where this next step in the weight function calculation is:

$$\Psi'(q_{j+1}) = \int dq_j \exp(w(q_{j+1}, q_j)) \Psi(q_j) \quad (4.30)$$

or in operator notation

$$\Psi' = \mathcal{T}\Psi. \quad (4.31)$$

A calculation of this kind is called a recursion relation, in that it works by giving step by step a new value of something, here Ψ . Whenever such a recursion calculation gives a fixed point, i.e. a result which does not change its form from recursion to recursion, one can infer the infinite recursion so that the problem is essentially solved.

For the moment, imagine that we were very lucky to find that Ψ' and Ψ were especially simply related: $\Psi'(q) = c\Psi(q)$, where c is a constant. Then every further iteration would simply multiply the wave function by another factor of c , and we would be all done. Since the normalization of wave functions does not matter, we have fortunately found a fixed point. In that case, Ψ and c would respectively have the interpretation of being an eigenfunction and eigenvalue of $\exp(-\mathcal{H})$.

It is hard to guess an eigenfunction. However, one can sometimes do almost that well by guessing that the wave functions belong to a class of functions, depending upon a few parameters. In this case, we shall guess that our wave function is described by two parameters,⁴ z and λ . If we were lucky and clever we might find that if Ψ belong to this class, so will Ψ' . However, the parameters for Ψ' will be z' and λ' , and have different values from the parameters for Ψ . In this case, the recursion relation would not have to find a whole new function, instead it must only express the new parameters in terms of the old. Let us see whether we can use this approach to solve for the partition function of this one-dimensional Gaussian chain.⁵

The problem we are doing looks Gaussian in nature. It seems quite reasonable to guess that a Gaussian form of Ψ might carry the day, and thus start from

$$\Psi(q) = ze^{-\lambda q^2/2}, \quad (4.32)$$

where λ is a constant to be determined, and z sets the normalization. Recall that the Gaussian problem seems to have much in common with the harmonic oscillator, and harmonic oscillators are known to have a ground state wave function of the form (4.32). Thus it seems quite a reasonable guess. To get Ψ' one uses Eqs. (4.28)–(4.32) and sets up the recursion relation

$$\begin{aligned} \Psi'(q) &= \int dp \exp \left[-\frac{1}{4}(q^2 + p^2) + Kqp \right] \Psi(p) \\ &= z \int dq \exp \left[-\frac{1}{4}q^2 - \frac{1}{4}(1+2\lambda)p^2 + Kqp \right] = z'e^{-\lambda' q^2/2}. \end{aligned} \quad (4.33)$$

Notice that the new result, Ψ' , is a Gaussian wave function with new values of the parameters z and λ . Here, the variance of the new Gaussian wave function is given by

$$\lambda' = \frac{1}{2} - \frac{K^2}{\lambda + 1/2}, \quad (4.34)$$

⁴ As we shall see in a moment it is a symmetrical Gaussian and the two parameters are related to the variance and the normalization of the Gaussian.

⁵This recursion approach is exactly the one used in renormalization group analysis, see Chapters 12, 13, and 14. Thus, we study it in a little detail here.

while the new normalization parameter is

$$z' = z \sqrt{\frac{2\pi}{\lambda + 1/2}}. \quad (4.35)$$

Note that λ' is different from λ . We have thus not yet found a fixed point. To obtain the fixed point demand that the λ and λ' have a common value, which we call λ^* . From the recursion, Eq. (4.34), we find

$$\lambda^* = \frac{1}{2} - \frac{K^2}{\lambda^* + 1/2}. \quad (4.36)$$

When we solve this quadratic equation, we find that there are two common values, namely

$$\lambda^* = \pm \sqrt{\frac{1}{4} - K^2}. \quad (4.37)$$

We demand that our wave function, Ψ be normalizable so that we must pick the positive root. We then find that λ^* has the value

$$\lambda^* = \sqrt{\frac{1}{4} - K^2} \quad (4.38)$$

corresponding to the positive square root. Since the Gaussian wave function gives the lowest eigenstate of the harmonic oscillator, we guess that the eigenstate we have just determined in the lowest energy eigenvalue. (It is!)

Equation (4.38) shows that the theory only makes sense when K is in the interval $[-1/2, 1/2]$. The two endpoints are kinds of *critical points* for the theory. (A critical point is a value of the coupling or couplings at which there is a qualitative change in behavior.)

The analysis we have just done, and especially result (4.38) strongly suggest that the one-dimensional Gaussian model only makes sense so long as $|K| \leq 1/2$. In fact if $|K|$ exceeds this limit, the Gaussian integrals diverge at infinite q -values, and the whole problem stops making sense. When there is any qualitative change in behavior of a many particle system we say that it undergoes a *phase transition*. The Gaussian model does so at the two points $K = \pm 1/2$. We shall return to this phase transition issue later.

Let us focus back onto the region where the calculations does make sense. From Eq. (4.33), we see that the lowest eigenvalue is

$$e^{-\epsilon_0} = \sqrt{\frac{2\pi}{\lambda^* + 1/2}} = \sqrt{\frac{4\pi}{1 + \sqrt{1 - 4K^2}}}. \quad (4.39)$$

Next we calculate the energy of the first excited state. We do this by using the standard trick of ladder operators⁶ which are also called creation and annihilation operators. The

⁶See P. A. M. Dirac, *The Principles of Quantum Mechanics*, third edition, The Clarendon Press (Oxford, 1947), Sec. 34.

latter operator has the form

$$a = uQ + ivP = uq + v \frac{d}{dq} \quad (4.40a)$$

while the creation operator is its Hermitian adjoint

$$a^\dagger = uQ - ivP = uq - v \frac{d}{dq}. \quad (4.40b)$$

Here, u and v are constant real coefficients which we have to compute. In the first form of writing, a is given as a linear combination of the quantum position operator, Q and the conjugate momentum operator P . The last form of writing gives the differential operator which defines a in the representation in which Q is diagonal. The operator, a is called an annihilation operator because it is zero when applied to the ground state wave function. The usual definition of the operators requires a commutation relation $[a, a^\dagger] = 1$, which then has the consequence that

$$uv = 1.$$

Our presumed ground state wave function is given by Eq. (4.32) with λ set equal to λ^* . Then the condition that $a\Psi = 0$ is the requirement

$$v\lambda^* = u.$$

Thus, we see that

$$u = (\lambda^*)^{1/2}, \quad v = (\lambda^*)^{-1/2}. \quad (4.41)$$

If a is an annihilation operator, it should reduce the eigenvalue of the Hamiltonian by one quantum unit, $\epsilon_1 - \epsilon_0$. In symbols,

$$ae^{-\mathcal{H}} = e^{-\epsilon_1 + \epsilon_0} e^{-\mathcal{H}} a. \quad (4.42)$$

To check Eq. (4.42), we evaluate both sides of the equation using $\exp(w)$ in place of $\exp(-\mathcal{H})$. In this way, we have written our Hamiltonian as a ‘matrix’ in the q representation. Since d/dq is an anti-symmetric operator,⁷ we find

$$\left((\lambda^*)^{1/2} q + (\lambda^*)^{-1/2} \frac{d}{dq} \right) e^{w(q,q')} = e^{(-\epsilon_1 + \epsilon_0)} \left[(\lambda^*)^{1/2} q' - (\lambda^*)^{-1/2} \frac{d}{dq'} \right] e^{w(q,q')}. \quad (4.43)$$

Calculate the derivatives, and cancel out the common factor of $\exp(w)$, so that Eq. (4.43) becomes

$$\left(\lambda^* - \frac{1}{2} \right) q + Kq' = e^{-\epsilon_1 + \epsilon_0} \left[\left(\lambda^* + \frac{1}{2} \right) q' - Kq \right],$$

⁷To get it to act to the left, you must integrate by parts, and that action changes the sign of the derivative.

which then gives us the result that we sought

$$e^{-\epsilon_1 + \epsilon_0} = \frac{1 - \sqrt{1 - 4K^2}}{2K}. \quad (4.44)$$

Because our approach has been algebraic in character, one can derive all the other eigenstates and eigenvalues by using the ladder operator technique of the text books.

Equation (4.44) gives the excitation energy of the lowest excitation from the ground state. This energy difference will be very important to us. We give it the name κ . Note that as K approaches its limiting, critical, value the energy difference, κ , goes to zero. Thus, at the critical points, the quantum system has a degenerate ground state. We shall see that this property is quite important in understanding how the critical behavior comes about. In particular, this result will prove quite useful in understanding the behavior of the correlations in this situation.

In any quantum mechanical system, there is only one possible way in which the ground state of the system can drastically change its character. This qualitative variation can only happen if some other state or states have an energy which crosses over the value of the ground state so that the situation becomes degenerate. Then the two states may mix and the mixing might change everything quite drastically and discontinuously. In our problem, this change can only occur when $|K| = 1/2$ so that the energy difference between the first two states becomes zero.

Figure 4.2 shows a picture of the behavior of this one-dimensional Gaussian chain. Just so long as $|K|$ is smaller than one half, the system sits one kind of ground state. We call this the ordinary phase. Then, at $|K| = 1/2$ a kind of critical state arises. As we shall see this will involve long ranged correlation. For $|K|$ larger yet, all integrals diverge and the Gaussian chain makes no sense at all. This situation is depicted in Fig. 4.2. This figure shows a *phase diagram*. A thermodynamic phase is a region of couplings in which the behavior of the system remains qualitatively unvarying. This happens for $|K| < 1/2$ for the Gaussian chain.

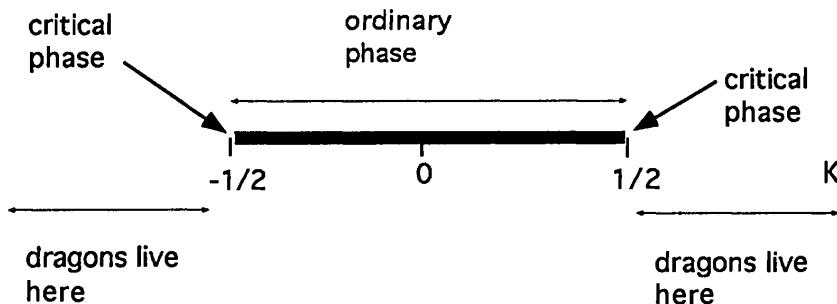


Fig. 4.2. Phase diagram for Gaussian chain problem. This diagram shows the space of coupling constants, here just the line of K 's, and shows what kind of phase appears at what point. We mark specially the boundaries between different phases. Here the boundaries are the points $K = \pm 1/2$ where the solution passes from good sense to nonsense. Notice that these are points at which the lowest two eigenvalues of the transfer matrix become degenerate.

4.5 Coherence Length

We have already emphasized the importance of the lowest two energy eigenstates in defining the qualitative properties of the linear chain problem. Let us carry this idea still further by calculating some space-dependent properties of the general one-dimensional system.

According to Eq. (4.15) the partition function can be calculated as

$$Z = \text{trace } e^{-N\mathcal{H}} = \sum_{\alpha} e^{-N\epsilon_{\alpha}}$$

in a chain of length N . If N is large, the sum is dominated by the lowest eigenvalue, so that the free energy is $\ln Z = -\beta F = -N\epsilon_0$. The first correction in the size of the system is given by the next lowest eigenvalue and gives:

$$\ln Z = -\beta F = -N\epsilon_0 + e^{-N(\epsilon_1 - \epsilon_0)} + \dots . \quad (4.45)$$

Equation (4.45) teaches us first that the correction term decays exponentially in the size of the system, if there is no degeneracy and the energy difference $\kappa = (\epsilon_1 - \epsilon_0)$ is strictly positive. This is our first hint of a quite general result, that there is a relation between spatial correlations and the value of κ . Here the correlations are caused by the periodic boundary conditions, which connect points at a distance $L = Na$. Here a is the distance between neighboring lattice sites so that L is the size of the system. The correction term is

$$e^{-N(\epsilon_1 - \epsilon_0)} = e^{-Na/\xi} = e^{L/\xi}, \quad (4.46)$$

where $L = Na$ is the total size of the system and, ξ , called the coherence length (or equivalently the correlation length), has the value

$$\xi = \frac{a}{\epsilon_1 - \epsilon_0}. \quad (4.47a)$$

We shall also use the notation κ for the excitation energy of the first excited state so that

$$\kappa = \epsilon_1 - \epsilon_0 = \frac{a}{\xi}. \quad (4.47b)$$

As κ goes to zero, the coherence length ξ goes to infinity.

In our work, we shall make a special fuss about the regions in the phase diagrams in which the coherence length, ξ , becomes large. In part, we do this because these cases are particularly interesting for particle physics. Particle physics describes the quantum behavior of systems with one dimension of time and many (usually three) dimensions of space. We often construct such a theory by having a $\mathcal{W}[q]$ with $q_{\mathbf{R}}$ defined on a higher dimensional lattice. The lattice is a construct aimed at keeping the theory finite and under control by having a countable number of degrees of freedom. But, in the end, of course, the resulting theory cannot make any reference to the lattice. After all, experiment gives us no hint that there is a regular lattice sitting under all the phenomena of particle physics. A lattice has preferred directions along its axes, and thus would produce a failure of rotational and

Lorentz invariance. Thus we wish to make the lattice disappear from all physical results. If one looks at correlations defined over distances much bigger than a lattice constant, a , then typically the underlying lattice is masked by the large scale of the effects under consideration. In short, to get a description of particle physics, we need to push statistical mechanics to situation in which the coherence length is very long. (Obviously there are additional criteria for a successful field theory based upon statistical mechanics, but the first condition is that the coherence length and the lattice constant must obey $\xi/a \rightarrow \infty$.)

The large size of ξ must be connected with a small value of the excited state energy. In making contact with field theory, we must look for situations in which the excitation energy $\epsilon_1 - \epsilon_0$ is small. One way of saying this is that we are looking for situation of quantum degeneracy or of near degeneracy. The degenerate situations occur when there is some exact internal symmetry of the system. Thus we are impelled to look at situations in which the classical variables q_R have some kind of symmetry built into them. In the relativistic theory, this situation occurs when there is a theory with an exact symmetry, utilizing some continuous variation of coordinates or internal symmetry variables. In such situations, the field theory usually generates particles without mass. Then, if the symmetry is slightly broken, the theory gives particles with mass. Typically, in scattering processes at larger values of the momentum transfer, the symmetry is restored and the theory is effectively massless. The energy of the massive particle is $\sqrt{p^2 + m^2}$, and goes to just, $|p|$, as the momentum p goes to infinity. Thus, massive particles arise from near-degeneracies and slightly broken symmetries. Massless particles, like the photon, arise from exact symmetries. We shall be very interested in both situations.

4.6 Operator Averages

We next look to other calculations, attempting to find other physical quantities. Imagine that we wish to calculate the average of a physical quantity defined at the site j of the lattice. Call the quantity $X(q_j)$. We can then represent this quantity by the diagonal operator \mathcal{X} such that

$$(q|\mathcal{X}|p) = X(q)\delta_{q,p} \quad (4.48)$$

and set up a calculation just like that in Eq. (4.10)

$$\langle X(q_j) \rangle = \text{trace}_{q_1} \text{trace}_{q_2} \cdots \text{trace}_{q_N} \prod_{j=1}^N e^{w(q_j, q_{j+1})} \frac{X(q_j)}{Z}.$$

We rearrange the traces into a matrix product once more as:

$$\begin{aligned} \langle X(q_j) \rangle &= \text{trace}_{q_N} [\text{trace}_{q_1}(q_N|\mathcal{T}|q_1) \text{trace}_{q_2}(q_1|\mathcal{T}|q_2) \cdots \text{trace}_{q_j}(q_j|\mathcal{T}|q_j) X(q_j) \\ &\quad \times \text{trace}_{q_{j+1}}(q_j|\mathcal{T}|q_{j+1}) \cdots \text{trace}_{q_{N-1}}(q_{N-2}|\mathcal{T}|q_{N-1})(q_{N-1}|\mathcal{T}|q_N)], \end{aligned}$$

which can then be simplified to

$$\langle X(q_j) \rangle = \text{trace}_{q_N} \text{trace}_{q_j} [(q_N | \mathcal{T}^j | q_j) X(q_j) (q_j | \mathcal{T}^{N-j} | q_N)].$$

Since X can also be written as a matrix, we find

$$\langle X(q_j) \rangle = \text{trace}_{q_N} \text{trace}_{q_j} \text{trace}_{p_j} [(q_N | \mathcal{T}^j | q_j) (q_j | \mathcal{X}(q_j) | p_j) (p_j | \mathcal{T}^{N-j} | q_N)],$$

so that finally the result can be written in terms of a quantum sum as

$$\langle X(q_j) \rangle = Z^{-1} \text{trace}\{e^{-(N-j)\mathcal{H}} \mathcal{X} e^{-j\mathcal{H}}\} \quad (4.49)$$

with $\exp(-\mathcal{H}) = \mathcal{T}$. Because a trace can always be cyclically rearranged $\text{trace } XY = \text{trace } YX$, we see that

$$\langle X(q_j) \rangle = Z^{-1} \text{trace}\{e^{-j\mathcal{H}} e^{-(N-j)\mathcal{H}} \mathcal{X}\} = Z^{-1} \text{trace}\{e^{-N\mathcal{H}} \mathcal{X}\}$$

so that the position j falls out of the average. We can then express the trace in terms over a diagonal sum over eigenstates $|\alpha\rangle$ of \mathcal{H} to find

$$\langle X(q_j) \rangle = Z^{-1} \sum_{\alpha} e^{-N\epsilon_{\alpha}} (\alpha | \mathcal{X} | \alpha). \quad (4.50)$$

For large N , the exponential $\exp(-N\mathcal{H})$ projects onto the ground state and Eq. (4.50) reduces to

$$\langle X \rangle = (0 | \mathcal{X} | 0), \quad (4.51)$$

so that *the average of any statistical operator can be written as the diagonal matrix element of the corresponding quantum operator in the ground state.*

As an example of the use of this formula let us calculate the average spin at a particular site in the linear Ising chain, described as in Eq. (4.17). Note that we are assuming that the coupling between neighboring spins is K , and that the magnetic field is zero. In this situation, we know the answer for the average spin. The problem has an invariance in which a change in the sign of all spins leaves all statistical weights quite unchanged. (This invariance is essentially time reversal symmetry.) Thus, the average of any given spin must be zero. Note that the spin operator is τ_3 . (See the discussion following Eq. (4.19).) Then, the average of the spin is, according to Eq. (4.50).

$$\langle \sigma_j \rangle = \frac{\text{trace}[e^{-N\mathcal{H}} \tau_3]}{\text{trace } e^{-N\mathcal{H}}}.$$

From Eq. (4.22) we read off the value of the Hamiltonian as

$$-\mathcal{H} = \tilde{K}_0 \mathbf{1} + \tilde{K} \tau_1.$$

Thus the average converts to

$$\langle \sigma_j \rangle = \frac{\text{trace}[e^{-N\tilde{K}\tau_1} \tau_3]}{\text{trace } e^{-N\tilde{K}\tau_1}}. \quad (4.52)$$

We give the evaluation of the traces as a homework exercise.

4.7 Correlation Functions

Now think about the correlation between two operators, at different points in our one-dimensional lattice. One can derive a quite general approach to calculate and understand correlation functions. Let us consider quantum operators \mathcal{P} and \mathcal{Q} placed respectively at the points j and k . These would represent two statistical quantities which depend upon q 's in the neighborhood of j and k respectively. Then the correlation function for the two operators at points j and k is, when k is bigger than j ,

$$\begin{aligned}\langle \mathcal{P}(j)\mathcal{Q}(k) \rangle &= \frac{1}{Z} \text{trace}\{\exp(-j\mathcal{H})\mathcal{P} \exp[-(k-j)\mathcal{H}]\mathcal{Q} \exp[-(N-k)\mathcal{H}]\} \\ &= \frac{1}{Z} \text{trace}\{\exp[-(N-k+j)\mathcal{H}]\mathcal{P} \exp[-(k-j)\mathcal{H}]\mathcal{Q}\} \\ &= \frac{1}{Z} \text{trace}\{\exp[-(N-r/a)\mathcal{H}]\mathcal{P} \exp(-r\mathcal{H}/a)\mathcal{Q}\}. \end{aligned} \quad (4.53)$$

In the last form of writing, once more, $r = (k-j)a$ is the distance between k and j , assuming $k > j$. Now we can expand in terms of eigenstates of \mathcal{H} so we can write

$$1 = \sum_{\alpha} |\alpha\rangle\langle\alpha|, \quad (4.54)$$

with $|0\rangle$ corresponding to the lowest eigenvalue, ϵ_0 , and $|1\rangle$ corresponding to the next lowest eigenvalue, ϵ_1 . We assume that both these eigenstates are non-degenerate. Then, by writing

$$e^{-\mathcal{H}} = \sum_{\alpha} |\alpha\rangle\langle\alpha| e^{-\epsilon_{\alpha}},$$

we find that our expression for the correlation function becomes:

$$\langle \mathcal{P}(j)\mathcal{Q}(k) \rangle = \frac{1}{Z} \sum_{\mu} \left\{ \exp\left(-\left(N - \frac{r}{a}\right)\epsilon_{\mu}\right) \left(\mu|\mathcal{P} \exp\left(-\frac{r\mathcal{H}}{a}\right)\mathcal{Q}| \mu\right) \right\}. \quad (4.55)$$

Let r , the distance between the sites, be fixed and consider the limit as the number of sites N goes to infinity. In the limit, only the lowest eigenvalue, μ counts so that we may make the replacement

$$e^{-N\mathcal{H}} \longrightarrow |0\rangle\langle 0| e^{-N\epsilon_0}$$

corresponding to our previous evaluation $Z = \exp(-N\epsilon_0)$.

We now find that the correlation function simplifies to

$$\langle \mathcal{P}(j)\mathcal{Q}(k) \rangle = \left\langle 0 \left| \mathcal{P} \exp\left(-\frac{r}{a}(\mathcal{H} - \epsilon_0)\right) \mathcal{Q} \right| 0 \right\rangle. \quad (4.56)$$

Use the completeness expansion (4.54) once more and find

$$\langle \mathcal{P}(j)\mathcal{Q}(k) \rangle = \langle 0|\mathcal{P}|0\rangle\langle 0|\mathcal{Q}|0\rangle + \sum_{\alpha>0} \langle 0|\mathcal{P}|\alpha\rangle \exp\left(-\frac{r}{a}(\epsilon_{\alpha} - \epsilon_0)\right) \langle \alpha|\mathcal{Q}|0\rangle,$$

so that

$$\langle [\mathcal{P}(j) - \langle \mathcal{P} \rangle][\mathcal{Q}(k) - \langle \mathcal{Q} \rangle] \rangle = \sum_{\alpha>0} \langle 0|\mathcal{P}|\alpha \rangle \exp\left(-\frac{r}{a}(\epsilon_\alpha - \epsilon_0)\right) \langle \alpha|\mathcal{Q}|0 \rangle. \quad (4.57)$$

Because ϵ_0 is the ground state energy the sum in Eq. (4.55) contains exponentials which decay with increasing r . In the limit as r/a becomes very large, only the slowest decay counts. If both the ground state and the first excited state are non-degenerate, we find:

$$\langle [\mathcal{P}(j) - \langle \mathcal{P} \rangle][\mathcal{Q}(k) - \langle \mathcal{Q} \rangle] \rangle = \langle 0|\mathcal{P}|1 \rangle \exp\left(-\frac{r}{a}(\epsilon_1 - \epsilon_0)\right) \langle 1|\mathcal{Q}|0 \rangle. \quad (4.58)$$

We can thus identify $(\epsilon_1 - \epsilon_0)$ with the previously defined quantity, κ , which was a dimensionless form of the inverse coherence length. We thus reach our answer:

$$\langle [\mathcal{P}(j) - \langle \mathcal{P} \rangle][\mathcal{Q}(k) - \langle \mathcal{Q} \rangle] \rangle = \langle 0|\mathcal{P}|1 \rangle \langle 1|\mathcal{Q}|0 \rangle \exp\left(-\frac{r}{\xi}\right) \quad (4.59)$$

where the correlation length, ξ , is given by our previous result (4.47)

$$\xi = \frac{a}{\epsilon_1 - \epsilon_0}.$$

4.8 Ising Correlations

We next extend the calculation we have just done by looking at the spin–spin correlation function in the linear Ising chain.

We set up our Ising calculation such that the partition function was computed as the sum over the spins $\sigma_1, \sigma_2, \dots, \sigma_j, \dots$ at sites $1, 2, \dots, N$. Thus our summation variables are the spin and the matrix representing the spin is, as we have already noted, τ_3 . Hence the correlation function can be written, according to Eq. (4.55), as

$$\langle \sigma_j \sigma_k \rangle = \frac{\text{trace}[\exp(-(N - r/a)\mathcal{H})\tau_3 \exp(-r\mathcal{H}/a)\tau_3]}{\text{trace } \exp(-N\mathcal{H})}. \quad (4.60)$$

Since

$$-\mathcal{H} = \tilde{K}_0 \mathbf{1} + \tilde{K} \tau_1,$$

the correlation function expression can be simplified to

$$\langle \sigma_j \sigma_k \rangle = \frac{\text{trace}\{\exp[(N - r/a)\tilde{K}\tau_1]\tau_3 \exp[(r/a)\tilde{K}\tau_1]\tau_3\}}{\text{trace } \exp(N\tilde{K}\tau_1)}.$$

The rest is easy. The quantum matrix τ_1 takes one of the two values $+1$ and -1 . The traces are then diagonal sums over eigenstates with these two values. In symbols

$$\langle \sigma_j \sigma_k \rangle = \frac{\sum_{\mu=\pm 1} \{\exp[(N - r/a)\mu\tilde{K}]\langle \mu|\tau_3 \exp[(r/a)\tilde{K}\tau_1]\tau_3|\mu \rangle\}}{\exp(N\tilde{K}) + \exp(-N\tilde{K})}.$$

Here, $|\mu\rangle$ is an eigenstate of τ_1 with eigenvalue μ . Each τ_3 changes an eigenvalue of τ_1 into its opposite so that our correlation function reads

$$\langle \sigma_j \sigma_k \rangle = \frac{\sum_{\mu=\pm 1} \{ \exp[(N - r/a)\mu \tilde{K}] \exp[-(r/a)\tilde{K}\mu] \}}{\exp(N\tilde{K}) + \exp(-N\tilde{K})}. \quad (4.61)$$

Since the dual coupling, \tilde{K} , and the direct coupling K are related by

$$\exp(-2\tilde{K}) = \tanh K, \quad (4.62)$$

expression (4.61) for the correlation function may also be written in terms of K as

$$\langle \sigma_j \sigma_k \rangle = \frac{(\tanh K)^{r/a} + (\tanh K)^{(N-r/a)}}{1 + (\tanh K)^N}. \quad (4.63)$$

For all finite values of K , if N goes to infinity and r/a remains fixed, the first terms in numerator and denominator will dominate and we find that the spin correlation function is

$$\langle \sigma_j \sigma_k \rangle = (\tanh K)^{r/a}. \quad (4.64)$$

Notice that this correlation function decays exponentially as:

$$\langle \sigma_j \sigma_k \rangle = e^{-r/\xi}. \quad (4.65)$$

The distance, ξ , measures the rate of the exponential fall-off in the correlation function. This correlation length is an extremely important quantity in statistical mechanics and plays a particularly large role in the area of intersection between statistical mechanics and field theory. In this example of the one-dimensional Ising model, the correlation length has the value

$$\xi = \frac{a}{-\ln \tanh K} = \frac{a}{2\tilde{K}}. \quad (4.66)$$

In our previous discussion we said that a/ξ was the excitation energy to the first excited state. Since the Hamiltonian is a constant plus $\tilde{K}\tau_1$ we recover our previous result.

Notice that ξ is dimensionally a length. Sometimes we have need of a dimensionless quantity which characterizes the long-ranged behavior. In these notes we shall use

$$\kappa = \frac{a}{\xi}, \quad (4.67)$$

as the appropriate dimensionless object. We have already noticed that κ is the excitation energy of the lowest excited state.

We have already noticed that one criterion for a successful field theory of elementary particles and fields, at least one based upon statistical mechanics, is that $\kappa \rightarrow 0$ so that the details of the lattice can disappear from the theory.)

The one-dimensional Ising case shows one way in which we can reach this limit of large coherence lengths. In Eq. (4.66) ξ/a goes to infinity if the coupling constant K becomes very large. In fact, in the limiting cases:

$$\frac{\xi}{a} \rightarrow \begin{cases} e^{2K}/2 & \text{as } K \rightarrow +\infty, \\ \ln K^{-1} & \text{as } K \rightarrow 0. \end{cases} \quad (4.68)$$

When the coupling between the spins is very large, spins tend to line up over a very large region of the lattice and therefore the coherence length becomes very large. Conversely, when the coupling is weak the correlation between even neighboring spins is quite weak and the correlation among distant points decays exponentially (and thus quite rapidly) with distance. In $d = 1$, the basic correlation decays exponentially as in Eq. (4.57) because the nearest neighbor interaction make for correlations which die away step by step as one goes to further and further sites. In three dimensions, the pattern of influence is less direct and correlations between spins set at a distance r apart tend to decay as $(a/r) \exp(-r/\xi)$ for large r .⁸

The one-dimensional problem is sufficiently simple so that we can essentially explain all aspects of it. The weak coupling form of the correlation function can be explained by doing a simple perturbation calculation. Imagine the simplest problem involving a coupling K : two sites one coupling, no magnetic field. We have, to second order in the coupling

$$Z = \sum_{\sigma\mu} \exp(L\sigma\mu) \approx \sum_{\sigma\mu} \left[1 + K\sigma\mu + \frac{K^2}{2} \right] = 4 + 2K^2. \quad (4.69)$$

By differentiating the partition function (4.63), we find the exact expression

$$\langle \sigma\mu \rangle = \frac{d}{dK} \ln Z$$

and then the approximate answer:

$$\langle \sigma\mu \rangle \approx K, \quad (4.70)$$

for small values of K .

The strong coupling limit is more complex. The main behavior at low temperatures is that spins line up as in the first panel of Fig. 4.3. If this were all that happened the spin–spin correlation function would not decay with distance. To get the decay one must consider the defects in this configuration, i.e. the effects of various spin reversals from the predominant pattern. At first sight one might think that the major effect would be the flipping of isolated spins as in the second panel of Fig. 4.3. However each such reversal costs the reversal of two bonds. Each bond reversal takes a factor of e^K in the partition function and replaces it by a factor of e^{-K} . The net cost of a reversal of a single isolated spin is that these bond reversals cost a probability factor of $\exp(-4K)$. Imagine that instead one reverses whole

⁸This behavior is a mean field theory result. Mean field theories are discussed in Chapters 10 and 11.

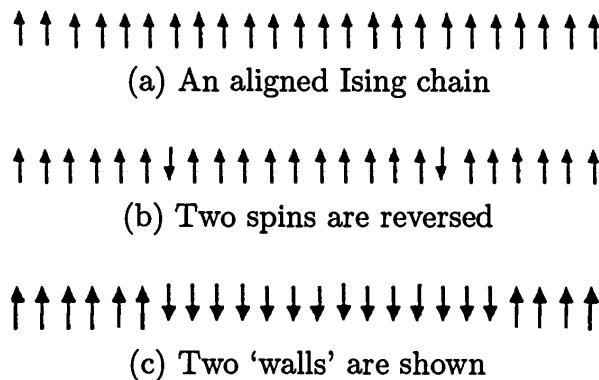


Fig. 4.3. Three kinds of spin configurations in a low temperature Ising chain. With nearest neighbor ferromagnetic interactions, the configuration in the first part is the one with the lowest energy. The other two parts show potential excitations of the system. Because the configuration in part c costs only half as much excitation energy as the one in part b, the production of walls is much more likely than spin reversals.

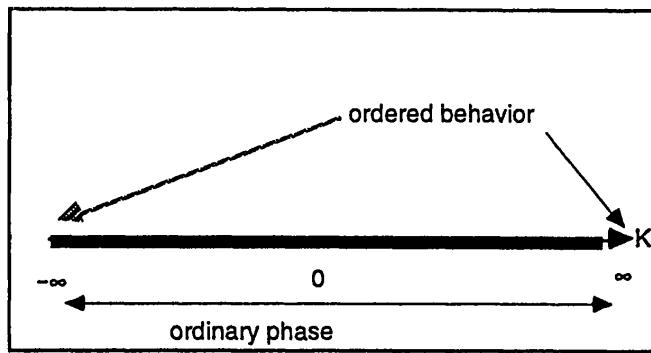


Fig. 4.4. Phase diagram for the One-Dimensional Ising model.

regions of spins as in of the third panel of Fig. 4.3. In this figure we see two points at which blocks are reversed. At each reversal (called a Bloch wall⁹) the system only loses the energy in one bond and thence must pay a probability cost of a factor of $\exp(-2K)$. Therefore at every site one has a possibility $\exp(-2K)$ of losing correlation. The net result is that the correlation length is proportional to $\exp(2K)$.

There is no qualitative difference between the different values of K , so long as these values are finite. For all finite K , the spin correlations decay exponentially with distance and the free energy is an analytic function of K . However, for K going to either plus infinity or minus infinity, the behavior is entirely different. The spin correlations do not fall off in space, while the partition function and free energy both go to infinity with $|K|$. The phase diagram for this system is shown in Fig. 4.4. There is a disordered phase for finite values of K . When the coupling is plus infinity, all the spins are exactly aligned so that we have a ferromagnetic phase. When the coupling goes to minus infinity, we have an antiferromagnetic phase in which successive spins point in opposite directions.

⁹C. Kittel, *Introduction to Solid State Physics*, 6th edition (Wiley, New York (1986)), p. 452 ff.

4.9 Two-Dimensional Ising Model

The same basic technique works for the two-dimensional Ising Model. If there is no magnetic field, the coupling can be written as

$$\mathcal{W}[\sigma] = \sum_{j=1}^{L_x} \sum_{k=1}^{L_y} (K_x \sigma_{j,k} \sigma_{j+1,k} + K_y \sigma_{j,k} \sigma_{j,k+1}). \quad (4.71)$$

This two-dimensional situation can be analyzed rather completely.¹⁰ If the coupling constants, K_x and K_y , are sufficiently large the system falls into one of two ordered states in which the spins point preferentially in one direction or the other. In this *ferromagnetic* situation one of the two states has $\langle \sigma_{j,k} \rangle$ greater than zero; the second has this average smaller than zero and this sign is maintained over the whole system. If one or both of the couplings get sufficiently small in magnitude, this ordering goes away and the system enters a disordered situation called a paramagnetic phase.¹¹ On the other hand, if both couplings are sufficiently large in magnitude, but negative, then the system enters an *antiferromagnetic* phase in which there is long range order of a different kind. Now the spins, $\sigma_{j,k}$ on sites with $j+k$ even will tend to have one sign and those with $j+k$ odd will tend to have the opposite sign. These different kinds of phases are depicted in Fig. 4.5 which is a phase diagrams that plots the position of these phases against K_x and K_y . In this section, we shall describe how the boundaries between the regions may be calculated exactly. We focus upon the transition from paramagnetic to ferromagnetic behavior.

Recall that the one-dimensional Ising model was converted into a quantum problem involving a Pauli spin matrix. Here we have a line of L_y Ising variables coupled to each other and each coupled to its x -direction neighbor in just the same manner as in the one-dimensional case. Thus, we expect our problem to be converted into L_y different Pauli matrices, each coupled to the other. As before we define a set of basis states, so as to build a quantum formulation. We write

$$|\{\sigma\}\rangle = |\sigma_1\rangle |\sigma_2\rangle \cdots |\sigma_k\rangle \cdots |\sigma_{L_y}\rangle, \quad (4.72)$$

where each $\{\sigma\}$ is the set of σ_k 's (L_y of them) each σ_k taking on the values $+1$ and -1 . The first, second, third ... of the states $|\sigma\rangle$ on the right hand side of Eq. (4.72) refer respectively to the spin on the site with k equal to $1, 2, 3, \dots$. We call $\tau_{1,k}$ the Pauli spin-flip operator τ_1 for the k th spin. In this representation, we can write the K_y term as the diagonal matrix

$$\langle \{\mu\} | \mathcal{T}_y | \{\sigma\} \rangle = \prod_{k=1}^{L_y} \delta(\sigma_k, \mu_k) e^{K_y \sigma_k \sigma_{k+1}}. \quad (4.73)$$

¹⁰The solution is a *tour de force* of Lars Onsager. See L. Onsager, Phys. Rev. **65**, 119 (1945). Expositions on the subject include: Kerson Huang, *Statistical Mechanics* (John Wiley and Sons, New York, 1965), Chapter 16; G. F. Newell and E. Montroll, Rev. Mod. Phys. **25**, 253 (1953).

¹¹There are two names for disordered phases in a magnet. If the magnetic susceptibility is positive, the material is called a paramagnet. In the magnetization points opposite to the applied field, the system is said to be diamagnetic. See D. Mattis, *The Theory of Magnetism* (Harper and Row, New York, 1965).

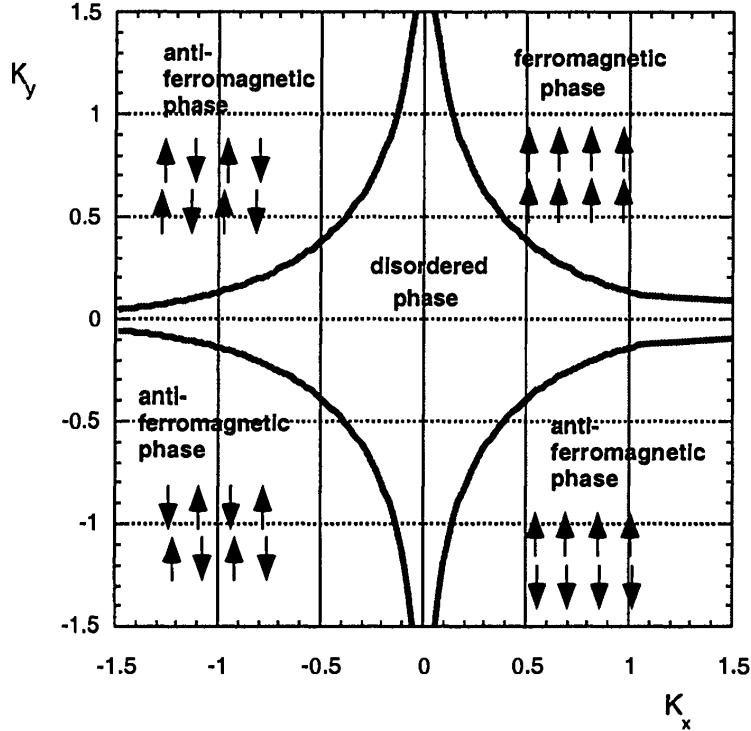


Fig. 4.5. Phase diagram for the two-dimensional Ising model. Four different ordered phases are shown. The nature of the ordering is indicated by the arrows, which represent spin vectors on a small piece of the lattice. In the ferromagnetic phase all the spins tend to line up as shown. The other three ordered phases have different kinds of opposing spin alignments. The lines drawn as the boundaries between the different phases. In addition, each line represents a special kind of phase, a *critically ordered* phase.

Thus, in a matrix-based notation

$$\mathcal{T}_y = \exp \left(\sum_{k=1}^{L_y} K_y \tau_{3,k} \tau_{3,k+1} \right). \quad (4.74)$$

The other part of \mathcal{W} is the coupling in the x direction. Here we have a sum of terms, each term referring to only one k -value. Therefore, the transfer matrix which arises from this part of the action is a product of terms, each one of which has exactly the same structure as the one we previously calculated for a single k -value. Specifically we find:

$$\langle \{\sigma_{j,k}\} | \mathcal{T}_x | \{\sigma_{j+1,k}\} \rangle = \sum_{k=1}^{L_y} e^{K_x \sigma_{j,k} \sigma_{j+1,k}}, \quad (4.75)$$

which gives us the matrix based expression

$$T_x = \exp \left(\sum_{k=1}^{L_y} (\tilde{K}_0 \mathbf{1} + \tilde{K}_x \tau_{1,k}) \right), \quad (4.76)$$

where the quantum couplings, \tilde{K} , are given as function of K_x by Eqs. (4.24b), i.e. $\tilde{K}_x = D(K_x)$. Thus, the entire problem has been converted into the quantum problem of finding the largest eigenvalue of the product

$$\mathcal{T} = \mathcal{T}_x \mathcal{T}_y. \quad (4.77)$$

It is not so easy to find this eigenvalue¹² but at least we have the comfort of translating one problem into another.

In one limit, we can immediately see that the quantum problem is one which can be cast into familiar form. Imagine that both K_y and \tilde{K}_x are small numbers. (We are thus saying that the coupling in the x -direction is very strong and tends to line up a whole row of spins. Then the weak y -coupling might possibly line up all the spins.) In this limit of couplings, it is permissible to recast \mathcal{T} by adding the exponents in \mathcal{T}_x and \mathcal{T}_y so as to produce

$$\mathcal{T} = e^{-\mathcal{H}}, \quad -\mathcal{H} = \exp \sum_{k=1}^{L_y} (\tilde{K}_0 \mathbf{1} + \tilde{K}_x \tau_{1,k} + K_y \tau_{3,k} \tau_{3,k+1}). \quad (4.78)$$

The error in adding the exponents is of order $K_y \tilde{K}_x$ and hence is negligible in the limit in which these couplings are small.

To solve the statistical mechanics problem, we have to find the ground state of the Hamiltonian, \mathcal{H} in Eq. (4.78). This Hamiltonian describes a chain of quantum spins coupled to an external x -direction magnetic field with coupling \tilde{K}_x . Also included, with strength K_y , is a coupling between the z -components of neighboring spins. Thus, the two-dimensional Ising model has been reduced to a one-dimensional quantum mechanics problem in which there are two different kinds of interactions which work against one another. The first kind, represented by the products of the τ_3 's represent an effect in which, for $K_y > 0$ the z - or third-component of the spins all line up. Therefore this term, when it produces its maximum effect, has the result of lining up all the spins so that the system falls into one of two quantum states, either

$$|\sigma_1 = +1) |\sigma_2 = +1) \cdots |\sigma_k = +1) \cdots |\sigma_{L_y} = +1) \quad (4.79a)$$

or alternatively

$$|\sigma_1 = -1) |\sigma_2 = -1) \cdots |\sigma_k = -1) \cdots |\sigma_{L_y} = -1). \quad (4.79b)$$

These states are both eigenstates of all of the τ_3 's. However, if K_x is positive but small, then \tilde{K}_x is big and so the \mathcal{T}_x -factor wins out. In this situation the ground state is an eigenstate of all the τ_1 's, this time with the eigenvalue of each of the τ_1 's being plus one.

There is, of course, a qualitative difference between these two kinds of states. In the first one, the spins are all lined up with each other and pointing in either the plus or minus z -direction. In the latter situation, the x -direction magnetic field has completely

¹²Onsager did it, but it was hard!

broken up the z -order. In the first situation there are two degenerate ground states; in the second a single ground state. This distinction persists even if neither K_y nor \tilde{K}_x are zero. Thus there are two kinds of situations, the ferromagnetic situation which we identify with degenerate ground states, qualitatively similar to the states (4.79) and the paramagnetic situation, which we identify as having a non-degenerate ground state. This situation applies to the transfer matrix of Eq. (4.78) and equally well to the more complex product matrix of Eq. (4.77). In both cases we have two phases: the ferromagnetic one in which the K_y term dominates, and the paramagnetic one in which \tilde{K}_x dominates.

We can sharpen our conclusion by looking at the algebraic structure of the transfer matrix.

Since the partial transfer matrix T_x is a description of basically the same kind of interactions as T_y it should not be a surprise that there is a symmetry relating these two operators. In particular, the algebraic structure of one, which is built upon $\tau_{1,k}$ is precisely the same as that of the other, built upon $\tau_{3,k}\tau_{3,k+1}$. To see this identify define

$$C_k = \tau_{1,1}\tau_{1,2} \cdots \tau_{1,k-1}\tau_{1,k}.$$

The \tilde{K}_x term has the algebraic structure

$$\sum_{k=1}^{L_y} \tilde{K}_x C_k C_{k+1},$$

except for an uninteresting additive constant. The K_y term has an identical looking structure

$$\sum_{k=1}^{L_y} K_y \tau_{3,k} \tau_{3,k+1}.$$

There is a complete symmetry between $\tau_{3,k}$ and C_n . The square of each is one. They commute if n is not equal to k . In the latter case they anticommute. The nontrivial product $\tau_{3,k}C_k = b_k$ also anti-commutes with all $\tau_{3,n}$ for $n < k$ and all C_n for $n > k$.¹³ Carry this argument a bit further, and you reach the correct conclusion that it is possible to interchange C_k and $\tau_{3,k}$ while maintaining the algebraic structure of all commutation relations. However, it is these relations which determine the eigenvalues of the operators in question. It then follows that the largest eigenvalue is (except for the constant K_0 term) a symmetrical function of K_y and \tilde{K}_x .

If there is going to be only one phase transition, it must occur where these two couplings are equal. Thus, the ferromagnetic phase must arise when $K_y > \tilde{K}_x$. The disordered phase arises when $K_y < \tilde{K}_x$. When these couplings are equal, we must have a critically ordered phase. This behavior is shown in Fig. 4.5. Thus, we have used the matrix formulation to infer the position of the line of phase transitions. Since \tilde{K} is the dual of K , this approach is called a duality argument. This argument was originally put forward by Kramers and Wannier.¹⁴

¹³See B. Kaufman, Phys. Rev. **76**, 1232 (1949) and also L. Onsager and B. Kaufman, Phys. Rev. **76**, 1244 (1949). E. H. Lieb T. Schultz and D. Mattis, Rev. Mod. Physics **36**, 856 (1964).

¹⁴H. Kramers and G. Wannier, Phys. Rev. **60**, 252, 263 (1941).

Homework

Problem 4.1 (Check the Partition Function Result). Calculate the partition function of the Ising Model with zero magnetic field from its definition for $N = 1, 2$, and 3 and 7 . Remember that the system has periodic boundary conditions. Compare your results with Eq. (4.25). (You might well want to do part of this problem on the computer.)

Problem 4.2 (Effects of a Magnetic Field). Redo the calculation (4.25) for the case in which a magnetic field is present, i.e. when $w(\sigma, \mu) = h(\sigma + \mu)/2 + K\sigma\mu$.

- (1) Find the partition function.
- (2) Find the free energy in the limit as N goes to infinity.
- (3) Calculate the magnetization as a function of K and h .
- (4) Find and plot the zero field magnetic susceptibility as a function of K .

Problem 4.3 (Ising Magnetization). Using the same form for w as above compute $\langle \sigma_j \rangle$ as a ground state average. Compare your result with the answer from the last problem.

Problem 4.4 (The Q -State Potts Model). Let the variable σ take on the values $1, 2, \dots, Q$ with Q being an integer. Consider a linear chain with one such variable per site and a nearest neighbor interaction among the sites. Let the total weight be the sum of individual weights, one for each bond, in which

$$w(\sigma, \mu) = K(Q\delta(\sigma, \mu) - 1).$$

Find the partition function for this problem. What is the value of $\langle \delta(\sigma_j, \sigma_{j+1}) \rangle$ for a system which has very large values of N . Is the answer a smooth function of K ?

Problem 4.5 (Correlations in the One-Dimensional Ising Model). Calculate the four-spin correlation function $\langle \sigma_j \sigma_k \sigma_m \sigma_n \rangle$ in the zero-field one-dimensional Ising model with nearest neighbor coupling K . Consider the case in which $m > l > k > j$. From your expression for this correlation function, calculate the derivative of $\langle \sigma_j \sigma_k \sigma_m \rangle$ with respect to h , evaluated at $h = 0$.

Problem 4.6 (Two-Spin Correlations). Calculate the two-spin correlation function $\langle \sigma_1 \sigma_2 \rangle$ for $h = 0$ to first order in the coupling K for $N = 1, 2$, and 3 . Compare your result with the answer in the limit $N \rightarrow \infty$.

Problem 4.7 (First Excited State of the Gaussian Model). Calculate a wave function for the first excited state of the Gaussian model. (Hint: think about the role of a^\dagger as a ladder operators. Using this wave function, show that Eq. (4.44) gives the correct form for the energy eigenvalue.)

Problem 4.8 (Trace Evaluation). Calculate the right-hand side of Eq. (4.52).

Part II

Random Dynamics

Chapter 5

Diffusion and Hopping

In this chapter, we describe the motion of a particle hopping at random on a lattice. We shall use this very simple situation to introduce the description of dynamical motions in mechanics. Our analysis will show that the typical motion of the particle is one in which it only slowly moves outward from its starting point. It goes forward and back and retraces its path many times so that, in the end, its net motion is quite slow indeed. This slow type of motion is called *diffusion*, and this chapter is all about diffusive motion. Thus random hopping and diffusion provide alternative ways of viewing the selfsame situation.

One way we shall analyze this motion is to look at the probability that the diffusing particle might, at a given time, be found at a particular point in space. In doing this analysis we shall follow a general prescription which has proven to be a very powerful method in the analysis of dynamical situations: First we define the conservation laws obeyed by the system, then identify a likely behavior for the current of the conserved quantity, and finally put that current into the conservation law to find a hydrodynamic equation. In the case considered here, the conserved quantity is the total probability of finding the particle someplace, and the resulting hydrodynamic equation is the partial differential equation called the *diffusion equation*.

5.1 Random Walk on a Lattice

Newton emphasized the importance of momentum conservation in the description of isolated systems. The conservation of momentum is, as we shall see, a very important ingredient in determining the motion of a Brownian particle. However, in this chapter, we shall not include the effects of momentum conservation. (Those effects will come in the next chapter.) Instead, we consider the somewhat more elementary problem posed by the motion of impurities on a lattice. Imagine a regular hypercubic lattice (as in Fig. 5.1) and a particle which is allowed to sit on any one of the lattice sites

$$\mathbf{r} = a(n_1, n_2, \dots, n_\mu, \dots, n_d), \quad (5.1)$$

where the n 's are integers, d is the dimensionality of the system, and a is the lattice constant, i.e. the distance between nearest neighbor lattice sites. An impurity particle in a real solid may get trapped for a while at some lattice site and then come into equilibrium with its environment. Then, after it has been sitting on the site for a time, it may hop to a neighboring site, where it sits for a while and equilibrates. As it equilibrates, the momentum which may have been gained to help it hop is lost so that it has no memory of its past. When it hops again, it jumps to a neighboring site picked at random from the nearest neighbors. This process is repeated again and again and the particle moves through the lattice.

Notice that we have not defined the mechanism which causes its hopping. The most likely process is one in which, while the particle is sitting on the site, a bunch of thermally excited sound waves arrive together at the site and thus accidentally bring the particle enough energy to hop to its neighbor. Alternatively the process may be quantum in nature and involve, in part, quantum tunneling. What causes the hopping will be not too relevant to our analysis. What we need instead is a good phenomenological description of the hopping process.

To analyze this situation in its simplest form, we introduce a simplified model in which the particle is assumed to hop to the next site after the time interval, τ . On each hop, the particle moves from a site to a randomly chosen nearest neighbor site. The change in position on the j th hop is written ξ_j , where ξ_j is a vector of magnitude a directed parallel to the possible vectors connecting nearest neighbors. (See Fig. 5.1.) There are $2d$ possible values of ξ_j , which are $\pm ae_\mu$ with e_μ being a unit vectors drawn parallel to the μ th axis. These random variables, ξ_j , are picked independently for each different value of j . At each j , the different possible value of ξ_j are chosen with equal probability. Thus they obey the condition that ξ_j and ξ_k are uncorrelated for different hops, that is if j is different from k .

$$\langle \xi_j \cdot \xi_k \rangle = \langle \xi_j \rangle \cdot \langle \xi_k \rangle . \quad (5.2a)$$

Further, because we choose ξ_j in such a way that a vector and its negative are equally likely, it follows at once that

$$\langle \xi_j \rangle = 0 . \quad (5.2b)$$

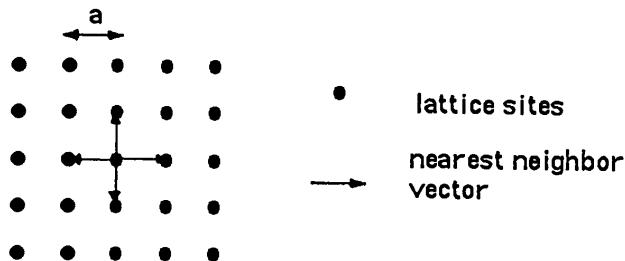


Fig. 5.1. The simple square lattice in two dimensions.

Thus, if j is different from k , the two vectors, ξ_j and ξ_k are uncorrelated. Since the length of all the ξ_j is a , we can find the average of $(\xi_j)^2$ and thus obtain

$$\langle \xi_j \cdot \xi_k \rangle = a^2 \delta_{j,k}. \quad (5.2c)$$

In the time interval $M\tau$, the particle hops M times and its displacement is

$$\mathbf{R} = \sum_{j=1}^M \xi_j. \quad (5.3)$$

Of course, the average displacement vector is zero

$$\langle \mathbf{R} \rangle = \sum_{j=1}^M \langle \xi_j \rangle = 0. \quad (5.4a)$$

However, the mean squared displacement is certainly nonzero.

$$\langle \mathbf{R} \cdot \mathbf{R} \rangle = \sum_{j,k=1}^M \langle \xi_j \cdot \xi_k \rangle = a^2 \sum_{j,k=1}^N \delta_{j,k}.$$

Thus the answer is that

$$\langle \mathbf{R} \cdot \mathbf{R} \rangle = a^2 M. \quad (5.4b)$$

Equations (5.4a) and (5.4b) together imply that for large M the particle really makes very little net progress. In M steps, it only progresses a distance which is of the order of $aM^{1/2}$. This slow progress should be compared with the behavior which arises when the different directions are weighted unequally so that

$$\langle \xi_j \rangle = \mathbf{u}\tau$$

with \mathbf{u} being the average velocity of the particle. In that case, $\langle \mathbf{R} \rangle = \mathbf{u}\tau N$, so that the displacement varies linearly with N . If there were a nonzero average of ξ_j this ‘velocity term’ would dominate the long term motion. But, in the situation we have picked, this regular motion is absent and we only have the much slower motion cased by the random walk. Figure 5.2 shows some random walks in two dimensions and lets us compare the resulting random motion with a regular ‘up and back’ walk which covers the same distance. Notice how much more compact are the random walks. They really are compressed into a small region of space.

5.2 Formulating This Problem

Let $\rho_{r/a,t/\tau}$ be the probability of finding a walker at the position r after a step which has been completed at time t . One can formally define this probability as

$$\rho_{\mathbf{r}/a,t/\tau}^L = \langle \delta_{\mathbf{R}(t),\mathbf{r}} \rangle. \quad (5.5)$$



Fig. 5.2. Two-dimensional Random Walks. We see three different random walks. The dark squares represent the beginning and the end of the walk. Each walk contains one thousand steps, with the same step-length. The walks each extend over a relative small distance, start to finish. This small distance should be contrasted with the distance which would be covered if the particles would move in a straight line. The straight line path it would cover sixteen page widths! Thus, random walks are so convoluted that they tend to fall into a quite small region of space.

Here $\mathbf{R}(t)$ is a vector which takes on values depending upon the values of the ξ_j . It is what is called a random variable. On the other hand \mathbf{r} is a prescribed vector which defines the position of the particle. It takes on values which are the sites on our lattice. The hypercubic lattice is defined by taking the lattice sites \mathbf{r} to be $a\mathbf{n}$, where a is the lattice constant and \mathbf{n} is a vector composed of d integers. Similarly the time t has values which are τ times an integer. Thus, we shall usually write this probability as $\rho_{\mathbf{n},M}^L$. The delta symbol on the right hand side of Eq. (5.5) gives a value one whenever the random vector falls on the lattice site, \mathbf{r} , and zero otherwise. The average of a quantity which gives a one, when a specific thing happens, and zero otherwise is just the probability of the thing happening. Thus, Eq. (5.5) defines the probability $\rho_{\mathbf{n},M}^L$ that our hopping particle will appear at the lattice site with a position vector $\mathbf{r} = a\mathbf{n}$ at the time $t = M\tau$.

The superscript ‘ L ’ in Eq. (5.5) reminds us that we are working with a lattice and that ρ^L is a probability defined on the lattice points. We shall be most interested in the behavior of this probability in the situation in which it is slowly varying in the spatial coordinate, \mathbf{r} . To handle that case, we introduce a continuum *probability density*, $\rho(\mathbf{r},t)$. Now let us assume that these densities are slowly varying, and then calculate the total probability in a region Ω from both probabilities. The region Ω is large enough to include many lattice sites, but small enough so that the probabilities vary very little over the region.

We have:

$$\int_{\mathbf{r} \in \Omega} d\mathbf{r} \rho(\mathbf{r}, t) = \sum_{\mathbf{r} \in \Omega} \rho_{\mathbf{r}/a, t/\tau}^L.$$

We take the two ρ 's out from under the summations and integrations that they are connected by a factor of the number of sites per unit volume. Since one site has a volume a^d

$$\rho(\mathbf{r}, t) = a^{-d} \rho_{\mathbf{r}/a, t/\tau}^L. \quad (5.6)$$

We can solve Eq. (5.5) quite explicitly to obtain the time dependence of the probability. To get started we need to know the value of ρ at some beginning time, say $t = 0$. Let us take as our initial data the statement that at $t = 0$ the particle is certainly at a specified point. For simplicity let us take this point to be $\mathbf{r} = 0$. In symbols

$$\rho_{\mathbf{n}, 0}^L = \delta_{\mathbf{n}, 0}.$$

At the time $t = M\tau$, with M being a positive integer, the particle has gone through M random steps and has a new position vector which is given by Eq. (5.3). Given this form of $\mathbf{R}(t)$ it is relatively easy to compute the average (5.5). To simplify the notation, we do this calculation in one dimension. It is easily generalized to any dimensionality. In one dimension each ξ takes on the two values $\pm a$. To take advantage of statistical mechanics tools, we would like to recast the right hand side of Eq. (5.5) as a sum of exponentials. This is easy since there is a fourier representation of the one-dimensional delta symbol as:

$$\delta_{n, m} = \int_{-\pi}^{\pi} \frac{dq}{2\pi} e^{iq(n-m)}, \quad (5.7)$$

whenever n and m are integers. Thus Eq. (5.5) may be written as

$$\rho_{\mathbf{r}/a, t/\tau}^L = \int_{-\pi}^{\pi} \frac{dq}{2\pi} \langle e^{iq(R(t)-r)-a} \rangle = \int_{-\pi}^{\pi} \frac{dq}{2\pi} e^{-iqr/a} \left\langle \prod_{j=1}^M e^{iq\xi_j/a} \right\rangle.$$

Since each ξ_j is independent of the others, the average of the product is just the product of the averages and that can be computed at once giving

$$\rho_{n, M}^L = \int_{-\pi}^{\pi} \frac{dq}{2\pi} e^{-iqn} [\langle e^{iq\xi_j/a} \rangle]^M = \int_{-\pi}^{\pi} \frac{dq}{2\pi} e^{-iqn} [\cos q]^M. \quad (5.8)$$

You are asked to evaluate this integral in homework Problem 5.7.

Equation (5.8) provides a nice but not fully explicit result. To get a little further notice that we can see one very sharp result from doing this integral. In this one-dimensional example, each of the M steps takes us either to the left or to the right. If M is even, we will have in total traversed an even number of steps; If M is odd we will have traversed an odd number. Then if $r = ma$ and $t = M\tau$, we get a nonzero result only for $\rho(r, t)$ only if n and M have the same evenness or oddness. Thus, quite explicitly:

$$\rho_{n, M}^L = 0 \quad \text{if} \quad n \neq M \mod 2. \quad (5.9a)$$

If the result is nonzero, the integral in (5.8) covers the same ground twice since the regions from $-\pi$ to $-\pi/2$ and the one from $\pi/2$ to π duplicate the integrand from $-\pi/2$ to $\pi/2$. When the integral is nonzero, it is

$$\rho_{n,M}^L = 2 \int_{-\pi/2}^{\pi/2} \frac{dq}{2\pi} e^{-iqn} [\cos q]^M. \quad (5.9b)$$

The result can be worked out further in the limit as the number of steps, M , gets to be very large. We do the calculation as a steepest descent integral, with the exponent being $iqn + M \ln \cos q$. This exponent has maxima at $q = 0$ and $q = \pi$. The steepest descent calculation applied to Eq. (5.9b) gives:

$$\rho_{n,M}^L = 2 \sqrt{\frac{1}{2\pi M}} \exp\left(-\frac{n^2}{2M}\right) \quad \text{for } n = M \pmod{2}. \quad (5.10a)$$

The equivalent expression in terms of dimensional variables is:

$$\rho_{r/a,t/\tau}^L = 2 \sqrt{\frac{\tau}{2\pi t}} \exp\left[-\frac{r^2\tau}{2ta^2}\right] \quad \text{for } n = M \pmod{2}. \quad (5.10b)$$

The result (5.10) indicates that after a time t the probability is spread out over a distance, r , of the order of

$$r = a \sqrt{\frac{t}{\tau}}. \quad (5.11)$$

Notice how this distance grows as the square root of the time. This growth rate, which we first saw in Eq. (5.4b), is characteristic of random walk behavior.

5.3 The Diffusion of Probability and Particles

We now look at precisely this same process from a different point of view. Recall that each site, \mathbf{r} , contains walkers which have come from the neighboring sites $\mathbf{r} + \xi$, where ξ is one of the $2D$ nearest neighbor vectors. Each hopping vector, ξ , has a likelihood $1/(2d)$ of being picked. This hopping took place during the proceeding time interval τ . In symbols, what we have just said is the equation,

$$\rho_{\mathbf{r}/a,1+t/\tau}^L = \frac{1}{2d} \sum_{\xi} \rho_{(\mathbf{r}-\xi)/a,t/\tau}^L. \quad (5.12)$$

We can use this expression to compute the probabilities in a very explicit fashion. For example, let us focus on a two-dimensional example in which, as before, at time 0 the site $\mathbf{r} = 0$ is the only one occupied. (See Fig. 5.3) Then at this time $\rho_{\mathbf{n},0}^L = \delta_{\mathbf{n},0}$. At the next time, all four of the sites neighboring to this one will have occupation probability $1/4$, with the result shown in Fig. 5.3 in which

$$\rho_{\mathbf{n},1}^L = \begin{cases} 1/4 & \text{for } \mathbf{n} = \pm(1, 0) \text{ or } \pm(0, 1), \\ 0 & \text{otherwise.} \end{cases}$$

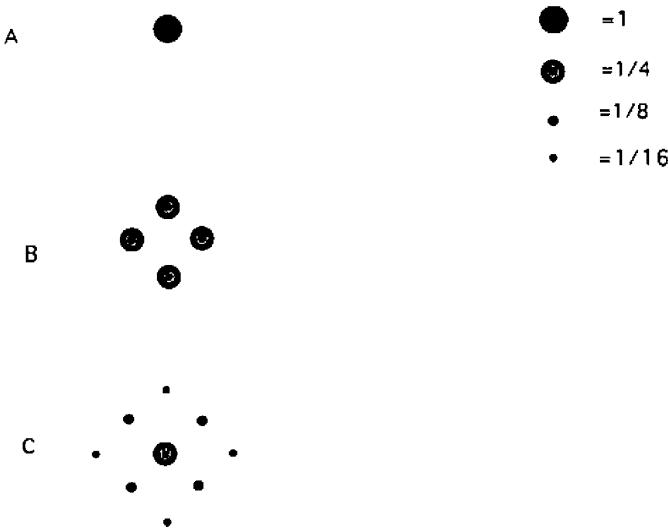


Fig. 5.3. Probabilities for occupation of a given site at three successive times. At the earliest time, A, the particle starts out at the center. After one step B is has a probability 1/4 of being at the neighboring sites. The next step, C, brings further outward motion.

The next few times are also shown on this figure. Notice that, as time goes on, ρ^L begins to spread out over the lattice. Once again all sites are divided into two groups: those with an even sum of n_μ and those with an odd sum. On even time steps ρ^L is nonzero at the first kind of sites; on odd steps it is nonzero at odd sum sites. Aside from this odd-even vanishing, after a few time steps ρ^L will become a slowly varying function of its spatial argument. It also changes very little with each successive time-step. (See Eq. (5.10)).

One can make use of this slow variation to convert Eq. (5.12) into a partial differential equation. We shall do it in a moment. It is easy. But before we do that, it is important to say why we are going to this partial differential equation. Imagine an experimentalist observing the diffusion of something, say Copper through some lattice of another material, say Gold. Our experimentalist is interested in the total amount of copper which gets from one region of the material to another. So this person wishes to take a macroscopic view in which instead of observing a particular lattice site, the observation is of a whole region containing many lattice sites. Similarly instead of looking for one hop, our imagined experimentalist is interested in the net result of many hops. So the person might well measure an average over many of our time intervals, τ . Because the diffusion process eventually leads to a flow over large regions of space, covering many lattice constants, it is important to have a good description of what is going on. But because the observer may be ignorant of or uninterested in the details of lattice structure, this information should not be $\rho_{n,M}^L$. Instead the right information is contained in a density $\rho(\mathbf{r}, t)$ defined so that $\rho(\mathbf{r}, t)d\mathbf{r}$ is the probability of finding a particular hopping atom in the element $d\mathbf{r}$ about the spatial point \mathbf{r} . A sharp connection between these quantities can be made when both vary slowly in space and time. In Eq. (5.6), we write

$$\rho(\mathbf{r}, t)a^d = \rho_{n,M}^L \quad \text{if } \mathbf{r} = a\mathbf{n}, t = M\tau. \quad (5.13)$$

In order to have this work with every cell in the lattice we must have $\rho_{n,M}^L$ be a slowly varying in its arguments.¹ We shall henceforth assume that ρ^L is indeed slowly varying.

To see the consequences of ρ 's smoothness multiply Eq. (5.12) by a^d and get the consequence

$$\rho(\mathbf{r}, t + \tau) - \rho(\mathbf{r}, t) = \sum_{\xi} \frac{\rho(\mathbf{r} - \xi, t) - \rho(\mathbf{r}, t)}{2d}. \quad (5.14)$$

No approximations have been made so far. To get the diffusion approximation, expand both side of the equation in the ‘small’ numbers τ and ξ and hold on to the first non-vanishing term on each side of the equation. On the left hand side, the lowest order non-vanishing term is first order. On the right one expands in a power series in ξ . The expansion gives

$$\tau \frac{\partial}{\partial t} \rho(\mathbf{r}, t) = \sum_{\xi} \frac{-\xi \cdot \nabla + (\xi \cdot \nabla)^2/2}{2d} \rho(\mathbf{r}, t).$$

The sum on the right is easily calculated. The first term just cancels out since $\langle \xi \rangle = 0$; the second order term is nonzero since the components of a given step obey Eq. (5.2c), which has the alternative expression

$$2d\langle \xi_{\mu} \xi_{\nu} \rangle = \sum_{\xi} \xi_{\mu} \xi_{\nu} = 2\delta_{\mu,\nu}.$$

Thus the continuum version of our equation of motion for the probability distribution reads

$$\tau \frac{\partial}{\partial t} \rho(\mathbf{r}, t) = \frac{a^2}{2d} \nabla^2 \rho(\mathbf{r}, t). \quad (5.15)$$

This conclusion is a consequence of the specific assumptions we have made, but there is a much more general conclusion which can be stated:

In a random walk, in the long run, the probability of finding the walker at the position \mathbf{r} at the time t obeys

$$\frac{\partial}{\partial t} \rho(\mathbf{r}, t) = \lambda \nabla^2 \rho(\mathbf{r}, t). \quad (5.16)$$

An equation of the form (5.16) is called a *diffusion equation*. The coefficient of the Laplacian term, λ , is called a *diffusivity*. Under the particular assumption we have made the value of the diffusivity is

$$\lambda = \frac{a^2}{2d\tau}. \quad (5.17)$$

¹Thus the configuration shown in Fig. 5.3 is unacceptable since at each step half the lattice sites will remain unoccupied. However, this is a trivial difficulty, easily fixed by averaging the initial occupation over some region of the lattice containing more than a few lattice sites, or by averaging the observation of ρ over some interval of space or some interval of time.

The diffusion equation, (5.16) arises quite often in physical systems. By definition, conserved quantities, like the probability discussed here, have the property that the total amount of the quantity remains independent of time. If the conserved quantity moves from place to nearby place, in response to gradients of that quantity, then it will almost always obey a diffusion equation.

5.4 From Conservation to Hydrodynamic Equations

A ‘hydrodynamic equation’ is a continuum partial differential equation which describes the limit of slowly varying flows in a nonequilibrium system. One example is the diffusion equation, discussed in the previous section. In this section, we shall discuss how the hydrodynamic equations follow from a conservation law plus an additional piece of information, called a *constitutive equation*, used to prescribe the current in the conservation law. We get two different kinds of hydrodynamics, one for charged particles, and the other for uncharged ones. Then we describe once more, but this time in d dimensions, the form of solutions to the diffusion equation.

Electrodynamics contains a conservation law for charge which can be expressed in the form

$$\frac{\partial}{\partial t} \rho(\mathbf{r}, t) + \nabla \cdot \mathbf{j}(\mathbf{r}, t) = 0, \quad \text{conservation law.} \quad (5.18)$$

Here, ρ is the charge density and \mathbf{j} is the current density. Exactly the same form of conservation law applies in our hopping case, except that ρ now has the meaning of the probability per unit volume for observing a hopping particle and \mathbf{j} represents the probability current for such hoppers. Of course, the integrated form of the conservation law

$$\frac{d}{dt} \int_{\Omega} d\mathbf{r} \rho(\mathbf{r}, t) = - \int_{\partial\Omega} d\mathbf{S} \cdot \mathbf{j}(\mathbf{r}, t) \quad (5.19)$$

follows directly from integrating Eq. (5.18) over a volume, Ω which is bounded by a surface $\partial\Omega$. Equation (5.19) says that the time derivative of the total amount of the conserved stuff in Ω is equal to the negative of the flux of stuff flowing out.

Notice that neither Eq. (5.18) nor Eq. (5.19) provide a theory which will enable us to find ρ . To get that one needs an additional relation called a constitutive equation which defines \mathbf{j} in terms of ρ . Thus we are required to understand the process which is driving a current through the system. In the electrodynamics of materials, there are several different constitutive equations, describing qualitatively different situations. Perhaps the most famous is Ohm’s law $\mathbf{j} = \sigma \mathbf{E}$, where σ is the electrical resistivity. This law effectively describes the low frequency response of a conductor. To describe the high frequency response, one needs to include the inertia of the charged particles. A charged particle gas is called a *plasma*. Consider a plasma with number density N/Ω and a charge per particle e and mass per particle m which is being accelerated by an electric field in an almost lossless

situation. Then the acceleration is $d\mathbf{j}/dt$ is then driven by the electric field according to

$$m \frac{d}{dt} \mathbf{j} = \frac{N}{\Omega} e^2 \mathbf{E} \quad \text{with } \nabla \cdot \mathbf{E} = 4\pi\rho.$$

The physical result of these assumptions is to give an oscillatory behavior for the charge density, described by the equation $(d^2/dt^2)\rho = -\omega^2\rho$. These oscillations called plasma oscillations have a frequency given by

$$\omega^2 = \frac{4\pi N}{m\Omega} e^2.$$

Different forms of the constitutive equations give different long distance behavior. But in all the cases studied to date there is some long-term behavior, which extends to far longer distances than the microscopic scale, and which can be described by partial differential equations. These partial differential equations are termed a hydrodynamic description.²

We can fit our hopping atoms into the usual hydrodynamic structure: conservation laws, constitutive equations, partial differential equations. Go back to the probability per site description of the hopping problem. Consider the geometry of this situation as it is given in Fig. 5.4. Notice then that in the time interval, τ , we have a situation in which $\rho_{\mathbf{n},m}$ changes to $\rho_{\mathbf{n},m+1}$ because particles have left the lattice site m . We would like to write a lattice form of the differential conservation law. To do this, we should interpret the flow out of the site m to occur via currents j_μ which are to be labeled by the centers of the bonds through which they flow. Thus a positive current j_μ at $\mathbf{n} + \mathbf{e}_\mu/a$ carries particle (or particle probability) away from our point while a positive current at j_μ at $\mathbf{n} - \mathbf{e}_\mu/2$ carries probability into our point. If we use the symbol j_μ^L for a lattice based current then the lattice conservation law reads:

$$\rho_{\mathbf{n},M-1}^L - \rho_{\mathbf{n},M}^L = - \sum_{\mu=1}^d \left[\mathbf{j}_\mu^L \left(\mathbf{n} + \frac{\mathbf{e}_\mu}{2}, M \right) - \mathbf{j}_\mu^L \left(\mathbf{n} - \frac{\mathbf{e}_\mu}{2}, M \right) \right]. \quad (5.20)$$

The superscript on \mathbf{j} stand for a lattice current. It does not have the same dimensions as an actual probability current. Our job will be to recast Eq. (5.20) into the form of a conservation law. It is mostly a job of putting in the appropriate factors of a and τ to get the dimensions right. Since M represents time steps measured in units of a time interval, τ , and since ρ and ρ^L are connected by a factor of a^d (see Eq. (5.6)), the left hand side of Eq. (5.20) is

$$\tau \frac{\partial}{\partial t} \rho(\mathbf{r}, t) a^d. \quad (5.21)$$

²Some of us at Chicago have been working recently on the motion of granular materials, e.g. sand. It is an open question about whether these materials do have a good and general hydrodynamic description which can be applied to characterize the motion of many grains of sand together. Jaeger, H. and Nagel, S., Science 255, 1523–1531 (1992). Y. Du, H. Li and L. P. Kadanoff, *Breakdown of Hydrodynamics in a One-Dimensional System of Inelastic Particles*, Phys. Rev. Lett. 74 (8) 1268–1271 (1995).

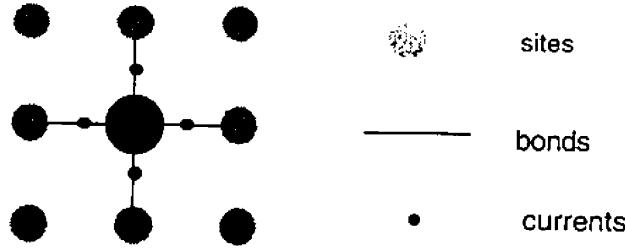


Fig. 5.4. Bonds and flows in two dimensions.

We must try to do something similar to the right hand side. Note that j_μ^L is a current integrated over a period of time τ . It also carries a current over a bond which carries all the current for the area pieced by the bond, an area a^{d-1} . Using this dimensional argument, define a continuum current

$$\mathbf{j}(\mathbf{r}, t) = \tau^{-1} a^{1-d} \mathbf{j}_{\mathbf{r}/a, t/\tau}^L, \quad (5.22)$$

where \mathbf{j} is the usual continuum current density. Substitute Eq. (5.21) and (5.22) into Eq. (5.20) and find the conservation law

$$\frac{\partial}{\partial t} \rho(\mathbf{r}, t) = -a^{-1} \sum_{\mu=1}^d \left[j_\mu \left(\mathbf{r} + \frac{a\mathbf{e}_\mu}{2}, t \right) - j_\mu \left(\mathbf{r} - \frac{a\mathbf{e}_\mu}{2}, t \right) \right].$$

If one expands this equation to first order in a power series in a , one rederives the basic conservation law (5.18). Our remaining task is to find the constitutive equation for j_μ .

We can calculate the value of the current. For each bond, the neighboring site in the direction of $-\mathbf{e}_\mu$ will send a particle along that bond with a probability $1/(2d)$ times the occupation probability of that site, thereby contributing a positive term to that current. A neighboring site in the opposite direction will send a particle along with probability $(1/2d)$ times its probability of being occupied, and thus make a negative contribution to the current. We then find that the current is:

$$j_\mu^L \left(\mathbf{n} + \frac{a\mathbf{e}_\mu}{2}, M \right) = \frac{\rho_{\mathbf{n}, M}^L - \rho_{\mathbf{n} + \mathbf{e}_\mu, M}^L}{2d}. \quad (5.23)$$

One then converts back to statements about continuum currents by using Eq. (5.22) and finding

$$j_\mu \left(\mathbf{r} + \frac{a\mathbf{e}_\mu}{2}, t \right) = \frac{a}{2d\tau} [\rho(\mathbf{r}, t) - \rho(\mathbf{r} + a\mathbf{e}_\mu, t)].$$

The assumption that ρ varies slowly in its spatial coordinate permits an expansion (essentially an expansion in a) which gives our constitutive equation:

$$\mathbf{j}(\mathbf{r}, t) = -\frac{a^2}{2d\tau} \nabla \rho(\mathbf{r}, t). \quad (5.24)$$

This equation says that whenever the density, ρ , varies from point to point, there is a current which carries particles in a direction which will smooth out the variation. It is this density-driven current which forms the basis of the diffusion phenomenon.

If one substitutes Eq. (5.24) into the exact discrete conservation law (5.18) one recovers the equation of motion (5.16). This argument has brought us back to familiar territory.

One can obtain a whole group of physical consequences directly from Eq. (5.16). We have used a continuum normalization of the probability density in Eq. (5.16) so that an integral over \mathbf{r} gives a total probability unity.

$$\int d\mathbf{r} \rho(\mathbf{r}, t) = 1.$$

Next we calculate the equations obeyed by averages of the position of the walkers, specifically, the two averages

$$\langle \mathbf{R}(t) \rangle = \int d\mathbf{r} \rho(\mathbf{r}, t) \mathbf{r}, \quad (5.25a)$$

$$\langle \mathbf{R}(t) \cdot \mathbf{R}(t) \rangle = \int d\mathbf{r} \rho(\mathbf{r}, t) \mathbf{r} \cdot \mathbf{r}. \quad (5.25b)$$

Form the moments of the diffusion equation indicated by the right hand side of Eqs. (5.25a) and (5.25b). In the first case one finds

$$\frac{d}{dt} \langle \mathbf{R}_\mu(t) \rangle = \frac{d}{dt} \int d\mathbf{r} \rho(\mathbf{r}, t) r_\mu = \lambda \int d\mathbf{r} r_\mu \nabla^2 \rho(\mathbf{r}, t). \quad (5.26)$$

Now demand that $\rho(\mathbf{r}, t)$ vanishes very rapidly as $\mathbf{r} \rightarrow \infty$ so that integrations by parts can be done in \mathbf{r} without giving any boundary terms. This enables us to rewrite the right hand side of Eq. (5.26) as

$$-\lambda \int d\mathbf{r} \nabla_\mu \rho(\mathbf{r}, t),$$

which is a perfect derivative and thus gives only boundary terms. In a very large system, these boundary terms vanish. Thus, the average position vector for the walker remains independent of time. This is an expected conclusion since there is no preferred direction in the problem and hence no direction in which the walkers can, on the average, go. The identical calculation gives an average for the position squared which is

$$\frac{d}{dt} \langle \mathbf{R}(t) \cdot \mathbf{R}(t) \rangle = \lambda \int d\mathbf{r} r^2 \nabla^2 \rho(\mathbf{r}, t) = -2\lambda \int d\mathbf{r} r_\mu \nabla_\mu \rho(\mathbf{r}, t). \quad (5.27)$$

One more integration by parts converts the right hand side to

$$2d\lambda \int d\mathbf{r} \rho(\mathbf{r}, t) = 2d\lambda.$$

Therefore the final result is that squared position grows as

$$\langle \mathbf{R}(t) \cdot \mathbf{R}(t) \rangle - \langle \mathbf{R}(0) \cdot \mathbf{R}(0) \rangle = 2d\lambda t. \quad (5.28)$$

Again we see that the square of a distance grows linearly in time. One can use the diffusion equation to determine the entire probability distribution. As before, we solve the problem by using a Fourier transform technique. We define the Fourier transform of ρ by writing the Fourier transform of ρ and its inverse as

$$\begin{aligned} G(\mathbf{q}, t) &= \int d\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \rho(\mathbf{r}, t); \\ \rho(\mathbf{r}, t) &= \int \frac{d\mathbf{q}}{(2\pi)^d} e^{i\mathbf{q}\cdot\mathbf{r}} G(\mathbf{q}, t). \end{aligned} \quad (5.29)$$

We use Eq. (5.14) starting from the initial condition that the particle is localized at $\mathbf{r} = 0$,

$$\rho(\mathbf{r}, 0) = \delta(\mathbf{r}). \quad (5.30a)$$

The equivalent statement in terms of G is that

$$G(\mathbf{q}, 0) = 1. \quad (5.30b)$$

The Fourier transformation enable one to replace the ∇^2 in the diffusion equation by $-q^2$ so that Eq. (5.14) becomes the statement

$$\frac{\partial}{\partial t} G(\mathbf{q}, t) = -\lambda q^2 G(\mathbf{q}, t). \quad (5.31)$$

Given the initial data of Eq. (5.30b), the solution of (5.31) is that

$$G(\mathbf{q}, t) = e^{-\lambda q^2 t}. \quad (5.32)$$

Thus the problem is reduced to doing a Gaussian integral to determine ρ via the second form of Eq. (5.29). One can complete squares as before and gets a rather direct generalization of the one-dimensional result, namely that

$$\rho(\mathbf{r}, t) = (2\pi\lambda t)^{-d/2} \exp\left[-\frac{r^2}{4\lambda t}\right]. \quad (5.33)$$

5.5 Distribution Functions

There is another interpretation of the diffusion equation which we might wish to emphasize at this point. Imagine that we had not one walker but many, with the different walkers labeled by the index $j = 1, 2, \dots, N$. Then we might deal with $\rho_j(\mathbf{r}, t)d\mathbf{r}$, the probability of finding the j th walker within the volume element, $d\mathbf{r}$, of the space point, \mathbf{r} . The average number of particles within a volume Ω is determined by the sum over all particles of this probability, and is

$$\int_{\Omega} d\mathbf{r} \sum_{j=1}^N \rho_j(\mathbf{r}, t).$$

For this reason, we define

$$f(\mathbf{r}, t) = \sum_{j=1}^N \rho_j(\mathbf{r}, t). \quad (5.34)$$

Here, f is called a distribution function. It behaves very much like the individual probabilities ρ_j , except it obeys a normalization condition which says that the total number of particles in the system is N :

$$\int_{\Omega} d\mathbf{r} f(\mathbf{r}, t) = N. \quad (5.35)$$

If there are many particles in the system, so that the fluctuation in the number within any fairly large region is quite small, we can think and speak about $f(\mathbf{r}, t)$ as if it were a deterministic quantity. Thus we say that the number of particles is determined as if $f(\mathbf{r}, t)d\mathbf{r}$ were the number of particles to be found within the volume element, $d\mathbf{r}$, about the space point, \mathbf{r} . Since every term in the sum (5.34) obeys the diffusion equation, and since this equation is linear, the sum obeys the diffusion equation. Thus, like ρ , f obeys

$$\frac{\partial}{\partial t} f(\mathbf{r}, t) = \lambda \nabla^2 f(\mathbf{r}, t), \quad (5.36)$$

with the very same value of the diffusion coefficient, λ , as before.

5.6 Cascade Processes and Securities Prices

To illustrate the concepts developed in this chapter let us consider a cascade process in time. The process is represented by a simple model in which the quantity of physical interest, call it S , is a function of time which is observed at discrete times $t_M = t_0 + M\tau$. The S 's at the different observation times are denoted by S_M . We then assume that S_M is modified in a step by step manner by a process in which S_{M+1} is produced from S_M by multiplication by a random variable

$$S_{M+1} = S_M e^{\xi_M}. \quad (5.37)$$

To make the calculation easy, we assume that the ξ_M 's are uncorrelated for different values of M . A model like this is called a *multiplicative random process*. The effect of such a process is to produce a cascade of changes which, in the end, will cause a huge variation in S .

It is possible to imagine several different applications of this kind of model. It might be that S_M is the price³ of a security (say a stock or bond⁴) observed after the elapse of M time

³We shall apply Eq. (5.37) to cases in which S_M should be interpreted as a positive quantity.

⁴An elementary discussion of the types of securities and strategies can be found in John C. Hull, *Options, Futures, and other Derivative Securities*, second edition (Prentice Hall, Englewood Cliffs, N.J., 1993).

steps from some initial time. It might be that S_M is the activity in a cosmic ray shower in which the basic step is one a single particle produces several. If we then follow the process from its inception through M steps we will see a cascading event in which many particles are produced. In hydrodynamic turbulence a piece of swirling fluid produces additional smaller swirls. This happens again and again as the turbulence cascades down to smaller and smaller spatial scales, possibly through a multiplicative process⁵ like (5.37).

For example in the case of securities, we imagine that the price is determined by a kind of random walk process. In each period of time, perhaps one week, the price of the security can either change (rise or fall) by a given percentage: ξ_M where ξ_M is a random variable describing the price change in the M th week. Each ξ_M is a random variable which takes on the value x with a probability $\rho(x)$.

These cascades are random walks, but with a difference. In these cases, the basic quantity of interest is a product of terms containing the random variable. For example take the security to have a well-determined price, S_0 , at time zero. After M steps we see:

$$S_M = S_0 \exp \left[\sum_{k=1}^M \xi_k \right]. \quad (5.38)$$

Because of the multiplicative structure in Eq. (5.38) S_M can have tremendous fluctuations if M is sufficiently large. Previously we said that fluctuations of some variable, S , would be small if the RMS fluctuations in S were small in comparison to the average of S and large if these RMS fluctuations were large in comparison $\langle S \rangle$. In a moment we shall show quite generally that if ξ_k is a fluctuating variable, then as M goes to infinity

$$\frac{\text{RMS}(S_M)}{\langle S_M \rangle} \longrightarrow \exp(rM), \quad (5.39)$$

where r is some positive growth rate. Thus, as M grows, the relative size of the fluctuations grow with exponential rapidity.

In statistical physics we distinguish between two kinds of statistical behavior produced by events with many steps and parts. The simpler kind of behavior is described by the phrase *self-averaging*. A self-averaging behavior is one in which the effects of the individual events add up to produce an almost deterministic outcome. An example of this is the pressure on a macroscopic surface. This pressure is produced by huge numbers of individual collisions, which produce a momentum transfer per unit time which seems essentially without fluctuations. The larger the number of collisions, the less is the uncertainty in the pressure.

In contrast multiplicative random processes all have a second behavior called *non-self-averaging*.⁶ When different markets or different securities are described by any kind of multiplicative random process, as we have described in this section, then the different

⁵This behavior is discussed in Chapter 8 of Uriel Frisch, *Turbulence* (Cambridge University Press, Cambridge, 1995).

⁶I take no responsibility for the unimaginative name.

securities can have huge and (mostly) unpredictable price swings. The larger the value of M , the more the uncertainty in price. There are other examples of measurements which do not self-average. For example the electrical resistance of a disordered quantum system at low temperature is determined in awful detail by the position of each atom. Change one atomic position and you might change the resistance by a factor of two. Here too the large number of individual units does not guarantee a certainly defined output.

Return to the large fluctuations in S_M . In one sense they are an obvious consequence of the multiplicative nature of the process. If you change the value of $\exp(\xi_1)$ by a factor of two each subsequent value of S_M also changes by the same factor. Thus the multiplicative system retains full memory of its past. We would like to calculate the effects of the large fluctuations. To do this imagine that we wish to calculate averages of the form: $\langle (S_M)^p \rangle$ where p is any number, not necessarily an integer. To obtain the RSM fluctuations, we should know this quantity for $p = 1$ and $p = 2$, but we can calculate it for all p without much extra work. From (5.37) we see that:

$$\langle (S_{M+1})^p \rangle = \langle (S_M)^p \rangle \langle e^{p\xi_{M+1}} \rangle = \langle (S_M)^p \rangle e^{\zeta_p}. \quad (5.40)$$

Here, ζ_p defines the growth rate of the p th moment of S_M . Since we have assumed that S_0 is not random but has a well defined value, the recursion relation (5.40) has the solution

$$\langle (S_M)^p \rangle = S_0^p e^{M\zeta_p}. \quad (5.41)$$

If each ξ_k is characterized by the probability distribution $\rho(x)$ then, the growth rate ζ_p is given by:

$$e^{\zeta_p} = \langle e^{p\xi_k} \rangle = \int dx \rho(x) e^{px}. \quad (5.42)$$

The indices ζ_p are called *Multifractal indices*. These indices define important properties of the fluctuations in a quantity like S_M . If the fluctuations grow only algebraically with M , then the indices will obey

$$\zeta_p = p\zeta_1.$$

In this case, the behavior of S_M is that of a simple fractal.⁷ If, on the other hand, the fluctuations grow exponentially in M , then ζ_p is a nonlinear function of p , and the form of that function gives considerable information about the nature of the fluctuations. In the linear case, the behavior of the fluctuating quantity is said to be fractal; in the nonlinear case we say that there is a multifractal behavior.

Now we prove that fluctuations diverge for large M . For any random variables, X , it is true that $\langle X^2 \rangle \geq \langle X \rangle^2$ since

$$\langle X^2 \rangle - \langle X \rangle^2 = \langle (X - \langle X \rangle)^2 \rangle \geq 0,$$

⁷B. B. Mandelbrot, *The Fractal Geometry of Nature*, W. H. Freeman, New York, 1983.

with equality holding if X does not fluctuate. Thus it follows that

$$\zeta_{2p} \geq 2\xi_p \quad (5.43)$$

with, once more, equality holding only if ξ_k has no fluctuations. Any function of p which obeys (5.43) is said to be convex.

The unbounded fluctuations are a consequence of the convexity of ξ_p . Equations (2.38) and (5.43) define the RMS fluctuations in S_M to be

$$\text{RMS}(S_M) = (\langle [S_M - \langle S_M \rangle]^2 \rangle)^{1/2} = S_0 \sqrt{e^{M\zeta_{2p}} - e^{2M\xi_p}}.$$

The ratio of this to $\langle S_M \rangle$ defines the relative size of the fluctuations. That ratio is:

$$\frac{\text{RMS}(S_M)}{\langle S_M \rangle} = \frac{\sqrt{e^{M\zeta_{2p}} - e^{2M\xi_p}}}{e^{M\xi_p}} = \sqrt{e^{M(\zeta_{2p}-2\xi_p)} - 1}.$$

Because of Eq. (5.42), we can estimate the fluctuations for large M and find

$$\frac{\text{RMS}(S_M)}{\langle S_M \rangle} \longrightarrow \exp[M(\zeta_{2p}/2 - \xi_p)]. \quad (5.44)$$

The convexity property of Eq. (5.43) ensures that the coefficient of M is a positive number, for all cases in which ξ_k fluctuates. Thus we have proven that, as M goes to infinity, so do the relative fluctuations.

Now we calculate a few histories in which we plot S_M as a function of M . The results are shown in Fig. 5.5. Our figures actually use the discrete probability distribution

$$\rho(x) = \frac{1}{2}\delta(x - r_0 - \sigma) + \frac{1}{2}\delta(x - r_0 + \sigma). \quad (5.45a)$$

However, the reader might wish to plot up the result which would arise from an alternative probability distribution. One alternative would be a Gaussian distribution

$$\rho(x) = \sqrt{\frac{1}{2\pi\sigma^2}} \exp\left(-\frac{(x - r_0)^2}{2\sigma^2}\right). \quad (5.45b)$$

Because the price has the Gaussian variables appear in an exponent, price fluctuations may be order of magnitude larger than the usual Gaussian fluctuations. Yet another alternative would be the exponential distribution.

$$\rho(x) = (2\sigma)^{-1} \exp\left[-\frac{|x - r_0|}{\sigma}\right]. \quad (5.45c)$$

In each case, r_0 controls the average rate of drift of the ‘log price’ variable, with larger r_0 causing a swifter upward drift. On the other hand, σ , controls the dispersion in the price-change. A larger value of σ indicates more fluctuations in these changes. In fact, σ is

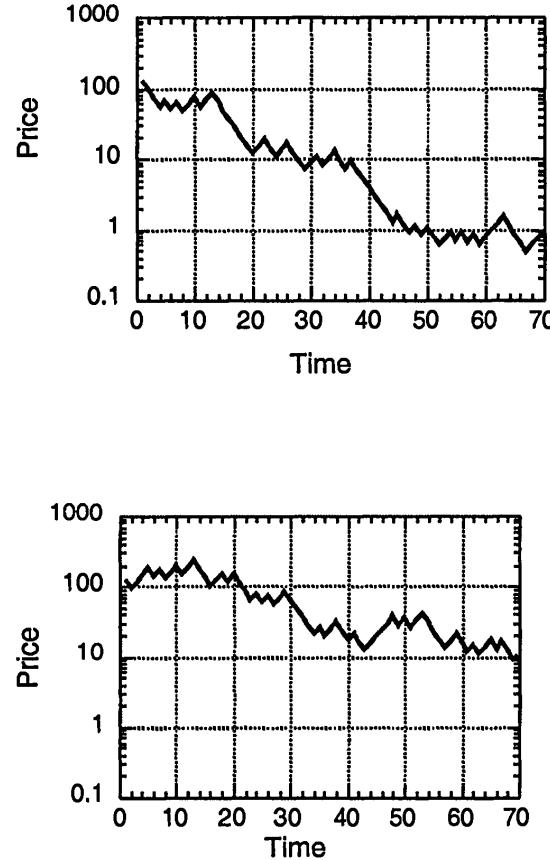


Fig. 5.5. Two Different Realizations of Behavior According to Eq. (5.45a). The price goes up or down in each step at random by a factor $\exp(\pm 0.25)/(2 \cosh(0.25))$. On the average the price remains constant in time. However, the actual behavior deviates wildly from the average. We use the distribution (5.45a), with the condition that the average over realizations of the price remain fixed.

the RMS fluctuation in the change. So the logarithm of S follows a kind of random walk with a per step mean drift r_0 and RMS fluctuation σ .

A brief calculation based upon Eq. (5.43) gives the values of the critical indices ζ_p controlling the growth. We find, after doing the appropriate integrals, that in the three cases, ζ_p has the respective values.

$$\zeta_p = pr_0 + \ln \cosh p\sigma \quad (5.46a)$$

$$\zeta_p = pr_0 + p^2\sigma^2/2 \quad (5.46b)$$

$$\zeta_p = pr_0 - \ln \sqrt{1 - p^2\sigma^2} \quad \text{for } |p| \leq \sigma^{-1}. \quad (5.46c)$$

In the last case if $|p|$ is larger than σ the average diverges so that ζ_p makes no sense.

In the stock analogy, an investor might be interested in the average or expected return from the security in question. Imagine making many investments of the type described by Eq. (5.37), and then ask what would be the average value of the investment after a certain period of time. Clearly the answer is that the average growth rate for each interval

is $\exp(\zeta_1)$. In order to make the three cases comparable, we set r_0 to give average growth rate zero.⁸ The result is then that the ζ 's have the value

$$\zeta_p = -p \ln \cosh \sigma + \ln \cosh p\sigma \quad \text{discrete possibilities} \quad (5.47a)$$

$$\zeta_p = (\sigma^2/2)p(p+1) \quad \text{Gaussian probabilities} \quad (5.47b)$$

$$\zeta_p = p \ln \sqrt{1 - \sigma^2} - \ln \sqrt{1 - p^2\sigma^2} \quad \text{for } |p| \leq \sigma^{-1} \text{ exponential probabilities.} \quad (5.47c)$$

Thus all the price models have the same average growth rate (zero) and the same dispersion in the logarithm of their price changes (given by σ). Now look at price patterns. Figure 5.5 plots typical time patterns of the value of these investments for the situation described by Eq. (5.45a) with $\sigma = 0.25$ and a starting price of 100. Although the average price (averaged over many many such histories) does nothing interesting, but in fact remains constant, we can see that the individual time histories are rather hectic. The price sometimes falls very low and stays there for quite a while. Alternatively there are periods in which the price is much higher than the average. The high price intervals are infrequent, but because they can be very high these infrequent events dominate the average. Typical investments are, as shown, quite different from the average and often quite a bit lower. These fluctuations will not, in our model, smooth out but continue to grow in time. Any signal with strong, long continued fluctuations, like that shown by our model prices is said to be *intermittent*. Intermittency is a feature of many statistical processes in the real world, including those describing turbulent systems.

As we have said, the wild variations shown in Fig. 5.5 are quite characteristic of a whole class of physical phenomena. These intermittent situations are characterized by exponentially increasing fluctuations of a physical quantity, using caused (as in our example) by a multiplicative process in which the quantity gets multiplied again and again by a randomly chosen, multiplier.⁹ Two physical situations in which such behaviors are particularly likely are in avalanches¹⁰ and in turbulence.¹¹ The usual statement of is that intermittency is a reflection of such strong fluctuations that a quantity like S , which may in the long run go to zero or infinity, has fluctuations such that $\langle S^p \rangle$ are in no way of the order of $\langle S \rangle^p$. (The geometrical version of intermittency is the statement that as time goes on $S(t)$ makes huge excursions toward large and small values, and goes by the name multifractality.) A large effort has been made to understand the implications of multifractality for statistical systems. The hypothesis described here would give many markets a multifractal behavior.

⁸If you wish, you could say that we are tracking the value of our investment relative to the average investment. This relative value must have an average equal to one.

⁹B. Mandelbrot, J. Fluid Mechanics **62**, 331 (1974), U. Frisch and G. Parisi in Turbulence and Predictability In Geophysical Fluid Dynamics and Climate Dynamics, edited by M. Ghil, R. Benzi and G. Parisi (North-Holland, Amsterdam, 1985), T. Halsey, M. Jensen, L. Kadanoff, I. Procaccia and B. Shraiman, Phys. Rev. **A33**, 1141 (1986).

¹⁰See for example Leo Kadanoff, Sidney Nagel, Lei Wu and Su-Min Zhou, Phys. Rev. **A39**, 6524 (1989).

¹¹R. Benzi, L. Biferale and G. Parisi, "On intermittency in a cascade model for turbulence", Physica **D65**, 163 (1993).

All three of the multifractal distributions are constructed by having $\ln S_M/S_0$ be a sum of M independent and identically distributed random variables. By the central limit theorem the probability that $\ln S_M$ will fall into the range between $\ln S$ and $\ln(S + dS)$ is given by the Gaussian expression:

$$\rho(S)dS = (d\ln S)(2\pi\beta_M)^{-1/2} \exp\left[-\frac{(\ln S - \alpha_M)^2}{2\beta_M}\right]$$

where α_M and β_M are respectively the mean and variance of $\ln S_M$. A behavior of this kind is said to be *log-normal*. Since we have defined the variance of a single step to always be σ^2 , the equation for the probability becomes

$$\rho(S) = (2\pi S^2 \sigma^2 M)^{-1/2} \exp\left[-\frac{(\ln S - \langle \ln S_M \rangle)^2}{2\sigma^2} M\right]. \quad (5.48)$$

Homework

Problem 5.1 (Fluctuation in Length of Random Walk). Calculate the RMS fluctuations in $\langle \mathbf{R}(t) \cdot \mathbf{R}(t) \rangle$ for a d -dimensional random walk. What is the behavior of these fluctuations in the limit as the number of steps goes to infinity?

Problem 5.2 (Probabilities in d -Dimensional Random Walk). Work out the result equivalent to Eq. (5.10) which applies to a system in d -dimensions.

Problem 5.3 (Landing Probabilities). Write a computer program to continue the calculation depicted in Fig. 5.3. Compare the resulting pattern from the one obtained from the diffusion Eq. (5.14). How closely do the results agree?

Problem 5.4 (Even and Odd). Replace equation by one in which the q integral goes from $-\pi$ to π . Calculate the effect produced by q 's close to $\pm\pi$ on the one-dimensional random walk's probability distribution. Discuss what your answer means.

Problem 5.5 (Gaussian Distributions). Find the solution to the diffusion equation in a system with no boundaries in d -dimensions if, at time zero, the distribution function $\rho(\mathbf{r}, t)$ is $\delta(r)$.

One good way to approach this problem is to take the Fourier transform of the equation. What is the form of the equation for the Fourier coefficients? What Fourier coefficients fit the initial data? What is the time-dependence of the coefficients? What is the distribution function $\rho(\mathbf{r}, t)$.

Problem 5.6 (Plots of Market Values). Make plots like those in Fig. 5.5 for the Gaussian and exponential distributions of ξ_k .

Problem 5.7 (Random Walk Probability Distribution). The right hand side of Eq. (5.8) can be integrated to give a fully explicit result for the probability expressed in terms of factorials.

- (a) Find that expression, using the binomial theorem.
- (b) Use the Sterling approximation to obtain an expression for the probability which holds when M is large.
- (c) Rederive Eq. (5.10) for the more general case of dimension d .

Problem 5.8 (Log-Normal Behavior of Markets). We have set up the probability distributions for the multifractal behavior so that $\log S_M$ is a sum of many independent terms,

$$\log S_M - \log S_0 = \sum_{k=1}^M \xi_k$$

of the time-variable, M . According to the central limit theorem, $\log S_M$ has a Gaussian behavior for large M . Here I ask you to calculate the typical behavior of these markets using Eq. (5.48).

- (a) Calculate the expectation value of $\ln S_M$ for the three probabilities listed in Eq. (5.45).
- (b) Calculate the variance of $\ln S_M$ for the three probabilities listed in Eq. (5.45).
- (c) What is the probability distribution for $\log S_M$, when M is large? What is the corresponding distribution for S_M ?
- (d) Find the median value of S_M . What time-development do you see? How does this compare to the average value of S_M ?

5.7 Reprints on Dynamics

The remainder of this chapter consists of reprints. The first two describe the development of a model, now described as diffusion limited aggregation or DLA. This model describes the motion of *mesoscopic* particles (i.e. particles much larger than an atom but still almost invisibly small). The model motion is very simple containing diffusion and then sticking. Nonetheless the objects produced by this motion are beautiful and complex. This model has proved to be very important. Inspired by DLA, many people constructed simple dynamical models of step by step changes which might occur in nature. (See the last paper in this chapter, ‘Chaos and Complexity’.) The models often turned out to be interesting, producing unexpected behaviors and often showing a fractal geometry. The whole exercise of studying the models became possible because they could easily be simulated on the computer.

5.7.1 Forest and Witten: Smoke Particle Aggregates

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LETTER TO THE EDITOR

Long-range correlations in smoke-particle aggregates

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Abstract. Ultrafine smoke particles stick together to form chain-like aggregates. We find that the particle density has long-range correlations of the same form in iron, zinc or silicon dioxide aggregates. The correlation data suggest a power-law spatial dependence giving a Hausdorff dimension between 1.7 and 1.9. We discuss the consistency of these results with a model based on percolation. We also compare our results with a random-walk model, which has a nominal Hausdorff dimension of 2.

1. Introduction

Certain extended physical systems (Fisher 1974) such as a fluid near its critical point have a fluctuating density $\rho(r)$ whose spatial correlations extend to arbitrarily long distance. In such cases the correlations typically obey a characteristic power law

$$\langle \rho(r)\rho(0) \rangle - \langle \rho(0) \rangle^2 \propto r^{-A} \quad (1)$$

over a large range of r . The exponents A in such power laws often have two striking features. First, in contrast to most power laws one encounters, A is usually not a simple fraction arising from dimensional considerations; it is ‘anomalous’. Second, A is typically unaffected by a continuous alteration of the parameters of the system: it is ‘universal’.

Recently ‘anomalous’ exponents like A have been discovered in a remarkably broad range of physical systems. The best known examples are extended matter at a second-order phase transition such as the liquid-gas critical point mentioned above. Here the observed power laws are manifestations of a symmetry known as the renormalisation group. This is a type of covariance of the system under spatial dilation. Long polymers (McKenzie 1976), the spin glass (Harris *et al* 1976) and connected clusters in a system near its percolation threshold (Kasteleyn and Fortuin 1969) appear to have ‘critical’ correlations in complete analogy to second-order phase transitions. Critical-point behaviour of a more general sort is thought (Mandelbrot 1977) to occur in the velocity autocorrelations of strongly turbulent fluids (Nelkin 1975, Abarbanel 1978), in the star density profile within star clusters and even in the spatial conformation of coastlines (Mandelbrot 1977).

We have observed that aggregates of ultrafine smoke particles can have long-range density correlations. Further, these correlations appear to have a characteristic exponent A which is both ‘anomalous’ and ‘universal’. In the systems we have studied,

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the smoke particles condense from the vapour produced by a hot filament or flame in a cool, dense gas (Wada 1967). The particles—approximately 40 Å in radius—stick together to form chain-like aggregates containing several thousand particles. Figure 1 shows an electron micrograph of a typical aggregate of Fe particles. Such particle aggregates have been observed in many studies of small metal particles (see, for

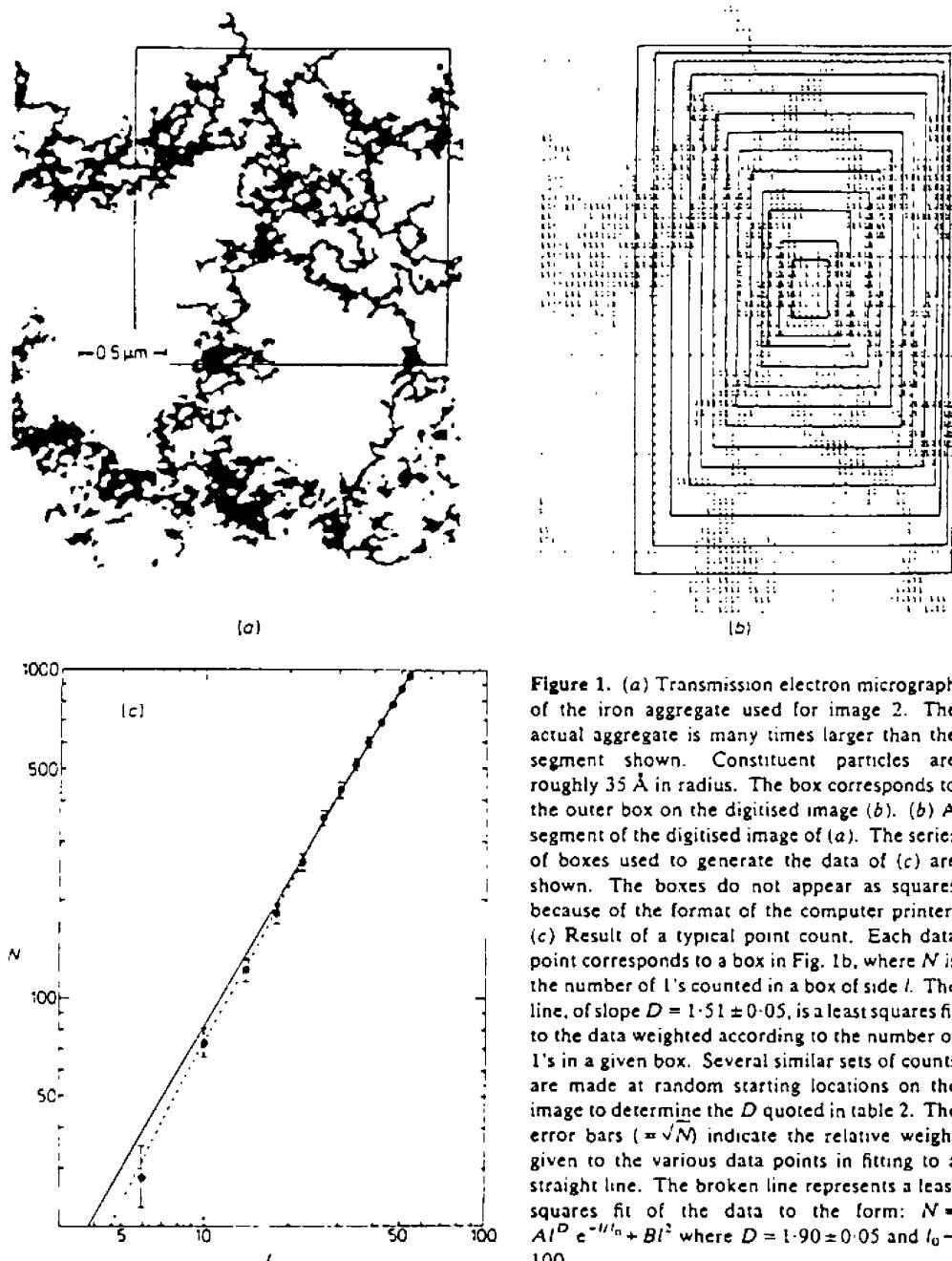


Figure 1. (a) Transmission electron micrograph of the iron aggregate used for image 2. The actual aggregate is many times larger than the segment shown. Constituent particles are roughly 35 Å in radius. The box corresponds to the outer box on the digitised image (b). (b) A segment of the digitised image of (a). The series of boxes used to generate the data of (c) are shown. The boxes do not appear as squares because of the format of the computer printer. (c) Result of a typical point count. Each data point corresponds to a box in Fig. 1b, where N is the number of 1's counted in a box of side l . The line, of slope $D = 1.51 \pm 0.05$, is a least squares fit to the data weighted according to the number of 1's in a given box. Several similar sets of counts are made at random starting locations on the image to determine the D quoted in table 2. The error bars ($\pm \sqrt{N}$) indicate the relative weight given to the various data points in fitting to a straight line. The broken line represents a least squares fit of the data to the form: $N = A/l^D e^{-B/l_0} + Bl^2$ where $D = 1.90 \pm 0.05$ and $l_0 = 100$.

example, Granqvist and Buhrman 1976). By measuring the density of particles as a function of position, we may determine the density autocorrelation function $\langle \rho(r)\rho(0) \rangle$. In several samples of iron, zinc and silicon dioxide aggregates produced under widely different conditions we found that the density profiles had power correlations as in equation (1) with A between 0.1 and 0.3.

In the analysis of our smoke-particle aggregates we employ the language of the Hausdorff dimension (Hausdorff 1919, Mandelbrot 1977) which is a convenient method of describing physical systems having dilation symmetry (Stanley *et al* 1976). An infinite set of points in space is said to have Hausdorff dimension less than or equal to D if it can be covered by $O(a^D)$ balls of radius a in the limit $a \rightarrow 0$. Such a set (in d -dimensional space) has density correlations of a power-law type with the exponent A equal to $d - D$.

2. Experimental results

We have analysed the density distribution in five different samples of aggregates, numbered 2–6. Samples 2–5, containing iron or zinc particles, were made in our laboratory by the procedure outlined below. Micrograph 6, obtained from a Cabot Corporation brochure (*Cabot Corporation* 1975†) showed aggregates of their 'Cab-O-Sil' powder. This commercial substance consists of SiO_2 particles produced in a flame process.

Figure 2 shows the apparatus used to make the iron and zinc aggregates. A 0.013 cm diameter tungsten wire electroplated with iron or zinc is rapidly heated by a short (250 ms) current pulse so that the plated metal vaporises. A dense gas (10^{-3} to

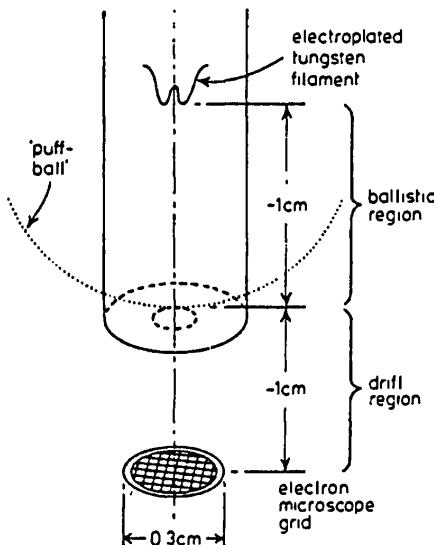


Figure 2. Schematic diagram of experimental apparatus used for production of metallic particle aggregates. The assembly is contained in a metal can with plumbing to admit helium gas. The can may be immersed in liquid nitrogen or helium.

† Cabot Corporation, 125 High Street, Boston, MA 02110, USA.

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10^{-1} of atmospheric number density) of helium confines the metal vapour so that it condenses into crystallites in a region close to the filament. These crystallites are the particles which make up our aggregates. They are roughly spherical and uniform in size, the mean radius being 35 Å, with a standard deviation of 15 Å, as determined via electron microscopy measurements.

The hot particles at first move rapidly away from the filament, but they soon come to rest in the gas ambient due to collisions with the gas atoms. The stopping distance for the different particles is nearly the same, and thus a thin spherical shell region with a high density of crystallites forms roughly 1 cm from the filament. The radius of the shell, or 'puff-ball' depends on the gas density: higher density makes a smaller puff-ball. It is in the puff-ball region that the particles stick together to form the aggregates we observe. The aggregates tend to be larger for higher gas temperature, and also when the puff-ball is smaller. Once formed, the aggregates settle slowly onto an electron microscope grid, which we later examine.

By placing electron microscope grids at various distances from the filament, we have determined that most of the aggregation occurs in the high-density puff-ball region, and that the aggregates do not change noticeably in size or shape even when allowed to fall distances of 3 cm or more. We have studied aggregates produced at widely varying temperatures and gas densities. We find that both iron and zinc have an equal ability for form chains under all conditions, in disagreement with observations made by Granqvist and Buhrman (1976). Thus magnetic forces do not play a dominant role in aggregate formation in our experiments.

Table 1 lists the five micrographs we have analysed in this study, along with the conditions under which they were made. The silicon dioxide is produced by the hydrolysis of silicon tetrachloride vapour in a flame of hydrogen and oxygen (*Cabot Corporation* 1975). The resulting aggregates are then allowed to cool and settle. We produced the first four samples under conditions favourable for forming many large aggregates; indeed, the connected aggregates extended far beyond the boundaries of the photographs. Only those that tended to lie flat on the microscope grid were photographed, as the depth of field of the transmission electron microscope is severely limited.

Next, each photograph was digitised by hand to produce a matrix of 'ones' and 'blanks' as shown in figure 1(b), the 'ones' ('blanks') corresponding to the presence (absence) of a particle. We analysed the digitised images with a computer in two different ways. The first method was motivated by the Hausdorff dimension approach of Mandelbrot (1977). A centre point on the image was picked at random, and then a

Table 1. Sample preparation.

Image matrix	Material	Gas density (cm^{-3})	Gas temperature (K)	Area of electron micrograph (μm^2)
2	Fe	$8 \cdot 1 \times 10^{17}$	295	9.2
3	Fe	$7 \cdot 3 \times 10^{16}$	77	3.1
4	Zn	$3 \cdot 2 \times 10^{17}$	77	7.7
5	Zn	$3 \cdot 2 \times 10^{17}$	77	7.7
6	SiO_2	—	—	1.2

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series of nested squares of different sizes was placed around it and the number of 'ones' in each square counted. This analysis, performed on a set of points with a Hausdorff dimension, would yield a power-law relationship between the length l of the square and the number of points N within it, namely $N \propto l^D$. For our images, we also obtained a power-law relation, with D varying in the range 1.5 to 1.6 with l varying over a factor-of-forty range in most cases. We found that our results were most reproducible when squares were chosen whose centres of mass coincided with their geometric centres. A typical series of such squares is shown in figure 1(b). Thus the computer would begin by defining at random a large square on the image, finding the centre of mass of the points within it, and moving the square until the centre of mass and the geometric centre coincided. Then the number of points inside was counted. Next a slightly smaller square was chosen concentric with the previous one. It was moved until its geometric centre and its centre of mass coincided, and so on. If the process resulted in a square being moved off the image or outside the previous square, the series was terminated. A value of D was computed for each series by least-squares fitting $\ln N$ against $\ln l$ to a straight line. In this weighted fit we assumed that as N increased, the relative uncertainty in N decreased roughly as $N^{-1/2}$. We verified the accuracy of this procedure by analysing a mathematical Hausdorff set known as a Koch curve (see, e.g., Mandelbrot 1977) with $D = \ln 3/\ln 2$. Our measuring method gave the correct D to within 1%—well within our statistical uncertainty (see table). We also analysed an image of points placed at random, and obtained the expected exponent, $D = 2$, to the same order of precision.

The accuracy of our method is limited by the finite total number of points in the image analysed; we have verified that the statistical variations in our measured exponents decrease when there are more points in the image. Another limitation on our precision arises from the finite size of our image. It is because of this finite size that our data span only a limited range of l .

We obtained results comparable with these by our second method of analysis, in terms of the density autocorrelation function. In this method we found the average density of occupied points in the digital image at a distance r from each occupied point, and this was done for all values of r (see figure 3(a)). In a set of points with a Hausdorff dimension, this average density should fall off with distance as r^{D-d} . Values of D for each image were found by plotting the logarithm of the average density against $\ln r$. Then D was obtained from the initial slope, as determined by equally weighted least-squares fitting. The errors quoted in table 2 give the range of D values whose χ^2 lay within a factor two of the minimum.

We verified the accuracy of this method using Koch curves and random images, as with our first method. We found that our results were reliable for distances r less than about a third of the image size. For larger distances the correlation function varied widely and depended sensitively on, for example, the size and location of the region sampled. These variations are due to the large, strongly correlated statistical fluctuations commonly encountered in correlation functions sampled over a region not much larger than the distance r (Jenkins and Watts 1968). We verified this idea by analysing a series of images, each with a Koch curve in a random position and orientation. These images were approximately the same size as our smoke images, and the Koch curves had $D = \ln 3/\ln 2 = 1.59$. If these images had been infinite, all would have had identical correlation functions. In the actual images the measured correlations fluctuate somewhat from image to image, and this gives a crude measure of the statistical uncertainties inherent in the sampling method. As in our smoke images, these fluctuations were

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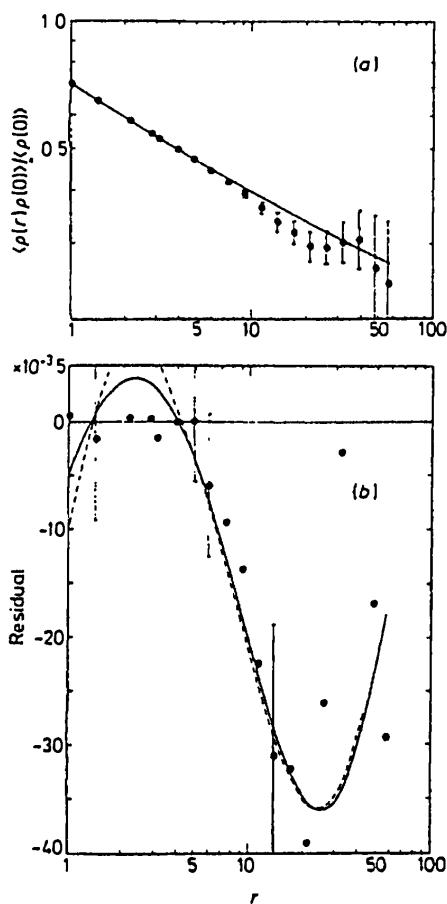


Figure 3. (a) Log-log plot of density autocorrelation divided by average density against distance r for the digitised image of figure 1(b). Unit of length is array element length in figure 1(b). The curve is of the form $Ar^{1.693-2} + B$, where the exponent, A and B were adjusted for a least-squares fit to the first four data points to obtain the initial slope. Error bars shown were obtained from the Koch curve study (see text). (b) Deviation of the data points from the line in (a) (horizontal line at 0). The full curve is of the form $Ar^{1.693-2} \exp(-r/15.8) + B$, where A and B were adjusted for a least-squares fit to the first 14 points. The broken curve is of the form $AK_0(r/15.8) + B$, where K_0 is the modified Bessel function.

highly correlated from point to point, so that one cannot infer the statistical uncertainties from the scatter of the data in a single image. We have assigned errors to our data points assuming that the relative error for a given distance r was the same as the relative spread of the data at that r in the Koch curve series. The error bars in figure 3 were drawn using this rough estimate.

We have summarised the results of these two methods in table 2. For each image we have listed the measured exponent D , with its statistical uncertainty, as obtained by each method. We have also indicated the approximate range of distance r sampled in each case. The exponent D for all these cases lies in the range 1.5 to 1.7. The exponents obtained by the point-counting method are systematically lower than those obtained from the density correlation method. We believe this is due to the breakdown of our power-law correlations in favour of an exponential decrease at large distances. Indeed, some type of exponential decrease is expected in an extended matter system for sufficiently large r (see, e.g., Duneau *et al* 1974). The effect of the exponential is to reduce the apparent D at large distances. The square-counting method weights the larger distances more heavily than does the correlation function method. Thus any exponential fall-off effects would cause the counting method to result in a smaller D , as we observe. We also see evidence for a more rapid fall-off at large distances by looking

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Table 2. Measurements of D .

Image matrix	Dimensions digitised image matrix	No of 'ones' in digitized image	Apparent D			
			Point counting ^a		D	Density auto-correlation ^b
			$N \propto L^D$	$N \propto L^D \times \exp(-L/r_0)$		
Real images						
2	70 × 96	1419	1.52 ± 0.04	1.90 ± 0.05	1.69 ± 0.02	1-12
3	97 × 120	2149	1.56 ± 0.02	1.90 ± 0.05	1.68 ± 0.01	1-12
4	96 × 120	1797	1.50 ± 0.04	1.85 ± 0.05	1.67 ± 0.02	1-7
5	94 × 119	2934	1.60 ± 0.04	1.85 ± 0.05	1.68 ± 0.02	1-13
6	50 × 49	523	1.55 ± 0.06 ^c	1.85 ± 0.05	1.55 ± 0.02	1-5.5
Test images						
Koch	79 × 77	2375	1.57 ± 0.02		1.55 ± 0.02	1-13
($D = 1.5850$)						
Random	100 × 100	2020	2.06 ± 0.02		2.00 ± 0.01	1-30
($D = 2$)						

^a Uncertainties are the standard deviations of fits to counts originating at several random sites on the image. The range of l in these fits was roughly 2-80.

^b Obtained by least-squares fit to a straight line on a log-log plot. The points spanning the range of r values indicated were equally weighted. Errors quoted are the nominal statistical errors of the fitted slope.

^c Range of l samples was 2-50.

at our power-law fits. There is often a slight downward curvature in our log-log plots. If we include exponential fall-off effects in our fitting, the fit to the data improves and the D values increase as expected. For fitting the correlation data we chose the functional form $\langle \rho(r)\rho(0) \rangle = Ar^{D-2} \exp(-r/r_0) + B$ where A , B , D and r_0 are fitted parameters. A corresponding form for the point count N as a function of the box size l is $N = A'l^D \exp(l/l_0) + B'l^2$. Here B and B' reflect the magnitude of the random background on our data, and r_0 and l_0 are characteristic length scales. Column 5 of table 2 reports the D values obtained using this fitting in the point-counting method. The nominal errors are based on the variations in D noted when several sets of data on a given image were approximately fitted. The broken line in figure 1(c) illustrates the improvement of the fits when the exponential fall-off was included. The l_0 values were typically about double the largest l value for each set of data. Evidently these data suggest an exponential fall-off, but they are also compatible with no such fall-off. The D values vary significantly depending on which functional form is chosen. The range of D values thus obtained overlaps the values from the correlation function method. The correlation function data may also be treated assuming exponential fall-off, as figure 3(b) illustrates. In this figure, we plot the residuals of the data from the line in figure 3(a). The full curve is the fit when exponential fall-off is included. Again the fit improves for large r , but the D values, taken from the initial slope, do not change significantly.

3. Discussion

Our results, though not conclusive, suggest that the particle distribution in these random aggregates arises from some type of critical process. For comparison we list in

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table 3 the D values which emerge in some model systems. One possible model for our system is based on percolation. In this model we imagine that the particles are ejected in random directions from a point source, and that they all slow to a stop in the same distance. In the spherical region where the particles stop, some will be close enough to touch. These touching particles stick together to form the aggregates we observe. If the particle density were large enough, percolating clusters would form. Under the right conditions one might preferentially observe these large clusters. The density correlations one measured would then be those within a percolating cluster. These correlations are known to have power-law behaviour (Kasteleyn and Fortuin 1969), and the exponent D is estimated (Stanley 1977) to lie near 1.8.

Table 3. Nominal D values for model systems.

Model	Field $\rho(r)$ (see equation (1))	$d = 2$	$d = 3$
Ising model (Brezin <i>et al</i> 1976) ^a	spin density	$\frac{2}{3}$	~ 1.96
Self-avoiding walk (McKenzie 1976) ^b	step density	$\sim \frac{4}{3}$	$\sim \frac{5}{3}$
Percolation (Stanley 1977) ^a	sites in percolating cluster	~ 1.8	~ 2

^a D is taken to be equal to $2 - \eta$, using η values from this reference.

^b D is taken to be equal to $1/\nu$ from this reference.

While our results are consistent with the above power-law picture, they are not good enough to rule out other interpretations. In fact, we have found a simple model with no critical exponent which fits our data nearly as well as the percolation model does. This model treats the aggregates as simple two-dimensional random walks. We assumed that the random walks consisted of nearest-neighbour steps on a hypothetical square lattice, and that the number of steps was not fixed, but exponentially distributed. The average density of points at a distance r from some step of such a walk is given by the modified Bessel function $K_0(2r/R)$ (Feller 1966), where R is the RMS average distance between any two steps (for r and R much larger than the lattice spacing). As with any two-dimensional random walk, the density has a logarithmic divergence for small distance. At large distances the density of these walks varies as $r^{-1/2} \exp(-2r/R)$. The result is that the apparent exponent D changes very slowly from 2 at small r to 1.5, before dropping rapidly at large r as a result of the exponential. We find (figure 3(b)) that our data fit this random-walk model nearly as well as they fit the power law.

The above discussion shows that the correlations we have observed need not imply a critical exponent. Of the two models we have proposed, though, the percolation model with its critical exponent seems the more plausible. In any case, it appears from our data that these random particle aggregates have density distributions of a general and long-range form. It is likely that these correlations can be explained by means of a simple model such as the ones we have proposed. Or it may be that these correlations are of a new type not previously seen. An experiment with larger samples and better statistics would settle the question. A wider range of materials and conditions should be studied to explore the generality of our finding.

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Acknowledgments

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5.7.2 Witten and Sander: Diffusion Limited Aggregation

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Diffusion-Limited Aggregation, a Kinetic Critical Phenomenon

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(Received 31 August 1981)

A model for random aggregates is studied by computer simulation. The model is applicable to a metal-particle aggregation process whose correlations have been measured previously. Density correlations within the model aggregates fall off with distance with a fractional power law, like those of the metal aggregates. The radius of gyration of the model aggregates has power-law behavior. The model is a limit of a model of dendritic growth.

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Gold black, Cab-o-SilTM, and coagulated aerosols¹ are aggregates of solid particles distinguished by their wispy appearance. The size of these aggregates far exceeds the range of forces holding them together²; it seems likely that the aggregation process can be understood without reference to the details of these forces. A class of aggregates were shown by Forrest and Witten³ to have density correlations of a power-law form. We show here that the formation conditions of these objects suggest a model which we simulate on a computer; the model is a discrete version of dendritic growth.⁴ The simulation produces model aggregates which also have power-law correlations. We compare the behavior of the model to other models which produce low-density objects: the Eden growth model,⁵ random animals,⁶ self-avoiding walks,⁶ and percolating clusters.^{4,7}

The aggregates which were studied by Forrest and Witten^{3,8} were formed when a metal vapor produced by heating a plated filament was quenched. Metal particles of average radius 40 Å condensed near the filament and streamed outward. The particles accumulated in a thin spherical shell (the "puff ball") of roughly a centimeter radius. In this region the particles are thought to coalesce. Then they drifted down to an electron microscope slide. The aggregates found on the slides contained on the order of 10^3 metal particles in a low-density mass. The particles appeared to coalesce *irreversibly* to form the aggregates, since these maintained their wispy shape even after drifting through the gas. We suppose that two particles in the puff ball stick together whenever their thermal motion brings them into contact.

The simplest model for the growth of such a

cluster of particles is the Eden model,⁵ a lattice model in which particles are added one at a time at random to sites adjacent to occupied sites. This process produces a relatively compact cluster whose density correlations are independent of distance in the limit of large size. The metal aggregates, by contrast, were reported³ to have correlations which fall off as a fractional power of distance. Thus they resemble random walks, percolating clusters, and other density profiles associated with critical phenomena.⁵⁻⁷ We present here a model for the observed aggregation which also exhibits fractional power-law behavior of the correlation function.

Our model is a variant of the Eden model whose initial state is a seed particle at the origin of a lattice. A second particle is added at some random site at large distance from the origin. This particle walks randomly until it visits a site adjacent to the seed. Then the walking particle becomes part of the cluster. Another particle is now introduced at a random distant point, and it walks randomly until it joins the cluster, and so forth. If a particle touches the boundaries of the lattice in its random walk it is removed and another introduced. A similar process was studied by Rosenstock and Marquardt.⁹ The exposed ends of our clusters tend to grow more rapidly than other perimeter sites because perimeter sites near the center are "shadowed"; our aggregates should be less compact than the Eden clusters.

Figure 1 shows a 3600-particle aggregate on a square lattice. Aggregates on a triangular lattice have the same general appearance. One may obtain information about the particle distribution from the density correlation function. The density $\rho(\vec{r})$ is defined to be 1 for the occupied sites

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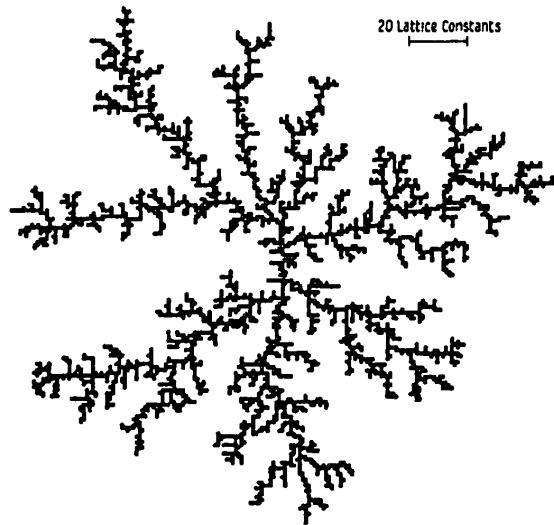


FIG. 1. Random aggregate of 3600 particles on a square lattice.

and 0 for the others. The correlation function in an N -particle aggregate,

$$C(r) = N^{-1} \sum_{r'} \rho(r') \rho(r' + r), \quad (1)$$

is an approximation to the ensemble average correlation function $\langle \rho(\vec{r}') \rho(\vec{r}' + \vec{r}) \rangle / \langle \rho(\vec{r}') \rangle$. This function is assumed to depend only on the distance r separating the two sites. Of course, this can only be true for r much less than the size of the aggregate. Figure 2 shows $C(r)$ averaged over directions and over six aggregates of roughly 3000 particles. It is clear from the fitted line that the data are consistent with a power law over distances from a few lattice spacings to the size of the cluster:

$$C(r) \sim r^{-0.343 \pm 0.004}. \quad (2)$$

The same exponent describes clusters on a triangular lattice; see Table I.

To check our computations we have measured³ $C(r)$ for a certain Koch curve, a geometric construction which is a Hausdorff set with a Hausdorff dimension¹⁰ D of $\ln 3 / \ln 2 = 1.585$. One expects the density of points in a Hausdorff set to have correlations of the form

$$\langle \rho(\vec{r}') \rho(\vec{r}' + \vec{r}) \rangle \sim r^{D-d} \equiv r^{-A}. \quad (3)$$

By definition, a Hausdorff set can be covered by a number of neighborhoods of radius a , $K(a)$, which varies as a^{-D} . The average number of points $N(a)$ within such a neighborhood must then

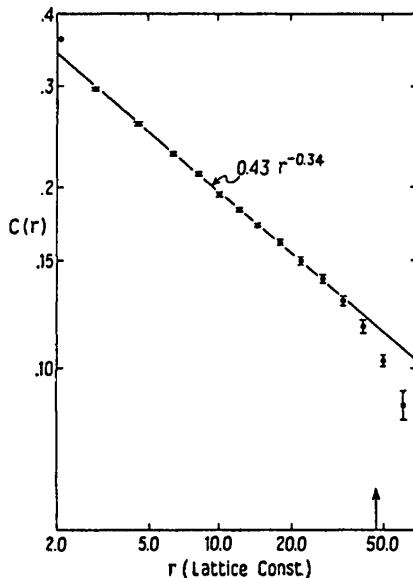


FIG. 2. The density correlation function averaged over six aggregates as a function of distance measured in lattice constants. The arrow marks the average radius of gyration. The solid line is a least-squares fit over the range $r=3$ to $r=27$. The error bars represent the spread of values among the six aggregates.

vary as a^D . Assuming that the neighborhoods may be chosen with arbitrary centers, one may relate the behavior of $N(a)$ to that of the correlations:

$$\begin{aligned} a^D \sim N(a) &= \int_0^a d^d r \langle \rho(\vec{r}) \rangle_{\text{origin occupied}} \\ &= \int_0^a d^d r \langle \rho(\vec{r}) \rho(0) \rangle / \langle \rho(0) \rangle, \end{aligned} \quad (4)$$

where d is the dimension of space. To yield this behavior the correlation function must obey Eq. (3).

To test the accuracy of our sampling procedure we generated images of the Koch curve and analyzed them with the same program used for the model aggregates. The resulting power-law fit confirms Eq. (3) as reported in Table I.

For the Koch curves and the model aggregates the measured $C(r)$ fall below the power-law line as r becomes comparable to the size of the aggregate. At short distances r the correlations of the model aggregates also differ from the power-law prediction. We believe this is a nonuniversal feature associated with the lattice.

The size R of a model aggregate should scale with the number of particles. Indeed, for neighborhoods of radius of order R , the contents $N(R)$

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TABLE I. Values of the correlation exponent A for diffusion-limited aggregation model and other systems.

	A	Two dimensions	Three dimensions
Diffusion-limited aggregation:			
Square lattice, average of six clusters of 2079–3609 particles in size (Fig. 2).	0.343 ± 0.004^a		
Triangular lattice, average of three clusters of 1500–2997 particles.	0.327 ± 0.01^a		
Radius of gyration, weighted average of A values inferred for six clusters of 999–3000 particles, Eq. (5).	0.299 ± 0.02^a		
Koch curve with $A = 2D = 0.416$, measured average correlation function of seven curves, translated and rotated at random.	0.42		
Metal-particle aggregates, correlations of particle density from micrographs, Ref. 3.	0.32 ± 0.01^b	1.32 ± 0.01^c	
Self-avoiding walk (flight), correlations of step density, Ref. 6.	0.667	1.33	
Percolation, from radius of gyration of clusters at threshold, Eq. (5), Refs. 5 and 7.	~ 0.2	0.9	
Random animals from radius of gyration, Eq. (5), Ref. 5.	0.46	1.18	

^aError range indicates statistical error only.

^bHere we interpret the measured two-dimensional density literally.

^cHere we interpret the measured density profile as the two-dimensional projection of a three-dimensional profile and infer the A value for the three-dimensional density.

must approach N . Since $N(a) \sim a^D$ for $a \leq R$, we expect

$$N \sim R^D = R^{d-A}. \quad (5)$$

Measurements of the radii of gyration of our aggregates support this prediction, as indicated in Table I.

Figure 2 suggests³ that our model aggregates are “critical” objects, having scale-independent correlations over an arbitrarily large range of distances. They are thus akin to self-avoiding walks, percolating clusters and order-parameter fluctuations near a phase transition. But in an important respect the model is different: The critical correlations here do not arise from an equilibrium ensemble but from an irreversible growth process. Indeed, our model is the discrete counterpart of the dendritic growth model of Langer and Muller-Krumbhaar.⁴ In this continuum model a substance (e.g., one species in a two-component solution) diffuses from infinity to

an absorbing surface. The density $u(\vec{r}, t)$ of the substance is constant on the surface (neglecting surface-tension effects) and zero at infinity. The rate of growth of the surface at r is proportional to the flux density ∇u there.

In our model the probability that a perimeter site at \vec{x} gains a particle at step n of the walk may also be expressed as a gradient of a quantity $u(\vec{r}, n)$, which gives the probability (in the ensemble of all random walks of length n) that there is an n th step and that it is at \vec{r} . The probability $u(\vec{r}, n)$ is proportional to the number of walks, $Z_n(\vec{r})$ arriving at \vec{r} in n steps. This $Z_n(\vec{r})$ satisfies the relation

$$Z_{n+1}(\vec{r}) = \sum_{\alpha=1}^c Z_n(\vec{r} + \vec{\alpha}), \quad (6)$$

where $\vec{\alpha}$ is one of the “ c ” nearest-neighbor vectors. To obtain the number of walks which have not visited perimeter sites \vec{x} , one sets $Z_n(\vec{x}) = 0$

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on the right side of Eq. (6), for these sites. This equation for Z_n implies a discrete diffusion equation for $u(\vec{r}, n) = Z_n(\vec{r})/c^n$:

$$\begin{aligned} u(\vec{r}, n+1) - u(\vec{r}, n) \\ = c^{-1} \sum_{\alpha=1}^c [u((\vec{r} + \vec{\alpha}), n) - u(\vec{r}, n)], \end{aligned} \quad (7)$$

with the boundary condition that $u = 0$ on perimeter sites. The left side of Eq. (7) is a discrete derivative in n and the right-hand side is the discrete Laplacian operator. The probability $v_{n+1}(\vec{x})$ that the perimeter site at \vec{x} grows in the $(n+1)$ th step is

$$\begin{aligned} v_{n+1}(\vec{x}) &= \sum_{\alpha=1}^c u_n(\vec{x} + \vec{\alpha})/c \\ &= c^{-1} \sum_{\alpha=1}^c [u((\vec{x} + \vec{\alpha}), n) - u(\vec{x}, n)]. \end{aligned} \quad (8)$$

This is a discrete gradient at \vec{x} . Thus our model is a discrete version of the dendritic growth model described above.

In the study of this system by Langer and Muller-Krumbhaar,⁴ they discovered that a smooth interface is unstable against wrinkling at all length scales; its growth depends on fluctuations in the diffusing field. Our findings describe the limit where these fluctuations are dominant.

The Monte Carlo study reported here may be extended to three or higher dimensions. We can study the effects of extending the size of the seed to simulate a finite tip radius of a dendrite. Realistic dendritic growth with surface tension can be simulated by making the sticking probability of particles smaller or larger for perimeter sites

with fewer or more neighbors. Finally, the model can be used to predict the time-dependent growth rate of real random aggregates, as well as their mechanical and transport properties.

The predicted features may appear in many processes, including gelation, condensation polymerization, and agglutination of biological molecules.

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5.7.3 Kadanoff: Chaos and Complexity

Chaos and Complexity: The Results of Non-linear Processes in the Physical World

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Abstract. The physical world contains an amazing variety of objects with intricate and complex geometrical properties. The laws of physics, on the other hand, are a set of rather simply-stated mathematical rules. So, how does simple law give rise to complex outcome? This paper suggests that complexity results from a natural process of organization in a chaotic environment. Three examples are given to illustrate this point. The first two are mathematical models: one called diffusion limited aggregation (DLA), and the other the avalanche model. The third example is drawn from the world of experimental physics and is convective turbulence.

I. Introduction

In recent decades, there has been a very considerable interest in the question of how complex spatial and temporal structures may arise from simple non-linear dynamical processes. The classic work of Kolmogorov [1] dealt with how a complex pattern of swirls shows up in turbulent hydrodynamic systems while Turing [2] addressed the evolution of structures in biochemical systems. Later on Katchalsky [3] and then Prigogine [4] described the formation of complex structures in dissipative systems. In solids, metallurgists explore a rich variety of different patterns [5-9] all generated dynamically. Dynamically produced objects can also occur in liquids as shown by Saffman and Taylor [10] and later workers [11-14]. In this note, I shall describe some recent work on structure formation in chaotic systems with the hope that these considerations might help one guess where the field is going.

In particular, I shall look at three examples of the dynamical formation of complex patterns in space and time.. The first, DLA, or diffusion limited aggregation was invented by Witten and Sander [15] as a mathematical model for the joining of carbon particles in the atmosphere to form pieces of soot.

This discussion will serve as an illustration of complex structure formation and as an introduction to the fractal [16] or scaling [17] concepts which have played a large role in the development of the area. We then turn to dynamical models of avalanches of the type originally proposed by P. Bak, C. Tang and K. Wiesenfeld [18] with the goal of showing how dynamical processes can lead to complex events of many different sizes. The distribution of events is described by the words 'self-organized criticality', which imply that the past events set in motion a chain of processes which will determine and limit the sizes of future events. The final example is the development of structure in convective turbulence as revealed by the experiments of Libchaber and coworkers [19]. Here the characteristics of the two previous examples are combined in that there is a complex spatial structure combined with events which are controlled by a feedback mechanism of the 'self-organizing' type.

2. DLA

DLA is a model in which an 'aggregate' sits on a lattice. This aggregate is just a connected group of occupied sites. (See Figure 1). Imagine a particle which comes in from infinity and move from site to neighboring site in the lattice. This particle is termed a 'random walker' since at each step the direction of its motion is picked at random. This step by step progress continues until the walker comes to a site which is next to an already occupied lattice site. At that point, the walker stops and joins the aggregate. In this way, the aggregate grows by one unit. Then another walker is released at infinity and the whole process begins once more. The structure that thereby forms is very light and consists mostly of holes. (See Figure 2)

Despite the randomness of the growth process, and despite the fact that the different structures produced by different realizations of this process may be quite different, nonetheless there are some rather simple and general laws

Figure 2 A DLA aggregate. The structure looks like a set of branches which occupy a very small fraction of the available area. Each branch is composed of sub-branches, looking like the main branches. These sub-branches are in turn composed of smaller units which look like the larger ones. This particular picture was produced by Michael Leibig by a process slightly different from the one described in the text.

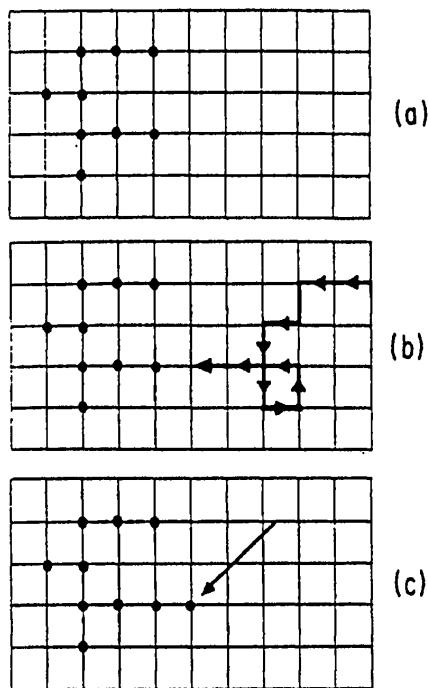
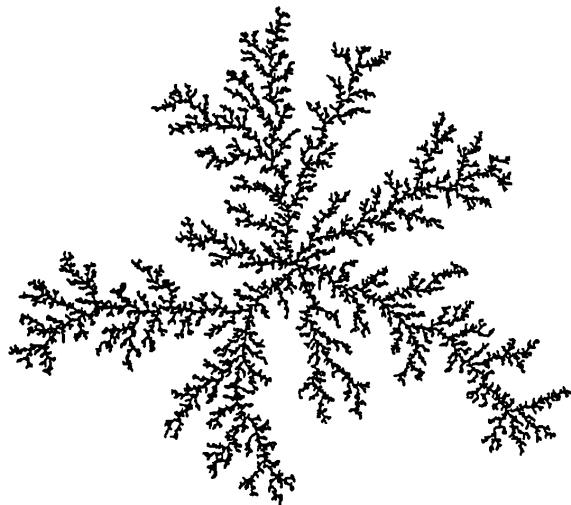


Figure 1 The DLA process. Part a shows the aggregate which occupies a region on the lattice. In Part b, a walker comes in from infinity, chooses a path at random, and comes to a stop when it gets to a site neighboring the aggregate. Part c shows the aggregate increased by one unit. After the walker comes to a stop, then the process starts all over again.



which govern the structures which are outcomes of this growth process. For example, as the mass of the cluster grows, its linear dimension grows as a power of that mass

$$\text{linear dimension} \sim M^x . \quad (1)$$

In two dimensions, x is about 0.6. In this usual terminology, (see Mandelbrot, ref 16) x^{-1} is called the fractal dimension of the aggregate. The density of the structure at a distance r from its initial starting point is given in terms of this fractal dimension by a 'scaling function' expression of the form

$$\text{density}(r) = r^{x^{-1}-d} \rho \left(\frac{r}{M^x} \right) \quad (2)$$

Notice that the first factor, which gives the typical density in the structure, goes down as r increases. The reason that the structure is so light and filled with holes is that the arms sticking out prevent the random walker from penetrating into the center of the object. Therefore the centers never quite get filled up. Thus the structure adjusts itself in precisely the proper manner so that it will allow itself to be partially filled but not totally filled. To see more of this adjustment process, turn to our next example:

3. Scaling and Universality in Avalanche Models

Bak, Tang, and Wiesenfeld [20] invented a cute dynamical model which shows how richly complicated events can arise in a relatively simple dynamical system. Let model sand [21] be arranged upon a model sandpile, built upon a regular d -dimensional lattice. A one-dimensional version of the model is shown in Figure 3. To start the cascade, one grain of sand is added to one of the columns, picked at random. In between additions, there are cascades of events in which sand falls downhill in response to a too-large local slope of the pile. In the particular model depicted in Figure 3, the sand falls over whenever the column in question stand more than two above its right-hand neighbor. In that case, two grains of sand 'fall over' and land on the two columns to the immediate right of the unstable site. If a grain of sand reaches the right-hand end of the system, it falls off and disappears from view. At any given time, all columns that can fall do so, simultaneously. Then, after this motion if in the new configuration, there are

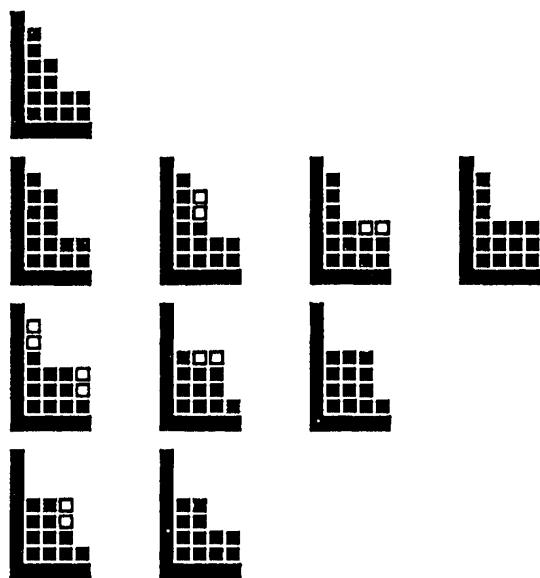


Figure 3 The Sand Model. This picture shows a short avalanche in progress in a small model sandpile. The first row shows the pile before the addition. The added grain is shown in black in the second row. Unstable grains are shown as boxes. They fall over until a stable configuration is finally reached.

any unstable columns, they fall and so on. Thus the system can sustain 'avalanches'. The cascade of events continues until no more columns are unstable. Then another grain of sand is added at random and the entire process begins once more. The algorithm for the model is shown in the box below:

An Avalanche Model
Square Sand stacked up in a region of size L
A. Add a Grain at a Random Site
(Avalanche begins)
B. If the Slope (Height Difference) is greater than 2, two grains from stack fall over. At right hand end, grains fall off Continue until no more stacks are unstable. (Avalanche Ends)
C. Return to A.

These avalanches in this system can be small or they can cover the entire system many times over. In a recent paper [22],, a group of us studied the nature of the probability distributions $p(X|L)$ for the probability that an event of size X will occur in a system with spatial extent L . We looked at two different quantities in some detail:

- a. The drop number D . In this case $X=D$ is the number of grains which fall off the end between two addition events.
- b. The flip number F . In this case X is the number of falling events which occur between two additions

These model sands slides can be considered to be an example of self-organized criticality. That is, the system organizes itself in such a way that it is marginally stable against the growth of an avalanche. An avalanche event, once started, has a finite probability for growing larger at every stage of its early existence. It also has some probability for growing smaller and dying. These two probabilities balance out so that events of all sizes occur in the sand pile.

It is interesting to ask the reason that the model pile organizes itself in such a fashion. To do this, we must look into the dynamics. Imagine that the pile were relatively flat so that the slides would almost always terminate after a few grains fell. Then, step by step as more sand were added the pile would become steeper and steeper. Conversely, if the pile were very steep, the addition of one grain would trigger a very large event in which many grains would move downhill and make the pile much less steep. The only type of configuration which would not disappear almost at once, is one of an intermediate steepness at which the pile is marginally stable. Thus, in this argument of Bak, Tang, and Wiesenfeld, the marginal stability is a necessary result of the nature of the underlying dynamics. (Notice incidentally, that the eventual result of a very large avalanche event is that much sand will fall off the end, reducing the slope and thus after-a-while bringing the avalanche to a halt.)

One could use the same kind of argument to describe the configurations produced by the DLA process. These configurations contain very long branches pointing outwards. If these branches were very long and thin, most of the walkers would hit the sides and the branches would fatten up. If, on the other hand, they were very thick, their tip ends would be liable to grow and stick out. As they became more exposed they would stick out further and there would be an increased likelihood that the walkers would land on them. In the end, the fat branches would produce much thinner structures.

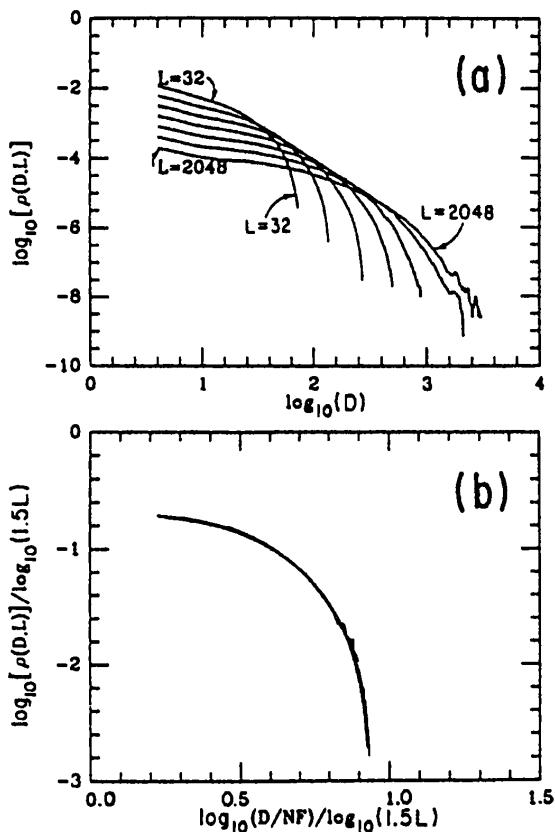


Figure 4. (from Kadanoff, et. al, reference 22. Figure 1.) Distribution of drop numbers in a one-dimensional model. The system size, L , ranges from 32 to 2048. Part a gives the raw data. Part b shows the best fit to these data using a result of the form of equation (3). This fit is very good indeed.

In both cases, the dynamics controls the result. However, in the avalanche model, the net result is not only a geometrical structure (a pile with a certain, marginally stable, slope) but also a distribution of event sizes. The produced distribution is one in which a whole range of events from very small ones to very large one will occur with appreciable probability. Figure 4a shows a probability distribution $\rho(D,L)$. This function describes the probability that in a stack of size L (see Figure 1) there will be an avalanche in which D grains of sand drop off the end. The beginning of the avalanche is defined by the addition of a new grain of sand at random, and the end occurs when all the grains stop moving. Notice that there is a tremendous range of events, from ones in which

essentially no grains fall off to ones in which the whole surface layer slides off.

Once again it is interesting to ask whether there is any simple law which fits the observed data. Does this avalanche process give any simple 'laws of nature'. Interestingly enough the answer is apparently 'yes'. All the data for large D and L shown in Figure 4a can be fit by a law of the form

$$\ln \rho(D/L) = f(\alpha) \quad (3)$$

$$\alpha = \frac{\ln D}{\ln L} \quad \text{for } L, D \gg 1$$

Thus if we plot $\ln \rho(D/L)/\ln L$ on the y axis against $\ln D/\ln L$ on the x axis, for sets of data taken at different values of L, we should expect that all the data would fall on a single curve. Figure 4b shows such a plot. Within the accuracy of the simulational work, all the data does fall onto a curve. Hence Eq (3) does provide a simple 'law' which summarizes the behavior of the avalanches.

It is even more remarkable to notice that this law remains true, with the very same form of the function $f(a)$, even when the model is changed somewhat by, for example, changing the rules by which the sand falls over. This property that the laws remain the same as the model is changed is called 'universality'. It is a characteristic and expected feature of models with self-organizing properties and large-sized events.

4. Turbulence in Thermal Convection

Recent experiments by Albert Libchaber's group [23,24] have shown how very beautiful and intricate structures may arise in situations in which one expects to observe hydrodynamic turbulence. The experiments in question involve a 'Rayleigh-Bénard' flow. In this flow, the fluid is set into motion by placing it in a box and heating it from below. The heated, and therefore less dense, fluid will rise. Correspondingly, the colder and more dense fluid will fall. The net effect that the whole fluid will move and carry heat from bottom to top.

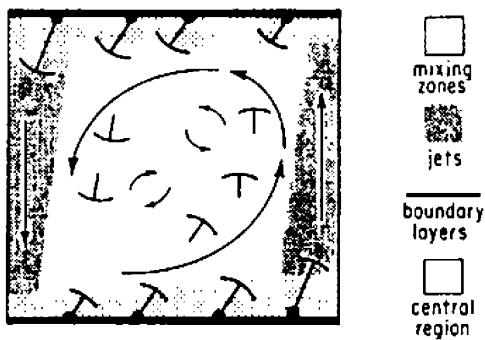
There is a dimensionless number which describes the strength of the forcing in this type of experiment. It is called the Rayleigh number and is given by

$$Ra = \frac{g\alpha\Delta L^3}{\kappa v} \quad (4)$$

Here, g is the acceleration of gravity, α is the volume thermal expansion coefficient, Δ is the temperature difference between the bottom and the top of the cell, κ and ν are respective the thermal diffusivity and the kinematic viscosity, and L is a characteristic size of the cell. More physically, $g\alpha\Delta$ is a typical size of the buoyant forces which are trying to get fluid into motion while κ and ν are measures of the contrary forces which are working to put the system into equilibrium. High values of Ra correspond to large forcings and indicate a situation in which the fluid is likely to be highly turbulent. The turbulence is easily seen for example (see reference 23) in a setup in which the working fluid is water in a rectangular tank with typical dimension about 20 cm and typical temperature difference Δ about 10 degrees centigrade. In that case, one can see a very chaotic pattern of motion within the tank. Measurements on an analogous system composed of low-temperature helium gas, where there is a better possibility for accurate measurement but a worse possibility for visualization, show scaling types of behavior roughly analogous to the ones discussed above. The environment is certainly very noisy and the measurements show many elements of randomness.

Nonetheless, the observation of the fishtank, as represented in the cartoon view of Figure 5 show considerable structure and regularity. There appear to be at least four different functional regions of the system:

A. Boundary Layer. This thin layer near the top and bottom of the tank contains fluid almost at rest. In these regions, heat is entering the tank via ordinary heat conduction processes.



Rayleigh-Bénard Cartoon

Figure 5. Cartoon of water tank. The bumps on top of the boundary layer are intended to depict the waves. Plumes and thermals are also roughly sketched in.

B. Central Region. This is a relatively quiet region near the center of the tank. The fluid undergoes a gentle regular circular motion together with a more random swirly motion in this region. Hot and cold umbrella-shaped objects called thermals carry heat through this region.

C Mixing Zone. Just above and below the boundary layers, one has a thicker region in which the motion and the temperature difference are much more violent and extreme than in the central region. Here mushroom-shaped structures containing hot (or cold) fluid rise (or fall). These 'plumes' differ from the thermals of the central region in that they are rooted to the boundary layers and have their motion fed from these layers.

D. Jet. Along the side walls there are orderly upwelling on hot fluid on one side and downward motion of cold fluid on the other.

This whole complex machine seems to be a self-regulating structure similar to those discussed in the DLA and avalanche sections. In particular, the amount of plume-like motion seems to regulate itself. There seem to be several parts of this regulatory system. These include: (See Figure 6)

1. The plumes and thermals which move respectively thorough the jets and the central region until they hit the top and bottom, whereupon they produce

2. Boundary layer waves. These are regions of increased thickness in the boundary layer which move rightward in the

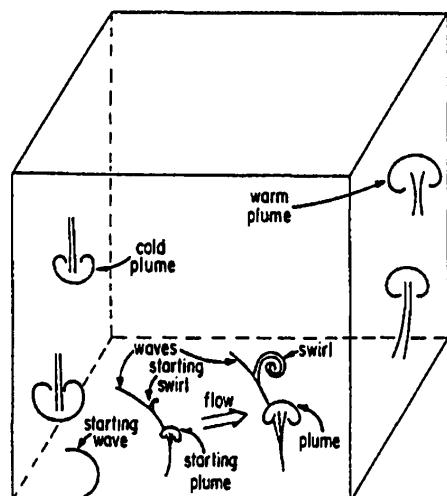


Figure 6. The processes in the water tank. (Taken from Zocchi, Moses, and Libchaber, ref. 23. This is the experimentalists' drawing of the life cycle of plumes.

bottom of the cell of Figure 5 and leftward at the top. Along the top of the bottom boundary layer waves there seem to be

3. Upwellings in the form of spray which then seem to rise and form into plumes.

4. 'Shocks'. In addition, when the boundary layer waves hit the side walls, they apparently produce splashes or shocks, strong temperature disturbances which form an apparently circular pattern and move through the central region. When these hit the boundary layers, they too produce boundary layer waves.

Thus the plumes, thermals, shocks, and waves seem to form a mutually regulating system somewhat like the kind of self-organized criticality discussed earlier in this note.

5. Conclusions

In this note, I have examined several examples in which physicists are attempting to explain observed phenomena by saying that dynamical systems can produce complicated objects via the repetition of simple elementary processes. Once this idea is pointed out it seems simple and inevitable. However, it may be that the organizational idea of Kolmogorov, Turing, Katchalsky, Prigogine, and all their followers is only the beginning of a rich subject of scientific study. We can make assertions about complexity and structure, but we are just beginning to touch the surface of the knowledge which can be gained in this way. One can hope that by following along the path trodden by such leading scientists as Professors Emeritus R. Kubo and H. Mori and, for example, Professors Y. Kuramoto, K. Kawasaki, M. Suzuki, K. Kaneko, Y. Sawada and many others, we shall begin to gain some understanding of how the beautiful simplicity of physical law can lead to the beautifully intricate structure of the world about us.

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Chapter 6

From Hops to Statistical Mechanics

Hamiltonian mechanics is the basis of the statistical mechanics described by Eqs. (1.1)–(1.8). A Hamiltonian is required in the formulation of either the classical or the quantum version of statistical mechanics. Given the Hamiltonian, one can have a probability distribution of the form

$$\rho = Z^{-1} e^{-\beta \mathcal{H}}. \quad (6.1)$$

In this chapter we wish to see how equilibrium statistical mechanics can arise from a non-equilibrium theory. We therefore start with a set of variables which at least potentially has a Hamiltonian character. A Hamiltonian structure is something very special. Not all differential equations can be cast into Hamiltonian form. To have this form, we must at least have variables which can serve as canonically conjugate coordinates and momenta as they appear in Hamilton's equations:

$$\begin{aligned} \frac{dq_\alpha}{dt} &= \frac{\partial \mathcal{H}}{\partial p_\alpha} \\ \frac{dp_\alpha}{dt} &= -\frac{\partial \mathcal{H}}{\partial q_\alpha}. \end{aligned} \quad (6.2)$$

However, the kind of hopping described in the last chapter is inherently inconsistent with Hamiltonian mechanics. We assumed that after each landing on a lattice site, the particle lost all memory of its previous location. Thus each particle carries with it one piece of information: its position — not the required two: position and momentum. For this reason, we cannot possibly have a Hamiltonian description of the hopping situation. Thus the equilibrium behavior of this system cannot shed much light on the source of a statistical mechanical equilibrium description in the usual kind of Hamiltonian system.

To get to statistical mechanics, we should have the canonical variable pair: position and momentum. The last chapter discussed hops in position. But, when a heavy particle sits in a noisy environment, it is continually bombarded by other particles. Each hit does not

immediately change the particle's position. However, many hits together can change the momentum quite substantially. If the hitting particles are moving fast enough, their effect upon the momentum may appear to be quite immediate. Now, we need to keep track of a momentum variable. Since if the system is left alone, it will be in thermal equilibrium at the temperature of the hitting particles. Then we shall have a probability of the form

$$\rho \sim \exp\left(-\frac{\beta p^2}{2M}\right), \quad (6.3)$$

with M being the mass of the heavy particle. Thus, if we want to have a description in terms of hops, we should study hops in momentum (and hence velocity) instead of the hops in position described in Chapter 5.

6.1 Random Walk in Momentum

Imagine a particle moving through a gas. The particle is assumed to be big and heavy in comparison to any molecule of the gas, but it is also assumed to be very much smaller than any macroscopic dimension. As Robert Brown observed when he watched pollen particles through the microscope, such a particle will move through the fluid in a jerky apparently random motion. We use the name 'Brownian particle' for any 'big' particle which is moved by random molecular collisions. As the Brownian particle moves it actually experiences several types of forces from the fluid:

First, collisions with the gas molecules produce a set of random knocks in momentum. If we wish to express these knocks in the form of an equation, they provide a contribution to the force like:

$$\frac{d\mathbf{P}}{dt} = \dots + \eta(t) + \dots, \quad (6.4)$$

where the ...'s represent terms which we do not wish to specify at the moment. Here, the random impulses described by the vector, $\eta(t)$, provide a set of many separate uncorrelated kicks to the momentum. Since we do not wish the kicks to send the particle in any preferred direction, we will choose the average kick to be zero

$$\langle \eta(t) \rangle = 0. \quad (6.5a)$$

Since we also wish to reflect the effect of many uncorrelated short duration collisions, we should choose $\eta(t)$ to have infinitely short time correlations, so that its components obey:

$$\langle \eta_\mu(t) \eta_\nu(t') \rangle = \Gamma \delta_{\mu,\nu} \delta(t - t'). \quad (6.5b)$$

The delta function in time arises because kicks are so short in comparison with our observation time that we cannot perceive their duration and structure.¹ The $\delta_{\mu,\nu}$ is a statement that kicks in different directions are uncorrelated. Finally the Γ is a kicking strength which we shall have to determine later. Alternatively, we can state the result of Eq. (6.5b) in terms of the impulse imparted to the particle in the interval between t and $t + \delta t$, which is

$$\mathbf{I} = \int_t^{t+\delta t} ds \eta(s). \quad (6.6)$$

From Eqs. (6.5), the mean squared impulse is given by

$$\langle I_\mu I_\nu \rangle = \Gamma \delta_{\mu,\nu} \int_t^{t+\delta t} ds = \Gamma \delta_{\mu,\nu} \delta t. \quad (6.7a)$$

The equilibrium we are seeking is one in which the momentum has a Gaussian distribution as in Eq. (6.3). So we wish to pick the probability distribution of $\eta(t)$ by the requirement that $\mathbf{P}(t)$, which is a time integral of η has a Gaussian distribution. Since we know that a sum of Gaussian terms is itself a Gaussian, we simply pick $\eta(t)$ to have a Gaussian distribution so both $\mathbf{P}(t)$ and I will have Gaussian probability distributions as well. Consequently

$$\langle \exp(i\mathbf{q} \cdot \mathbf{I}) \rangle = \exp(-\Gamma \delta t q^2 / 2). \quad (6.7b)$$

However the random kicks cannot be the whole story. The kicks in Eq. (6.4) will produce a random walk in momentum space. The kicking will — if allowed to run unchecked over a long period of time — produce unboundedly large values of the kinetic energy. To prevent this unwanted outcome, we must introduce a frictional force which will slow down the particles. A study of the hydrodynamics of particles moving thorough a fluid shows that if there is no external force upon them, their momentum obeys a frictional law:

$$\frac{d\mathbf{P}}{dt} = -\frac{\mathbf{P}}{\tau} + \dots, \quad (6.8)$$

where τ is a relaxation time determined by the viscosity of the fluid. This relaxation is the second kind of force produced by the collisions. We can put (6.4) and (6.8) together and solve the resulting equation:

$$\frac{d\mathbf{P}}{dt} = -\frac{\mathbf{P}}{\tau} + \eta(t), \quad (6.9)$$

¹Hydrodynamicists have long been interested in what are called *passive scalars* — particles which diffuse as they are carried along by the motion of a fluid. This situation is the generalization of Einstein's Brownian motion problem to the case in which the fluid is motion. In 1968, R. Kraichnan set up a model involving very rapidly changing velocities. In his paper, Physics of Fluids 11, 945 (1968), he exhibited a solution for the correlation between the densities at different points in the fluid. Since then, there has been a great deal of discussion of how this result can be generalized. A summary of the discussions can be found in *Turbulent Excursions*, L. P. Kadanoff, Fluid Motion, News and Views, Nature, Vol. 382, July 11, 1996.

to obtain

$$\mathbf{P}(t) = \mathbf{P}(t_0) \exp\left(-\frac{t-t_0}{\tau}\right) + \int_{t_0}^t dt' \eta(t') \exp\left(-\frac{t-t'}{\tau}\right). \quad (6.10a)$$

This equation expresses the value of $\mathbf{P}(t)$ expressed in terms of $\mathbf{P}(t_0)$, with t_0 being an arbitrary time. Sometimes, it is useful to have the form which arises when this starting time t_0 is set back to minus infinity so that (6.10a) becomes:

$$\mathbf{P}(t) = \int_{-\infty}^t dt' \eta(t') \exp\left(-\frac{t-t'}{\tau}\right). \quad (6.10b)$$

One can now start to evaluate physical quantities. For example, by using Eq. (6.4) we find that if we fix the value of the momentum at time zero, we can find the average momentum at the time t from Eq. (6.10a) as:

$$\langle \mathbf{P}(t) \rangle = \mathbf{P}(0) \exp\left(-\frac{t}{\tau}\right). \quad (6.11)$$

Thus the friction reduces the average momentum to zero with exponential decay and a time constant, τ . Now, we start to convince ourselves that the momentum defined by Eq. (6.9) really has a Gaussian probability distribution — as predicted by Boltzmann.²

To find the actual probability distribution for η , one writes a generating function for the averages of momentum as $\langle \exp(i\mathbf{q} \cdot \mathbf{P}(t)) \rangle$. On one hand, this generating function can be evaluated from the Boltzmann distribution (6.1) as:

$$\langle \exp[i\mathbf{q} \cdot \mathbf{P}(t)] \rangle = \exp\left(-\frac{Mq^2}{2\beta}\right). \quad (6.12)$$

But, by using Eq. (6.7b) we see

$$\langle \exp(i\mathbf{q} \cdot \mathbf{P}(t)) \rangle = \left\langle \exp\left[iq_\mu \int_{-\infty}^t ds \eta_\mu(s) \exp\left[-\frac{t-s}{\tau}\right]\right] \right\rangle. \quad (6.13a)$$

Because of the Gaussian nature of \mathbf{P} we can use Eq. (3.6) to compute the average of the exponential in Eq. (6.13a) to be:

$$\exp(i\mathbf{q} \cdot \mathbf{P}(t)) = \exp\left[-\frac{q_\mu q_\nu \Lambda_{\mu,\nu}(t)}{2}\right] \quad (6.13b)$$

with

$$\Lambda_{\mu,\nu}(t) = \int_{-\infty}^t dw \int_{-\infty}^t ds \langle \eta_\mu(w) \eta_\nu(s) \rangle \exp\left\{-\left[\frac{t-s}{\tau}\right] - \left[\frac{t-w}{\tau}\right]\right\}.$$

Equation (6.13b) may be further evaluated using the force correlation function (6.5b). The integral becomes elementary and gives the result:

$$\Lambda_{\mu,\nu} = \delta_{\mu,\nu} \int_{-\infty}^t dw \Gamma \exp\left\{-\left[\frac{2(t-w)}{\tau}\right]\right\} = \delta_{\mu,\nu} \Gamma \tau / 2 \quad (6.13c)$$

²See the discussion in Abraham Pais, *Subtle is the Lord, the Science and Life of Albert Einstein*, Oxford, 1982, Chapters 4 and 5.

so that finally (6.10a) simplifies to

$$\langle \exp[i\mathbf{q} \cdot \mathbf{p}(t)] \rangle = \exp\left(-\frac{q^2\Gamma\tau}{4}\right). \quad (6.14)$$

The quadratic structure of the right hand side of Eq. (6.14) is a signal that, as expected, the Gaussian impulses, η , do indeed give a Gaussian probability distribution. (Look back at Eq. (3.3) we want an answer of the form (6.3). Using Eqs. (3.3) and (6.3), we are led to an identification of the constants in the two Gaussians, according to:

$$\Gamma\tau = 2MkT \quad (6.15)$$

Equation (6.15) is a profound result.³ Given a big particle moving through a fluid with a frictional relaxation having a time constant, τ , one can predict the mean squared rate at which momentum is being added to the particle, Γ , via collisions with the little particles in the environment. (It is quite natural that there is a relation between the friction and the kicks, since they are determined by precisely the same process of multiple collisions between our special particle and the much lighter, faster particles in the gas.⁴)

Equation (6.15) can also be interpreted as a condition that our particle be in equilibrium. Here τ represents a rate at which momentum is being removed by the environment while Γ represents a balancing mean squared rate at which momentum is being added.

6.2 The Diffusion Equation Again

A simpler version of the argument which led to Eq. (6.10b) gives a correlation equation for the momenta at different times, which is

$$\langle P_\mu(t)P_\nu(t') \rangle = \langle P_\mu(t')P_\nu(t') \rangle \exp\left(-\frac{|t-t'|}{\tau}\right) = (MkT)\delta_{\mu,\nu} \exp\left(-\frac{|t-t'|}{\tau}\right). \quad (6.16)$$

Since, in non-relativistic mechanics,

$$\mathbf{P} = M \frac{d\mathbf{R}}{dt},$$

Equation (6.16) may also be expressed as an expression for position correlations:

$$\frac{d}{dt} \frac{d}{dt'} \langle R_\mu(t)R_\nu(t') \rangle = \frac{kT}{M} \delta_{\mu,\nu} \exp\left(-\frac{|t-t'|}{\tau}\right). \quad (6.17)$$

Two integrations of Eq. (6.17) over the interval $[0, s]$ gives the position structure function

$$\langle [R_\mu(s) - R_\mu(0)][R_\nu(s) - R_\nu(0)] \rangle = \frac{2kT\tau}{M} \delta_{\mu,\nu} \left[s - \tau + \tau \exp\left(-\frac{s}{\tau}\right) \right]. \quad (6.18)$$

³Equation (6.15) is a form of the fluctuation-dissipation theorem, derived in the next chapter.

⁴See Abraham Pais, *Subtle is the Lord, the Science and Life of Albert Einstein*, Oxford, 1982, pages 17–20. One portion of Einstein's work on Brownian motion can be found in English translation in *Investigations on the Theory of the Brownian Movement*, by Albert Einstein, Ph.D., edited by R. Fürth (Dover Publications, Inc., 1956).

In general correlation functions formed from differences of the form

$$X(t+s) - X(t)$$

and their powers are called structure functions. They are particularly important in situations like the one considered here in which correlations can get very large for large time-separations.

To check the result, Eq. (6.18), note the left hand side of Eq. (6.18) must vanish as s^2 for small values of s . A power series expansion of the right hand side shows that the term of order s^0 and s each vanish leaving the first nonzero term being the one proportional to s^2 .

In actual Brownian motion the particle which is being hit shows a diffusive behavior over long periods of time. In our model problem, in the limit as s goes to infinity, Eq. (6.18) reads:

$$\langle (R_\mu(s) - R_\mu(0))(R_\nu(s) - R_\nu(0)) \rangle \longrightarrow \frac{2kT\tau}{M} \delta_{\mu,\nu} s. \quad (6.19)$$

A comparison with Eq. (5.28) shows that the long time behavior is indeed diffusive with a diffusivity:

$$\lambda = \frac{kT\tau}{M}. \quad (6.20)$$

Einstein realized that Eq. (6.20) provided an excellent opportunity to, for the first time, see in a quantitative fashion the effects of microscopic motion. The diffusivity, λ , can be measured by looking at the displacement of the Brownian particle, specifically by measuring the time dependence of the mean squared displacement. The mass of the particle and the temperature are also directly measurable. The relaxation time, τ , can be computed using ordinary hydrodynamics in terms of the macroscopic viscosity, η , and the particle radius. At once the Boltzmann constant, k , becomes accessible to macroscopic measurement. If k were the same for different gases and different kinds of Brownian particles, the statistical theory of fluids and the atomic theory of matter would be partially verified. If not, it would be disproved. Experiment showed k is a constant of nature.

6.3 Time Dependence of Probability

Now consider the probability function $\rho(\mathbf{p}, \mathbf{r}, t)$ defined so that $\rho(\mathbf{p}, \mathbf{r}, t)d\mathbf{p} d\mathbf{r}$ is the probability for finding the particle within the phase space volume $d\mathbf{p} d\mathbf{r}$ about the phase space point \mathbf{p}, \mathbf{r} . This probability is defined as

$$\rho(\mathbf{p}, \mathbf{r}, t) = \langle \delta(\mathbf{P}(t) - \mathbf{p})\delta(\mathbf{R}(t) - \mathbf{r}) \rangle. \quad (6.21a)$$

Here, \mathbf{p} and \mathbf{r} are just numbers which define the values of the momentum and the position for which we are calculating the probability, ρ . On the other hand, $\mathbf{P}(t)$ and $\mathbf{R}(t)$ are something quite different. They are random variables which depend upon the random kicks,

$\eta(\cdot)$. These random kicks in turn define the process by which the particle moves through the fluid. We shall use $\rho(\mathbf{p}, \mathbf{r}, t)$ as our basic calculational quantity in the situations in which we can think of the system as containing one particle. If there are N particles labeled by an index j we shall instead use

$$f(\mathbf{p}, \mathbf{r}, t) = \sum_{j=1}^N \langle \delta(\mathbf{P}_j(t) - \mathbf{p}) \delta(\mathbf{R}_j(t) - \mathbf{r}) \rangle h^3, \quad (6.21b)$$

where, of course, $\mathbf{P}_j(t)$ and $\mathbf{R}_j(t)$ are the momentum and position of the j th particle and h^3 is our conventional normalization of all classical phase space densities. If all the particles behave in the same way,

$$f(\mathbf{p}, \mathbf{r}, t) = N\rho(\mathbf{p}, \mathbf{r}, t)h^3. \quad (6.22)$$

The name of $f(\mathbf{p}, \mathbf{r}, t)$ is the *one-particle distribution function*.

We would like to write an equation for the time dependence of $\rho(\mathbf{p}, \mathbf{r}, t)$ which will take into account the physical effects of friction and random knocking considered up-to-now. (We consider ρ instead of f because the notation is simpler.) In addition we would like to generalize the problem slightly by looking directly at the coordinate vector which obeys a Hamiltonian equation of motion:

$$\frac{d\mathbf{R}}{dt} = \frac{\mathbf{P}}{M} = \frac{\partial \mathcal{H}(\mathbf{P}, \mathbf{R})}{\partial \mathbf{P}}. \quad (6.23a)$$

Similarly, in addition to the forces we have already considered we would like to add an explicitly potential force $-\nabla U$ so that the equation for the momentum is:

$$\frac{d\mathbf{P}}{dt} = -\frac{\partial \mathcal{H}(\mathbf{P}, \mathbf{R})}{\partial \mathbf{R}} + \eta(t) - \frac{\mathbf{P}}{\tau}. \quad (6.23b)$$

Here the Hamiltonian \mathcal{H} is given as a sum of kinetic and potential energy terms

$$\mathcal{H}(p, r) = \frac{\mathbf{p}^2}{2M} + U(r). \quad (6.24)$$

We want to derive an equation for the time derivative of ρ . In the last chapter, we calculated the probability by using $\exp(i\mathbf{q} \cdot \mathbf{R})$ as a generating function. (See the argument leading up to Eq. (5.33)). But now ρ depends upon two variables. In this situation, it is somewhat easier to use an approach in which we imagine that we are calculating the average of some arbitrary function of momentum and coordinates at time t . We write this observable as $O(\mathbf{p}, \mathbf{r})$. This average of the observable at time t is

$$\langle O \rangle(t) = \int d\mathbf{p} dr O(\mathbf{p}, \mathbf{r})\rho(\mathbf{p}, \mathbf{r}, t). \quad (6.25)$$

Our strategy is to calculate the time derivative of the average in Eq. (6.25). We choose the function $O(\mathbf{p}, \mathbf{r})$ to be totally independent of time. Then all of the time dependence we can see in the average must be a result of the time-dependence of ρ .

Why are we describing things in terms of probabilities? Is it not true that classical mechanics is completely deterministic? There are two possible reasons for using a probability distribution. If the motion is driven by a random variable like η , probabilities are the natural formulation of the problem. Even if the system is deterministic, often we do not have sufficient information to define the initial state of the system. Then we use the probability

$$\rho_0(\mathbf{p}, \mathbf{r}) = \rho(\mathbf{p}, \mathbf{r}, 0) \quad (6.26)$$

to describe the initial configuration of the system.

For now, we stick to the case in which all the randomness comes from initial conditions. We want to calculate averages like $\langle O \rangle$. We have already mentioned that we can do this by considering an equation for the time-dependence of ρ .

Alternatively, one can proceed by solving the equations for $\mathbf{P}(t)$ and $\mathbf{R}(t)$. Since these obey first order equations in time, we need one piece of initial data for every variable, specifically the values of $\mathbf{P}(0)$ and $\mathbf{R}(0)$. The later-time variables ($\mathbf{P}(t)$ and $\mathbf{R}(t)$) are functions of these starting variables. Thus we can interpret ($\mathbf{P}(t)$ and $\mathbf{R}(t)$) as being stochastic variables precisely because the probabilities of $\mathbf{P}(0)$ and $\mathbf{R}(0)$ are given by the initial probability ρ_0 . Thus, one can calculate the average defined by Eq. (6.25) by calculating an average based upon ρ_0 , namely

$$\langle O \rangle(t) = \int d\mathbf{p} d\mathbf{r} O(\mathbf{P}(t), \mathbf{R}(t))\rho(\mathbf{p}, \mathbf{r}, 0) = \langle O(\mathbf{P}(t), \mathbf{R}(t)) \rangle_0. \quad (6.27)$$

In Eq. (6.27), \mathbf{p} and \mathbf{r} are the momentum and the position of the particle at time 0. The last form of writing Eq. (6.27) is intended to be a concise reminder that the result is calculated in terms of averages over the initial values of the variables.

Equations (6.25) and (6.27) are formulas from classical physics. The first of these is very much like the Schrödinger representation of quantum mechanics in that all the time dependence is in the ‘state’ function, $\rho(\mathbf{p}, \mathbf{r}, t)$. In contrast, Eq. (6.27) is like the Heisenberg representation of quantum mechanics since all the time dependence is to be found in the ‘operators’, $\mathbf{P}(t)$ and $\mathbf{R}(t)$.

6.4 Time Dependence in Deterministic Case

We will first use these two expressions to calculate the time derivative of ρ in the case in which the motion is completely deterministic. It pays to do our job in a rather general fashion. For this reason, we shall say that ρ is a probability distribution in some general set of coordinates x_α and that the average of an observable is

$$\langle O \rangle_t = \int d\mathbf{x} O(\mathbf{x})\rho(\mathbf{x}, t),$$

where

$$\rho(\mathbf{x}, t) = \langle \delta(\mathbf{x} - \mathbf{X}(t)) \rangle$$

with X_α is a position or momentum random variable, or perhaps a function of these variables.

The time derivative of the average is:

$$\frac{d}{dt}\langle O \rangle(t) = \int d\mathbf{x} O(\mathbf{x}) \frac{\partial}{\partial t} \rho(\mathbf{x}, t). \quad (6.28)$$

Now let us imagine that each X_α has a time derivative

$$\frac{d}{dt} X_\alpha(t) = V_\alpha(\mathbf{X}(t)), \quad (6.29)$$

we call V_α a *generalized velocity*.

In the Hamiltonian case, if X_μ refers to a coordinate variable, \mathbf{r}_μ

$$V_{\mathbf{p}} = -\frac{\partial \mathcal{H}}{\partial \mathbf{r}},$$

while if it is a momentum

$$V_{\mathbf{r}} = -\frac{\partial \mathcal{H}}{\partial \mathbf{p}}.$$

The ‘Heisenberg representation’ of Eq. (6.27) is, for the Hamiltonian system, the statement that $\langle O \rangle(t) = \langle O(\mathbf{X}(t)) \rangle_0$ so that the time dependence is also given by

$$\frac{d}{dt}\langle O_t \rangle = \left\langle V_\alpha(\mathbf{X}(t)) \frac{\partial}{\partial X_\alpha(t)} O(\mathbf{X}(t)) \right\rangle_0 = \int d\mathbf{x} \rho(\mathbf{x}, t) V_\alpha(\mathbf{x}, t) \frac{\partial}{\partial x_\alpha} O(\mathbf{x}),$$

where we understand that we are supposed to sum over repeated Greek indices (that is α). After an integration by parts,⁵ we have the expression

$$\frac{d}{dt}\langle O \rangle(t) = - \int d\mathbf{x} O(\mathbf{x}) \frac{\partial}{\partial x_\alpha} [\rho(\mathbf{x}, t) V_\alpha(\mathbf{x}, t)]. \quad (6.30)$$

We should, however, notice that $O(\mathbf{x})$ can be any function at all. If Eqs. (6.28) and (6.30) are both going to be true then the coefficients of $O(\mathbf{x})$ in these two equation must be equal to one another. If we shift everything to the same side of the equation, we find:

$$\frac{\partial}{\partial t} \rho(\mathbf{x}, t) + \sum_\alpha \frac{\partial}{\partial x_\alpha} [V_\alpha(\mathbf{x}) \rho(\mathbf{x}, t)] = 0. \quad (6.31)$$

Thus is our general result. It will enable us to find the time derivative of the probability in any deterministic situation.

In a Hamiltonian situation, Eq. (6.31) can be further simplified. It is a consequence of Liouville’s theorem (or simply of the Hamiltonian structure of the system), that the sum

$$\sum_\alpha \frac{\partial}{\partial x_\alpha} V_\alpha(\mathbf{x}, t) = \sum_\mu \frac{\partial^2 \mathcal{H}}{\partial p_\mu \partial q_\mu} - \sum_\mu \frac{\partial^2 \mathcal{H}}{\partial q_\mu \partial p_\mu} = 0. \quad (6.32)$$

⁵We set up the observables to vanish at the boundary of the x -domain so that there are no surface terms.

Consequently in the Hamiltonian case, Eq. (6.31) reduces to

$$\frac{\partial}{\partial t}\rho(\mathbf{x}, t) + \sum_{\alpha} V_{\alpha}(\mathbf{x}) \frac{\partial}{\partial x_{\alpha}} \rho(\mathbf{x}, t) = 0. \quad (6.33)$$

Equations (6.31) and (6.33) describe the probability for observing something with the coordinate \mathbf{x} moving along with a fluid having a velocity, \mathbf{V} . Equation (6.31) is the more general result. Equation (6.33) describes the particular case in which the fluid is incompressible. The incompressibility condition is that the divergence, given by Eq. (6.32), is zero.

We can write Eq. (6.33) in much more explicit form by writing in the \mathbf{p} 's and \mathbf{r} 's of Hamiltonian mechanics.

$$\frac{\partial}{\partial t}f(\mathbf{p}, \mathbf{r}, t) + \left[\frac{\partial \mathcal{H}(\mathbf{p}, \mathbf{r}, t)}{\partial \mathbf{p}} \cdot \frac{\partial}{\partial \mathbf{r}} - \frac{\partial \mathcal{H}(\mathbf{p}, \mathbf{r}, t)}{\partial \mathbf{r}} \cdot \frac{\partial}{\partial \mathbf{p}} \right] f(\mathbf{p}, \mathbf{r}, t) = 0. \quad (6.34)$$

Here, we have written the equation in terms of $f(\mathbf{p}, \mathbf{r}, t)$ because f is slightly more general than ρ in that it can refer to a situation in which several particles are moving independently of one another. Then f is proportional to the number of particles. For the one particle case, f and ρ are essentially the same since $\rho = f/h^d$, with d being the dimension of the system.

6.5 Equilibrium Solutions

Notice first of all that (6.34) is a linear equation for $f(\mathbf{p}, \mathbf{r}, t)$. Often we can solve, or at least begin-to-solve linear equations. (Nonlinear equations are much harder!) It is a partial differential equation involving derivatives with respect to all the arguments of $f(\mathbf{p}, \mathbf{r}, t)$. The first term in square brackets represents the effect of our particle moving under the influence of the Hamiltonian⁶ \mathcal{H} . This Hamiltonian describes the energy of the particle in question, leaving out the influence of the particle which might bump into it. In our case, we imagine that this Hamiltonian is not arbitrary but is given by a sum of a specified kinetic energy and an unspecified potential energy, $U(\mathbf{r})$. The latter might perhaps be given by an electrostatic or gravitational energy. It might also include forces required to hold the particles in their container.

We are after simple, time-independent, solutions of Eq. (6.34). To find these, we write Eq. (6.28) in the equivalent form

$$\frac{\partial}{\partial t}f = \{\mathcal{H}, f\}. \quad (6.35)$$

⁶In many particle systems, it is often true that the interactions between particle produce an ‘effective Hamiltonian’, H , which depends upon the distribution function $f(\mathbf{p}, \mathbf{r}, t)$. This idea was much developed by Lev Landau and P. W. Anderson. We shall not follow up on this idea now. Anderson’s point of view can be found in ‘Concepts in Solids’, P. W. Anderson, W. A. Benjamin, Inc. (1963). See also L. D. Landau, J. Phys. U.S.S.R. 5, 71 (1941).

We have rewritten the hand side of (6.34) by using a notation which involves the Poisson bracket of \mathcal{H} and f . The Poisson bracket of any pair of functions of \mathbf{p} and \mathbf{r} is defined by

$$\{A, B\} = \frac{\partial A(\mathbf{p}, \mathbf{r})}{\partial r_\mu} \frac{\partial B(\mathbf{p}, \mathbf{r})}{\partial p_\mu} - \frac{\partial B(\mathbf{p}, \mathbf{r})}{\partial r_\mu} \frac{\partial A(\mathbf{p}, \mathbf{r})}{\partial p_\mu}, \quad (6.36)$$

with a summation over $\mu = 1, 2, \dots, d$ understood. Equation (6.35) is a very important result giving the time-dependence of the distribution function for any classical system.

The reader will recall that such brackets play a crucial role in classical mechanics. This bracket is antisymmetrical in its arguments:

$$\{A, B\} = -\{B, A\}. \quad (6.37)$$

In addition because of the nature of the bracket as a derivative, it obeys the chain rule that for any function of the quantity B :

$$\{A, f(B)\} = f'(B)\{A, B\}. \quad (6.38)$$

From Eq. (6.37)

$$\{A, A\} = -\{A, A\} = 0. \quad (6.39)$$

Now we see from Eq. (6.38) that the bracket of A with any function of A vanishes,⁷ specifically:

$$\{A, f(A)\} = 0. \quad (6.40)$$

There are two additional properties of these brackets which we shall not use now, but are important in their general theory. These additional properties are the Jacobi identity

$$\{\{A, B\}, C\} + \{\{C, A\}, B\} + \{\{B, C\}, A\} = 0, \quad (6.41)$$

which holds for any A, B, C depending on \mathbf{p} and \mathbf{q} and the statement that the bracket is a linear function of its arguments, namely that if r and s are constants

$$\{A, sB + tC\} = s\{A, B\} + t\{A, C\}. \quad (6.42)$$

The reader will recall that the general properties (6.37) and (6.39)–(6.42) hold also for the commutators of quantum mechanics.

⁷For a functions of only one variable there is no content to saying that two function $A(x)$ and $B(x)$ are functions of one another. But if A and B depend upon two or more variables, they might or might not be functions of one another. Thus if $A(x, p) = x$ and $B(x, p) = p$, then A and B are not functions of one another. Conversely, if $A(x, p) = xp$ and $B(x, p) = 1 + x^2 p^2$, then $B = 1 + A^2$ so that B is a function of A .

But, let us come back to the specifics of Eq. (6.35). We would like to find a time-independent solution of that equation to compare with the usual result of statistical mechanics, which gives an equilibrium solution of the form $\exp(-\beta\mathcal{H}(\mathbf{p}, \mathbf{r}))$ when \mathcal{H} is independent of time. We are thus looking for

$$f(\mathbf{p}, \mathbf{r}, t) = z^{-1} \exp \left[-\frac{\mathcal{H}(\mathbf{p}, \mathbf{r})}{kT} \right] = z^{-1} \exp \left[-\frac{\mathbf{p}^2}{2mkT} - \frac{U(\mathbf{R})}{kT} \right], \quad (6.43)$$

as a time-independent solution of Eq. (6.35). This solution works. Equation (6.40) shows that the bracket on the left is zero. This is a very interesting result because it shows that our primary conclusion from equilibrium statistical mechanics, Eq. (6.43), can in part be reached via a dynamical argument.

I say ‘in part’ because the solution is not unique. The $\{f, \mathcal{H}\}$ term describes how a quite general Hamiltonian induces a change in f via a change in the coordinates of the particles. When we get to collisions, we shall have to include other terms. In the jargon this $\{f, \mathcal{H}\}$ — part of the equation describes a *conservative* system, with conservative referring to the existence of a time-independent \mathcal{H} . Consider the situation in which $H(p, q)$ — or any other function of \mathbf{p} and \mathbf{q} with no explicit time dependence — is conserved. By this we mean that its total time derivative is zero

$$\frac{d}{dt} \mathcal{H}(\mathbf{p}(t), \mathbf{r}(t)) = \frac{\partial \mathcal{H}}{\partial \mathbf{p}} \frac{d\mathbf{p}}{dt} + \frac{\partial \mathcal{H}}{\partial \mathbf{r}} \frac{d\mathbf{r}}{dt} = 0. \quad (6.44)$$

In that case, *any* f which depends upon H will make the left hand side of Eq. (6.35) vanish. The exponential form shown in Eq. (6.43) is the simplest example of such a function, but there are other examples like H^2 or

$$\frac{1}{\exp[\beta(\mathcal{H} - \mu)] + 1}. \quad (6.45)$$

One can imagine more general situations in which f depends upon additional conserved quantities, N and \mathbf{G} and \mathbf{L} and (Here N might be the number of particles, \mathbf{G} might be the total momentum, \mathbf{L} the angular momentum. There are sometimes other conserved quantities as well.) The arguments about equilibrium we have given still hold. If $f = F(\mathcal{H}, N, \mathbf{G}, \mathbf{L}, \dots)$, this F is a solution to Eq. (6.35). For example if \mathcal{H} is independent of \mathbf{r} , i.e. if the potential $U(\mathbf{r})$ is constant, the momentum, \mathbf{p} , is conserved. Then there is a class of equilibrium solutions of Eq. (6.35) in which

$$f(\mathbf{p}, \mathbf{r}, t) = F(\mathbf{p}), \quad (6.46)$$

for any function, F , of \mathbf{p} . So, on one hand, we reach the very important conclusion that

A conservative system has a equilibrium distribution function which is an almost arbitrary function of all the conserved quantities, subject to only a few constraints like positivity, integrability, and smoothness.

The arguments we have given apply to all conservative systems with time-independent Hamiltonians, and correctly specify equilibrium solutions to all these problems. The statements are also true in quantum mechanics, when the $\mathcal{H}, \mathbf{G} \dots$ are replaced by quantum operators.

On the other hand, we do not think that the Brownian particle has an equilibrium distribution function which is any old function of \mathcal{H} . We have specifically constructed the kicks on the particle so as to produce a Gaussian behavior in \mathbf{p} . The fault in our argument is that we have not included collisions in our equation for the time dependence of the distribution function. As we shall see in the following section, their inclusion will produce a unique equilibrium solution.

6.6 Back to Collisions

To include collisions of our Brownian particle we shall have to take into account the effects of the frictional force (described by the term $-\mathbf{p}/\tau$ in the time derivative of the momentum) and also the random kicks (described by η). When all this is done, we shall have an equation of motion for $f(\mathbf{p}, \mathbf{r}, t)$ which includes both Hamiltonian effects and collision processes. Our equation will look like a generalization of (6.35), namely:

$$\frac{\partial}{\partial t} f + \{\mathcal{H}, f\} = \left. \frac{\delta f}{\delta t} \right|_{\text{collisions}} . \quad (6.47)$$

We define the collision term on the right to be $\delta f/\delta t$, rather than df/dt since this term is not a time derivative of anything. We say right now the value of the collision term on the right hand side of (6.47) as it is produced by our collision model. Then, just below, we follow up by giving its derivation. For the case in which the collisions consist of many random kicks, the collision term takes the form:

$$\left. \frac{\delta f(\mathbf{p}, \mathbf{r}, t)}{\delta t} \right|_{\text{collisions}} = \nabla_{\mathbf{p}} \cdot \left\{ \left[\frac{M}{\beta\tau} \nabla_{\mathbf{p}} + \frac{\mathbf{p}}{\tau} \right] f(\mathbf{p}, \mathbf{r}, t) \right\} . \quad (6.48)$$

The combination of (6.47) and (6.48) is called the *Fokker–Planck equation*. The collision term has two kinds of physics in it. The first term in the square bracket represents a process in which momentum changes its value little by little so there is diffusion in momentum space. This process is mathematically identical to the coordinate space diffusion we have already described. The only difference is that ordinary diffusion is described by a time derivative being equal to a spatial Laplacian, while here we have a Laplacian in \mathbf{p} . We recognize the other term, the one with \mathbf{p}/τ as being descriptive of a process in which particles with nonzero momentum are having a relaxation process carrying the momentum back to the value of zero. This relaxation also occurs because of collisions with the fluid background. These collisions tend to slow down rapid particles.

To derive Eq. (6.48) we go back to the derivation of Eq. (6.31) via Eq. (6.30). We can recognize that what we need is a contribution for the change in the value of the observable

$O(\mathbf{p}, \mathbf{r})$ produced by the collision-induced change in \mathbf{p} . Imagine that we look at changes over the small interval δt . In this interval, the collision have changed \mathbf{p} by the amount

$$\delta\mathbf{p} = -\mathbf{p}\frac{\delta t}{\tau} + I; \quad I = \int_t^{t+\delta t} ds \eta(s). \quad (6.49)$$

As a result the observable has changed by an amount:

$$\delta\langle O \rangle(t) = \int d\gamma \delta t O(\mathbf{p}, \mathbf{r}) \frac{df(\mathbf{p}, \mathbf{r}, t)}{dt} \Big|_{\text{collisions}} \quad (6.50)$$

where $d\gamma$ is an integral over the one-particle phase space, defined in Eq. (2.27). This form of the rate of change describes how the collision terms works to change $\langle O \rangle$. To actually find the rate of change, notice that collisions directly change the momentum as in Eq. (6.49). Thus the change in the observable is equivalently given by

$$\begin{aligned} \delta\langle O \rangle(t) &= \left\langle \int d\gamma [O(\mathbf{p} + \delta\mathbf{p}, \mathbf{r}) - O(\mathbf{p}, \mathbf{r})] \right\rangle \\ &= \int d\gamma \left[\left\langle O \left(\left(1 - \frac{\delta t}{\tau}\right) \mathbf{p} + I, \mathbf{r} \right) \right\rangle - O(\mathbf{p}, \mathbf{r}) \right] f(\mathbf{p}, \mathbf{r}, t). \end{aligned} \quad (6.51)$$

Notice the $\langle \rangle$, which stands for an average over the different realizations of the random forcing. In Eq. (6.51) we have to average over the random variable. Most of that averaging is included in $f(\mathbf{p}, \mathbf{r}, t)$. In fact that probability function includes averages over $\eta(s)$ for all s less than t . The remaining average is for the $\eta(s)$ included in I , that is the randomness for s in the period between t and $t + \delta t$. It is that averaging which is advertised by the brackets, $\langle \rangle$.

The $\mathbf{p}\delta t/\tau$ term does not care about the averaging and gives a contribution to the rate of change in the observable which is

$$\int d\gamma \left[-\frac{\mathbf{p}}{\tau} \cdot \nabla_{\mathbf{p}} O(\mathbf{p}, \mathbf{r}) \right] f(\mathbf{p}, \mathbf{r}, t) = \int d\gamma O(\mathbf{p}, \mathbf{r}) \nabla_{\mathbf{p}} \cdot \left[\frac{\mathbf{p}}{\tau} f(\mathbf{p}, \mathbf{r}, t) \right].$$

To get the contribution to the time derivative, we look once more for the coefficient of $O(\mathbf{p}, \mathbf{r})$. In this way, we derive the second term in the square brackets on the right hand side of Eq. (6.48). There is nothing new here, we have just retraced the argument which led to Eq. (6.31) for the specific term $-\mathbf{p}/\tau$.

The remaining term comes from the random force in Eq. (6.51). This term requires a slightly new argument. We put the \mathbf{p} into an exponent via a process of Fourier transformation. The exponentiation is done by writing:

$$O(\mathbf{p}, \mathbf{r}) = \int d\mathbf{q} e^{i\mathbf{q} \cdot \mathbf{p}} \tilde{O}(\mathbf{q}, \mathbf{r})$$

and then look at the contribution of the I to the rate of change of $\langle O \rangle$ in Eq. (6.51). This contribution is

$$\lim_{\delta t \rightarrow 0} \int d\gamma \int d\mathbf{q} e^{i\mathbf{q} \cdot \mathbf{p}} \tilde{O}(\mathbf{q}, \mathbf{r}) \frac{\langle e^{i\mathbf{q} \cdot I} \rangle - 1}{\delta \tau} f(\mathbf{p}, \mathbf{r}, t). \quad (6.52)$$

Since the average is a Gaussian one, we know how to calculate it and we have already done so in Eq. (6.7b), which says

$$\langle e^{i\mathbf{q} \cdot \mathbf{I}} \rangle = e^{-\Gamma \delta t q^2 / 2}.$$

An expansion to first order in δt now converts expression (6.52) into the form

$$\int d\gamma \int d\mathbf{q} e^{i\mathbf{q} \cdot \mathbf{p}} \tilde{O}(\mathbf{q}, \mathbf{r}) (-\Gamma q^2 / 2) f(\mathbf{p}, \mathbf{r}, t).$$

In the further evaluation of this function q^2 is replaced by $-\nabla_p^2$ acting upon $\exp(i\mathbf{q} \cdot \mathbf{p})$, which is then converted, via an integration by parts, into derivatives acting on f . The final result is the expressions (6.52) has the value

$$\int d\gamma O(\mathbf{p}, \mathbf{r}) \frac{\Gamma}{2} \nabla_p^2 f(\mathbf{p}, \mathbf{r}, t). \quad (6.53)$$

The coefficient of $O(\mathbf{p}, \mathbf{r})$ in Eq. (6.53) may be recognized as the diffusion term within the square brackets of Eq. (6.48). When we put in the value of Γ given by Eq. (6.15), we finally derive the full equation of motion for the Brownian motion model, as given by Eqs. (6.47) and (6.48).

6.7 From Fokker–Planck to Equilibrium

Equations (6.47) and (6.48) are the outcome of a long and rather hard calculation. We should spend some effort to understand them. We have already seen that, in the absence of the collision terms, the equilibrium solution to Eq. (6.47) would have $f(\mathbf{p}, \mathbf{r}, t)$ be any function, say F of the Hamiltonian $\mathcal{H} = \mathbf{p}^2/(2M) + U(\mathbf{r})$. Any $F(\mathcal{H}(\mathbf{p}, \mathbf{r}))$ will make the left hand side of (6.47) be zero. But this equation also has a right hand side. This side describes the exchange of energy with an ‘outside world’ of gas atoms or molecules. This outside world is considered to be weakly coupled to our ‘inside world’, the single particle. As a result of our rather specific picture of how the energy exchange occurs, we have reached a specific form of this exchange term. If we substitute just any function of $\mathbf{p}^2/(2m)$ into that right hand side it will not be zero. For example say we substitute into Eq. (6.48) the expression

$$f(\mathbf{p}) = z^{-1} \exp \left[-b \left(\frac{\mathbf{p}^2}{2M} + U(\mathbf{r}) \right) \right],$$

with b not necessarily equal to β . Then the left hand side vanishes but the collision term becomes

$$\frac{\delta f(\mathbf{p}, \mathbf{r}, t)}{\delta t} \Big|_{\text{collisions}} = \nabla_{\mathbf{p}} \cdot \left\{ \left[\frac{M}{\beta \tau} \nabla_{\mathbf{p}} + \frac{\mathbf{p}}{\tau} \right] f(\mathbf{p}, \mathbf{r}, t) \right\} = -\nabla_{\mathbf{p}} \cdot \left[\left(\frac{b}{\beta} - 1 \right) \cdot \frac{\mathbf{p}}{\tau} f(\mathbf{p}, \mathbf{r}, t) \right].$$

This expression is certainly not zero unless the inverse temperature of our particle, b , is equal to the inverse temperature (β) of the sea of particles kicking at it. So here we see the collision term forcing the system to the right equilibrium. There is a way of writing the

collision term which shows quite immediately the form of the equilibrium solution. Just write the collision term as

$$\begin{aligned} \left. \frac{\delta f(\mathbf{p}, \mathbf{r}, t)}{\delta t} \right|_{\text{collisions}} &= \frac{M}{\beta\tau} \nabla_{\mathbf{p}} \cdot \{ e^{-\beta\mathcal{H}} \nabla_{\mathbf{p}} [e^{\beta\mathcal{H}} f(\mathbf{p}, \mathbf{r}, t)] \} \\ &= \frac{M}{\beta\tau} \nabla_{\mathbf{p}} \cdot [\nabla_{\mathbf{p}} + \beta \nabla_{\mathbf{p}} \mathcal{H}] f(\mathbf{p}, \mathbf{r}, t). \end{aligned} \quad (6.54)$$

In this form of writing a glance shows that $f \sim \exp(-\beta\mathcal{H})$ makes the collision term vanish. Thus the correct equilibrium solution can be obtained directly from the Fokker–Planck equation (6.47) and (6.48).

This conclusion can be stated in terms which apply to a whole host of similar calculations:

Let a given system not be conservative, but is instead be weakly coupled to some ‘outside world’, which is in statistical equilibrium. Assume that there are some quantities conserved within the system itself. But our given system transfers the conserved quantities up and back to the ‘outside world’ via the weak coupling. In that case, if the given system is left undisturbed it eventually relaxes to a situation described by a probability distribution function which depends upon the conserved quantities, but in a very special fashion. The distribution function is an exponential function of all the exchanged extensive conserved quantities, i.e.

$$\rho = \text{const.} \times \exp[-\beta\mathcal{H} - \alpha N + \beta \mathbf{v} \cdot \mathbf{G}]. \quad (6.55)$$

Here, β , α and $\beta \mathbf{v}$ are constants which describe the relative willingness of the system to give up energy, particles, and momentum to the outside world.

Thus the extensive conserved quantities play a crucial role in the formulation of statistical mechanics. The logarithm of the probability is proportional to a linear combination of these extensive quantities. We have to specify that they be the extensive ones since if \mathcal{H} is conserved so is \mathcal{H}^2 , but it is \mathcal{H} that appears in (6.55). There are other, non-extensive conserved variables. But, they usually vary in a wildly discontinuous fashion from one point in the phase space to the next. They are left out in this formulation of statistical mechanics. As we go along, we shall have to be more specific about the conserved quantities so that we can define the theory more precisely.

Notice that something wonderful has happened. We have seen a plausible dynamical argument which gives the equilibrium form of distribution functions and have constructed the argument so that it might apply to many different systems. In short, we have outlined a program of calculation which would take one from dynamics to equilibrium statistical mechanics.

6.8 Properties of Fokker–Planck Equation

There is considerably more to be said about the Fokker–Planck equation. First of all, notice that it agrees with the conservation laws for the total number of particles and the total probability of finding a particle in the system. In one sense, it must agree with that since all the processes which we took into account conserve particle number. But it does make sense to follow it all through and see the consequences of particle conservation. The total particle number is

$$N = \int \frac{d\mathbf{r} d\mathbf{p}}{h^d} f(\mathbf{p}, \mathbf{r}, t) \quad (6.56)$$

and the total probability is

$$1 = \int d\mathbf{r} d\mathbf{p} \rho(\mathbf{p}, \mathbf{r}, t).$$

As we know, the conservation law can be stated in differential form as

$$\frac{\partial}{\partial t} \rho(\mathbf{r}, t) + \nabla \cdot \mathbf{j}(\mathbf{r}, t) = 0, \quad (6.57)$$

where the particle density and current are respectively:

$$\rho(\mathbf{r}, t) = \int \frac{d\mathbf{p}}{h^3} f(\mathbf{p}, \mathbf{r}, t), \quad \mathbf{j}(\mathbf{r}, t) = \int \frac{d\mathbf{p}}{h^3} f(\mathbf{p}, \mathbf{r}, t) \nabla_p \mathcal{H}. \quad (6.58)$$

The second expression has not been given in this set of lectures before. It says that the current of particles is the sum over all momentum of a number per unit interval of momentum, $d\mathbf{p} h^{-3} f$, times the velocity of each such particle. And according to Hamiltonian mechanics, that velocity is $\nabla_p \mathcal{H}(\mathbf{p}, \mathbf{r}, t)$ which \mathcal{H} is an effective Hamiltonian or energy which describes the single particle motion. Equation (6.58) can be derived by integrating Eq. (6.47) over all \mathbf{p} . After an integration by parts the left hand side turns into the left hand side of Eq. (6.57). Because the collision term is a perfect derivative, its momentum integral vanishes and out comes Eq. (6.57).

By the same logic as we call $\mathbf{j}(\mathbf{r}, t)$ a particle current we can write the entire Fokker–Planck equation as a conservation law in momentum. Notice that one can put Eqs. (6.47) and (6.48) together in the form

$$\frac{\partial}{\partial t} f + \{\mathcal{H}, f\} + \nabla_{\mathbf{p}} \cdot \mathbf{J}(\mathbf{p}, \mathbf{r}, t) = 0. \quad (6.59)$$

Here $\mathbf{J}(\mathbf{p}, \mathbf{r}, t)$ represents a current which carries particles up and down through momentum space in the system. That is $\mathbf{J}(\mathbf{p}, \mathbf{r}, t)$ represents the density of matter or probability carried per unit interval of time in this system. It has the value

$$\mathbf{J}(\mathbf{p}, \mathbf{r}, t) = -\frac{M}{\beta\tau} [\nabla_{\mathbf{p}} f(\mathbf{p}, \mathbf{r}, t) + f(\mathbf{p}, \mathbf{r}, t) \nabla_{\mathbf{p}} \beta \mathcal{H}(\mathbf{p}, \mathbf{r}, t)]. \quad (6.60)$$

The vanishing of this current will ensure that this system is in equilibrium.

So far we have been considering a dilute gas of particles. The particles represented by the distribution function $f(\mathbf{p}, \mathbf{r}, t)$ are dilute enough so that we have to worry about neither the interaction between the particles nor the possible effects of the quantum statistics they obey. Now let us consider these particles to be non-interaction but identical. For the moment let them obey fermi statistics. We know that in a fermion system it is impossible for any two particles to be in the same quantum state. But $f(\mathbf{p}, \mathbf{r}, t)$ represents the number of particles which sit in the state defined by its approximate momentum \mathbf{p} and its approximate position \mathbf{r} . Therefore, when the particles scatter as in the last term in (6.60) the scattering must be proportional to the density of scattering particles $f(\mathbf{p}, \mathbf{r}, t)$ and also the density of final states available for them, $[1 - f(\mathbf{p}', \mathbf{r}', t)]$. Here \mathbf{p}' is the final momentum of the particles and \mathbf{r}' their final position. Since the particles do not change either their momentum or their position much in the scattering, \mathbf{p}' and \mathbf{r}' may be replaced by \mathbf{p} and \mathbf{r} and this term becomes:

$$-\frac{M}{\beta\tau}\{[1 - f(\mathbf{p}, \mathbf{r}, t)]f(\mathbf{p}, \mathbf{r}, t)\nabla_{\mathbf{p}}\beta\mathcal{H}(\mathbf{p}, \mathbf{r}, t)\}. \quad (6.61a)$$

For bosons, according to Einstein (again 1905), scattering processes are enhanced if there are already particles in the final state. The scattering rate as the particles are slowed by moving through the fluid is, for this case:

$$-\frac{M}{\beta\tau}\{[1 + f(\mathbf{p}, \mathbf{r}, t)]f(\mathbf{p}, \mathbf{r}, t)\nabla_{\mathbf{p}}\beta\mathcal{H}(\mathbf{p}, \mathbf{r}, t)\}. \quad (6.61b)$$

In general, we write formulas like this by using an upper sign for bosons and a lower one for fermions, so that the answer for both cases together is

$$-\frac{M}{\beta\tau}\{[1 \pm f(\mathbf{p}, \mathbf{r}, t)]f(\mathbf{p}, \mathbf{r}, t)\nabla_{\mathbf{p}}\beta\mathcal{H}(\mathbf{p}, \mathbf{r}, t)\}. \quad (6.61c)$$

Thus, if we modify the process of frictional slowdown in Eq. (6.60) in the form of (6.61c) we find that the collision term in the Fokker–Planck equation now involves the current in momentum

$$\mathbf{J}(\mathbf{p}, \mathbf{r}, t) = -\frac{M}{\beta\tau}\{\nabla_{\mathbf{p}}f(\mathbf{p}, \mathbf{r}, t) + \{[1 \pm f(\mathbf{p}, \mathbf{r}, t)]f(\mathbf{p}, \mathbf{r}, t)\nabla_{\mathbf{p}}\beta\mathcal{H}(\mathbf{p}, \mathbf{r}, t)\}\}. \quad (6.62)$$

It is no harder to argue about the effect of statistics on the first term in Eq. (6.62). In fact, the statistics do not change the result at all, at least in our model. Think about fermions. Let the random force take a particle from a momentum \mathbf{p} to a new momentum \mathbf{p}' . In this model all the particles undergo exactly the same momentum changes. That being so, as ‘our’ particle is lifted into a state with momentum \mathbf{p}' , at the same time, any other particle which might be in that state moves off to another momentum state. Thus the process gets around the exclusion principle. As a result, Eq. (6.62) is the full answer for the current in momentum.

As we have notice, a sufficient condition for equilibrium is that \mathcal{H} is independent of time, that $f(\mathbf{p}, \mathbf{r}, t)$ depends only upon $\mathcal{H}(\mathbf{p}, \mathbf{r})$, and that the current (6.62) vanishes. So let

us assume that $f(\mathbf{p}, \mathbf{r}, t) = F(\mathcal{H}(\mathbf{p}, \mathbf{r}))$, and see what might be the condition for vanishes of \mathbf{J} . From (6.62)

$$\mathbf{J}(\mathbf{p}, \mathbf{r}, t) = -\frac{M}{\beta\tau} [\nabla_{\mathbf{p}} \mathcal{H}(\mathbf{p}, \mathbf{r})] \left\{ \frac{d}{d\mathcal{H}} F(\mathcal{H}) + \beta[1 \pm F(\mathcal{H})]F(\mathcal{H}) \right\}.$$

The condition for vanishing \mathbf{J} is that

$$\frac{d}{d\mathcal{H}} F(\mathcal{H}) + \beta[1 \pm F(\mathcal{H})]F(\mathcal{H}) = 0.$$

Divide by F^2 and find:

$$\frac{d}{d\mathcal{H}} F^{-1} = \beta[F^{-1} \pm 1].$$

which can be solved at once to find that the distribution function has the value:

$$f(\mathbf{p}, \mathbf{r}, t) = \frac{1}{\exp(\beta\mathcal{H} - \beta\mu) \mp 1}. \quad (6.63)$$

Equation (6.63) is the correct expression for the equilibrium distribution function of a non-interacting but degenerate gas of particles. This expression involves one new parameter, μ , which is called the chemical potential.

Homework

Problem 6.1 (Deriving Position Correlation Function). Do the two definite integrals of Eq. (6.17) to obtain Eq. (6.18).

Problem 6.2 (Equal Time Correlations). Prove our statement that ‘At equal times the correlation of a position, $\mathbf{r}(t)$, and a momentum, $\mathbf{p}(t)$, vanish’. by using classical statistical mechanics and the usual Hamiltonian (6.24).

Problem 6.3 (Time Correlation Functions). Calculate the correlation between $\mathbf{p}(t)$ and $\mathbf{r}(t')$ in Brownian motion. Assume that the Brownian particle has been in motion for a long time so that everything has settled down to its long-time behavior.

Problem 6.4. Calculate the time dependence of the $\langle \mathcal{H} \rangle$ for a situation in which a Brownian particle moves through a gas which abruptly changes its temperature from T_0 to T_1 at the time $t = 0$. Assume that \mathcal{H} contains only a kinetic energy term. Before this change occurs, assume that the Brownian particle has been in motion for a long time in a gas at temperature T_0 so that everything has settled down to its long-time behavior.

Problem 6.5. Discuss the form of the Brownian motion formulas appropriate for the case in which the particle in motion is relativistic.

Problem 6.6 (Rederive Collision Term). Equation (6.48) was derived by a Fourier transform technique. Rederive this same result by using an expansion in I . What happens if the random variables are not Gaussian?

6.9 Reprints on Organization

Recently people have wondered how the behavior of dynamical system, working out their simple dynamical laws, can give rise to complexity. This thinking has led to two ‘big ideas’.⁸ The first is that instead of being stable or unstable a dynamical system would tend to push itself toward a place where it was just on the edge of stability. It would then hang there. This idea, called the marginal stability hypothesis appeared in the first reprint below⁹ and also in the parallel publication.¹⁰ Both papers cover somewhat the same territory, but because the latter has a technical solid state perspective, I omit it from this book. It is, however, interesting to notice how statistical physics draws ideas from the other parts of physics.

Next, Per Bak, Chao Tang, and Kurt Wiesenfeld¹¹ suggested that there were important analogies between the marginal stability reached at the critical point of a phase transition¹² and the complex self-organized features which arise from the marginal stability of a dynamical system. They called this point of view SOC for ‘self-organized criticality’.

But, SOC was a suggestion, not a fact. The inventors suggested that it would be found in the piling up of sand poured slowly onto a heap. Would that work out? I include two recent papers asking that question. In one¹³ theoretical analysis of a sandpile model clearly supports the SOC hypothesis. In the other experiments¹⁴ on granular materials show that landslide ruin the delicate marginal behavior demanded by the theory. So the final word has yet to be said.

It is very likely that some system will indeed show SOC. It may be true that even granular materials do so.¹⁵ But we still do not know how robust that behavior will be. And we certainly do not know if SOC is closely connected with the mechanisms by which nature produces complexity.

⁸For a historical treatment see P. Bak, *How Nature Works*, Copernicus, New York, 1996.

⁹Chao Tang, Kurt Wiesenfeld, Per Bak, Susan Coppersmith and Peter Littlewood, ‘Phase Organization’, Phys. Rev. Lett. 58, pp. 1161–1164 (1987).

¹⁰S. N. Coppersmith and P. B. Littlewood, ‘Pulse Duration Memory Effects and Deformable Charge-Density Waves’, Phys. Rev. B 36, pp. 311–317 (1987).

¹¹Per Bak, Chao Tang and Kurt Wiesenfeld, ‘Self-Organized Criticality, An Explanation of 1/f Noise’, Phys. Rev. Lett. 59, pp. 381–384 (1987).

¹²See Chapters 10 and below.

¹³J. M. Carlson, J. T. Chayes, E. R. Grannan and G. H. Swindle, *Self-Organized Criticality and Singular Diffusion*, Phys. Rev. Lett. 65 pp. 2547–2550 (1990).

¹⁴H. M. Jaeger, Chu-heng Liu and Sidney R. Nagel, ‘Relaxation at the Angle of Repose’, Phys. Rev. Lett. 62 pp. 40–43 (1989).

¹⁵K. Frette, et al., *Nature* 379, 49 (1996).

6.9.1 Chao Tang *et al.*: Phase Organization

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Phase Organization

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We describe the selection mechanism for novel pattern formation in a driven chain of nonlinear oscillators. Phase organization arises as a consequence of dynamical selection of minimally stable states.

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Understanding the behavior of complex (many-degrees-of-freedom) systems continues to present a great challenge to physicists. The standard statistical mechanics is a powerful theory for equilibrium and uniform systems; however, for nonequilibrium systems possessing spatio-temporal structure there is no general theory — indeed, it is not even clear what quantities might characterize the physics of such systems. Recently a large step has been taken towards the understanding of these complex systems, in large part because of the study of simple low-dimensionality discrete dynamical equations. It is now realized that (1) simple nonlinear maps can have very rich time series and very complex structures can be produced from very simple algorithms; (2) there exist universality classes, such that very different systems possess identical scaling properties. The hope is that the study of these simple deterministic models can help us pose and answer more general questions in complex systems; this approach is in some sense the obverse of the statistical point of view.

To date, significant progress has been made in understanding complex systems whose behavior can be captured by few “effective degrees of freedom” (EDF)¹; in contrast, very little is known in general about high-EDF

behavior. Systems where few-EDF models appear inadequate include spin-glasses, arrays of coupled maps,² spatio-temporal chemical oscillators,³ neural networks,⁴ large-aspect-ratio fluid convention,⁵ and a video feedback system.⁶ In this Letter, we study a high-EDF system displaying complex dynamics and interesting organizing behavior. In contrast with these other complex systems, ours is simple enough to completely characterize theoretically. Our hope is that this will stimulate progress toward a general characterization of high-EDF behavior.

The model consists of an array of N balls of mass m , each connected to its neighbors by springs with force constant K . The array is subject to a sinusoidal potential and driven by a time-periodic square-wave force $E(t)$. The equation of motion is

$$m\ddot{y}_j = -\gamma\dot{y}_j + K(y_{j+1} - 2y_j + y_{j-1}) - A \sin(2\pi y_j) + E, \quad j = 1, 2, \dots, N, \quad (1)$$

where y_j is the position of the j th ball, γ is the damping constant, and A the amplitude of the potential. In the static case ($m = \gamma = E = 0$), Eq. (1) is the Frenkel-Kontorova model which has been studied extensively.⁷

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Of particular interest for our purpose is that the Frenkel-Kontorova model has a very large number ($\sim e^N$) of stable configurations—in our problem there is a similarly large number of stable time-periodic stationary states and a hierarchy of metastable states.

What is a phase-organized state? It is a time-periodic state with the property shown in Fig. 1: A snapshot at an instant just before the pulse is turned off shows the majority of balls sitting at maxima of the periodic potential. The phase of ϕ of a ball is its distance from the nearest-potential minimum; a configuration is *phase organized* when $\phi = \frac{1}{2}$ for most of the balls at the falling edge of a pulse. Remarkably, in the appropriate parameter regime (weak springs and large damping), simulations reveal that the phase-organized states are always reached for sufficiently random initial conditions even though these states are measure zero (as N goes to infinity) with respect to the total number of stable states. This phenomenon was first discovered in the context of the pulse-duration memory effect in charge-density waves,⁸ where experiments show a macroscopic manifestation of this microscopic organization. We will return to this point briefly later on.

Our goal is to understand the selection mechanism leading to phase organization. We accomplish this by writing down a “Poincaré map” for Eq. (1). By studying the set of fixed points we recognize a “topological” selection for *marginally stable* states and identify the subset of *minimally stable* states as the phase-organized states. The dynamics then selects for these latter states, and reveals the existence of a hierarchy of metastable, “almost” phase-organized configurations.

In the limit of strong damping, weak coupling, and high field ($\gamma \gg m, E > A \gg K$), we approximate Eq. (1) by the mapping⁹

$$\begin{aligned} z_j(n) &= y_j(n) + k[y_{j+1}(n) - 2y_j(n) + y_{j-1}(n)] + F \\ &\equiv y_j(n) + k\mathcal{D}y_j(n) + F, \end{aligned} \quad (2a)$$

$$y_j(n+1) = \text{nint}[z_j(n)], \quad (2b)$$

where $y_j(n)$ and $z_j(n)$ are the positions of the j th ball just before the n th pulse is turned on and off, respectively, and $\text{nint}(x) = \text{int}(x + 0.5)$ is the nearest integer of x . The parameters k and F are the effective nearest-neighbor coupling and external force, respectively, and are related to the parameters in Eq. (1).⁹ Equation (2b)

says that when the pulse is off each ball falls directly into its nearest potential minimum, while Eq. (2a) says that during the pulse the balls are depinned from their minima and their motion is determined by the pulse force F and the nearest-neighbor elastic interaction leading in general to a net drift current. That Eq. (2) captures the essential physics of Eq. (1) is supported by extensive numerical simulations of both the iterative map and the ordinary differential equations; a derivation of a closely related map for $m=0$ is possible within the context of perturbation theory.¹⁰ The chief effect of the approximation leading to Eq. (2) is that simulations of the mapping typically lead to more perfect phase organization than do the corresponding ordinary differential equations. In what follows, we focus on the iterative map since its dynamical properties can be completely characterized by analytic means.

Without loss of generality, we take F to be an integer and rewrite Eq. (2) as

$$y_j(n+1) = y_j(n) + F + \text{nint}[k\mathcal{D}y_j(n)]. \quad (3)$$

Applying the operator \mathcal{D} to both sides and denoting the “curvature” $\mathcal{D}y_j(n)$ as $C_j(n)$ yields

$$C_j(n+1) = C_j(n) + \mathcal{D}\text{nint}[kC_j(n)]. \quad (4)$$

Equation (4) is a nonlinear diffusion equation on the *lattice* phase space Z^N . In contrast with linear diffusion, the competition between diffusion (pulse on) and local relaxation (pulse off) allows the chain to stably maintain nonzero curvature configurations. The fixed-point condition $C_j(n+1) = C_j(n)$ implies

$$\text{nint}[kC_j(n)] = m + l, \quad j = 1, 2, \dots, N, \quad (5)$$

where m and l are integers. For periodic or free boundary conditions, only $m = l = 0$ is allowed, so that the set of fixed-point solutions is given by

$$-1/2k \leq C_j < 1/2k, \quad j = 1, 2, \dots, N. \quad (6)$$

Since k is small, this defines a large (compact) hypercube in $\{C_j\}$ space. Any point in or on this cube is an allowed solution¹¹ and represents a stable time-periodic solution of Eq. (1); it can be proven that there are no attractors outside this cube. The origin is located at the center of the cube and is the most stable configuration, in that it requires the largest (finite) perturbation to violate



FIG. 1. Snapshot of a phase-organized solution of Eq. (1) just before the field is switched off, showing the positions of the balls relative to the sinusoidal potential; $N=55, m=1, \gamma=100, K=1, A=100, E=305, T_{\text{on}}=5, T_{\text{off}}=2$, free boundary conditions. Only an eight-ball portion of the chain is shown.

Eq. (6). Points on the surface of the cube are "marginally stable" (this is a slight misuse of terminology) since at least one of the C_j 's only barely satisfies Eq. (6), i.e., $C_j = \pm \text{int}[1/(2k)]$, while points at the corners of the cube are also *minimally stable* since every C_j barely satisfies Eq. (6).

Thus, based only on the topology of the solution set, we see that the marginally stable states are preferred. Starting with any initial condition outside the cube, the diffusive nature of Eq. (4) drives trajectories toward the origin, until it hits the cube where it "sticks." One expects that trajectories will hit the surface states with roughly uniform probability, but this is not the case. Rather, the dynamics funnels trajectories toward the corners: If one starts with initial conditions sufficiently far from the cube, the system will arrive at a corner state with probability 1. To understand this selection, one must probe beyond this topological picture, and look at the dynamics outside the cube.

Not only are the corner states minimally stable, but they also correspond to states having perfect phase organization. This follows from Eqs. (2) and (6): One sees immediately that these solutions correspond to $z_j = \frac{1}{2} \pmod{1}$ for all j . Thus, each time the pulse is switched off, all the balls are sitting on the tops of the potential! Before giving an explanation for this selection of corner solutions, we note that there is a hierarchy of "almost" fixed points wherein only a tiny fraction of the C_j 's change each iteration of Eq. (4). These metastable configurations consist of local domains (subchains) which satisfy Eq. (5) with nonzero m and l , with different domains having different values of m and l . If we consider only the lower-dimensionality phase space for a subchain, the set of possible metastable configurations defines a nested sequence of hypercubes indexed by m . Again, the corners of these nested hypercubes are dynamically preferred.

We now explain the dynamical mechanism underlying the selection of the corner states. Imagine a plot of C_j vs j after each time iteration n (see Fig. 2). Then the stable (metastable) corner states correspond to each C_j being one of the values $\pm 1/2k$ [$\pm (2m+1)/2k$]. Consider a very random initial configuration of C_j 's, say C_j distributed uniformly between $-c$ and $+c$ where $c \gg 1/k$. Then for times less than $O(1/k)$, Eq. (4) acts essentially like ordinary diffusion with diffusion constant k , and the shortest wavelength spatial components die out so that neighboring C_j 's are likely to have values within $\sim 1/k$ of each other—in fact, it is natural to break the $j-C_j$ plane into horizontal strips such that $2m-1 < 2kC_j < 2m+1$ for each integer m . At this point, the nonlinear function nint in Eq. (4) comes to play an important role, driving each C_j toward the *borders* of these horizontal strips. To see this, suppose that C_{j-1} and C_j are the m th strip with C_{j+1} in the $(m-1)$ th. Then $\text{nint}(kC_j) = -1$ and C_j will move

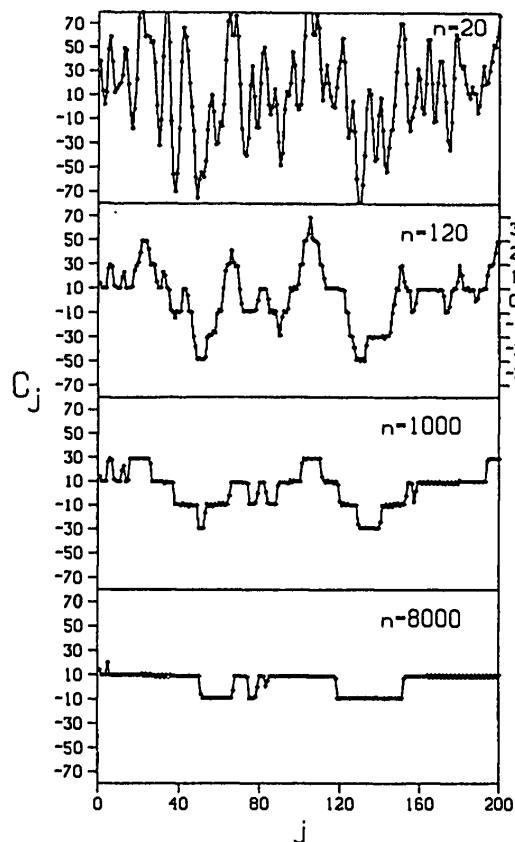


FIG. 2. Curvature C_j of a chain of 200 masses at four times, as Eq. (4) evolves toward a phase-organized state, with $k = 0.05$ and free boundary conditions. From a random initial condition the system quickly evolves toward a metastable state, then slowly relaxes toward a stable corner state. Integers on the right denote the strip index m , as described in the text.

down one unit. As long as its neighbors remain in their strips, C_j will continue to move downward until it just enters the $(m-1)$ th strip. But now $\text{nint}(kC_j) = +1$, and C_j will move upward one unit, again crossing the border, then down, then up, etc.; so, once C_j reaches the border of a strip, it stays there. By the same argument one easily shows that if C_{j-1} , C_j , and C_{j+1} lie within two neighboring strips, C_j will move to the border of the two strips and stay there. Finally, if the triple are all in the same strip, or in three consecutive strips, C_j will not move. Consequently, there is a tendency for the C_j 's to cluster about the border lines of the strips. This is illustrated by the time series shown in Fig. 2. Note that any of these border lines corresponds to phase-organized behavior, though the system has not reached a *bona fide* stable configuration at this stage.

The time scale for this clustering process is $\sim 1/k$ since the width of the strips is $1/k$. After this clustering, the system only very slowly relaxes to one of the stable

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corner states, since only the edges of a cluster can have significant change under Eq. (4). This slow "leaking" process towards a stable state takes a time $O(N/k)$.

We now discuss some ramifications of the picture developed above.

First, the fact that the dynamics selects configurations of minimal stability has significant implications for the statistical mechanics of this system. The usual approach would be to seek some global free energy, e.g., the total elastic energy of the chain, and assume a probability density that peaks at the energy minimum. In fact, precisely the *opposite* situation applies here: The most stable (minimum-energy) configuration is the state *least* likely to be observed; the minimally stable (maximum-energy) configurations should be most heavily weighted.

Next, we can extend our analysis to include the effect of quenched randomness modeled by the addition of random constants α_j to Eq. (2a). In fact, it was simulations on this random system that first detected the phenomenon of phase organization.⁹ This complication is nonessential to the problem since the rigid translation

$$y_j \rightarrow y_j - \beta_j, \quad z_j \rightarrow z_j - \beta_j,$$

where

$$k \mathcal{D}\beta_j = \alpha_j$$

eliminates the α_j . (This is analogous to the nonessential nature of randomness in the 1D spin-glass problem.¹²) The corner states still are selected, and are phase organized. In effect, the α_j 's change the potential from sinusoidal to irregular, but the selected states are still those where the balls sit at potential maxima at the instant the pulse is turned off.

Finally, we revisit the original realization of this model, namely the pulse-duration memory effect in charge-density waves (CDW's). A discussion of the relevance of Eqs. (1) and (2) to CDW's appears in Ref. 9. Recall that periodic voltage pulses cause the CDW to "learn" the length of the pulse. For a "dirty" CDW, the pulses bring the system to some metastable state, so that changing the pulse duration (i.e., changing k in our model) causes the CDW to "relearn" since the structure of the metastable state space has changed. This relearning process has been observed experimentally. However, for a clean enough CDW we can expect a different behavior,

since the training pulses may bring the CDW directly to one of the stable corner states. Then, decreasing k (i.e., shortening the pulse) simply expands the stable hypercube, so that the system is already in a stable configuration and no relearning will occur, though increasing k instead will give the familiar effect.

In conclusion, we have studied a periodically pulsed, weakly coupled dissipative many-body system. This high-EDF system displays spontaneous self-organization with a selection mechanism which can be fully characterized. This collective behavior is not due to a long-range correlation (like that in second-order phase transitions), but rather due to a very local dynamical rule; we expect this rule to play a role in a wide class of complex dynamical systems.

We thank Vic Emery and Laszlo Mihaly for useful discussions. This work was supported by the Division of Materials Sciences, U.S. Department of Energy, under Contract No. DE-AC02-76CH00016.

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¹¹For periodic boundary conditions on y_j , there is an extra constraint on Eq. (6), i.e., $\sum_j C_j = 0$. Thus, the allowed solutions are the intersection of the hypercube with this hyperplane; however, this constraint does not change the general picture for large N .

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6.9.2 Bak *et al.*: Self-Organized Criticality

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Self-Organized Criticality: An Explanation of $1/f$ Noise

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We show that dynamical systems with spatial degrees of freedom naturally evolve into a self-organized critical point. Flicker noise, or $1/f$ noise, can be identified with the dynamics of the critical state. This picture also yields insight into the origin of fractal objects.

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One of the classic problems in physics is the existence of the ubiquitous " $1/f$ " noise which has been detected for transport in systems as diverse as resistors, the hour glass, the flow of the river Nile, and the luminosity of stars.¹ The low-frequency power spectra of such systems display a power-law behavior $f^{-\beta}$ over vastly different time scales. Despite much effort, there is no general theory that explains the widespread occurrence of $1/f$ noise.

Another puzzle seeking a physical explanation is the empirical observation that spatially extended objects, including cosmic strings, mountain landscapes, and coastal lines, appear to be self-similar fractal structures.² Turbulence is a phenomenon where self-similarity is believed to occur both in time and space. The common feature for all these systems is that the power-law temporal or spatial correlations extend over several decades where naively one might suspect that the physics would vary dramatically.

In this paper, we argue and demonstrate numerically that dynamical systems with extended spatial degrees of freedom naturally evolve into self-organized critical structures of states which are barely stable. We suggest that this self-organized criticality is the common underlying mechanism behind the phenomena described above. The combination of dynamical minimal stability and spatial scaling leads to a power law for temporal fluctuations. The noise propagates through the scaling clusters by means of a "domino" effect upsetting the minimally stable states. Long-wavelength perturbations cause a

cascade of energy dissipation on all length scales, which is the main characteristic of turbulence.

The criticality in our theory is fundamentally different from the critical point at phase transitions in equilibrium statistical mechanics which can be reached only by tuning of a parameter, for instance the temperature. The critical point in the dynamical systems studied here is an attractor reached by starting far from equilibrium: The scaling properties of the attractor are insensitive to the parameters of the model. This robustness is essential in our explaining that no fine tuning is necessary to generate $1/f$ noise (and fractal structures) in nature.

Consider first a one-dimensional array of damped pendula, with coordinates u_n , connected by torsion springs that are weak compared with the gravitational force. There is an infinity of metastable or stationary states where the pendula are pointing (almost) down, $u_n \approx 2\pi N$, N an integer, but where the winding numbers N of the springs differ. The initial conditions are such that the forces $C_n = u_{n+1} - 2u_n + u_{n-1}$ are large, so that all the pendula are unstable. The pendula will rotate until they reach a state where the spring forces on all the pendula assume a large value $\pm K$ which is just barely able to balance the gravitational force to keep the configuration stable. If all forces are initially positive, then the final forces will all be K . Of course, the array is also stable in any configuration where the springs are still further relaxed; however, the dynamics stops upon reaching this first, maximally sensitive state. We call such a state locally minimally stable.³

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What is the effect of small perturbations on the minimally stable structure? Suppose that we "kick" one pendulum in the forward direction, relaxing the force slightly. This will cause the force on a nearest-neighbor pendulum to exceed the critical value and the perturbation will propagate by a domino effect until it hits the end of the array. At the end of this process the forces are back to their original values, and all pendula have rotated one period. Thus, the system is stable with respect to small perturbations in one dimension and the dynamics is trivial.

The situation is dramatically different in more dimensions. Naively, one might expect that the relaxation dynamics will take the system to a configuration where all the pendula are in minimally stable states. A moment's reflection will convince us that it cannot be so. Suppose that we relax one pendulum slightly; this will render the surrounding pendula unstable, and the noise will spread to the neighbors in a chain reaction, ever amplifying since the pendula generally are connected with more than two minimally stable pendula, and the perturbation eventually propagates throughout the entire lattice. This configuration is thus unstable with respect to small fluctuations and cannot represent an attracting fixed point for the dynamics. As the system further evolves, more and more more-than-minimally stable states will be generated, and these states will impede the motion of the noise. *The system will become stable precisely at the point when the network of minimally stable states has been broken down to the level where the noise signal cannot be communicated through infinite distances. At this point there will be no length scale in the problem so that one might expect the formation of a scale-invariant structure of minimally stable states.* Hence, the system might approach, through a self-organized process, a critical point with power-law correlation functions for noise and other physically observable quantities. The "clusters" of minimally stable states must be defined dynamically as the spatial regions over which a small local perturbation will propagate. In a sense, the dynamically selected configuration is similar to the critical point at a percolation transition where the structure stops carrying current over infinite distances, or at a second-order phase transition where the magnetization clusters stop communicating. The arguments are quite general and do not depend on the details of the physical system at hand, including the details of the local dynamics and the presence of impurities, so that one might expect self-similar fractal structures to be widespread in nature: The "physics of fractals"⁴ could be that they are the minimally stable states originating from dynamical processes which stop precisely at the critical point.

The scaling picture quite naturally gives rise to a power-law frequency dependence of the noise spectrum. At the critical point there is a distribution of clusters of all sizes; local perturbations will therefore propagate

over all length scales, leading to fluctuation lifetimes over all time scales. A perturbation can lead to anything from a shift of a single pendulum to an avalanche, depending on where the perturbation is applied. The lack of a characteristic length leads directly to a lack of a characteristic time for the resulting fluctuations. As is well known, a distribution of lifetimes $D(t) \sim t^{-\alpha}$ leads to a frequency spectrum

$$S(\omega) = \int dt \frac{t D(t)}{1 + (\omega t)^2} \approx \omega^{-2+\alpha}. \quad (1)$$

In order to visualize a physical system expected to exhibit self-organized criticality, consider a pile of sand. If the slope is too large, the pile is far from equilibrium, and the pile will collapse until the average slope reaches a critical value where the system is barely stable with respect to small perturbations. The "1/f" noise is the dynamical response of the sandpile to small random perturbations.

To add concreteness to these considerations we have performed numerical simulations in one, two, and three dimensions on several models, to be described here and in forthcoming papers. One model is a cellular automaton, describing the interactions of an integer variable z with its nearest neighbors. In two dimensions z is updated synchronously as follows:

$$\begin{aligned} z(x,y) &\rightarrow z(x,y) - 4, \\ z(x \pm 1, y) &\rightarrow z(x \pm 1, y) + 1, \\ z(x, y \pm 1) &\rightarrow z(x, y \pm 1) + 1, \end{aligned}$$

if z exceeds a critical value K . There are no parameters since a shift in K simply shifts z . Fixed boundary conditions are used, i.e., $z=0$ on boundaries. The cellular variable may be thought of as the force on an individual pendulum, or the local slope of the sand pile (the "hour glass") in some direction. If the force is too large, the pendulum rotates (or the sand slides), relieving the force but increasing the force on the neighbors. The system is set up with random initial conditions $z \gg K$, and then simply evolves until it stops, i.e., all z 's are less than K . The dynamics is then probed by measurement of the response of the resulting state to small local random perturbations. Indeed, we found response on all length scales limited only by the size of the system.

Figure 1 shows a structure obtained for a two-dimensional array of size 100×100 . The dark areas indicate clusters that can be reached through the domino process originated by the tripping of only a single site. The clusters are thus defined operationally—in a real physical system one should perturb the system locally in order to measure the size of a cluster. Figure 2(a) shows a log-log plot of the distribution $D(s)$ of cluster sizes for a two-dimensional system determined simply by our counting the number of affected sites generated from a

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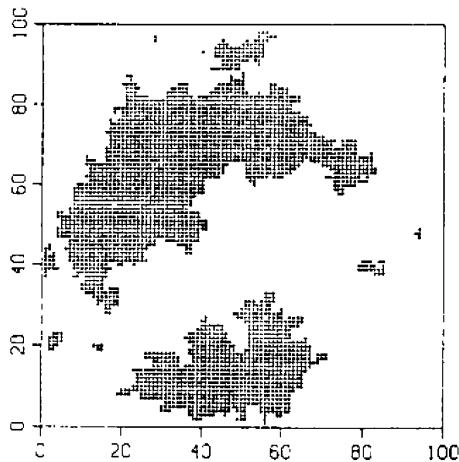


FIG. 1. Self-organized critical state of minimally stable clusters, for a 100×100 array.

seed at one site and averaging over many arrays. The curve is consistent with a straight line, indicating a power law $D(s) \sim s^{-\tau}$, $\tau \approx 0.98$. The fact that the curve is linear over two decades indicates that the system is at a critical point with a scaling distribution of clusters.

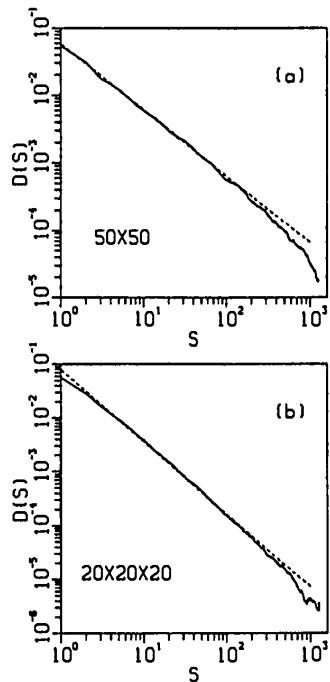


FIG. 2. Distribution of cluster sizes at criticality in two and three dimensions, computed dynamically as described in the text. (a) 50×50 array, averaged over 200 samples; (b) $20 \times 20 \times 20$ array, averaged over 200 samples. The data have been coarse grained.

Figure 2(b) shows a similar plot for a three-dimensional array, with an exponent of $\tau \approx 1.35$. At small sizes the curve deviates from the straight line because discreteness effects of the lattice come into play. The falloff at the largest cluster sizes is due to finite-size effects, as we checked by comparing simulations for different array sizes.⁵

A distribution of cluster sizes leads to a distribution of fluctuation lifetimes. If the perturbation grows with an exponent γ within the clusters, the lifetime t of a cluster is related to its size s by $\tau^{1+\gamma} = s$. The distribution of lifetimes, weighted by the average response s/t , can be calculated from the distribution of cluster sizes:

$$D(t) = \frac{s}{t} D(s(t)) \frac{ds}{dt} \approx t^{-(\gamma+1)\tau+2\gamma} \equiv t^{-\alpha}. \quad (2)$$

Figure 3 shows the distribution of lifetimes corresponding to Fig. 2 (namely how long the noise propagates after perturbation at a single site, weighted by the temporal average of the response). This leads to another line indicating a distribution of lifetimes of the form (2) with $\alpha \approx 0.42$ in two dimensions (50×50), and $\alpha \approx 0.90$ in three dimensions. These curves are less impressive than the corresponding cluster-size curves, in particular in three dimensions, because the lifetime of a cluster is much smaller than its size, reducing the range over

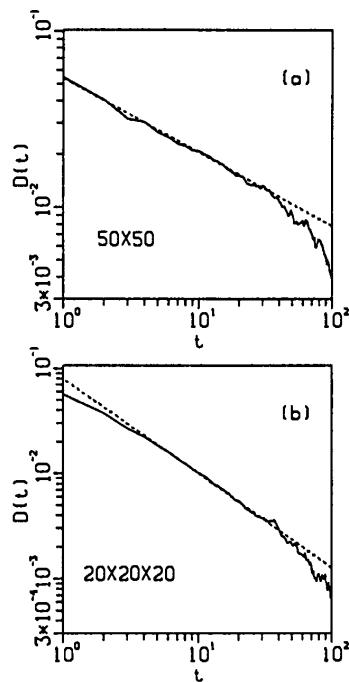


FIG. 3. Distribution of lifetimes corresponding to Fig. 2. (a) For the 50×50 array, the slope $\alpha \approx 0.42$, yielding a "1/f" noise spectrum $f^{-1.58}$; (b) $20 \times 20 \times 20$ array, $\alpha \approx 0.90$, yielding an $f^{-1.1}$ spectrum

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which we have reliable data. The resulting power-law spectrum is $S(\omega) \approx \omega^{-2+\alpha} \approx \omega^{-1.58}$ in 2D and $\omega^{-1.1}$ in 3D.

To summarize, we find a power-law distribution of cluster sizes and time scales just as expected from general arguments about dynamical systems with spatial degrees of freedom. More numerical work is clearly needed to improve accuracy, and to determine the extent to which the systems are "universal," e.g., how the exponents depend on the physical details. Our picture of $1/f$ spectra is that it reflects the dynamics of a self-organized critical state of minimally stable clusters of all length scales, which in turn generates fluctuations on all time scales. Voss and Clarke⁶ have performed measurements indicating that the noise at a given frequency f is spatially correlated over a distance $L(f)$ which increases as f decreases. We urge that more experiments of this type be performed to investigate the scaling proposed here.

We believe that the new concept of self-organized cri-

ticality can be taken much further and might be the underlying concept for temporal and spatial scaling in a wide class of dissipative systems with extended degrees of freedom.

We thank George Reiter for suggesting that these ideas might apply to the problem of turbulence. This work was supported by the Division of Materials Sciences, U. S. Department of Energy, under Contract No. DE-AC02-76CH00016.

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6.9.3 Carlson et al.: Singular Diffusion

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Self-Organized Criticality and Singular Diffusion

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We suggest that certain open driven systems self-organize to a critical point because their continuum diffusion limits have singularities in the diffusion constants at the critical point. We rigorously establish a continuum limit for a one-dimensional automaton which has this property, and show that certain exponents and the distribution of events are simply related to the order of the diffusion singularity. Numerically we show that some of these results can be generalized to include a class of sandpile models which are described by a similar, but higher-order, singularity.

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A wide variety of open dissipative dynamical systems are seen to exhibit scale-invariant characteristics reminiscent of traditional equilibrium systems at a critical point. Bak, Tang, and Wiesenfeld¹ introduced the first class of systems of this kind, the cellular automata referred to as "sandpiles." In the absence of intrinsic spatial inhomogeneities these systems generate avalanches of all sizes—the so-called "self-organized criticality" (SOC)—due to a dynamical threshold instability associated with the local slope of the pile. In an attempt to describe the anomalously large fluctuations exhibited by these and related systems, others have studied correlations in a diffusion equation with nonlinear corrections, driven by a white noise.² Inherent in this analysis is the *assumption* that these systems are at a critical point (associated with the critical angle of repose) and that the leading nonlinearities determine the critical exponents which describe the scaling behavior. However, a direct connection between any self-organizing model and these simple driven diffusions has not been made. So far the continuum equations which exhibit some form of scale invariance fail to capture the singular nature of the threshold criterion which governs the local evolution of the SOC models, and they do not explain the evolution of the system to a critical point.

In this Letter we explain why certain open driven systems organize to a critical point. Our key result is that continuum diffusion limits of certain self-organizing models exist and have the interesting feature of possessing diffusion "constants" which not only depend on the local density of the conserved quantity, but which in fact have a *singularity* at the critical point. With a pole in the diffusion constant, the boundary-value problem corresponding to the open driven system exhibits a boundary-layer phenomenon, and as the system size diverges the solution converges to the critical point (the pole) everywhere but on a vanishing fraction of the system. Additionally, the solution of the boundary-value problem can be used to extract information about the distribution of events in the original system. The analytical work in this paper will focus on a simple, but until now unstudied, model which exhibits SOC (nontrivial

scaling properties without the tuning of a parameter). Using simulations we will show that many of our results can be generalized to describe other systems such as sandpiles.

We begin by describing the self-organizing model which succumbs to rigorous analysis. The model is designed to mimic the way that regions of high slope diffuse to regions of low slope during an avalanche.³ We consider a finite one-dimensional lattice with a non-negative integer height $h(i)$ associated with each site $i = 1, \dots, N$. The system evolves continuously in time, such that for a fixed positive integer h_c we have the following: (i) If $h(i) \geq h_c$, then at rate 1, $h(i) \rightarrow h(i) - 1$ and $h(j) \rightarrow h(j) + 1$, where j is the nearest site $j > i$ with $h(j) < h_c$. (ii) The same transition rate holds for $j < i$. As in the sandpile models, the dissipation and driving mechanisms are associated with the boundary conditions of the finite system. Here we assume that the right boundary is open and the left boundary is closed, so that if there is no such j satisfying the above conditions then in (i) the grain leaves the system, and in (ii) the transition is suppressed. We drive the system by injecting new grains at rate α at site $i = 1$, which instantly hop to the first site j with $h(j) < h_c$. Since configurations with $h(i) < h_c - 1$ or $h(i) > h_c$ for any i are transient, each site can be in one of only two states. Taking $h_c = 1$ we have a *two-state model* with site values 1 (occupied) or 0 (vacant): 1's hop at rate 1 to the nearest 0 on the right and on the left; 1's fall off the right edge, are blocked on the left edge, and are injected at the first site $i = 1$ at rate α .

The advantage of working with the two-state model is that the continuum limit can be obtained rigorously for a closed system (a torus), where the spatially averaged density $\langle \rho \rangle$ of 1's is conserved. Two features make analysis of this model tractable. First, product measure with constant density $\langle \rho \rangle$ is invariant (i.e., each site is independently occupied with a 1 with probability $\langle \rho \rangle$). Second, the process is reversible (i.e., detailed balance is satisfied) for the family of equilibria ($0 \leq \langle \rho \rangle \leq 1$). Note that at density $\langle \rho \rangle$, the expected jump size is (formally $N = \infty$) $\sum_{k=1}^{\infty} k \langle \rho \rangle^{k-1} (1 - \langle \rho \rangle) = (1 - \langle \rho \rangle)^{-1}$,

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which diverges as $\langle \rho \rangle \rightarrow 1$. This fact is a strong indication of a singular diffusion constant, and will play an important role in driving the open system toward the critical point. We can interpret the 0's as being domain walls which locally bound the size of a jump. The density of 0's, $p_0 = 1 - \langle \rho \rangle$, is the order parameter in the two-state model, where $p_0 \rightarrow 0$ as $\langle \rho \rangle$ approaches the critical point ($\langle \rho \rangle \rightarrow 1$). A similar, although less trivial, critical behavior was observed in sandpiles in Ref. 3.

The exact form of the diffusion constant can be deduced from a simple calculation assuming product measure and a linear profile in the density with constant slope 2ϵ . The diffusion constant is then given by $D(\rho) = I/2\epsilon$, where I is the current through a plane separating two sites:

$$I = \sum_{k=0}^{\infty} \left[\prod_{i=0}^k [\rho + (2i+1)\epsilon] - \prod_{i=0}^k [\rho - (2i+1)\epsilon] \right]. \quad (1)$$

For each k the first term is associated with current flow in the positive direction, and the second term with the negative direction. The terms are the probabilities that all sites from the plane to the k th site to the left (or right) are occupied, in which case the k th particle can jump through the plane at rate 1. Keeping terms to $O(\epsilon)$ in (1) we obtain the resulting diffusion constant

$$D(\rho) = (1+\rho)/(1-\rho)^3, \quad (2)$$

which depends on the local density ρ , and has a third-order pole at $\rho = 1$. With a great deal more work the following theorem can be proved, establishing that the continuum limit of the two-state model is

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x} \left(D(\rho) \frac{\partial \rho}{\partial x} \right). \quad (3)$$

Stripped of technical details, the theorem states that if we consider the system as a random measure with mass $1/N$ at each occupied site, scaling site separation by $1/N$ and the transition rates by N^2 (standard diffusion scaling), then as $N \rightarrow \infty$ this random measure approaches a deterministic density which solves the diffusion equation (3) with the diffusion constant given by (2).

Theorem.—On the discrete torus $T_N = \{1, \dots, N\}$ denote the configuration at time $N^2 t$ by η_t , where $\eta_t(i) = 1$ if site i is occupied. Given an initial density profile $\kappa(x)$ on the continuum torus $T = [0, 1]$ which is uniformly bounded away from 1, start the system on T_N with this profile: $P(\eta_0(i) = 1) = \kappa(i/N)$, independent of other sites. To each occupied site associate a mass $1/N$. As $N \rightarrow \infty$, with spatial rescaling this random measure converges to the deterministic density $\rho(t, x)$ which satisfies (2) and (3), with $\rho(0, x) = \kappa(x)$. The convergence is in the weak sense—for any smooth function ψ on the torus T ,

$$\lim_{N \rightarrow \infty} N^{-1} \sum_{i=1}^N \psi \left(\frac{i}{N} \right) \eta_t(i) \rightarrow \int_T \psi(x) \rho(t, x) dx$$

in distribution.

Remark.—A complete proof of the theorem is given in Ref. 4, and is based on the techniques developed in Ref. 5 for establishing hydrodynamic limits.

Although Eq. (3) was derived for the closed system, we will use it to derive the behavior of the open driven system⁶ for large N , where the appropriate boundary conditions are

$$\rho(1) = 0, \quad \rho'(0) D(\rho(0)) = -\alpha N, \quad (4)$$

where α is a constant. The first condition is associated with the open boundary on the right. The second condition is simply a flux-balance condition at the left boundary. Note that the driving rate is proportional to N because we rescale a system of size N into the unit interval in order to use the hydrodynamic equation (doubling the size of a one-dimensional diffusive system with fixed flux and then rescaling to the original size is equivalent to doubling the flux in the original system). Asymptotically for large N , the solution to the boundary-value problem is

$$\rho_N(x) \approx 1 + \frac{1 - \sqrt{4\alpha N(1-x)+1}}{2\alpha N(1-x)}. \quad (5)$$

In spite of the fact that (3) was derived for a closed system, (5) is in very good agreement with numerical results for the time-averaged configuration of the original system (see Fig. 1). The presence of the “boundary layer” at the open boundary with thickness that vanishes as $N \rightarrow \infty$ is explained by noting that for any specified density $\hat{\rho} < 1$ and for any (large) N , there will be a site at $x_N = k_N/N$ with density approximately $\hat{\rho}$. The flux condition $\rho'(x_N) = -\alpha N D(\hat{\rho})^{-1}$ implies that the slope of the profile at x_N diverges as N , implying the boundary-layer thickness scales like $1/N$.

Scaling properties follow immediately from the above

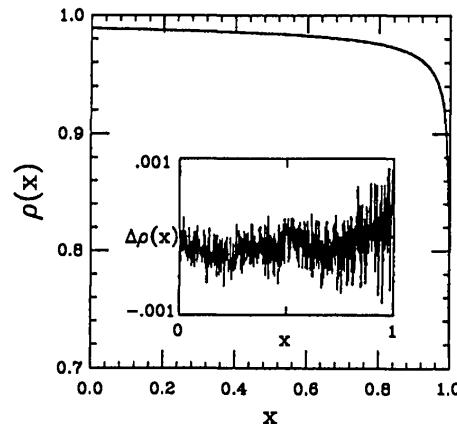


FIG. 1. The numerical and analytical profiles (both shown in the main figure) for the two-state model are essentially coincident. The inset is the difference between them. The analytical result is given by Eq. (5) with $\alpha = 1$, while the numerical results are obtained as the time average of a system of corresponding size $N = 8192$.

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considerations: (1) The thickness Δ of the boundary layer scales like $\Delta \sim N^{-1}$. (2) The mean density $\bar{\rho}_N = \int_0^N \rho_N(x) dx$ converges to the critical point $\rho_c = 1$ as $\bar{\rho}_N \sim 1 - 2/\sqrt{aN}$. This implies the density of zeros $p_0(N) = 1 - \bar{\rho}_N$ scales like $p_0(N) \sim 2/\sqrt{aN}$. (3) The steady-state distribution of jump sizes can be calculated assuming product measure locally. In a system of N sites, the probability $P(k, N)$ that a 1 will hop $k < N$ sites in an event is given by

$$P(k, N) = [1 - p_0(N)]^{k-1} p_0(N). \quad (6)$$

The comparison between these results and simulations of the open system are excellent.

Because $p_0(N) \sim 2/\sqrt{aN}$, the distribution of events will scale with the number of sites. From (6) we derive finite-size scaling $P(k, N) = N^{-\beta} g(k/N^\nu)$ in the limit of large N , obtaining the universal curve

$$g(z) = A e^{-Az}, \quad (7)$$

with $A = 2/\sqrt{a}$ and $\nu = \frac{1}{2}$.

These results can be extended to other systems. For example, an obvious generalization of the two-state model to higher dimensions, in which each 1 moves to the

nearest 0 in a randomly selected direction, satisfies the d -dimensional generalization of (3). The general singular diffusion equation that we consider is of the form

$$\frac{\partial \rho}{\partial t} = \nabla \cdot [D(\rho) \nabla \rho]. \quad (8)$$

The exponents characterizing the scaling behavior depend on the order of the pole at ρ_c in the diffusion constant and on the boundary conditions, but not on any analytic factors which are bounded away from zero and infinity. Therefore, we consider the diffusion constant

$$D(\rho) = 1/(\rho_c - \rho)^\phi. \quad (9)$$

We will solve (8) for the simple case of a source at the center of a d -dimensional disk, where $\rho = \rho(r)$ and the boundary conditions are

$$\rho(1) = 0, \quad \rho'(0) D(\rho(0)) = -\alpha_N. \quad (10)$$

Here α_N is the rescaled driving rate which depends on both dimension and how the system is being driven. Note also that in order to have a well posed boundary-value problem in $d \geq 2$ the flux condition at $r=0$ must be replaced by a similar condition at a radius $\delta \geq 0$, which we incorporate into α_N in the solutions below: for $d=1$,

$$\rho(r) = \begin{cases} \rho_c - [\rho_c^{-(\phi-1)} + \alpha_N(\phi-1)(1-r)]^{-1/(\phi-1)}, & \phi \neq 1, \\ \rho_c[1 - e^{-\alpha_N(1-r)}], & \phi = 1; \end{cases} \quad (11a)$$

for $d=2$,

$$\rho(r) = \begin{cases} \rho_c - [\rho_c^{-(\phi-1)} - \alpha_N(\phi-1)\ln(r)]^{-1/(\phi-1)}, & \phi \neq 1, \\ \rho_c[1 - r^{\alpha_N}], & \phi = 1; \end{cases} \quad (11b)$$

for $d \geq 3$,

$$\rho(r) = \begin{cases} \rho_c - \left\{ \rho_c^{-(\phi-1)} - \frac{\alpha_N(\phi-1)}{d-2}[1-r^{2-d}] \right\}^{-1/(\phi-1)}, & \phi \neq 1, \\ \rho_c[1 - e^{-\alpha_N(1-r^{2-d})/(d-2)}], & \phi = 1. \end{cases} \quad (11c)$$

Scaling relations are immediate. For example, in one dimension, where $\alpha_N = aN$, the density of zeros is given by

$$p_0(N) \sim \begin{cases} N^{-1/(\phi-1)}, & \text{if } \phi \neq 1, 2, \\ N^{-1} \text{ if } \phi = 1, \\ N^{-1} \ln N \text{ if } \phi = 2. \end{cases} \quad (12)$$

Substituting (12) into (6), the corresponding distribution of jump sizes $P(k, N)$ is obtained (with the product-measure assumption). In each case finite-size scaling leads to a universal curve of the form (7), where the exponents β and ν are equal, and given by the same exponents as that of the order parameter p_0 in Eq. (12), with logarithmic corrections in the case $\phi = 2$. It is worth noting from (11) that, given a source at the origin, convergence to the critical point [i.e., $\rho(r) \rightarrow \rho_c$ as $N \rightarrow \infty$] occurs only if α_N diverges as $N \rightarrow \infty$. With a constant driving rate α , scaling a system with N^d sites onto the unit disk yields $\alpha_N = \alpha N^{2-d}$, which does not diverge for

$d \geq 2$. In this case there is a finite characteristic jump distance, and finite-size scaling is not observed. To observe SOC in $d \geq 2$, we could take a driving rate at the origin diverging faster than N^{d-2} in the unrescaled system, or a constant driving rate could be applied to a larger set of sites (e.g., on part of the boundary as is the case in certain sandpile models). In the latter case, one would have to solve a different boundary-value problem, but we expect that the scaling behavior would be the same as that arising from (11) with the proper α_N .

We will now provide evidence that equations of the form (8) also underlie other self-organizing models. We consider the one-dimensional limited local sandpile models⁷ in which n grains of sand fall to the right whenever the local slope $z(i)$ exceeds the threshold z_c . As shown in Ref. 3, there are domain walls [any site i with $z(i) \leq z_c - n$] which bound avalanches, much like 0's bound jumps in the two-state model. When this model is run on a torus, total slope is conserved. Furthermore,

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there is a critical slope $s_c < z_c$ so that if the mean slope $\langle s \rangle = (1/N) \sum_{i=1}^N z(i) < s_c$, then domain walls persist, while if $\langle s \rangle > s_c$ they become extinct. This implies that as $\langle s \rangle \uparrow s_c$ the density of domain walls approaches zero, so that the length scale on which slope is transported via avalanches diverges, suggesting a singular diffusion constant.

We verify the singular diffusion in sandpiles on both a closed and an open set, taking $z_c = n - 2$ (for which $s_c = \frac{1}{2}$). First, we start the system on a torus with average slope $\langle s \rangle$ and observe the relaxation rate of a long-wavelength sinusoidal perturbation as a function of $\langle s \rangle$. For large systems a log-log plot of relaxation rate versus $s_c - \langle s \rangle$ has a slope of -4 (inset to Fig. 2), indicating that the diffusion constant diverges as $\langle s \rangle \rightarrow s_c$ with the order of the singularity being $\phi = 4$. Second, Fig. 2 shows that the time-averaged slope profile on the open system (note the presence of a sharp boundary layer) agrees well with the solution (11) with ρ replaced by s and with $d = 1$, $\phi = 4$, and an optimally selected constant α ($\alpha_N = \alpha N$). From (12), we obtain the corresponding density of domain walls which scales like $N^{-1/3}$, consistent with simulations in Ref. 3. While the agreement of the profiles in Fig. 2 is impressive, so that scaling properties of the solution should apply to the system, the boundary conditions (10) do not accurately describe the sandpile model, in which there is no flux of slope through the right boundary. Instead, the boundary layer is driven by an effective potential⁸ acting at the left edge which arises from an asymmetry of the rules at that boundary (see Ref. 3) and which scales with N . A similar asymmetry (potential) yields the slight decrease in the profile at the right edge.

To conclude, we have introduced a two-state model which exhibits SOC, for which we have rigorously established the existence of a diffusion limit with a singular diffusion constant. The boundary-value problem corresponding to the rescaled open driven system in one dimension has a solution which converges to the diffusion singularity as the system size diverges. In higher dimensions appropriate scaling of the driving rate yields similar results. Scaling properties follow directly from the solution. In addition, numerical evidence indicates that singular diffusion also occurs in a class of sandpile models. We suggest that singular diffusion provides a cogent framework on which to address the issue of how self-organizing systems find their critical points.

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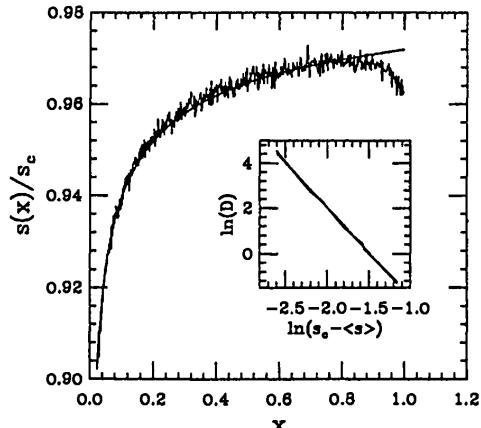


FIG. 2. Numerical and analytical slope profiles for the limited local sandpile model on an open system scaled into the unit interval ($N=2048$). The inset illustrates the relaxation rate (i.e., the diffusion constant D since the primary mode relaxes like e^{-Dx}) of a sinusoidal perturbation as a function of distance from the critical point in the closed system. In both cases we find that the sandpile model is associated with a singular diffusion equation of the form (8), where the order of the pole $\phi = 4$ in (9).

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⁶Technically the theorem does not apply to the driven system because the proof requires reversibility. Also, the theorem only holds when the density is bounded away from 1, while here we will find that the steady-state density converges to 1 like $N^{-1/2}$. Nevertheless, we expect the hydrodynamic limit to apply in the interior of the driven system since simulations show that the variance of $N^{-1} \sum_{i=1}^N \psi(i/N) \eta_i(i)$ vanishes as $N \rightarrow \infty$.

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⁸This suggests that with a large number of sites N , sandpiles should be approximately described by a singular diffusion equation: $\partial \rho / \partial t = -\nabla \cdot [D(\rho) \nabla \rho] - \nabla [F_N(x) \rho]$, where F_N is the force due to the potential. Numerically, solutions yield profiles which are qualitatively the same as those shown in Fig. 2, but the form of F_N is unclear.

6.9.4 Jaeger *et al.*: Experimental Studies

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Relaxation at the Angle of Repose

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We have investigated the distribution of avalanches which occur when the slope of a sandpile exceeds the metastable slope given by the angle of repose. In contradiction to recent models by Bak, Tang, and Wiesenfeld for the dynamics of granular systems, we do not observe power-law distributions. We also find that the slope of a sandpile decays as $\log(t)$ when vibrations are introduced. We propose a simple model for this effect.

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Sandpiles have often been used as a metaphor for other phenomena in physics. As children we have played with sand and it is only natural to believe that we can intuit the processes underlying the shape and dynamics of these structures. Thus de Gennes¹ has compared the motion of vortices in superconductors to avalanches in sandpiles, and Souletie² has argued that spin-glasses and sandpiles behave in a similar manner. Dry, noncohesive, granular material like sand can flow, resembling a liquid, but also, like a solid, can sustain under the influence of gravity a finite "angle of repose," θ_r . This is the angle between the horizontal and the free surface of the sandpile after a land slide has restored the pile to a metastable equilibrium slope. As early as 1773 the connection between θ_r and the static internal friction of a given material was developed by Coulomb.³ The analogies mentioned above were made because it is tempting to think of a phase transition occurring at θ_r : For slopes such that $\theta < \theta_r$, no flow of sand can occur and the pile appears to be a solid whereas for $\theta > \theta_r$, the top layers of sand flow freely downhill. Most recently Bak, Tang, and Wiesenfeld⁴ introduced the idea of "self-organized criticality" in terms of a model of how they expected a sandpile to behave. Clearly their ideas may have much wider applicability than to just sandpiles, but it is this analogy which makes their model so intuitively appealing. Their idea rests on the assumption that θ_r is a critical angle. If the angle θ of the free surface is increased continuously (e.g., by adding more material to the top or by tilting the base of the pile), the pile will organize itself such that its average slope will be the angle of repose θ_r by unloading excess material through avalanches. Bak, Tang, and Wiesenfeld predict a self-organized state at θ_r characterized by long-range spatial and temporal correlations and giving rise to a typical " $1/f$ " power spectrum of the fluctuations around the steady-state particle flow. They further suggest an analogy between the nonequilibrium behavior of sandpiles and traditional critical phenomena and find a power-law dependence for the relaxation from a supercritical state $\theta > \theta_r$, back to the critical state.⁵

Motivated by the above conjectures we have investigated the nature of particle flow along the free surface in

a model system for granular materials: "sandpiles" consisting of spherical glass beads or rough aluminum-oxide particles. We report here on the power spectrum for fluctuations as well as on relaxation properties.

We have performed the experiment in two basic configurations [see Fig. 1(a)]. The average slope of the free surface was varied either by turning a semicircular drum (i.e., tilting the free surface of the pile) partially filled with granular material, or by randomly adding particles to the top surface of a pile contained in a box with one open side. The semicircular drum of width 8 cm and radius 5 cm had an angular velocity $\Omega = 1.3^\circ/\text{min}$. Several box geometries were used having a width of ap-

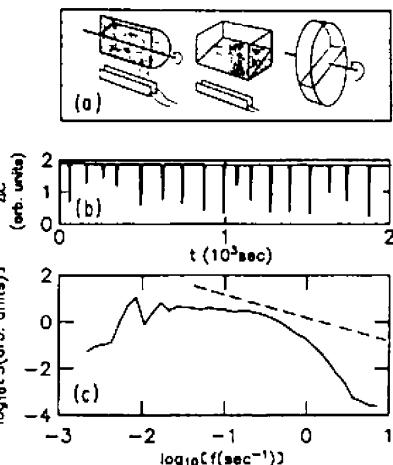


FIG. 1. (a) Schematic diagram of the three experimental configurations (left to right): A rotating semicircular drum, an open box with sand added from the top, and a closed cylindrical drum. In the first two the sand falls through a pair of capacitor plates. (b) The time trace of a typical sequence of avalanches in a rotating drum ($\Omega = 1.3^\circ/\text{min}$) with spherical glass beads. ΔC is the change in capacitance due to the flow of the beads through the capacitor. (c) The power spectrum, $S(f)$, for the above time trace. Dashed line shows a $1/f$ power spectrum for comparison.

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proximately 5 cm and aspect ratios (width/length) ranging from $\frac{1}{3}$ to 3. In the drum we used spherical glass beads of average diameter 0.54 ± 0.08 mm. For the open box we used smaller beads, 0.07 ± 0.01 mm average diameter, to keep the momentum transfer as low as possible when the particles hit the surface of the pile. The results in both configurations were insensitive to the particle size although for the very small particles the experiments were performed in a drybox since special care had to be taken to prevent cohesion due to moisture. We also performed the experiment with rough aluminum-oxide particles of diameter 0.5 ± 0.1 mm.

The flow of particles over the open edge of the drum or box was detected by a parallel-plate capacitor through which the particles flowed. The corresponding time sequence of capacitance changes, ΔC , was detected by a bridge circuit and fed into a spectrum analyzer. Capacitance changes directly correspond to changes in the flow rate of particles. The resolution was sufficient to detect even the passage of only a few particles at a time.

We show, in Fig. 1(b), a typical time trace and, in Fig. 1(c), the corresponding power spectrum obtained with the rotating drum using the spherical glass beads. Similar results were obtained with the open box and for the case of rough aluminum-oxide particles. Each inverted spike in Fig. 1(b) corresponds to a major avalanche, in almost all cases spanning the whole free surface of the system. The avalanches start at an angle $\theta_m \equiv \theta_r + \delta$ (where δ is typically a few degrees) and return the pile to its metastable state at θ_r . The distributions for the Δt interval between avalanches and their width τ are sharply peaked near their average values as shown in Fig. 2. The nearly uniform spacing of avalanches, $\langle \Delta t \rangle = \langle \Delta \theta \rangle / \Omega$, corresponds to the broadened peak at $f = 1/\langle \Delta t \rangle$ in the power spectrum. The roll off at high frequencies above $f = 1/\langle \tau \rangle$ is due to the finite width τ of the individual avalanches. Its average power-law decay, close to f^{-3} , is explained by variations between rec-

tangular and triangular pulse shapes of individual events. In the relevant frequency range, between $1/\langle \Delta t \rangle$ and $1/\langle \tau \rangle$, the spectra appear frequency independent. This finding is in conflict with Bak, Tang, and Wiesenfeld who predicted power-law behavior, $f^{-\theta}$, with $\theta \approx 1$. Such behavior would have followed from a power-law distribution of widths τ implying events over a wide range of time scales. Instead we find that the power spectrum is indicative of a linear superposition of global, system-spanning avalanches with a narrowly peaked distribution of time scales.

This situation is a direct consequence of the existence of a nonzero value of δ . The phenomenon was first explained as dilatation by Reynolds⁶ in 1885. For particles to slide on the surface, θ , (which corresponds to the metastable configuration after an avalanche) must be exceeded by an additional amount δ to allow for clearance with the profile of the underlying layer.⁷ As long as effects from the retaining walls of the container can be neglected we find $\langle \theta_r \rangle = 26^\circ$ (39°) and $\langle \delta \rangle = 2.6^\circ$ (5°) for glass beads (aluminum-oxide particles), independent of container or grain size. These values for $\langle \delta \rangle$ agree with calculations by Bagnold⁷ who also predicted the periodic occurrence of avalanches in the steady state. We believe that the observation of a wide spread of values for Δt by Evesque and Rajchenbach⁸ is due to wall effects in a comparatively narrow system.

Since θ_m is inherently unstable, the hysteresis, δ , is easily reduced to zero by the application of mechanical vibrations to the system. By adjusting the intensity of the vibrations one can span the transition from solidlike to liquidlike behavior of the granular material in a very controlled way. We induced vibrations by a speaker mechanically coupled to the system. This configuration allowed us in a convenient way to address whether $1/f$ fluctuations in the steady-state particle flow for $\Omega = \text{const}$ could be recovered if $\delta \rightarrow 0$. It also allowed us to investigate, for $\Omega = 0$, the time dependence of $\theta(t)$ as the average angle of the free surface relaxes under the influence of the vibrations.

Figure 3 shows the variation of the power spectrum as the vibration intensity in the drum is increased. The spectra show that increasing intensity leads to a broader distribution of time scales, yet no universal power-law behavior emerges. Instead the fall off in the curve broadens smoothly as the intensity is increased and at the highest vibration intensity the spectrum can be approximated by $f^{-0.8}$ over a limited range. If a finite value of δ were the main reason for the absence of universal power-law dependence, that dependence should have emerged for vibration intensities even smaller than that corresponding to the top curve in Fig. 3. Clearly the introduction of noise does not bring the system closer to a critical state. The transition that occurs appears to be more similar to a first-order transition than to a critical point.

We have studied the nature of the particle flow by in-

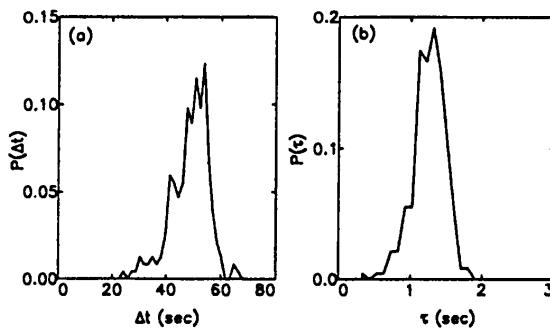


FIG. 2. (a) The distribution of intervals between avalanches, $P(\Delta t)$, and (b) the distribution of avalanche durations, $P(\tau)$, for a run using glass beads in the rotating drum ($\Omega = 3.2^\circ/\text{min}$).

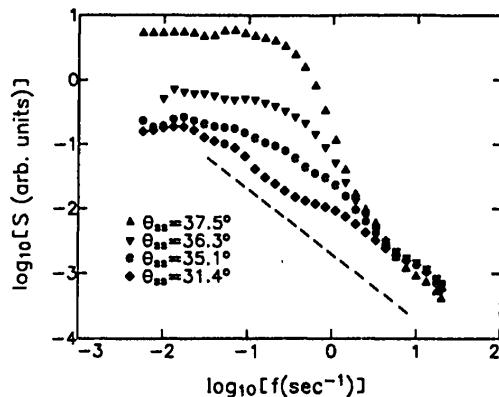


FIG. 3. The power spectra for avalanches of aluminum-oxide particles in a rotating drum ($\Omega = 1.3^\circ/\text{min}$) for different vibration intensities (increasing from top to bottom) parametrized by the steady-state angle, θ_{ss} . Dashed line shows a $1/f$ power spectrum for comparison. Similar results were found for spherical beads.

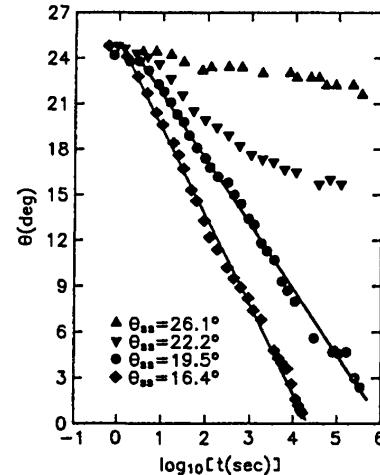


FIG. 4. The relaxation of θ in a stationary drum with glass beads. Vibration intensities increase from top to bottom. Straight lines indicate $\log(t)$ behavior.

vestigating the dependence of the average slope on vibration intensity and rotation speed Ω . The data were taken both in the semicircular drum and in a fully circular drum with no opening for particles to leave [Fig. 1(a)]. This second configuration had radius 15 cm and width 10 cm and allowed continuous rotation without refilling. The steady state of the system at constant speed Ω and constant nonzero vibration intensity is characterized by an angle θ_{ss} . Switching off the vibrations thus is a way to prepare the system in a supercritical state, $\theta > \theta_{ss}$, and one can then observe the relaxation to the steady state as the vibrations are turned back on. Such relaxation is shown in Fig. 4 for the case $\Omega = 0$ (stationary drum) and initial condition $\theta(t=0) = \theta_r$. The model of self-organized criticality predicts^{4,9} a power-law dependence on t while our data cannot be fitted by a power law with reasonable parameters over any wide interval of time, even for small intensities. Instead the data for high vibration intensity are consistent with a $\log(t)$ dependence over many decades. For smaller intensities the curves follow a $\log(t)$ behavior over several decades but turn over to a slower decay rate at very large times.

To make such dependence plausible, consider a simple model based on the notion that the vibration intensity plays the role of an effective temperature. In analogy with electrical conduction we relate the particle flow j to an applied field E by a conductivity σ whose T dependence is governed by an effective rate of escape from random trapping sites. For the rotating drum we replace j by $d\theta/dt$ and E by θ . The motion of particles is impeded by the barriers posed by neighboring beads and the corresponding random potential will be a complicated function of the local configurations. Here, however, we

are interested in the average effective barrier height U as the angle θ is varied. Expanding to first order around the experimental starting value $\theta(t=0) = \theta_r$, we have $U \approx U_0 + U_1(\theta_r - \theta)$. Since we know that spontaneous flow sets in at θ_m we require $U(\theta_m) = 0$ which gives $\delta \equiv \theta_m - \theta_r = -U_0/U_1$. Assuming now an effective temperature T_{eff} due to the mechanical vibrations, we obtain a rate of escape over the barrier exponentially dependent on the ratio U/kT_{eff} . This leads to

$$\frac{d\theta}{dt} = -A\theta e^{\beta(\theta-\theta_r)},$$

where $A \equiv A_0 \exp(-U_0/kT_{eff})$ and $\beta \equiv U_1/kT_{eff}$ are independent of θ . The equation can be solved analytically for $\theta(t)$ in terms of the exponential integral function¹⁰ $E_1(\beta\theta)$. For $\beta\theta \gg 1$ and, up to logarithmic corrections in θ/θ_r , the solution is well approximated by $\theta = \theta_r - (1/\beta)\ln(\beta A\theta_r t + 1)$. This reproduces the logarithmic dependence on t seen in Fig. 4 for times larger than $t_0 \equiv 1/\beta A\theta_r$, and also gives a good fit for shorter times.

For small vibration intensities the assumption that mechanical vibrations mimic an effective temperature fails when kT_{eff} becomes less than U . In contrast to thermal fluctuations we expect the mechanical energy distribution to be cut off sharply above a finite value corresponding to the maximum vibration intensity. Particles therefore get stuck when $\beta(\theta_r - \theta) < c$, where c is some constant of order unity, and the logarithmic decay seen in Fig. 4 flattens out. Also at very long times it becomes difficult to determine the angle θ precisely since the profile of the free surface starts to deviate from a straight line. θ in Fig. 4 is therefore the average angle,

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measured along the center portion of the free surface to exclude boundary effects. At long times, when most particle flow downhill has ceased, convective motion in the bulk may become important.¹¹

In conclusion, we find that the simple, intuitive picture of θ_c as the critical angle of the system has to be modified and that the direct analogy between the dynamics of sandpiles and physical systems exhibiting a critical point, suggested by Bak, Tang, and Wiesenfeld, is not well founded. Perhaps other systems can be found which would show such critical behavior. Under steady-state conditions the angle θ oscillates between θ_c and θ_m . However, the observation that $\theta(t) \propto T_{\text{eff}} \log(t)$ when there is a finite vibration intensity suggests that the relaxation of the free surface in sandpiles might be related to phenomena such as flux creep in superconductors¹² and slow relaxation processes in glasses. In addition, further investigation of the question of whether the models introduced by Bak, Tang, and Wiesenfeld have universal properties is currently under way.¹³ Finally, an understanding of the dynamics of particle flow in sandpiles is important not only for its use as a metaphor to other physical systems but also because granular materials are widely used in industrial processes. Although much is known about the time-independent bulk flow properties of granular materials very little is known about the instabilities and fluctuations that occur in these flow patterns. Dynamical effects of this kind are suspected of being responsible for the collapse of grain silos.¹⁴ Only recently have attempts been made^{14,15} to investigate such problems. Studies of what happens at the surface of sandpiles may be one way of making accessible the underlying physics of granular material.

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T. Witten, L. Wu, and S.-M. Zhou for many stimulating discussions. We are particularly grateful to R. Behringer for informing us of his work prior to publication. This work was supported in part by NSF Materials Research Laboratory Grant No. DMR 8519460.

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⁹This is predicted in the limit of zero vibration intensity.

¹⁰M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1972), p. 228.

¹¹J. Rajchenbach and P. Evesque, to be published.

¹²M. Tinkham, *Introduction to Superconductivity* (Krieger, Huntington, NY, 1980), p. 174.

¹³L. P. Kadanoff, S. R. Nagel, L. Wu, and S.-M. Zhou, to be published.

¹⁴D. G. Schaeffer, *J. Differential Equations* **66**, 19 (1987).

¹⁵R. P. Behringer, private communication.

Chapter 7

Correlations and Response

In this chapter, we discuss one of the most remarkable and general features of statistical mechanics:

In a system described by conventional classical statistical mechanics, there is a simple relationship between correlations among the fluctuating quantities and the response to changing a parameter in the Hamiltonian.

There is also a dynamical version of the same idea:

In a system described by conventional classical statistical mechanics, there is a simple relationship between the time-dependent correlations among the fluctuating quantities and the response to changing a parameter in the Hamiltonian in a time-dependent fashion.

This last is most commonly used as what is called a *fluctuation-dissipation* theorem. The word ‘fluctuation’ refers to a correlation function while the word ‘dissipation’ describes the long-run result of a response to an external disturbance.

In this chapter, we shall start with discussions of the response in a time-independent situation and then go into the analogous time-dependent problem. We finish off by actually evaluating some time-dependent correlation functions in a simple diffusive situation. Our analysis closely follows the work of Kadanoff and Martin.¹

7.1 Time Independent Response

Notice that each of the parameters, like K and h , which appear in the Ising problem, play a double role. On one hand they define the nature of the problem, by determining the statistical weight to be used in all summations. They describe the couplings among the different degrees of freedom in the problem. When we wish to emphasize this aspect

¹LPK Essays A2, *Hydrodynamic Equations and Correlation Functions*, L. P. Kadanoff and P. C. Martin, Ann. Phys. 24, 419 (1963).

of their role, we shall call them *coupling constants*. But they have another role. If you differentiate the log of the partition function with respect to one of these ‘couplings’, say the local magnetic field $h(j, k)$, you generate an average of the local magnetization $\sigma_{j,k}$. If you differentiate the resulting average with respect to a h at a different point, you get a correlation between two σ ’s.

Thus, each of the coupling constants is coupled to a fluctuating quantity like $\sigma_{j,k}$. Because of the analogy with quantum mechanics, we call the local fluctuating quantities operators. So changing these couplings generates averages of the operators. Repeated changes generate correlation functions. When we wish to emphasize this part of the role of coupling constants, we call these quantities not couplings, but *fields*.

The dual role of the couplings constants is reflective of the dual role played by all the basic operators in classical mechanics, quantum mechanics, and statistical mechanics. (In the classical situations, the ‘operators’ are any functions of p ’s and q ’s.) In each case the Hamiltonian, which defines the problem is an operator. It is usually expressed as a function of the basic operators, the p ’s and q ’s. Operators also constitute the observables of the theory. Each field is also important, since correlation functions can be computed as derivatives of the partition functions with respect to local fields.

For many purposes, it is painful to write lists of field and coupling constants like the h, K which appears in our discussion of the Ising model. We shall often simplify our notation by writing instead of a specific list a vector $\mathbf{K} = (h, K, \dots)$. In using this notation we write the α th coupling as K_α and the conjugate operator as O^α . Thus, the action for the system is:

$$W = \sum_\alpha K_\alpha O^\alpha. \quad (7.1a)$$

Most often the local operators depend upon the spatial position, \mathbf{r} , as does the magnetization operator $\sigma_{j,k}$ in the Ising model. In that case it is more convenient to separate out the \mathbf{r} -dependence explicitly by writing

$$W = \sum_\alpha \sum_{\mathbf{r}} K_\alpha(\mathbf{r}) O^\alpha(\mathbf{r}). \quad (7.1b)$$

In discussing the results of changes in the Hamiltonian, it is most convenient to think about small changes in K , according to

$$K_\alpha \rightarrow K_\alpha + h_\alpha. \quad (7.2)$$

Here h_α is small. We shall differentiate with respect to this variable and then set it equal to zero in all of our final expressions. Corresponding to the change in the couplings, there is also a change in the action and the Hamiltonian

$$W[\mathbf{K}] \rightarrow W[\mathbf{K}] + \sum_\alpha h_\alpha O^\alpha, \quad (7.3a)$$

$$\mathcal{H} \rightarrow \mathcal{H} - \sum_\alpha h_\alpha \frac{O^\alpha}{\beta}. \quad (7.3b)$$

We have already calculated many response and correlation functions using expressions of the form (7.3a). Here, we shall simply list some results as they are derived from differentiating the partition function, $Z = \text{Tr} \exp W$, or its logarithm, which is $-\beta$ times the free energy, F :

The average of a single operator is given by

$$\langle O^\alpha \rangle = \frac{\partial}{\partial h_\alpha} \ln Z. \quad (7.4)$$

If one differentiates Eq. (7.4) once more, one finds

$$\langle O^\alpha O^\beta \rangle = \langle O^\alpha \rangle \langle O^\beta \rangle + \frac{\partial^2}{\partial h_\alpha \partial h_\beta} \ln Z. \quad (7.5)$$

This equation can be rewritten by using as our basic operator the quantity describing fluctuations in O^α , i.e.

$$\delta O^\alpha = O^\alpha - \langle O^\alpha \rangle. \quad (7.6)$$

Thus we find after a rearrangement of terms

$$\langle \delta O^\alpha \delta O^\beta \rangle = \frac{\partial^2}{\partial h_\alpha \partial h_\beta} \ln Z. \quad (7.7)$$

Equation (7.7) is a result from classical physics. It does not work in a quantum mechanical situation unless the Hamiltonian, O^α , and O^β all commute.

The next result comes from three derivatives:

$$\langle \delta O^\alpha \delta O^\beta \delta O^\gamma \rangle = \frac{\partial^3}{\partial h_\alpha \partial h_\beta \partial h_\gamma} \ln Z. \quad (7.8)$$

Finally, we give the expression for the fourth order correlation function

$$\begin{aligned} \langle \delta O^\alpha \delta O^\beta \delta O^\gamma \delta O^\nu \rangle &= \langle \delta O^\alpha \delta O^\beta \rangle \langle \delta O^\gamma \delta O^\nu \rangle + \langle \delta O^\alpha \delta O^\gamma \rangle \langle \delta O^\nu \delta O^\beta \rangle + \langle \delta O^\alpha \delta O^\nu \rangle \langle \delta O^\beta \delta O^\gamma \rangle \\ &\quad + \frac{\partial^4}{\partial h_\alpha \partial h_\beta \partial h_\gamma \partial h_\nu} \ln Z. \end{aligned} \quad (7.9)$$

Equations (7.3) establish a relation between operators and fields. For every member h_α of a set of fields h there is a corresponding operator O^α so that derivatives with respect to h_α (with all the other h 's fixed) corresponds to putting in an extra factor of O^α . We shall see in the next section that the variable conjugate to the particle number is the chemical potential μ . It is normalized by multiplication by a temperature factor, β , so that, for example,

$$N \rightarrow \beta^{-1} \left. \frac{\partial}{\partial \mu} \right|_{\beta, \Omega}. \quad (7.10)$$

7.2 Hamiltonian Time-Dependence

Equations (7.4)–(7.9) above are essentially review for us. Now we turn to the time dependence generated by a Hamiltonian. As we recall from the last chapter, one can write equations for the time-dependence of the operators using Poisson brackets, defined in Eq. (6.36). This ‘Heisenberg representation’ has the probability, ρ , independent of time and the operators obeying

$$\frac{d}{dt}O^\alpha = \{O^\alpha, \mathcal{H}\} + \frac{\partial}{\partial t}O^\alpha. \quad (7.11a)$$

The bracket term describes how the value of the operator changes because of the time-dependence of the momenta and coordinates. If the operator is not just a function of momenta and coordinates but also has an explicit time-dependence, then that time-dependence is taken in account in the second term of Eq. (7.11a).

In contrast, one can use² a ‘Schrödinger representation’ in which the operators are independent of time but the probability density obeys

$$\frac{d}{dt}\rho = -\{\rho, \mathcal{H}\}. \quad (7.11b)$$

There is a more general way of doing the time-dependence, called the ‘interaction representation’. Split the entire Hamiltonian into two parts $\mathcal{H} = \mathcal{H}_0 + \mathcal{V}(t)$. Consider operators with no explicit time-dependence, and take \mathcal{H}_0 also to contain no explicit dependence upon t . Use the equations of motion

$$\frac{d}{dt}O^\alpha = \{O^\alpha, \mathcal{H}\}. \quad (7.12a)$$

Part of the time dependence is given to the probability density

$$\frac{d}{dt}\rho = -\{\rho, \mathcal{V}\}. \quad (7.12b)$$

Equation (7.12) is analogous to the interaction representation used in quantum field theory.

The Poisson bracket is defined as:

$$\{A, B\} = \frac{\partial A}{\partial q_\alpha} \frac{\partial B}{\partial p_\alpha} - \frac{\partial A}{\partial p_\alpha} \frac{\partial B}{\partial q_\alpha},$$

with a sum on α understood. Specific properties of these brackets include a set of relations closely analogous to the properties of commutators used in quantum theory, namely those

²In Problem 7.2 we ask for a derivation of the equivalence of the different representations. One can get the derivation with the very same mathematics which is used in the standard quantum mechanics texts.

given by Eqs. (6.37)–(6.41)

$$\{A, B\} = -\{B, A\} \quad (7.13a)$$

$$\{A, BC\} = \{A, B\}C + \{A, C\}B \quad (7.13b)$$

$$\{A, uB + vC\} = u\{A, B\} + v\{A, C\} \quad (7.13c)$$

$$\{F(A), B\} = F'(A)\{A, B\} \quad (7.13d)$$

for any operators A, B and C and any numbers u and v any function, $F(A)$, which depends upon the operator A . If A and B go to zero rapidly enough when the q 's and p 's go to infinity, then one has

$$\text{Tr}\{A, B\} = 0. \quad (7.14)$$

Here the Tr is an integral over phase space. See Problem (7.4).

The final part of the set-up for our problem is the evaluation of a statistical average of our Poisson bracket: The result is:

$$\langle\{A, B\}\rangle = \text{Tr}\left[\{A, B\}\frac{\exp(-\beta\mathcal{H})}{Z}\right] = -\beta\langle A\{B, \mathcal{H}\}\rangle = -\beta\left\langle A\frac{dB}{dt}\right\rangle, \quad (7.15)$$

for operators without any explicit time dependence.

Now we can start our calculation. Imagine that we have some operator, O^α , with no explicit time-dependence, developing in the presence of a Hamiltonian which is

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{V}(t). \quad (7.16a)$$

The $\mathcal{V}(t)$ term is explicitly time-dependent. We can expand it in terms of the basic operators in the theory:

$$\mathcal{V}(t) = -h_\nu(t)\frac{O^\nu(t)}{\beta}. \quad (7.16b)$$

The time-dependence of the results arise because the fields $h_\nu(t)$ are explicitly functions of time. To make our calculation work, we want \mathcal{H}_0 to have no explicit time dependence. We assume that $h_\nu(t)$ is zero for times earlier than t_0 and then use Eq. (7.12)

$$\frac{d}{dt}\rho = -\{\rho, \mathcal{V}\} = h_\nu(t)\frac{\{\rho, O^\nu(t)\}}{\beta}. \quad (7.17)$$

To lowest order in $h_\nu(t)$ the probability density is its value at t_0 :

$$\rho_0 = \frac{\exp(-\beta\mathcal{H}_0)}{Z}.$$

An integration of Eq. (7.17) gives the next-order result, for times, t , greater than t_0 :

$$\rho(t) - \rho_0 = \int_{t_0}^t ds h_\nu(s)\frac{\{\rho_0, O^\nu(s)\}}{\beta}. \quad (7.18)$$

To finish the calculation, calculate the average of $O^\alpha(t)$ for $t > t_0$. This average is

$$\langle O^\alpha(t) \rangle = \text{Tr} \rho(T) O^\alpha(t) = \text{Tr} [\rho_0 O^\alpha(t)] + \text{Tr} \left[O^\alpha(t) \int_{t_0}^t ds h_\nu(s) \frac{\{\rho_0, O^\nu(s)\}}{\beta} \right]. \quad (7.19)$$

Since \mathcal{H}_0 gives the time dependence of the operators, and since ρ_0 is a function of \mathcal{H}_0 one can rewrite the lowest order term in h_ν as an average at t_0 and find:

$$\begin{aligned} \langle O^\alpha(t) \rangle - \langle O^\alpha(t_0) \rangle &= \text{Tr} \left[O^\alpha(t) \int_{t_0}^t ds h_\nu(s) \frac{\{\rho_0, O^\nu(s)\}}{\beta} \right] \\ &= - \int_{t_0}^t ds \frac{h_\nu(s)}{\beta} \text{Tr}[\rho_0 \{O^\alpha(t), O^\nu(s)\}]. \end{aligned}$$

Notice that the value of $\langle O^\alpha(t_0) \rangle$ is precisely the equilibrium average determined by \mathcal{H}_0 . We demand that $h(s)$ go to zero rapidly as s goes to minus infinity. We then set t_0 equal to minus infinity and find our final result:

$$\delta \langle O^\alpha(t) \rangle = - \left\langle \int_{-\infty}^t ds h_\nu(s) \frac{\{O^\alpha(t), O^\nu(s)\}}{\beta} \right\rangle, \quad (7.20)$$

where $\delta \langle O^\alpha(t) \rangle$ stands for the deviation of the average from its value in the unperturbed system described by \mathcal{H}_0 . Thus, Eq. (7.20) describes the change in the average produced by a additional term in the Hamiltonian.

Equation (7.20) is expressed in terms of the Poisson brackets which give dynamical behavior. However, it is easy to convert the equation into an expression involving correlation functions. Use Eq. (7.15) and find

$$\delta \langle O^\alpha(t) \rangle = \int_{-\infty}^t ds h_\nu(s) \left\langle O^\alpha(t) \frac{d}{ds} O^\nu(s) \right\rangle_0, \quad (7.21)$$

where the average on the right is taken with the unperturbed density matrix, ρ_0 . Thus the result is that the correlation function

$$C_{\alpha,\nu}(t-s) = \langle O^\alpha(t) O^\nu(s) \rangle \quad (7.22)$$

appears directly in a calculation of the response since the response is

$$\delta \langle O^\alpha(t) \rangle = \int_{-\infty}^t ds h_\nu(s) \frac{d}{ds} C_{\alpha,\nu}(t-s). \quad (7.23)$$

Fourier analysis is most helpful in understanding the relation between (7.22) and (7.23). The correlation function is written as a time Fourier transform³

$$C_{\alpha,\nu}(t-s) = \int \frac{d\eta}{2\pi} S_{\alpha,\nu}(\eta) \exp(-i\eta(t-s)). \quad (7.24)$$

³This discussion, and indeed much of this chapter, is drawn from the paper by P. C. Martin and L. P. Kadanoff, LPK: Essays. The notation in that paper uses $\chi''_{\alpha,\nu}(\omega)$ instead of $S_{\alpha,\nu}(\omega)$. Notice that the form of S is dependent upon the time translational invariance which permits the use of the frequency variable ω . If the system also has spatial translational invariance, we can label each operator by a point in space, and then can also do a spatial Fourier transform to generate $S_{\alpha,\nu}(\mathbf{q}, \omega)$.

We have used η for the frequency variable since we would like to reserve ω as a symbol for the time-dependence of the field $h_\nu(s)$, which we write as

$$h_\nu(s) = h_\nu(0) \exp(-i\omega s). \quad (7.25)$$

We take ω to have a positive imaginary part, perhaps infinitesimally small, to make $h_\nu(t)$ go to zero as t goes to minus infinity. A substitution of Eq. (7.25) into (7.23) then gives:

$$\delta\langle O^\alpha(t)\rangle = \chi_{\alpha,\nu}(\omega)h_\nu(t). \quad (7.26)$$

Thus, $\chi_{\alpha,\nu}(\omega)$ describes the strength of the frequency dependent response. It is called a response function. Its value is given by Eqs. (7.24) and (7.25) as

$$\chi_{\alpha,\nu}(\omega) = \int \frac{d\eta}{2\pi} S_{\alpha,\nu}(\eta) \frac{\eta - \omega}{\eta - \omega}. \quad (7.27)$$

In this expression, ω lies in the upper half of the complex plain while η is real. The integral is well-defined and even analytic in ω in the entire upper half plain. Equation (7.27) gives a very general structure for causal responses to disturbances. A response is said to be ‘causal’ if it occurs only after the beginning of the disturbance which caused it.

7.3 Sum Rules

The low frequency form of the response is particularly simple. At zero frequency Eqs. (7.24) and (7.27) combine to give

$$\chi_{\alpha,\nu}(0) = \int \frac{d\eta}{2\pi} S_{\alpha,\nu}(\eta) = C_{\alpha,\nu}(0). \quad (7.28)$$

This is a statement in symbols of what we have already given in words: the correlation function is the zero frequency response. Notice that the integral of the dissipation function S over all frequencies gives the response χ at zero frequency. In this form the result is known as the fluctuation-dissipation theorem.

Let us focus our attention upon two different observables: the particle density $\rho(\mathbf{r}, t)$ and the particle current $\mathbf{j}(\mathbf{r}, t)$ respectively defined in terms of the particle position and momentum operators ($\mathbf{R}_k(t)$ and $\mathbf{P}_k(t)$) as:

$$\rho(\mathbf{r}, t) = \sum_{k=1}^N \delta(\mathbf{r} - \mathbf{R}_k(t)), \quad (7.29a)$$

$$\mathbf{j}(\mathbf{r}, t) = \sum_{k=1}^N \delta(\mathbf{r} - \mathbf{R}_k(t)) \frac{\mathbf{P}_k(t)}{m}. \quad (7.29b)$$

The particle conservation law reads

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0, \quad (7.30)$$

To describe the correlation functions constructed from ρ and \mathbf{j} we use notation like $C_{\rho\rho}$, $C_{\rho\mathbf{j}}$ and $C_{\mathbf{j}\mathbf{j}}$. Each of these correlation functions depends upon space and time difference variables. Thus we have:

$$\langle \delta\rho(\mathbf{r}, t)\delta\rho(\mathbf{w}, s) \rangle = C_{\rho\rho}(\mathbf{r} - \mathbf{w}, t - s).$$

In a system with space and time translational invariance, one can write a Fourier transform representation for every correlation function formed from two operators. In particular one can define $S_{\rho\rho}(\mathbf{q}, \omega)$ via

$$\langle \delta\rho(\mathbf{r}, t)\delta\rho(\mathbf{w}, s) \rangle = \int \frac{d\omega}{2\pi} \int \frac{d\mathbf{q}}{(2\pi)^d} S_{\rho\rho}(\mathbf{q}, \omega) \exp[i\mathbf{q} \cdot (\mathbf{r} - \mathbf{w}) - i\omega(t - s)]. \quad (7.31)$$

Here $\delta\rho$ stands for the deviation of the particle density from its equilibrium value.

Given these definitions, one can use the conservation law to relate current correlations to density correlations. Specifically, one has:

$$\omega S_{\rho\rho}(\mathbf{q}, \omega) = \mathbf{q} \cdot S_{\mathbf{j}\rho}(\mathbf{q}, \omega), \quad (7.32a)$$

$$\omega S_{\rho\mathbf{j}}(\mathbf{q}, \omega) = \mathbf{q} \cdot S_{\mathbf{j}\mathbf{j}}(\mathbf{q}, \omega), \quad (7.32b)$$

$$\omega^2 S_{\rho\rho}(\mathbf{q}, \omega) = \mathbf{q} \cdot S_{\mathbf{j}\mathbf{j}}(\mathbf{q}, \omega) \cdot \mathbf{q}. \quad (7.32c)$$

One can calculate some equal time correlations in a translationally invariant classical fluid. The density-density correlation function is hard. But the current, current correlation function is much easier to calculate because it is related to momentum correlations. We have:

$$C_{j_\mu j_\nu}(\mathbf{r} - \mathbf{w}, 0) = \left\langle \sum_{k=1}^N \delta(\mathbf{r} - \mathbf{R}_k(t)) \frac{P_{k\mu}(t)}{m} \sum_{l=1}^N \delta(\mathbf{w} - \mathbf{R}_l(t)) \frac{P_{l\nu}(t)}{m} \right\rangle. \quad (7.33)$$

A classical, time-independent situation is described by a Boltzmann distribution in which all momenta are uncorrelated with one another and with particle positions. Therefore our correlation function reduces to

$$C_{j_\mu j_\nu}(\mathbf{r} - \mathbf{w}, 0) = \left\langle \sum_{k=1}^N \delta(\mathbf{r} - \mathbf{R}_k(t)) \frac{P_{k\mu}}{m} \delta(\mathbf{w} - \mathbf{R}_k(t)) \frac{P_{k\nu}}{m} \right\rangle.$$

The average momentum squared is mkT . Each term in the sum contributes the same amount and thus

$$C_{j_\mu j_\nu}(\mathbf{r} - \mathbf{w}, 0) = \frac{N}{m\beta} \delta(\mathbf{w} - \mathbf{r}) \delta_{\mu,\nu} \langle \delta(\mathbf{r} - \mathbf{R}_k(t)) \rangle.$$

The final average has an integral over all space which has the value unity. Since it is spatially uniform this average is $1/\Omega$. Our final sum evaluation of the equal time correlation function is thus:

$$C_{j_\mu j_\nu}(\mathbf{r} - \mathbf{w}, 0) = \frac{\rho}{m\beta} \delta(\mathbf{w} - \mathbf{r}) \delta_{\mu,\nu}. \quad (7.34)$$

From the Fourier transform representation of C we find

$$\int \frac{d\eta}{2\pi} S_{j_\mu j_\nu}(\mathbf{q}, \eta) = \frac{\rho}{m\beta} \delta_{\mu, \nu}. \quad (7.35)$$

Take the scalar product of Eq. (7.35) with \mathbf{q} on both indices and find

$$\int \frac{d\eta}{2\pi} \eta^2 S_{\rho\rho}(\mathbf{q}, \eta) = \frac{\rho}{m\beta} q^2. \quad (7.36)$$

7.4 Non-Interacting Particles

Let us calculate this correlation function for non-interacting particles as described by a Boltzmann distribution. Since the particles are non-interacting, there is no correlation between different particles. Therefore Eq. (7.29a) gives

$$\begin{aligned} \langle \delta\rho(\mathbf{r}, t)\delta\rho(\mathbf{w}, s) \rangle &= \left\langle \sum_{k=1}^N \delta(\mathbf{r} - \mathbf{R}_k(t))\delta(\mathbf{w} - \mathbf{R}_k(s)) \right\rangle \\ &= N\langle \delta(\mathbf{r} - \mathbf{R}_k(t))\delta(\mathbf{w} - \mathbf{R}_k(s)) \rangle. \end{aligned} \quad (7.37)$$

The particles do not interact with anything. Therefore particle number k will retain its momentum \mathbf{p} for all time. If the particle is at $\mathbf{R}_k(t)$ at time t it is at $\mathbf{R}_k(t) + (s-t)\mathbf{P}_k/m$ at time s . Thus the right hand side is

$$\begin{aligned} &= N\langle \delta(\mathbf{r} - \mathbf{R}_k(t))\delta(\mathbf{w} - \mathbf{R}_k(t) - (s-t)\mathbf{P}_k/m) \rangle \\ &= N\langle \delta(\mathbf{r} - \mathbf{R}_k(t))\delta(\mathbf{w} - \mathbf{r} - (s-t)\mathbf{P}_k/m) \rangle. \end{aligned}$$

There are two averages here. The first averages the position over all possible places within the volume, Ω and gives

$$\langle \delta(\mathbf{r} - \mathbf{R}_k(t)) \rangle = \Omega^{-1}.$$

The second is an average over momentum with the usual Boltzmann probability distribution. This Gaussian distribution gives

$$\begin{aligned} \langle \delta\rho(\mathbf{r}, t)\delta\rho(\mathbf{w}, s) \rangle &= \frac{N}{\Omega} \langle \delta(\mathbf{w} - \mathbf{r} - (s-t)\mathbf{P}_k/m) \rangle \\ &= \frac{N}{\Omega} \left(\frac{1}{2\pi m k T} \right)^{d/2} \int d\mathbf{p} e^{-\beta p^2/2m} \langle \delta(\mathbf{w} - \mathbf{r} - (s-t)\mathbf{p}/m) \rangle. \end{aligned} \quad (7.38)$$

We replace N/Ω by the equilibrium particle density ρ and find the final result

$$\langle \delta\rho(\mathbf{r}, t)\delta\rho(\mathbf{w}, s) \rangle = \rho |(s-t)|^{-d} \left(\frac{m\beta}{2\pi} \right)^{d/2} \exp \left(-\frac{\beta m |\mathbf{w} - \mathbf{r}|^2}{2|s-t|^2} \right). \quad (7.39)$$

We calculate a spatial fourier transform to rewrite this result as

$$\langle \delta\rho(\mathbf{r}, t)\delta\rho(\mathbf{w}, s) \rangle = \rho \int \frac{d\mathbf{q}}{(2\pi)^d} \exp[i\mathbf{q} \cdot (\mathbf{r} - \mathbf{w}) - \mathbf{q}^2(s - t)^2/(2m\beta)],$$

which in turn can be written as a full Fourier transform as given in Eq. (7.31) with:

$$S_{\rho\rho}(\mathbf{q}, \omega) = \chi_0(\mathbf{q}, \omega) = \rho \sqrt{\frac{2\pi m\beta}{|\mathbf{q}|^2}} \exp\left(-\frac{m\beta\omega^2}{2\mathbf{q}^2}\right). \quad (7.40)$$

We use the notation $\chi_0(\mathbf{q}, \omega)$ for this Fourier transform in the noninteracting system.

7.5 Plasma Behavior

We imagine a gas with Coulomb forces. The gas is composed of N discrete particles with mass m and charge e confined to a region with volume Ω . The charge density is Ne/Ω ; the particle density, ρ , is N/Ω . This density is grainy because the charge is contained in point particles. In addition there is a uniform background of charge of the opposite sign with charge density $-Ne/\Omega$.

That is the problem. Now let us consider our approach. Imagine that the system were excited by applying an electrical potential to it. The electrical potential couples to the charges in a term:

$$\int d\mathbf{r} e\phi(\mathbf{r}, t)\rho(\mathbf{r}, t),$$

where ϕ is a scalar potential for the electromagnetic field and $e\rho$ is the operator which represents the local density of charge. As a coulomb system, the scalar potential is given by:

$$\phi(\mathbf{r}, t) = \phi_0(\mathbf{r}, t) + \int d\mathbf{s} v(\mathbf{r} - \mathbf{s}) \left[e\rho(\mathbf{s}, t) - \frac{eN}{\Omega} \right]. \quad (7.41)$$

The potential v is the standard coulomb interaction, with the form

$$v(\mathbf{r}) = \int \frac{d\mathbf{q}}{(2\pi)^d} \frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{q^2}. \quad (7.42)$$

Thus, $v(\mathbf{r})$ has values proportional to

$- \mathbf{r} $	in one dimension	(7.43)
$-\ln \mathbf{r} $	in two dimensions	
$1/ \mathbf{r} $	in three dimensions	
$1/ \mathbf{r} ^{d-2}$	for all dimensions	

In one and two dimensions, the potential contains an infinite constant, which we have implicitly subtracted away.

We are ready to start the calculation. Imagine that we calculate the response to an external electric field, $\mathbf{D}(\mathbf{r}, t) = iq\phi_0(\mathbf{r}, t)$ where ϕ_0 is an external scalar potential. This potential has the form

$$\phi_0(\mathbf{r}, t) = \phi_{00} e^{i\mathbf{q}\cdot\mathbf{r}-i\omega t}.$$

Notice then that the extra term in the action is

$$-\beta \int d\mathbf{r} \phi_0(\mathbf{r}, t) \left[e\rho(\mathbf{r}, t) - \frac{Ne}{\Omega} \right].$$

If we had non-interacting particles this response would be given by a change in the charge density which is:

$$\delta\rho(\mathbf{r}, t) = -\chi_0(\mathbf{q}, \omega)e\phi_0(\mathbf{r}, t)\beta. \quad (7.44)$$

Here $\chi_0(\mathbf{q}, \omega)$ is the response function for non-interacting particles. It is obtained by substituting the non-interacting form (7.40) for $S_{\rho\rho}$ into the dispersion relation (7.27) for $\chi_0(\mathbf{q}, \omega)$.

The Coulomb force has a very long range. Each particle feels the forces produced by lots and lots of other particles. In this situation, we can in our first thinking about the subject, only take into account the average value of the produced field. This approach is called the mean field approximation. When we consider the average response, ignoring the fluctuations in the produced fields, we find from Eq. (7.41)

$$\phi(\mathbf{r}, t) = \phi_0(\mathbf{r}, t) + \int d\mathbf{s} v(\mathbf{r} - \mathbf{s})e\delta\rho(\mathbf{s}, t). \quad (7.45)$$

Here, $\phi(\mathbf{r}, t)$ is the total scalar potential in the system. It has two sources. First, there is the part, ϕ_0 , produced by charges external to the system. Secondly, the particles respond to the field by moving about some. The result of the motion is a average charge density which, like $\phi_0(\mathbf{r}, t)$, has wave vector \mathbf{q} and frequency ω . Then Eq. (7.45) reads

$$\phi(\mathbf{r}, t) = \phi_0(\mathbf{r}, t) + \frac{1}{q^2}e\delta\rho(\mathbf{r}, t). \quad (7.46)$$

The mean field approximation is the statement:

The charge density in the system, responds to the total field ϕ in exactly the same way as free particles would respond to an applied field ϕ_0 .

In symbols:

$$\delta\rho(\mathbf{r}, t) = -\chi_0(\mathbf{q}, \omega)e\phi(\mathbf{r}, t)\beta. \quad (7.47)$$

Thus, when we substitute (7.47) into (7.45) we come to our result:

$$\phi(\mathbf{r}, t) = \frac{\phi_0(\mathbf{r}, t)}{1 + e^2\beta\chi_0(\mathbf{q}, \omega)/q^2}. \quad (7.48)$$

Another form of the same result is:

$$\delta\rho(\mathbf{r}, t) = -\frac{q^2\chi_0(\mathbf{q}, \omega)e\beta\phi_0(\mathbf{r}, t)}{q^2 + e^2\beta\chi_0(\mathbf{q}, \omega)}. \quad (7.49)$$

To interpret these results first consider the limit in which ω goes to zero. Then, according to Eq. (7.27),

$$\chi_{\alpha,\nu}(0) = \int \frac{d\eta}{2\pi} S_{\alpha,\nu}(\eta)$$

and if we use expression (7.40) we get find that the value of the response function at zero frequency is $\chi_0(\mathbf{q}, 0) = \rho$, leaving us with an expression in which

$$\phi(\mathbf{r}, t) = \frac{\phi_0(\mathbf{r}, t)}{1 + q_s^2/q^2}, \quad (7.50)$$

with $q_s^2 = \beta\rho e^2$. Here, q_s has the physical meaning of an inverse screening length.

To see how this works out, imagine that the unperturbed field was the same as produced by a point charge at the origin:

$$\phi_0(\mathbf{r}, t) = e \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{q^2} = e \frac{1}{4\pi|\mathbf{r}|}. \quad (7.51)$$

Then the full field is the same expression as in Eq. (7.51) with each component multiplied by the factor in Eq. (7.50) so that

$$\phi(\mathbf{r}, t) = e \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{q^2 + q_s^2} = e \frac{e^{-q_s|\mathbf{r}|}}{4\pi|\mathbf{r}|}. \quad (7.52)$$

(We have done this calculation in three dimensions since that is a case in which the integrals are particularly simple.) The field in Eq. (7.51) extends a long, long distance from the origin. The field in Eq. (7.52) is cut off exponentially at a distance, called the screening length, given by q_s^{-1} .

This screening has a very direct physical interpretation. Imagine placing a charge in the plasma. By definition a plasma contains charges free to move. Here the moving particles have charge e . To balance out these particles there is a ‘jelly’ containing an equal and opposite charge uniformly distributed over the whole system. This balancing charge stays still and does not move at all. A test charge placed in the plasma will tend to attract particles with the opposite sign of charge and will tend to push away charges with the same sign of charge. The end result is that there is a small region near the test charge in which there is a buildup of opposite charge. That screening region will contain a charge of just large enough to compensate the test charge. This charged region is called a screening cloud. Its size is the screening length we have already defined. The net result is that from far away, the test charge plus the screening cloud look like an uncharged region. As one penetrates the screening cloud, one sees less and less screening and more and more of the test charge.

All this describes the behavior of a plasma, a gas in which particles are free to move. The alternative word for such a gas is a conductor, meaning a material which can support

the motion of electrical currents. On the other hand, one can find many materials in which charges are not free to move over long distances. For example, salt (NaCl) is a crystal in which positive ions (Na^+) and negative (Cl^-) sit on the sites of a regular lattice. Both kinds of charge can move a little in response to an applied field. This kind of material is called a dielectric or an insulator. There is some reduction (by a factor of the dielectric constant) of the field produced by a test charge within the material, but there is never perfect screening within this dielectric material. Return to the plasma. We have now analyzed its low frequency response behavior. Let us ask in contrast what happens to the charges in the limit of high frequency. Go back to Eq. (7.27), written as

$$\chi_{\rho,\rho}(\mathbf{q}, \omega) = \int \frac{d\eta}{2\pi} S_{\rho,\rho}(\mathbf{q}, \eta) \frac{\eta}{\eta - \omega}$$

and expand under the integral in a power series in η/ω . The first few orders are:

$$\chi_{\rho,\rho}(\mathbf{q}, \omega) = - \int \frac{d\eta}{2\pi} S_{\rho,\rho}(\mathbf{q}, \eta) \left[\frac{\eta}{\omega} + \frac{\eta^2}{\omega^2} + \frac{\eta^3}{\omega^3} + \dots \right]. \quad (7.53)$$

Most gases have parity invariance in which a change of the sign of a vector leaves all physical quantities unchanged. We assume this property for our plasma and thus demand $S_{\rho,\rho}(\mathbf{q}, \eta) = S_{\rho,\rho}(-\mathbf{q}, \eta)$. Since the space-time correlation function which defines $S_{\rho,\rho}(\mathbf{q}, \eta)$ must be an even function of its arguments, we now have $S_{\rho\rho}(\mathbf{q}, \eta) = S_{\rho,\rho}(-\mathbf{q}, -\eta)$. Thus, the odd terms vanish in Eq. (7.53) and we find that in the limit as $\omega \rightarrow \infty$,

$$\chi_{\rho,\rho}(\mathbf{q}, \omega) \rightarrow - \int \frac{d\eta}{2\pi} S_{\rho,\rho}(\mathbf{q}, \eta) \frac{\eta^2}{\omega^2}.$$

The integral is evaluated in (7.36) which then gives us

$$\chi_{\rho,\rho}(\mathbf{q}, \omega) \rightarrow - \frac{\rho}{m\beta\omega^2} q^2. \quad (7.54)$$

Thus, in the high frequency limit Eq. (7.48) implies

$$\phi(\mathbf{r}, t) = \frac{\phi_0(\mathbf{r}, t)}{1 - \omega_p^2/\omega^2}, \quad (7.55)$$

with $\omega_p^2 = e^2 \rho / m$. The frequency, ω_p , is called the plasma frequency.

Equation (7.55) indicates that an infinitesimal disturbance with a frequency close to ω_p will produce a large total electric field. The same analysis shows that there is a tendency to produce particularly large charge fluctuations at that frequency. The analysis is accurate when the produced frequency is high. Therefore, what we are seeing is a system which has a natural tendency to oscillate or ‘ring’ at this high frequency. Such ringing has been observed in the plasma which surrounds the earth. The oscillations are produced by the following mechanism: Imagine that the charged particles with charge e all move with respect to the background particles. The latter remain at rest. They then pull the other particles back toward them. The particles pick up speed, move in to the background particles, and shoot right by them. Then the whole story starts again. A natural oscillation is produced which eventually stops because of damping mechanisms which we have not included here.

Homework

Problem 7.1 (Quantum Fluctuations).

- (1) Explain in words why Eq. (7.7) does not work in a quantum situation.
- (2) Show that it does not work by considering the Hamiltonian:

$$-\beta\mathcal{H} = K\tau_3 + h_1\tau_1 + h_2\tau_2.$$

Problem 7.2 (The Different Representations). In the Hamiltonian formulation of classical mechanics, give an example of a nontrivial operator which has an explicit time-dependence.

Show that the different representations: Heisenberg, Schrödinger, and interaction all give the same answers for the time dependence of any average.

Problem 7.3 (The Unit Operator). The unit operator is defined as a non-fluctuating quantity which always has the value 1. Please see what becomes of the relations (7.4)–(7.9) when one of the operators inside the average is the unit operator.

Problem 7.4 (Trace Theorem). Derive Eqs. (7.14) and (7.15).

Problem 7.5 (Self-Correlations in a Non-interacting system). Use the results of Sec. 7.4 to find the average of powers of the particle separation, specifically $|w - r|^2$ and $|w - r|^4$, as a function of $t - s$. Use a dimensional argument to get the order of magnitude of the result.

Problem 7.6 (Another Sum Rule). Derive an equation for

$$\int \frac{d\eta}{2\pi} \eta S_{\rho\rho}(\mathbf{q}, \eta)$$

by using arguments like the one which led to Eq. (7.36)

Problem 7.7 (Sum Rule Example). Calculate

$$\int \frac{d\eta}{2\pi} \eta^2 S_{\rho\rho}(\mathbf{q}, \eta)$$

by using the expression for S given in Eq. (7.40).

Part III

More Statistical Mechanics

Chapter 8

Statistical Thermodynamics

In this chapter we consider the relationship between statistical mechanics and thermodynamics. The subject which lies between these two disciplines is called *statistical thermodynamics*. In our development of this area of intersection, we shall be particularly interested in the meaning of several of the basic variables specifically the chemical potential, temperature, and entropy. We start with the chemical potential. We define it and then use this definition by looking at the barometer formula, which predicts the density of molecules in the atmosphere as a function of height. We then describe some different formulations of statistical mechanics, defined by averaging over different sets (or *ensembles*) of states. The different ensembles give us natural definitions of entropy, free energy, and pressure. This ensemble point of view gives us a natural framework for discussing temperature as the quantity which determines the partition of energy between two weakly-coupled containers. We thus see why two bodies in equilibrium with one another should have the same temperature. Finally, we describe how the discussion of temperature can be modified to apply to the chemical potential.

8.1 The Chemical Potential Defined

In this chapter, we shall again make use of the one particle distribution function, $f(\mathbf{p}, \mathbf{r}, t)$, which is defined to be proportional to the probability that we will find a particle with momentum \mathbf{p} at the space point \mathbf{r} . Consider again the situation of Brownian motion in which there are N particles bouncing around, independently buffeted by the repeated collisions with much smaller particles. If we are looking at N individual particles, $f(\mathbf{p}, \mathbf{r}, t)$ is related to the probability density, ρ_j , for the individual particle by:

$$\frac{f(\mathbf{p}, \mathbf{r}, t)}{w} = \sum_{j=1}^N \rho_j(\mathbf{p}, \mathbf{r}, t) = \left\langle \sum_{j=1}^N \delta(\mathbf{P}_j(t) - \mathbf{p}) \delta(\mathbf{R}_j(t) - \mathbf{r}) \right\rangle. \quad (8.1)$$

(For more information see the discussion around Eq. (6.21).) Once again we have put in an entirely gratuitous factor of $w = h^3$ in order to make the transition to the quantum mechanical case easier.¹ According to the analysis we have just given when the system is allowed to find its equilibrium behavior, it constructs an exponential of the Hamiltonian, $\mathcal{H}(\mathbf{p}, \mathbf{r})$, in the form

$$f(\mathbf{p}, \mathbf{r}) = \exp(\beta\mu) \times \exp(-\beta\mathcal{H}(\mathbf{p}, \mathbf{r})) \quad (8.2)$$

where the constant, $\exp(\beta\mu)$, is picked to give f the appropriate normalization. Since this is just an adjustable constant, we may write it in any way we choose just so long as we leave some suitable thing left to adjust. Here we follow the conventional notation, and define the normalization by using a new thermodynamic variable called the *chemical potential*, μ . Alternatively we might say that the density of particles is proportional to $\exp(\beta\mu)$, which is called a *fugacity*.

Equation (8.2) is a rather specific result which applies when the Hamiltonian includes all the important interactions among particles and with the environment. To illustrate the use of this result, we consider once again the case in which \mathcal{H} is the sum of a kinetic energy and a potential energy $U(\mathbf{r})$. For example, if the particle is moving in the gravitational field near the earth, the gravitational potential energy is

$$U(\mathbf{r}) = -mg \cdot \mathbf{r} \quad (8.3)$$

with \mathbf{g} being the acceleration of gravity. The content of Eq. (8.2), which then becomes $f(\mathbf{p}, \mathbf{r}) = \exp[-\beta\mathbf{p}^2/(2m) - \beta U(\mathbf{r}) + \beta\mu]$ is that the \mathbf{r} dependence is totally given by the appearance of \mathbf{r} in the potential energy. This applies to a weakly interacting particle. But, we can say something much more general:

For all bodies which are in thermodynamic equilibrium have their behavior described by such thermodynamic parameters as the inverse temperature, β , and the chemical potential, μ . The β appears because the energy of the system is conserved; the μ because the number of particles is conserved. If there is more than one type of conserved particle, there will be a chemical potential associated with each of the conserved species. When there are several large bodies in weak contact with one another, so that they might be exchanging particles and energy, they will be in equilibrium with one another only if the β 's and each kind of chemical potential for the different bodies are precisely equal. If they are not equal the sign of the difference determine the direction of flow of the correspond conserved quantity. Energy in the form of heat will flow from the hotter (lower β) body to the colder, and particles will flow from higher chemical potentials to lower.

¹If one were only doing classical systems one could leave w out and the only thing which would change is that an extra, additive constant would appear in the chemical potential.

Thus, in this way of approaching the subject, the form of expression (8.3) is fixed by the fact that different spatial regions of the fluid are in equilibrium, so their neither β nor μ may vary in space.²

8.2 Barometer Formula

The density of particles $n(\mathbf{r}, t)$ is defined so that $n(\mathbf{r}, t)d\mathbf{r}$ is the number of particles within a volume of size $d\mathbf{r}$ about the point \mathbf{r} . The definition of f then tells us that n is the momentum integral of f , i.e.

$$n(\mathbf{r}, t) = \int d\mathbf{p} f(\mathbf{p}, \mathbf{r}, t)/w. \quad (8.4)$$

According to Eq. (8.3) this density can be calculated for an equilibrium system with molecules moving through as potential $U(\mathbf{r})$ as

$$n(\mathbf{r}) = K e^{-\beta U(\mathbf{r})} \quad (8.5)$$

where the \mathbf{r} -independent constant is

$$K = e^{\beta\mu} (2\pi m k T)^{3/2} h^{-3}. \quad (8.6)$$

with k being the Boltzmann constant.

In an equilibrium system which has no space-dependent potential, the density is constant through the containing volume, Ω and has the value N/Ω . Thus, in a equilibrium classical system, the chemical potential has the value

$$\mu = kT \ln \left[\frac{N}{\Omega} h^3 (2\pi m k T)^{-3/2} \right] \quad (8.7)$$

This information about the exact value of the chemical potential is not too important for us right now. Instead, we care mostly that the constant, K , in Eq. (8.5) does not vary in space. Therefore, we do know the dependence of the density upon position. For one species, say Nitrogen molecules, the density is

$$n(\mathbf{r}) = n(\mathbf{0}) \exp \left(-\frac{mgh}{kT} \right), \quad (8.8)$$

where h is the height and m the mass of the molecule. In this exponential decay formula, we see that the density of nitrogen molecules decreases by a factor of e for each increase of height by an amount equal to the scale height, which is

$$h_0 = \frac{kT}{mg}. \quad (8.9)$$

²In our actual atmosphere, the temperature does vary from place to place. Typically, above the earth, the temperature falls to some value like -30°C . Thus β can vary by the order of $\pm 10\%$ within the nearer regions of the earth's atmosphere. This variation is caused by solar heating and radiative cooling which continually provide outside sources and sinks of energy and prevent the earth's atmosphere from coming to equilibrium. In equilibrium, our analysis would be easier but there could be no rain or snow or variability in the weather.

Equation (8.8) is called the barometer formula. It is roughly but not exactly true in the actual atmosphere. It would be correct were the gases in the atmosphere given enough time to come to thermodynamic equilibrium. But, instead, hot gas rises off the surface of the earth and moves upward without having enough time to come into thermal equilibrium with its surroundings. The temperature variations thus produced make Eq. (8.8) not fully accurate.

8.3 Sharing Energy

A thermodynamic system can gain or lose energy in two different ways. First, the system can do work. If a gas within a container pushes against a piston and does work by pushing the piston outward, the energy of the gas decreases by the amount of work done

$$dE = -p d\Omega ,$$

where p is the pressure, assumed constant, and $d\Omega$ is the change in volume. Even if the volume does not change, the amount of energy within the system may change as heat flows into and out of our system. Heat is usually described as energy in the form of disorderly atomic or molecular motion. Changes in the amount of heat energy are generally denoted by δQ so that the energy balance equation is

$$\delta Q = dE + p d\Omega , \quad (8.10)$$

where δQ is the amount of heat entering our system.

Classical thermodynamics starts with Eq. (8.10). This is the first law of thermodynamics which states that if you keep track of the heat entering a leaving a given system, you have in net a conservation of energy. The next part of thermodynamics is the second law. This is based upon asking which quantities in this equation can be determined if we know the ‘state’ of the system. Empirically, if we have a one component gas, we can define the situation in the gas if we know the temperature of the gas, T , its number of particles, N , and the volume in which the system is confined, Ω . Once these three quantities are defined everything else about the system is fully characterized. Thus, for example, the energy and the pressure are function of these quantities: $E = E(T, N, \Omega)$ and $p = p(T, N, \Omega)$. Once the system is characterized we say that we know the *state* of the system.

Equation (8.10) is written for the case in which no particles enter or leave the system. The generalization of that equation to a situation in which the number of particles, N , is changed is

$$\delta Q = dE + p d\Omega - \mu dN . \quad (8.11)$$

The coefficient, μ , in this relationship describes the amount of heat you put in when you add one particle to a system while holding the energy and volume fixed. It is, of course, the very same chemical potential as appeared in our previous discussion.

Each of the changes $dE, d\Omega, dN$ and the right hand side of Eq. (8.11) are changes in quantities which are completely determined once you know the full thermodynamic information about the present state of the system. Quantities like these which depend upon the state of the system but not its past history are called *state functions*. The energy, the pressure, the chemical potential, N , and Ω are all state functions. There is no state function corresponding to the amount of heat within the system. One can add an arbitrarily large amount of heat to the system, without changing its internal state, if in the process one makes the system do a correspondingly large amount of work. These cycles which add heat and do work are the basic mechanism of all engines. Hence there is no statistical function Q corresponding to the change δQ . (That is why one uses a ‘ δ ’ rather than a ‘ d ’ notation for this change.)

However, the changes δQ are not arbitrary. According to the second law of thermodynamics, there are two more state functions for systems in thermodynamic equilibrium. These are first the temperature, T , and the entropy, S . When everything is changing so slowly that it is reasonable to apply thermodynamic concepts, the heat flow is related to the change in S via

$$\delta Q = T dS. \quad (8.12)$$

Equation (8.12) is a succinct statement of the second law of thermodynamics. The content of this equation is that the entropy, defined in this manner, is a state function. As we shall see in a moment, S directly measures the amount of disorder in the system. Equations (8.11) and (8.12) together give an equation which we shall use as the font of much thermodynamic wisdom:

$$TdS = dE + p d\Omega - \mu dN \quad (8.13)$$

for any changes which keep the system in equilibrium. We shall have several equivalent reformulations of the laws of thermodynamics. (The first of these was given in our introductory outline, as Eq. (1.10).) To keep track of these, we collect them in a tabular form in Table 8.1:

Equation (8.13) is a thermodynamic statement of the definition of entropy. Instead of approaching the entropy solely in the thermodynamic mode, we in addition define it in

Thermodynamic function	Function of	Differential	Relation to previous function
$S = \text{entropy}$	E, N, Ω	$TdS = dE + pd\Omega - \mu dN$	
$F = \text{free energy}$	T, N, Ω	$dF = -SdT - pd\Omega + \mu dN$	$F = E - TS$
$p = \text{pressure}$	T, μ	$dp = \frac{S}{\Omega}dT + \frac{N}{\Omega}d\mu$	$p\Omega = \mu N - E + TS$

Table 8.1. Thermodynamic functions and their derivatives.

terms of statistical mechanics. We define a statistical mechanical entropy, S in terms of the volume of phase space available to the system via the statement:

$$\exp \left[\frac{S(E, N, \Omega)}{k} \right] = \int d\Gamma_N \delta(H(p, q) - E), \quad (8.14a)$$

where $d\Gamma_N$ is defined by the Eq. (1.4).

$$(1.4) \quad d\Gamma_N = \frac{1}{W_N} \prod_{j=1}^N d\mathbf{p}_j d\mathbf{q}_j = \frac{1}{N!} \prod_{j=1}^N \frac{d\mathbf{p}_j d\mathbf{q}_j}{h^3}$$

and k is the Boltzmann constant. Equation (8.14a) is another definition of the entropy. As we shall see, this definition gives an entropy with exactly the same properties as the thermodynamic entropy. We shall call the subject which derives from the definition (8.14a) as *statistical thermodynamics* to distinguish it from the more classical approach to thermodynamics, which derives from Eq. (8.13). Notice that Eq. (8.14a) defines S as a state function, which is expressed as $S(E, N, \Omega)$. The corresponding quantum mechanical definition of entropy is even more instructive. Recall that, according to our overview, to go from classical to quantum statistical mechanics one replaces $d\Gamma_N$ by a sum over states at fixed N and then H by the energy eigenvalue E_α . Unfortunately, the resulting expression

$$\exp \left[\frac{S(E, N, \Omega)}{k} \right] = \sum_\alpha \delta(E - E_\alpha)$$

makes hardly any sense. The sum of delta functions is a very bumpy function which is zero almost everywhere but which has infinitely high peaks at some very closely spaced set of values. To make the entropy smoother, we define a smoothed out delta function

$$\delta_\Delta(E) = \begin{cases} 0 & \text{if } E > 0 \\ \Delta^{-1} & \text{if } 0 > E > -\Delta \\ 0 & \text{if } E < -\Delta \end{cases}$$

Here Δ is picked to be a rather small positive energy which is nonetheless much larger than the distance between energy levels. With this choice, and the alternative definition of entropy

$$\exp \left[\frac{S(E, N, \Omega)}{k} \right] = \sum_\alpha \delta_\Delta(E - E_\alpha), \quad (8.14b)$$

we get an expression which is very easily interpreted. The sum on the right measures the number of energy levels between $E - \Delta$ and E divided by the energy interval, Δ . Thus the entropy can be interpreted by saying that

$$\exp \left(\frac{S(E, N, \Omega)}{k} \right)$$

is the number of states available to the system at a given value of E . Or more precisely, it is the number of states per unit interval of energy. Strictly speaking these two definitions give quantities which differ by a factor of Δ . However, the actual number of states is so huge and so rapidly growing with E that the factor Δ simply counts for nothing in comparison. Consequently we say that

$$\exp(S/k) \text{ is the number of states available to the system.}$$

We also use the same words for the classical case despite the fact that there are no states in classical mechanics. Instead we are really counting the available volume in phase space divided by the volume of the basic quantum phase-space cell: h^{3N} .

We recall a factor like this $\exp(S/k)$ from our discussion of the probabilistic behavior of the energy in Sec. 3.7. In that discussion we saw — in a simple example — that the entropy, S , is a rapidly growing function of E . We also saw that we could calculate the partition function:

$$Z(\beta, N, \Omega) = \int d\Gamma_N \exp(-\beta H(p, q))$$

as an energy integral. That energy integral was a fight between an entropy which grows very rapidly in E and an energy factor $-\beta E$ which falls off very rapidly. Exactly this same calculation may be done quite generally by writing the partition function in terms of an energy integral

$$Z(\beta, N, \Omega) = \int d\Gamma_N \exp(-\beta H(p, q)) \int dE \delta(H(p, q) - E),$$

rearranging as

$$Z(\beta, N, \Omega) = \int dE \int d\Gamma_N \delta(H(p, q) - E) \exp(-\beta E)$$

and then carrying it into the form:

$$Z(\beta, N, \Omega) = \int dE' \exp \left[\frac{S(E', N, \Omega)}{k} \right] \exp(-\beta E'). \quad (8.15)$$

This equation merits our attention. From the definition of probabilities in classical statistical mechanics we see that we can interpret the integrand in Eq. (8.15) by saying that

$$\exp \left[\frac{S(E', N, \Omega)}{k} \right] \frac{\exp(-\beta E')}{Z(\beta, N, \Omega)},$$

is the probability of observing a system which is known to have the temperature β to have its energy equal to E' . The integral in (8.15) is easily evaluated. It contains two factors:

$$\exp \left[\frac{S(E', N, \Omega)}{k} \right] \quad \text{and} \quad \exp(-\beta E').$$

The first counts the number of ways that our system can realize an energy equal to E' . As in our earlier calculation, this factor grows rapidly as E' is increased. On the other

hand, the temperature factor decreases exponentially with E' . These two work against one another, with the first factor winning for small E' and the second for large E' . In both limits, the integrand goes strongly to zero. In between, somewhere, there is a point where the integrand reaches a maximum. As we shall see, that maximum is very, very sharp. This maximum contribution to the integral comes when the exponent reaches an extreme value, i.e. when its slope is zero, and that happens when

$$\frac{\partial S(E', N, \Omega)}{\partial E'} \Big|_{N, \Omega} - \frac{1}{T} = 0. \quad (8.16)$$

Equation (8.16) is not something new. It is a direct consequence of the first line of Table 8.1 and shows that our statistical definition of entropy (and temperature) can agree with the thermodynamic definitions of these quantities.

We finish up the calculation by finding the partition function. The integral over E' in Eq. (8.15) is very strongly peaked around a single number

$$E' = E(\beta, N, \Omega). \quad (8.17)$$

To see this sharp peaking, define a difference in energy from the average as

$$\Delta E = E' - E(\beta, N, \Omega) \quad (8.18)$$

contributions to the integral. We once more follow through the approach for obtaining and evaluating a quasi-Gaussian integral. Start by expanding the exponent in Eq. (8.15) in a Taylor series in ΔE . The first term in the expansion vanishes in virtue of the extremal condition (8.16), and the integral becomes:

$$Z(\beta, N, \Omega) = \exp \left[\frac{S(E(\beta, N, \Omega))}{k} \right] \exp(-\beta E(\beta, N, \Omega)) \int d\Delta E \exp \left(-\frac{C^{-1} \Delta E^2}{2} \right). \quad (8.19)$$

In the final integrand C^{-1} is a abbreviation for the Taylor expansion coefficient

$$\begin{aligned} C^{-1} &= -\frac{\partial^2 S(E, N, \Omega)}{(\partial E)^2} \Big|_{N, \Omega}, \\ C^{-1} &= -\frac{\partial T^{-1}}{\partial E} \Big|_{N, \Omega}, \\ C &= T^2 \frac{\partial E}{\partial T} \Big|_{N, \Omega}, \end{aligned} \quad (8.20)$$

where this coefficient is to be evaluated at the energy, $E(\beta, N, \Omega)$, defined by the peak in the integral. We have again made use of the first line in Table 8.1 to rewrite the derivative. Notice that C must be non-negative for the state to be stable.

The reason that the integral may be evaluated in this manner is that the number of particles in the system, N , is quite large. We imagine doing this calculation for a large

system by holding the intensive quantities N/Ω (density) and E/N (energy per particle) fixed and letting N increase without limit. Then, E, Ω, N , and S are each extensive in that they grow proportionally with N as the system grows larger but its internal properties, say β and N/Ω , are held fixed. It follows from the definition (8.20) that unless something very special happens, C grows proportionally with N . Therefore the logarithm of the first two terms in Eq. (8.19) are each proportional to N . On the other hand, the integral gains its main contribution while ΔE is of order $C^{1/2}$, that is of order $N^{1/2}$. The integral has the value $\sqrt{2\pi C}$ which is completely dominated by the other two terms in the expression. The latter terms are, after all, exponential in N . Thus, to lowest order, we find that the partition function has the value given by Eq. (8.19):

$$Z(\beta, N, \Omega) = \exp \left[\frac{S(E(\beta, N, \Omega))}{k} \right] \exp[-\beta E(\beta, N, \Omega)]. \quad (8.21)$$

Equation (8.21) gives an important relation between the partition function and the entropy. It is one of the main points in statistical thermodynamics.

We conclude this argument by saying why C must not be negative. There are two arguments for this. One is thermodynamic in character. The quantity C , as we have defined it, is proportional to the specific heat at constant volume.³ However, if this quantity is negative, the system becomes unstable against processes which subtract energy from one part of it and add energy to another.⁴ The second argument uses statistical mechanics. According to Eq. (2.25), the derivative on the second line of (8.20) must be proportional to $\langle (H - \langle H \rangle)^2 \rangle$. Since the average of a non-negative quantity must be non-negative, C must be positive. Consequently the whole approach does indeed make sense.

8.4 Ensemble Theory

We have been talking our way around a part of statistical mechanics called ensemble theory. This is the theory of how to use statistical mechanics to define averages in various situations. The sets of configurations or of quantum states used in the average is called an ensemble, and hence the whole subject is called ensemble theory. There are many, many different ways to define averages. However, there are three which are most commonly used. The canonical ensemble,⁵ is the one defined in the introductory section, having the classical probability

³The derivative is also taken at constant particle number, N . However, in much of the discussions of classical thermodynamics it is assumed that no material objects are entering or leaving the volume under consideration so that constant N is implied.

⁴Classical thermodynamics contains a whole host of beautiful arguments based upon three ideas: (a) energy is conserved. (b) the matter we observe is stable. (c) The stability of a closed system implies that you cannot extract useful work from it and leave it unchanged. The first of these ideas is the statement that you can have no perpetual motion machines of the first kind. The last militates against perpetual motion machines of the second kind. We shall not begin to make use of the rich and beautiful arguments which you can construct, by saying that these kinds of machines cannot exist.

⁵Canon is an adjective meaning standard or usual, as in canon law.

Ensemble	Normalizing factor	ln of normalizing factor	Relative to previous factor
microcanonical	$\chi(E, N, \Omega)$	$S(E, N, \Omega)/k$, $S = \text{entropy}$	
canonical	$Z(\beta, N, \Omega)$	$-\beta F(\beta, N, \Omega)$ $F = \text{free energy}$	$Z = \int dE \exp(-\beta E) \times \chi(E, N, \Omega)$
macrocanonical	$\Xi(\beta, \mu, \Omega)$	$\beta \Omega p(\beta, \mu)$	$\Xi = \sum_N \exp(\beta \mu N) \times Z(\beta, N, \Omega)$
grand canonical		$p = \text{pressure}$	

Table 8.2. The relation among the different thermodynamic functions defined by the ensembles.

distribution

$$\rho(x)d\Gamma_N = \frac{d\Gamma_N}{Z(\beta, N, \Omega)} \exp(-\beta H(p, q)) \quad \text{Canonical Distribution} \quad (8.22)$$

with x being an abbreviation for all the p and q variables in the system. In this ensemble we hold the particle number, N , fixed and integrate over all energies. We have also implicitly defined an ensemble called the *microcanonical ensemble*, in which both E and N are held fixed:

$$\rho(x)d\Gamma_N = \frac{d\Gamma_N}{\chi(E, N, \Omega)} \exp(-\beta H(p, q)) \delta(E - H(p, q)) \quad \text{Microcanonical Distribution .} \quad (8.23)$$

Here the quantity $\chi(E, N, \Omega)$, called the structure function, is defined by the condition that the probability (8.23) be properly normalized. Using this condition, it follows that

$$\chi(E, N, \Omega) = \int d\Gamma_N e^{-\beta H(p, q)} \delta(E - H(p, q)) = \exp\left(\frac{S(E, N, \Omega)}{k}\right) \quad (8.24)$$

is just an exponential of our old friend the entropy. Tables 8.1 and 8.2 are used to collect the definitions of some of the thermodynamic quantities defined by the different ensembles so that they may be used as needed.

The canonical ensemble defines a thermodynamic function called the free energy, $F(\beta, N, \Omega)$. From thermodynamic arguments, one can show that F defines the amount of energy in the system available to be converted into useful work. According to Table 8.2, F is defined from the partition function via $\ln Z = -\beta F$. Equation (8.21) reproduces the thermodynamic definition:

$$F(\beta, N, \Omega) = E - TS(E, N, \Omega) \quad (8.25)$$

which is listed in Table 8.1. That table also gives the value of δF as it is determined from Eq. (8.25) and the previously described equation for dS . The energy in Eq. (8.25) is a function of β , N , and Ω which is determined by the construction described around Eq. (8.19). This last equation then gives the value of E .

The last ensemble used is called the grand canonical ensemble or macrocanonical ensemble. In this case, we sum over all possible values of the numbers of particles in the system using the weight

$$\rho_N(x)d\Gamma_N = \frac{d\Gamma_N}{\Xi(\beta, \mu, \Omega)} \exp(-\beta H + \beta\mu N)$$

Macrocanonical Distribution . (8.26)

The $\exp(\beta\mu N)$ controls the sum over N . The grand partition function, Ξ , which appears as a normalization constant is defined, as usual, by the condition that the total probability be unity so that

$$\Xi(\beta, \mu, \Omega) = \sum_N \int d\Gamma_N \exp(-\beta H + \beta\mu N) = \sum_N \exp[-\beta F(\beta, N, \Omega) + \beta\mu N]. \quad (8.27)$$

In an argument which we should now find familiar, for large systems, this sum is dominated by a relatively small range of N , near the extremum of the sum. To determine this maximum, differentiate the exponent with respect to N and find:

$$\frac{\partial F(\beta, N, \Omega)}{\partial N} = \mu \quad (8.28)$$

which implicitly determines N as a function of μ , β and Ω . Since N is an extensive function, it must be linear in the volume and thus has the form:

$$N = \Omega n(\beta, \mu). \quad (8.29)$$

By the same argument as we have given several times, the sharpness of the maximum in the sum over N in Eq. (8.27) ensures that, for a large system, $\ln \Xi$ is proportional to the quantities in the exponent at the maximum value. Hence,

$$\ln \Xi(\beta, \mu, \Omega) = -\beta F(\beta, N, \Omega) + \beta\mu N, \quad (8.30)$$

where N is given by Eq. (8.28) and has the form indicated in Eq. (8.29). The transformation (8.28) which takes us from a function of one set of variables to one of another, via an extremal principle is called a Legendre transformation. The same type of transform takes one from E to S .

One more step is needed to complete the data in Table 8.2. Because the right hand side of Eq. (8.30) is extensive so is the left. Write this left as $\Omega g(\beta, \mu)$. Then differentiate Eq. (8.30) with respect to Ω at fixed β and μ . The result is

$$g(\beta, \mu) = \left. \frac{\partial}{\partial \Omega} [-\beta F(\beta, N, \Omega) + \beta\mu N] \right|_{N, \beta}.$$

Since the Legendre transform construction makes the derivative with respect to N vanish we then see

$$g(\beta, \mu) = -\beta \frac{\partial}{\partial \Omega} F(\beta, N, \Omega).$$

To complete the discussion one looks to Eq. (8.13) which gives the derivative of the free energy at fixed particle number and temperature as the pressure, p , and leaves us with the result $g = \beta p$, from which it follows that:

$$\ln \Xi(\beta, \mu, \Omega) = \beta p(\beta, \mu) \Omega = -\beta F(\beta, N, \Omega) + \beta \mu N = S/k - \beta E + \beta \mu N. \quad (8.31)$$

Thus, we have gotten to the identity

$$p\Omega = TS - E + \mu N. \quad (8.32)$$

We have now completed our definitions of statistical quantities in terms of their thermodynamic counterparts.

To use the statistical mechanics, we must know when to use the different ensembles. If the system is large, the answer is easy. All ensembles give exactly the same results. In this case, the choice of ensemble is determined by conceptual simplicity or by calculational convenience. However, statistical mechanics may also be applied to small systems. If we have a small system with fixed volume which exchanges neither particles nor energy with its environment, then one will describe the system by using the microcanonical ensemble. If one makes the walls of the system permeable to energy (heat) and then keep it in contact with some large system, then the large system may be said to have some temperature, $1/\beta$, and the small system will be effectively described by the canonical ensemble at that temperature. One can imagine relaxing the constraints still further and letting the walls leak particles. Perhaps they could be a slightly permeable membrane. In that case, the outer world would be a large system and its concentration of particles would be described by a chemical potential. Like the temperature, the chemical potential will equalize for two systems in contact. Thus, our small system would, in this case, be described by the grand canonical ensemble defined by the temperature and chemical potential of its surroundings.

8.5 Temperatures and Energy Flow

This argument given above is almost enough to show us that statistical mechanics and thermodynamics are equivalent. Additional argumentation in that direction would show that the work term, $pd\Omega$, plays exactly the same role in both approaches. To really make the connection, however, we must show that the temperature has the same meaning in statistical thermodynamics as in classical thermodynamics.

Thermodynamics is not by any means a simple subject. And temperature is not a simple concept. At one level, temperature is defined as an integrating factor in the equation for the heat flow, (8.11). At a simpler level, temperature is defined by the direction of heat flow. Given two such systems, called A and B , it is easy to see which one of these isolated systems

has a higher temperature — without making use of any theory. Just bring the two into a form of weak contact in which they can slowly exchange energy but no other conserved quantity. In this kind of contact, systems with higher values of temperature always give up energy in the form of heat to systems with lower temperatures. Observation will then tell us which of the following three cases holds:

$$\begin{array}{ll} \text{heat flows from } A \text{ to } B & \text{so that we say } T_A > T_B \\ \text{no heat flows} & \text{so that we say } T_A = T_B \\ \text{heat flows from } B \text{ to } A & \text{so that we say } T_A < T_B . \end{array} \quad (8.33)$$

In a moment, we shall describe how this relation between energy flow and temperature is derived from statistical mechanics. For now, I just point out that (8.33) makes good sense. For example, it implies the usual rule that the only way two bodies can be in equilibrium with one another is if they have the same temperature. It furthermore says that temperature provides what the mathematician call an ordering relation among different bodies in equilibrium. Specifically the temperature enables us to order all these things one linear scale, called hotness, so that

heat will flow from body A to body B if and only if A is hotter than B .

Then we can get a whole group of nontrivial statements as for example: if heat flows from A to B and also from B to C , then if we brought A into contact with C , heat would flow from A to C . Thus this part of thermodynamics provides a linear ordering of things as hotter or colder. To know how to assign a number (like three degrees Kelvin or ninety degrees Fahrenheit) to the temperature of some object, one must make use of some relation like Eq. (8.11). Then the definition will ensure, for example, that for a ideal gas the change in average energy is directly proportional to change in temperature.

To see one part of Eq. (8.33) imagine that we have a system composed of two weakly coupled classical subsystems, A and B , in equilibrium. Let subsystem A have a Hamiltonian $H^A(\mathbf{x}^A)$ and number of particles, N^A while subsystem B is similarly described by quantities labeled with superscripts B . (Here \mathbf{x} is an abbreviation for a large number of p and q variables.) We hold the number of particles in each subsystem fixed and hide factors involving the numbers as much as possible. Assume that the entire system has energy E . Then, we make use of the microcanonical ensemble to find that the subsystem A has energy E^A . This probability will be proportional to the average of $\delta(E^A - (H^A(\mathbf{x}^A)))$, so that according to Eq. (8.23) the probability is

$$\begin{aligned} \rho(E^A) &= \int d\Gamma^A \int d\Gamma^B \delta(E - (H^A(\mathbf{x}^A) + H^B(\mathbf{x}^B))) \delta(E^A - (H^A(\mathbf{x}^A))) / \chi(E) \\ &= \int d\Gamma^A \delta(E^A - (H^A(\mathbf{x}^A))) \int d\Gamma^B \delta(E - E^A - H^B(\mathbf{x}^B)) / \chi(E) \\ &= \frac{1}{\chi(E)} \exp \left[\frac{S^A(E^A) + S^B(E - E^A)}{k} \right]. \end{aligned} \quad (8.34)$$

This probability reaches a maximum when the exponent on the last line of Eq. (8.34) has a maximum. The maximum is attained when the derivative of the exponent vanishes or when

$$\frac{\partial S^A(E^A)}{\partial E^A} = \frac{\partial S^B(E - E^A)}{\partial E}. \quad (8.35)$$

But Eq. (8.35) is in turn the condition that E^A be adjusted so that the temperatures of the two subsystems are precisely equal. (See Eq. (8.16).) Thus the probability calculation shows that the most likely event is one in which the two temperatures are the same. Since the systems are, by hypothesis, large ones the most probable event is, by overwhelming odds, the only event that will be seen.

Thus, we have shown that the statistical approach to entropy and temperature satisfies one of the crucial thermodynamic requirements, the statement from (8.33) that two bodies which are in equilibrium with each other will have the same temperature. To complete the discussion we must figure out a statistical argument for the direction of heat flow. There is nothing in the statistical thermodynamics which we have defined so far which will determine this sign. Another postulate is necessary. We assert and assume that

In the natural course of time development, an isolated system will move from less probable to more probable configurations. Hence, as time goes on, the total entropy of the system will increase.⁶

In this argument we have also made use of a relation which gives the probability in terms of the entropy, as

In a large system in thermodynamic equilibrium, the probability of a given configuration is proportional to the number of accessible states in phase space. That number, in turn, is given as $e^{S/k}$, where S is the entropy, and k is a state function.

We also assume that, if we have a system composed of two subsystems which interact weakly, the entropy of the joint system is the sum of the entropies of the subsystems. Then the remaining parts of Eq. (8.33), which define the direction of heat flow, follow at once. Thus, we have shown that the main properties of the thermodynamic temperature and entropy also are true for the statistically defined temperature and entropy.

Just as β has an interpretation, is interpreted in terms of the willingness of the system to give up particles. We can quote what we said for temperature, almost word for word. Every isolated system, containing some kind of particle whose number is conserved, which

⁶There has been a big argument about the status of this second law of thermodynamics. The trouble is that classical and quantum mechanics each obey time reversal invariance. Thus statistical mechanics must include time reversal invariance since it is built from invariant theories. But entropy does only increase. It never decreases. To reconcile these different observations, we must presume that the thermodynamic situations which show a substantial entropy increase are ones which are very, very unlikely. In contrast, the equilibrium configurations are much more likely. Following this line of argument, one would say that it is possible to start from an equilibrium state and go to a non-equilibrium one — with a corresponding decrease in entropy — but this behavior is very unlikely. In practice, it is never observed for large systems.

has come to statistical equilibrium can be described by giving the value of its chemical potential. Given two such large systems, called A and B , it is easy to see which one of these isolated systems has a higher chemical potential — without making use of any theory. Just bring the two into a form of weak contact in which they can slowly exchange particles of the given type but no other conserved quantity. In this kind of contact, systems with higher values of the chemical potential always give up particles of the given type to particles with the lower value of the chemical potential. (If the chemical potential is exactly equal, fluctuations will produce particle exchange but the number of particles exchanged will not be proportional to the numbers of particles in the subsystems, but instead much smaller.)

Homework

Problem 8.1. Find the value of the chemical potential for the nitrogen in the air at standard temperature and pressure. What would be the value if the h^3 were left out of its definition?

Problem 8.2 (Entropy for a Perfect Gas). Calculate the entropy for a noninteracting monatomic gas. Show that it is extensive.

Problem 8.3 (Direction of Heat flow). Below Eq. (8.35), I said “Then the remaining parts of equation (8.33), which define the direction of heat flow, follow at once.” Fill in the argument.

Chapter 9

Fermi, Bose, and Other

9.1 Quantum Formulation

In this chapter, we consider additional applications of the statistical mechanics developed in the previous chapter. In particular, we are going to treat systems of non-interacting but degenerate quantum particles. These systems can be described by their *single particle states*, or *modes*. As before, we label the different modes by the index ν . In the quantum mechanics of non-degenerate particles, the density is low enough so that the probability for any occupation of a single particle state is quite small. Therefore, it is very unlikely indeed that more than one particle will be found in any given mode. In this case, one may proceed as if the particles were distinguishable one from the other. In the quantum mechanics of distinguishable particles, one sets up a set of basis states by saying which mode is occupied by each of the particles. Then a general states is a linear superposition of these basis states. This approach is conceptually forbidden for identical and indistinguishable particles. The reason is that two basis states which differ from one another only by a permutation of particles are, for identical particles, really the same basis state.

This identity becomes important as soon as there is a substantial probability that two particles might try to enter a single quantum state. For these cases one must use the quantum theory of identical particles. In that case, one can only say how many particles occupy each of the single particle states but not which particle is in which state. Thus one sets up basis states by saying that there are n_ν particles in the ν th mode. Since that single particle state has energy ϵ_ν the total energy of the basis state is

$$H = \sum_\nu \epsilon_\nu n_\nu, \quad (9.1a)$$

while the total number of particles is

$$N = \sum_\nu n_\nu. \quad (9.1b)$$

There are then two cases: Bose–Einstein statistics and Fermi–Dirac statistics. In the latter case, there can be no more than one particle occupying each single particle

state so

$$n_\nu = 0 \text{ or } 1 \quad \text{Fermi case} \quad (9.2)$$

while in the other situation all integer values of n are possible

$$n_\nu = 0 \text{ or } 1 \text{ or } 2 \dots \quad \text{Bose case.} \quad (9.3)$$

To do the general quantum theory of interacting degenerate particles is often very difficult. However, if the particles do not interact, the basis states we have just described are the eigenstates of the Hamiltonian and thus can be directly used for further calculations.

9.2 Statistical Mechanics of Non-Interacting Degenerate Particles

So we turn to statistical mechanics. For degenerate systems one thinks of the basic process involved as adding or subtracting a particle. If one adds a particle to the ν th single particle state then one adds an amount of energy $\delta H = \epsilon_\nu$, and — naturally — a number of particles $\delta N = 1$. It is difficult to handle the combined addition of particles and energy in the canonical ensemble, because this ensemble naturally refers to a fixed number of particles. In contrast, it is relatively easy to handle this combined addition in the grand canonical ensemble. In this ensemble, the probability of finding the system in a quantum state $|\alpha\rangle$ is

$$\rho(\alpha) = \frac{\exp(-\beta H_\alpha + \beta \mu N_\alpha)}{\Xi}. \quad (9.4)$$

Now each state $|\alpha\rangle$ is specified by giving the number of particles in each of the single particle states:

$$|\alpha\rangle = |n_1, n_2, \dots, n_\nu, \dots\rangle \quad (9.5)$$

and the sum over α is a sum over all possible sets of n_ν 's. But notice that the probability given by (9.4) can be factorized into pieces describing the different single particle states

$$\rho(\alpha) = \frac{1}{\Xi} \prod_\nu [\exp(-\beta \epsilon_\nu + \beta \mu)]^{n_\nu}. \quad (9.6)$$

Since the probability is a product over the different single particle states, these modes are independent of one another. Thus, one can focus attention upon one of them and then get the final answer by composing the answers for the individual modes.

Notice the normalizing constant, Ξ , in Eq. (9.6). This constant is called the *grand partition function*. Note from Eq. (8.32) that $\ln \Xi$ has the value $\beta p\Omega$. Now, turn to calculating this thermodynamic or statistical quantity.

First do fermions, they are simpler. Think of a situation with but one mode. There are but two possibilities: either the mode is occupied or it is empty. The two probabilities are:

$$n_\nu = 0; \text{ mode empty; probability } \frac{1}{\xi_\nu}, \quad (9.7a)$$

$$n_\nu = 1; \text{ mode occupied; probability } \frac{e^{-\beta(\epsilon_\nu - \mu)}}{\xi_\nu}. \quad (9.7b)$$

Here ξ_ν is the normalizing factor — the ‘grand’ partition function — for this tiny subsystem. This factor is determined by the condition that the sum of the two probabilities must be one so that

$$\xi_\nu = 1 + e^{-\beta(\epsilon_\nu - \mu)}. \quad (9.7c)$$

The full grand partition function is given as a product over modes of the single-mode functions, ξ_ν .

There is hardly anything more to compute. The probability that the state will be occupied is the same as the average of n_ν ,

$$\langle n_\nu \rangle = \frac{1}{1 + e^{\beta(\epsilon_\nu - \mu)}}. \quad (9.8)$$

The squared fluctuations in the occupation number is given by

$$\langle (n_\nu - \langle n_\nu \rangle)^2 \rangle = \langle n_\nu^2 \rangle - 2\langle n_\nu \langle n_\nu \rangle \rangle + \langle n_\nu \rangle^2 = \langle n_\nu \rangle - \langle n_\nu \rangle^2. \quad (9.9)$$

The last line follows because the quantum operator n_ν has eigenvalues 0 and 1 and therefore obeys $n_\nu^2 = n_\nu$. In this way, we get to our final result

$$\langle (n_\nu - \langle n_\nu \rangle)^2 \rangle = \langle n_\nu \rangle [1 - \langle n_\nu \rangle]. \quad (9.10)$$

Thus the fluctuations become very small in two limits: if the state is almost always empty, $\langle n_\nu \rangle \approx 0$, and equally when the state is almost always full, $\langle n_\nu \rangle \approx 1$. For this non-interacting system, the complete partition function must be the product over all modes of the one-mode result (9.7c). Hence the logarithm of the grand partition function is given by

$$\ln \Xi = \beta p \Omega = \sum_\nu \ln \{1 + e^{-\beta(\epsilon_\nu - \mu)}\}. \quad (9.11)$$

Bosons present no problem either. Instead of (9.7) one finds that the probability of finding the mode excited to its n th level is

$$\rho(n) = \frac{e^{-\beta n(\epsilon_\nu - \mu)}}{\xi_\nu}, \quad (9.12a)$$

with a normalization condition that the sum over all n gives unity so that

$$\xi_\nu = \sum_{n=0}^{\infty} e^{-\beta n(\epsilon_\nu - \mu)}.$$

Since this is just a sum of a geometric series, we can easily add it up and find

$$\xi_\nu = \frac{1}{1 - e^{-\beta(\epsilon_\nu - \mu)}}, \quad (9.12b)$$

for $\epsilon_\nu > \mu$. If this condition is not satisfied, the sum does not converge and the averaging process makes no sense.

One can now calculate the average of all powers of n_ν . The best way of doing it is via a generating function. Define

$$z = e^{-\beta(\epsilon_\nu - \mu)}$$

and notice that

$$\xi_\nu = \frac{1}{1 - z}$$

generates simple expressions for these averages since

$$\langle n_\nu^p \rangle = \frac{1}{\xi_\nu} \left[z \frac{d}{dz} \right]^p \xi_\nu. \quad (9.13)$$

After a moment's calculation one finds

$$\langle n_\nu \rangle = \frac{1}{e^{\beta(\epsilon_\nu - \mu)} - 1}. \quad (9.14)$$

The right hand side of this expression must be non-negative since the left hand side is an average of a non-negative quantity. Thus we must demand that the chemical potential be less than the energy of the lowest mode:

$$\epsilon_0 > \mu. \quad (9.15)$$

A further small calculation gives the mean squared fluctuation in the occupation number to have the value:

$$\langle (n_\nu - \langle n_\nu \rangle)^2 \rangle = \langle n_\nu \rangle [1 + \langle n_\nu \rangle]. \quad (9.16)$$

The partition function for the entire system can, once again, be computed as the product of the partition functions for the individual models so that

$$\ln \Xi = \beta \rho \Omega = - \sum_\nu \ln [1 - e^{-\beta(\epsilon_\nu - \mu)}]. \quad (9.17)$$

9.3 The Non-Degenerate Limit

All of these formulas should be compared with their counterparts in the case in which the system is non-degenerate. This limit is approached by letting $\langle n_\nu \rangle$ be very small in comparison with unity or, alternatively, by letting the chemical potential go to minus infinity. In this limit, we find from Eq. (9.8) (for fermions) or Eq. (9.13) (for bosons) that the average number of particles in the single particle state ν is

$$\langle n_\nu \rangle = e^{-\beta(\epsilon_\nu - \mu)} \quad (9.18)$$

while the formula for the pressure, as derived from Eq. (9.7c) or (9.17)

$$\ln \Xi = \beta p \Omega = \sum_\nu e^{-\beta(\epsilon_\nu - \mu)} = \sum_\nu \langle n_\nu \rangle = N. \quad (9.19)$$

The last equality follows from the fact that the sum over all modes of the number of particles in each mode must be the total number of particles. Since N/Ω is the density of particles, n , we recover the fact that in the non degenerate limit the pressure is determined by the familiar formula.

$$p = nkT. \quad (9.20)$$

The average occupation, $\langle n_\nu \rangle$, has a very natural interpretation in terms of the one particle distribution function, $f(\mathbf{p}, \mathbf{r})$. Recall that the distribution function is proportional to the number of particles which can be found in the neighborhood of the point in phase space \mathbf{p}, \mathbf{r} . Then, the total number of particles is given as the phase space integral of f in the form

$$N = \int \frac{d\mathbf{p} d\mathbf{r}}{h^3} f(\mathbf{p}, \mathbf{r}). \quad (9.21a)$$

In parallel, consider $\langle n_\nu \rangle$ for the case in which the system is translationally invariant. In that situation, the label ν is replaced by an a momentum label, \mathbf{p} . If the energy levels are close to one another, then the sum over n can be replaced by a phase space integral of the form

$$\sum_\nu \rightarrow \int \frac{d\mathbf{p} d\mathbf{r}}{h^3}.$$

Since $\langle n_\nu \rangle$ depends upon the momentum, we find

$$N = \int \frac{d\mathbf{p} d\mathbf{r}}{h^3} \langle n_{\mathbf{p}} \rangle. \quad (9.21b)$$

A comparison of the two forms of (9.21) shows that in the classical limit, the occupation number $\langle n_\nu \rangle$ is essentially the same as the distribution function, $f(\mathbf{p}, \mathbf{r})$. In fact, this identification works in the entire semi-classical domain when the wavelengths contained in

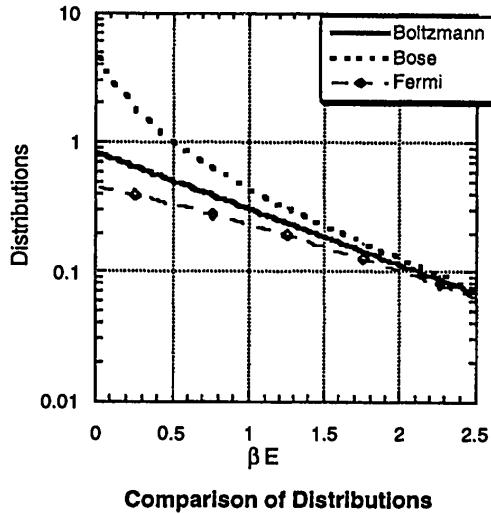


Fig. 9.1. Comparison of different distributions for the same value of $\beta\mu$. Here we plot the average number of particles in a mode with energy E . In comparison to the Boltzmann case, the Bose situation is one in which there is more chance for a large occupation for the state. In contrast, in the Fermi case, there is a smaller chance that the state will be occupied.

$f(\mathbf{p}, \mathbf{r})$ are very large in comparison to the typical or important values of the quantum wave length, h/p .

It is instructive to compare the three cases of Fermi–Dirac statistics, Bose–Einstein statistics, and the non-degenerate situation of Boltzmann statistics. In Fig. 9.1 we plot $\langle n_\nu \rangle$ as a function of its argument, $z = \beta(\epsilon_\nu - \mu)$. In the fermion case, this argument can be negative and then $\langle n_\nu \rangle$ saturates at a value close to one. In the boson case, z cannot be negative and in fact the occupation number approaches infinity as this mode's energy approaches the value of the chemical potential from above. As shown in Fig. 9.1 both forms reduce to the Boltzmann expression when the dimensionless energy is large.

9.4 Degenerate Fermions

Nature offers us several examples of degenerate fermion systems. One familiar example is the electrons in an atom, which are tightly bound by the Coulomb field produced by the nucleus and by the other electrons. Another rather similar example occurs within the atomic nucleus in which the protons and neutrons are each fermions bound in the self-consistent potential produced by the strong-interaction forces among them. In these last two examples, the degenerate systems are each composed of only a few hundred particles. Nonetheless, for some purposes, statistical mechanics does apply to each of the cases.

But both electrons and nucleons form extended systems, comprising arbitrarily many particles. For these systems statistical mechanics must work well. All of our usual solid materials contain degenerate electrons.

Another example of a degenerate extended system is a neutron star in which neutrons and protons are bound by gravitational forces and then convert into one another via the

weak interactions. Effectively, this system contains up to six kinds of degenerate fermions. There are two spin components each of neutron and proton and two more of neutrino. The electrons in a metal provide another example in which there are two kinds of degenerate fermions given by the two possible values of the electronic spin. In the latter example, the nucleons are bound up into atomic nuclei. These nuclei may act as either bosons or fermions depending upon their total content of nucleons. However, each of these atomic nuclei is bound into place in a particular position in the crystal lattice of the solid. Because of this localization, the statistics of the nuclei do not play an important role in most of the properties of the metal.

As our first example of fermion behavior, consider the electrons in a metal. Consider an oversimplified model in which the electrons act as noninteracting particles with spin one half. Thus, each electronic excitation is characterized first by its momentum, \mathbf{p} , which takes on the values

$$\mathbf{p} = \frac{\hbar}{L}(\nu_1, \nu_2, \nu_3) \quad (9.22a)$$

with the ν 's being integers, and second by the z -component of its spin which takes on the two values

$$\sigma_z = \pm 1. \quad (9.22b)$$

Because the particles do not interact, each stable excitation in the system can be labeled by these two kinds of quantum numbers. The Hamiltonian can be written as

$$\mathcal{H} = \sum_{\sigma=\pm 1} \sum_{\mathbf{p}} n_{\mathbf{p},\sigma} \epsilon_{\mathbf{p},\sigma}. \quad (9.23)$$

Here, $\epsilon_{\mathbf{p}\sigma}$ is the energy of an excitation with these quantum numbers. In the non-relativistic situation, the free particle energy takes the form:

$$\epsilon_{\mathbf{p}\sigma} = \frac{(\mathbf{p} - e\mathbf{A}/c)^2}{2m} + e\phi - \mu_B \sigma_z \mathbf{B}_z \quad (9.24)$$

where ϕ is a scalar potential, \mathbf{A} , is a vector potential, e is the charge on the particle and \mathbf{B} is the magnetic field. In what follows, we shall ignore the presence of the electromagnetic potentials, but consider only the coupling of the spin to the magnetic field. In writing this coupling, we have used the symbol μ_B in the magnetic coupling. The subscript is intended to distinguish this quantity from the chemical potential.

In Eq. (9.23) $n_{\mathbf{p}\sigma}$ is the quantum mechanical operator which represents the number of fermions in the single particle state. This number has only two possible values: zero and one, and correspondingly, the eigenvalues of each $n_{\mathbf{p}\sigma}$ can only be 0 or 1. In a situation described by statistical mechanics, we think about $\langle n_{\mathbf{p}\sigma} \rangle$, where $\langle \rangle$ represents an average in the grand canonical ensemble. From our earlier analysis, (see Eq. (9.8)) this average has the value:

$$\langle n_{\mathbf{p}\sigma} \rangle = \frac{1}{1 + \exp \beta(\epsilon_{\mathbf{p}\sigma} - \mu_\sigma)}. \quad (9.25)$$

In Eq. (9.25) we have introduced a chemical potential which depends upon the spin label σ . When we do this, we are implicitly assuming that the number of fermions with each kind of spin is conserved so that we need a separate chemical potential to keep track of each species. Starting with expression (9.25) one can compute the average number of particles with spin σ as

$$\langle N_\sigma \rangle = \sum_{\mathbf{p}} \langle n_{\mathbf{p}\sigma} \rangle = \int d\mathbf{p} \left(\frac{L}{h} \right)^3 \langle n_{\mathbf{p}\sigma} \rangle, \quad (9.26)$$

so that the density of particles with spin σ is

$$n_\sigma = \frac{\langle N_\sigma \rangle}{L^3} = \int \frac{d\mathbf{p}}{h^3} \langle n_{\mathbf{p}\sigma} \rangle. \quad (9.27)$$

Thus, we can think of $\langle n_{\mathbf{p}\sigma} \rangle$ as being the probability per unit volume of finding a particle with a given value of the momentum and spin. Thus, a distribution function which includes the spin dependence may be defined as

$$f_\sigma(\mathbf{p}, \mathbf{r}, t) = \langle n_{\mathbf{p}\sigma} \rangle. \quad (9.28)$$

(To confirm this result compare with our earlier (see Eqs. (6.21b) and (6.56)) expression for the distribution function.)

Equation (9.27) gives one thermodynamic quantity, the density of particles with a given spin, in terms of the single particle distribution function defined by Eq. (9.26). The analogous relations for momentum and energy density are

$$\langle \mathbf{g}(\mathbf{r}, t) \rangle = \text{momentum density} = \sum_{\sigma} \int \frac{d\mathbf{p}}{h^3} \mathbf{p} f_\sigma(\mathbf{p}, \mathbf{r}, t), \quad (9.29a)$$

$$\langle \epsilon(\mathbf{r}, t) \rangle = \text{kinetic energy density} = \sum_{\sigma} \int \frac{d\mathbf{p}}{h^3} \epsilon_{\mathbf{p}} f_\sigma(\mathbf{p}, \mathbf{r}, t). \quad (9.29b)$$

We shall also make use of the expression for the pressure which comes from Eq. (9.11) which implies¹

$$\beta p = \sum_{\sigma} \int \frac{d\mathbf{p}}{h^3} \ln \{1 + \exp[-\beta(\epsilon_{\mathbf{p}} - \mu)]\}. \quad (9.29c)$$

It is instructive to look at the results of equilibrium theory, as described by Eq. (9.25), for these different quantities for the simple case in which the kinetic energy is just

$$\epsilon_{\mathbf{p}} = \frac{\mathbf{p}^2}{2m}. \quad (9.30)$$

¹The results (9.26)–(9.29c) can be extended to interacting systems in the limit of low temperature. Lev Landau put together a whole theory about these systems, called Fermi liquid theory. This theory is reported for example in the books by P. Nozière and D. Pines, *The Theory of Fermi Liquids*, W. A. Benjamin, Inc. New York (1966).

We wish to specialize to the case of *degenerate fermions* in which the particles are so crammed into the single particle states that, for many momenta, the occupation numbers are near their saturation value of one. This degeneracy will occur when the chemical potential is a large positive number. (For the moment let us focus on the simplest case in which the chemical potential is independent of spin). More precisely we require that the dimensionless combination $\mu/(kT)$ is much bigger than unity. When this happens, the energy μ is called the Fermi energy and denoted by ϵ_F . Physically, ϵ_F represents the maximum likely value of the energy of a single particle in the system. The *Fermi sphere* is the region of momentum with $p^2/(2m) < \epsilon_F$. Therefore it is the set of all momenta with magnitude less than the *Fermi momentum*, which has the value $p_F = \sqrt{2m\epsilon_F}$.

To see how this interpretation works, look at expression (9.25) for the distribution function and the corresponding graph, Fig. 9.1. This expression shows that the momentum space can be divided into three parts. When ϵ_p is smaller than the Fermi energy, and enough smaller so that $(\epsilon_p - \epsilon_F)/(kT) \ll -1$, then we have almost filled states, and this implies $1 - \langle n_{p\sigma} \rangle \ll 1$. We then say that the state is fully occupied. States which obey this condition are said to be part of the Fermi sea and the set of momenta which satisfy this condition are said to make up the Fermi sphere.

The opposite case is the one in which the energy is sufficiently higher than the Fermi energy so that the state is very likely to be empty. These unfilled states have $(\epsilon_p - \epsilon_F)/(kT) \gg -1$ so that the occupation is very small, $\langle n_{p\sigma} \rangle \ll 1$.

Neither almost filled states nor almost empty ones have a very important role in the behavior of the degenerate Fermion system. Nothing can change in these extreme situations. The active states, the ones which can easily change their occupation numbers, have intermediate values of the occupation probabilities and therefore have

$$|\epsilon_p - \epsilon_F| \sim kT \text{ implies active states.} \quad (9.31)$$

It is very easy to calculate the thermodynamic quantities in the limit of zero temperature. For example, Eq. (9.26) gives the total density of particles, the number per unit volume as the volume of the Fermi sphere, divided by \hbar^3 , times a factor of two which counts the number of spin components. In symbols,

$$n = \sum_{\sigma=\pm 1} n_\sigma = 2 \int_{p < p_F} \frac{d\mathbf{p}}{\hbar^3} = 2 \frac{4\pi}{3\hbar^3} p_F^3 = \frac{8\pi}{3\hbar^3} (2m\mu)^{3/2}. \quad (9.32a)$$

Since we are integrating a vector quantity over a symmetrical sphere, the total momentum defined by Eq. (9.29) vanishes. The total energy is given by a calculation almost identical to the one in (9.32) to be

$$\frac{\langle E \rangle}{L^3} = \frac{8\pi}{5\hbar^3} (2m)^{3/2} \mu^{5/2}. \quad (9.32b)$$

For degenerate fermions, μ is a positive number. Thus as the temperature goes to zero, both the energy density and the particle-density approach fixed values.

In contrast, in the classical limit, the energy per unit volume is proportional to nkT . This result arises because everything moves more and more slowly as the temperature decreases. In this highly degenerate situation, nothing slows down. Instead all the single particle states up to a certain energy value are filled, and all those above that value are empty. In this situation, the energy per unit volume does not go to zero with temperature but instead has the value

$$\frac{\langle E \rangle}{L^3} = \frac{3}{5}\mu n \left[1 + \text{const} \left(\frac{kT}{\mu} \right)^2 + \dots \right]. \quad (9.33)$$

Notice that the main term is temperature independent, with a correction proportional to temperature squared and then terms of higher order, not shown.

Finally, the pressure is given by Eq. (9.29c) to be a similar kind of integral

$$p = 2 \int_{p < p_F} \frac{dp}{h^3} (\mu - \epsilon_p) = \frac{2}{5}\mu n. \quad (9.34)$$

This result could have been obtained more directly by using the thermodynamic relation (see Table 8.1)

$$dp = \frac{S}{\Omega} dT + n d\mu.$$

Thus,

$$\left. \frac{\partial p}{\partial \mu} \right|_T = n. \quad (9.35)$$

At zero temperature, both p and n go to zero as μ goes to zero. Hence (9.34) can be obtained by integrating (9.35) with the aid of Eq. (9.32b).

There is an important physical consequence of Eqs. (9.33) and (9.34). These equations describe a system with a much larger kinetic energy and pressure than would be possible in the classical limit. In classical statistical mechanics, both energy and $p\Omega$ are proportional to T and are in fact of order $Nk_B T$. Hence as the temperature goes to zero the system ‘slows down’ and both energy and pressure go to zero. In contrast, in degenerate fermion systems, such slowing down is quite impossible because the exclusion principle forces particles into states of higher kinetic energy. Then both E and $p\Omega$ are of order $N\mu$, since μ is the typical free energy per particle. This is a very large energy or pressure and makes the resulting metal (or neutron star) very resistant to compression. In fact the strength of materials under compression depends upon the resistance of the electrons to compression. The very stability of the neutron star or metal depends upon the fermion nature of the constituent particles.

9.5 Degenerate Bosons I. Photons and Phonons

The chemical potential, μ , appears in our formulas for distribution functions because of the conservation of particle number. Different values of μ reflect situations in which there

is a different number of particles per unit volume. When the particles are photons, which are not conserved, then there is no chemical potential. Instead of (9.14) the distribution function takes the simpler form

$$\langle n_\nu \rangle = \frac{1}{e^{\beta\epsilon_\nu} - 1}. \quad (9.36)$$

This expression can be used to compute the statistical properties of a gas of photons. Photons moving in a box have modes which can be labeled by a polarization index and a momentum \mathbf{p} (which is \hbar times a wave vector \mathbf{k}). The energy of the photon is

$$\epsilon_\nu = pc = \hbar ck. \quad (9.37)$$

The total energy of the photons in the box will then be

$$E = \sum_\nu \langle n_\nu \rangle \epsilon_\nu. \quad (9.38a)$$

A parallel calculation gives the flow of energy in photons through a unit area of the box as

$$\text{flux} = \sum_\nu dS \cdot \frac{c\mathbf{p}}{p} \langle n_\nu \rangle \epsilon_\nu. \quad (9.38b)$$

Here the combination $c\mathbf{p}/p$ gives the velocity of the photon while velocity times energy is the flux. The two calculations described by these formulas are very similar. We shall only carry out the first of these.

One can replace the sum over modes by sum over polarizations times a sum over momentum states. As usual the latter is the volume of the system times an integral over \mathbf{p} divided by \hbar^3 . As a result Eq. (9.38a) reduces to

$$\frac{E}{\Omega} = 2 \int \frac{d\mathbf{p}}{\hbar^3} \frac{1}{e^{\beta cp} - 1} cp. \quad (9.39a)$$

The factor of two arises because there are two polarization states for each momentum. An alternative and equivalent form is one in which the integration is done over the vector wave vector, \mathbf{k} , which describes the space-dependence of the cavity modes. This form

$$\frac{E}{\Omega} = 2 \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{e^{\beta c\hbar k} - 1} hck \quad (9.39b)$$

is useful because it has a simple classical interpretation. Take \hbar to zero in Eq. (9.39b). Notice that as x goes to zero, the expression $e^x - 1$ may be expanded in a power series in x and becomes simply proportional to x . Thus Eq. (9.39b) becomes

$$E = \beta^{-1} 2\Omega \int \frac{d\mathbf{k}}{(2\pi)^3} . \quad (9.40)$$

The coefficient of β^{-1} on the right hand side of Eq. (9.40) is just the sum over modes, \sum_ν .

Thus, Eq. (9.40) has the very reasonable interpretation that the energy of a cavity containing electromagnetic radiation is $k_B T$ times the number of modes. This result can be interpreted as an oscillation of an elastic medium which has $k_B T/2$ kinetic energy per mode and $k_B T/2$ of potential energy. However as one can see from Eq. (9.40), there are an infinite number of modes of electromagnetic radiation in a cavity and hence the energy is infinite. This infinity was quite embarrassing for classical physics. This embarrassment is mitigated by the fact that the energy density of a cavity is not quite directly observable. On the other hand, the flux defined by Eq. (9.38b) is directly observable and is, according to this same classical methodology, equally infinite. This difficulty was one of the troubles which showed the need for a replacement or extension of classical physics. These difficulties showed that classical physics could not be a complete descriptor of familiar objects in our everyday world, and that a new theory (quantum physics) would be required to understand any everyday object.

However, in our more modern view, there is no problem. Go back to Eq. (9.39), use as the variable of integration $x = \beta pc$, so that the integral becomes:

$$\frac{E}{\Omega} = \frac{2}{\beta^4 c^3} \int \frac{dx}{h^3 e^x - 1} x = \frac{8\pi}{\beta^4 c^3 h^3} \int_0^\infty x^2 dx \frac{1}{e^x - 1}. \quad (9.41)$$

Notice that the final integral is finite. As x goes to infinity, the integral converges because of the exponential in the denominator. As x goes to zero we expand the exponential in the denominator and see that the integrand becomes x^2 , which certainly gives a finite result. Since the integral is just a finite constant, the net result is that the energy is proportional to h^{-3} . The inverse power of h is a hint that the classical limit might be very funny indeed. The energy is also proportional to β^{-4} or alternatively to T^4 . The flux has this same power of temperature.

It was Max Planck who first introduced the notion that electromagnetic radiation might appear as quanta. The flux, Eq. (9.38b) also contains a factor of T^4 . This behavior was seen in earlier experiments which led to the Stefan–Boltzmann law which says that the flux of energy has the form σT^4 . This temperature dependence followed from a simple thermodynamic argument. But Planck was able to obtain the intensity as a function of wavelength. That Planck was able to get the right wave-length dependence led people to follow his line of thinking, even though it seemed strange and arbitrary at the time. In the long run, this line of thinking led to quantum mechanics and quantum field theory.

9.6 Degenerate Bosons II. One-Dimensional Phonons

The oscillations of electromagnetic waves in a cavity are bosons. It is also true that all kinds of oscillatory modes in condensed systems behave as bosons. For example, sound wave oscillations in a solid or liquid act as Bosons, and at low temperatures, the degenerate character of these bosons manifest themselves. To see this kind of oscillation in its simplest manifestation, we consider a set of one-dimensional particles labeled by $j = 1, 2, \dots, N$ which each have a mass m . They are arranged in a line and have a coordinate x_j together

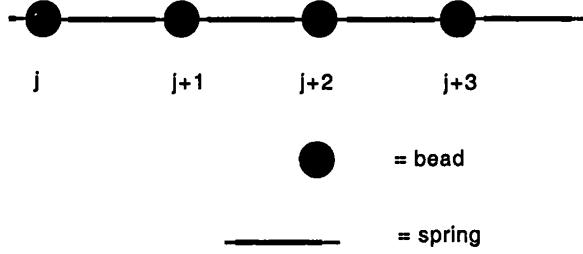


Fig. 9.2. Beads connected by springs. The motion of these beads is described by a linear theory in which the different eigenmodes are labeled by a momentum.

with a momentum p_j . They are coupled by springs connecting the immediately neighboring particles as in Fig. 9.2. The spring constant is written $m\omega_0^2$ and the unextended length of the spring is a . The actual position of the j th particle is $ja + x_j$ so that x_j has the interpretation of the displacement of the particle from its equilibrium position ja . The total Hamiltonian for the system is

$$H = \sum_{j=1}^N \frac{1}{2} \left[\frac{p_j^2}{m} + m\omega_0^2(x_{j+1} - x_j - a)^2 \right]. \quad (9.42)$$

This Hamiltonian is interpreted by saying that the system obeys periodic boundary conditions:

$$x_{j+N} = x_j. \quad (9.43)$$

Because the system is translationally invariant in time, one expect that the basic modes if the system will have the time dependence in which x_j is proportional to $\exp(-i\omega t)$. Similarly because of the spatial invariance, one expects that the space dependence of the modes will be one in which the displacement x_j is proportional to $\exp(ikja)$ since ja is the lowest order expression for the position of the j th lattice site. In summary, we pick the j th displacement to obey

$$x_j(t) = A(k) \exp(ikja - i\omega_k t) \quad (9.44)$$

in the eigenmode labeled by k . Here ω_k is the mode-frequency and $A(k)$ is the amplitude of the mode. In the usual way, we notice that the periodic boundary condition requires that k must have the form

$$k = \frac{2\pi\nu}{Na}, \quad (9.45a)$$

where ν is an integer. Then Eq. (9.45a) will ensure that (9.43) is obeyed. Since there are only N degrees of freedom, there can be no more than N modes. Thus not all ν 's give distinct modes. Notice that if k is replaced by $k + 2\pi/a$, according to Eq. (9.44), the

displacement does not change. Thus, ν 's differing by N must give exactly the same mode. For this reason, we supplement Eq. (9.45a) by the additional restriction

$$-\frac{N}{2} < \nu \leq \frac{N}{2}. \quad (9.45b)$$

The Hamiltonian (9.42) implies the equation of motion:

$$\frac{d}{dt}x_j = \frac{\partial}{\partial p_j}H = \frac{p_j}{m}, \quad (9.46a)$$

$$\frac{d}{dt}p_j = -\frac{\partial}{\partial x_j}H = m\omega_0^2(x_{j+1} + x_{j-1} - 2x_j). \quad (9.46b)$$

One uses a mode in the form given by Eq. (9.44) and finds

$$-i\omega_k x_j = \frac{p_j}{m}, \quad (9.47a)$$

$$-i\omega_k p_j = -2m\omega_0^2 x_j(1 - \cos ka). \quad (9.47b)$$

As a result the modal frequency obeys

$$\omega_k = \omega_0 \sqrt{2(1 - \cos ka)} = 2\omega_0 |\sin(ka/2)|. \quad (9.48)$$

Given this frequency, one can go ahead exactly as in the photon case. Equation (9.38) remains as before. Then Eq. (9.39b) is replaced by

$$\frac{E}{Na} = \int_{-\pi/a}^{\pi/a} \frac{dk}{2\pi} \frac{\hbar\omega_k}{e^{\beta\hbar\omega_k} - 1}. \quad (9.49)$$

One can consider two limits. In the limit of high temperatures (equivalent to the limit in which \hbar goes to zero) one can expand the denominator in (9.49) in a power series in $\hbar\omega_k$ and find, to the lowest order, that

$$\frac{E}{Na} = \int_{-\pi/a}^{\pi/a} \frac{dk}{2\pi} \beta^{-1}, \quad (9.50)$$

so that the average energy is $k_B T$ times the number of modes. In this lattice system, as contrasted to the vacuum, the number of modes is finite. The other limit is low temperatures, which tends to pick out small values of the frequency. The frequency gets small when k gets small. From Eq. (9.48), in this limit, the phonon system has ω_k equal to ck . In this case c is the speed of sound and is equal to $\omega_0 a$.

$$\frac{E}{Na} = 2 \int_0^\infty \frac{dk}{2\pi} \frac{1}{e^{\beta\hbar ck} - 1} hck = (\beta^2 \hbar c)^{-1} \int_0^\infty \frac{dx}{\pi} \frac{1}{e^x - 1} x, \quad (9.51)$$

so that in this one-dimensional example, the energy is proportional to T^2 . In three dimensions, there are two more factors of k in the phase space integral and then two more factors of T in the energy.

9.7 Degenerate Bosons III. Bose Phase Transition

Yet another interesting calculation can be done for degenerate Bose systems. Imagine a situation in which there are a group of particles with no internal degrees of freedom confined to a three-dimensional box of side L . The formulation is very simple. The energy is $p_\nu^2/(2m)$ while the momentum is

$$\mathbf{p}_\nu = \frac{\hbar}{L}(v_1, v_2, v_3). \quad (9.52)$$

The total number of particles is

$$N = \sum_\nu n_\nu \text{ with } n_\nu = \frac{1}{e^{\beta\epsilon_\nu - \beta\mu} - 1}. \quad (9.53)$$

Since this average number of particles in the single particle state ν must be positive, we must have

$$\mu \leq \epsilon_\nu \quad (9.54)$$

for all of the single particle states, ν .

As before, we replace the sum by an integral and find that the density of particles, n , obeys

$$n = \frac{N}{\Omega} = \int \frac{d\mathbf{p}}{h^3} \frac{1}{e^{\beta\epsilon_p - \beta\mu} - 1}. \quad (9.55)$$

We go through the usual story of changing variables to get a dimensionless integration variable and end up with the expression

$$n = 4\pi \left(\frac{m}{\beta h^2} \right)^{3/2} \int_0^\infty dx x^2 \frac{1}{\exp(\frac{x^2}{2} - \beta\mu) - 1}. \quad (9.56)$$

Notice that as $\beta\mu$ goes upward toward zero, this integral increases. It reaches its maximum value at $\mu = 0$ when

$$n = n_{\max} = 4\pi \left(\frac{mk_B T}{h^2} \right)^{3/2} \int_0^\infty dx x^2 \frac{1}{\exp(x^2/2) - 1}. \quad (9.57)$$

However, the result (9.57) seems decidedly strange. This is a theory of non-interacting Bosons. If we have a box full of such particles what should prevent us from adding more? How can it possibly be that the density reaches a maximum value? Did we make an error?

The right answer is that we made an error in going from the sum (9.53) to the integral (9.56). Notice that the zero-momentum term in the sum is

$$n_0 = \frac{1}{e^{-\beta\mu} - 1}. \quad (9.58)$$

For small $-\beta\mu$ this number of particles in the lowest mode may be as large as we wish. In fact, by choosing

$$-\beta\mu \sim \frac{1}{N} \sim \frac{1}{L^3}, \quad (9.59)$$

we can make the number of particles in this lowest mode be of the same order as the total number of particles in the system. The number in the next higher state will be much smaller. In particular the next state has energy

$$\epsilon = \frac{\hbar^2}{2mL^2} \quad (9.60)$$

and hence the number of particles in the first excited state will be of order

$$n_1 = \frac{kT}{\frac{\hbar^2}{2mL^2} - \mu} \quad (9.61)$$

since for a large system L^3 will be bigger than L^2 , the μ in the denominator will be negligible and hence the number of particles in the first state will be

$$n_1 \approx \frac{2mL^2k_B T}{\hbar^2}, \quad (9.62)$$

which will be much smaller than the number of particles in the system. The contribution from all the higher modes can be estimated as the integral which we have already calculated. In short

$$N = n_0 + \Omega n_{\max} \quad (9.63)$$

and the number of particles in the lowest mode may be increased without limit to drive the overall density as high as we wish.

Thus we see that there are two kinds of qualitatively different behaviors in the degenerate bose system. If $-\beta\mu$ remains positive, there is a normal situation in which each of the modes remains occupied by only a small fraction of the particles in the system. Then the system is said to be a *normal Bose fluid*. Conversely, for a fixed value of the temperature, if the density is higher than n_{\max} , then the system has a finite fraction its entire number of particles in a single mode. In this *Bose condensed state*, one might expect to see many manifestations of the quantum nature of that single, macroscopically occupied, mode.

In the real world this change of behavior is observed in the highly degenerate bose system formed by liquid He⁴. For temperatures above a critical temperature, T_c , which is at about 2.18 K, the system behaves as a usual liquid. If, for example, it is pushed through a channel it is slowed down by ordinary viscous drag. But below this critical temperature, it becomes a ‘superfluid’ and can move through a channel without any drag whatsoever. This dissipationless motion is the expected manifestation of the quantum mechanical state which is macroscopically occupied. The noninteracting Bose gas described above only mimics

rather weakly the actual properties of helium, but it does show a transition roughly like the normal to superfluid transition. This qualitative change in behavior is also called a *Bose transition*.

Atomic systems at very low temperatures show a Bose transition. In this case, the interactions are much weaker so that the non-interacting theory just described might be substantially more accurate.

We shall argue in the next chapter that qualitative changes in physical behavior, called ‘phase transitions’, are always accompanied by infinities in thermodynamic derivatives. This phase transition of the non-interacting bose gas is no exception. The simplest infinity can be seen in the derivative $(\partial n / \partial \mu)|_T$ in the normal region in which $\beta\mu$ is nonzero. According to Eq. (9.56) this derivative has the value

$$\left(\frac{\partial n}{\partial \mu}\right)_T = -4\pi \left(\frac{mk_B T}{h^2}\right)^{3/2} \int_0^\infty dx x^2 \frac{1}{[\exp(\frac{x^2}{2} - \beta\mu) - 1][\exp(-\frac{x^2}{2} + \beta\mu) - 1]}. \quad (9.64)$$

In the limit of small $\beta\mu$ the integral contributes mostly when x is small, of order $\sqrt{-\beta\mu}$. Replace the integration variable, by x divided by this characteristic value. Then the integral is

$$\left(\frac{\partial n}{\partial \mu}\right)_T = \frac{4\pi}{\sqrt{-\beta\mu}} \left(\frac{mk_B T}{h^2}\right)^{3/2} \int_0^\infty dx \left(\frac{2x}{\frac{x^2}{2} + 1}\right)^2. \quad (9.65)$$

Notice how the thermodynamic derivative diverges as $-\beta\mu$ goes to zero.

This example illustrates three important characteristic features of phase transition problems:

- (1) There is a qualitative change in the behavior of the system at the phase transition. Here the difference is the macroscopic number of particles which occupy the lowest mode of the system.
- (2) There are singularities in thermodynamic quantities at the phase transition. These usually take the form of infinities in derivatives of thermodynamic expressions. Here $(\partial n / \partial \mu)_T$ is infinite.
- (3) The singularities usually take the form of powers of the quantities which measure the deviation from criticality. Here $-\beta\mu$ measures that deviation and $(\partial n / \partial \mu)_T$ goes to infinity as $1/\sqrt{-\beta\mu}$.

9.8 Entropies

It is rather easy to calculate the entropy of a Boltzmann, or Fermi, or Bose gas.

First do the Boltzmann case. Imagine that we have N particles to distribute among M modes. These modes are picked as a subset of all the modes in the system, so that they all have about the same properties. Thus will have rough equal value of the average

occupation number, $f_\nu = N/M$. The first particle can go into any one of those states, as can the second, and the third, and . . . Each particle has M possibilities. The total number of possibilities is M^N . The number of possibilities is the exponential of S/k_B so that the contribution of these particles and states to the entropy is:

$$\frac{S_M}{k_B} = N \ln M. \quad (9.66a)$$

In this expression, and others below S_M stands for the contribution to the entropy from these modes. However, if the particles are really identical, then we have, in writing Eq. (9.66a), overcounted the number of different possibilities. Imagine for a moment that we do have labels on the different particles. With these labels, we might see the first particle might go into any one of the N occupied states, the second into $N - 1$ slots, the third into $N - 2$, etc. In total the labeling has given us $N!$ ways of filling up the states. For identical particles, all these possibilities are just one possibility. Therefore we have to subtract from the result (9.66a) the overcounting, $\ln N!$ According to the Sterling approximation, for large N , $N! \approx N \ln N/e$, with e being the base of the natural logarithms. With this amendment Eq. (9.66a) becomes:

$$\frac{S_M}{k_B} = N \ln \left(\frac{eM}{N} \right). \quad (9.66b)$$

So far we have used the large number of modes as a device for simplifying the analysis. Now, we would like to calculate the contribution as a sum over modes. To make this conversion, we write instead of M a sum over quantum modes, and take the occupation per mode to be $N/M = f_\nu$. Thus our formula for the entropy is, in the Boltzmann case,

$$\frac{S_M}{k_B} = - \sum_\nu f_\nu \ln \left(\frac{f_\nu}{e} \right).$$

In this equation, the sum extends over the limited number of modes under consideration. However, once the result is expressed as a sum over some modes, it can immediately be extended to a sum over all modes

$$\frac{S}{k_B} = - \sum_\nu f_\nu \ln \left(\frac{f_\nu}{e} \right) \quad \text{Boltzmann.} \quad (9.67)$$

Equation (9.67) was derived by considering a sum over a small proportion of the entire number of modes in the system. But we may extend the calculation to apply to all modes, and thus this equation gives the entropy for any weakly interacting system of Boltzmann particles.

The Fermion case works much the same way. Imagine again a large number, M , of rather similar states which are in total occupied by a number of particles N . The occupation number is again $f_\nu = N/M$. We take these M modes and divide them into two classes, N being full and $(M - N)$ empty. There are M ways to place the first particle, $M - 1$ for

the second, with a total of N factors. Thus the total number of ways is $M!/(M - N)!$. However, we have to divide by $N!$ since our argument introduces (once again!) an entirely inadmissible distinction among the particles. The new result is that

$$\frac{S}{k_B} = \ln \frac{M!}{N!(M - N)!}.$$

We take N and M to be large, and simplify the result with the aid of Sterling's formula. One then finds

$$\frac{S}{k_B} = \sum_{\nu} [-f_{\nu} \ln f_{\nu} - (1 - f_{\nu}) \ln(1 - f_{\nu})] \quad \text{Fermions.} \quad (9.68)$$

This formula also applies to the calculation of the total entropy in any weakly interacting fermion system.

We could derive the entropy for a boson system by using a combinatorial analysis once again. But for simplicity, let's just apply normal algebra. Let n_{ν} be the number of particles in mode ν . Once again we consider a restricted set of M essentially similar modes. Of course, this number is a positive integer which obeys the restriction that the sum of all the n_{ν} 's is the total number of particle N .

$$\exp\left(\frac{S_M}{k_B}\right) = \left[\prod_{\nu=1}^M \sum_{n_{\nu}=0}^{\infty} \right] \delta\left(\sum_{\mu} n_{\mu}, N\right), \quad (9.69)$$

where the δ requires the arguments, two integers, to be equal to one another. Now use the integral relation for the delta symbol

$$\delta(m, 0) = \int_{-\pi}^{\pi} \frac{dq}{2\pi} \exp(iqm).$$

To express (9.69) as

$$\exp\left(\frac{S}{k_B}\right) = \int_{-\pi}^{\pi} \frac{dq}{2\pi} \exp(-iqN) \prod_{n_{\nu}=0}^{\infty} \exp(iqn_{\nu}). \quad (9.70)$$

If we change the contour of integration just a bit so that q moves just a bit into the upper half plain, then each sum over n_{ν} is easily calculated as a geometric series and we find

$$\sum_{n=0}^{\infty} \exp(iqn) = \frac{1}{1 - \exp(iq)}$$

and consequently Eq. (9.70) gives

$$\exp\left(\frac{S}{k_B}\right) = \int_{-\pi}^{\pi} \frac{dq}{2\pi} \exp(-iqN)(1 - \exp(iq))^{-M}. \quad (9.71)$$

The power may be expanded by using the binomial theorem which implies

$$(1 - \exp(iq))^{-M} = \sum_{N=0}^{\infty} \exp(Niq) \frac{(M+N)!}{N! M!}.$$

An elementary integration then gives the combinatorial formula, here algebraically derived,

$$\exp\left(\frac{S}{k_B}\right) = \frac{(M+N)!}{N! M!}. \quad (9.72)$$

One more application of the Sterling approximation now gives us the final result for the entropy

$$\frac{S}{k_B} = - \sum_{\nu} [f_{\nu} \ln f_{\nu} - (1 + f_{\nu}) \ln(1 + f_{\nu})] \quad \text{Bosons}. \quad (9.73)$$

Homework

Problem 9.1 (Fermi and Bose). Given two single particle modes with wave functions ϕ_1 and ϕ_2 . What are the wave functions for the possible three-boson states involving these wave functions? If there are two spatial modes and the fermions have spin 1/2, what are the possible states and wave functions of three fermions?

Problem 9.2 (Specific Heat of Fermion Systems). Define an energy as measured from the Fermi energy for a fermion system as

$$E^* = \sum_{\nu} (\epsilon_{\nu} - \mu) \frac{1}{\exp(\beta(\epsilon_{\nu} - \mu)) + 1}.$$

Consider the partial derivative of E^* with respect to temperature at fixed μ . How does this quantity dependent upon T for small T and very large positive μ .

Problem 9.3 (Bose Condensation). We argued that in three dimensions, a non-interacting bose system would be forced to enter a bose condensed state if we could get the density high enough. How does this argument work in one dimension? In two dimensions?

Problem 9.4 (Pressure for Bosons). Calculate the pressure in a degenerate bose gas.

Problem 9.5 (Neutrinos as Degenerate Fermions). Assume that some part of the universe contains (in a big box) equal numbers of three different kinds of massless neutrinos each with spin 1/2. These form a highly degenerate fermion system at a negligibly low temperature. Write down the relation among entropy, energy density, pressure, and particle density for this system.

Problem 9.6 (Higher Order Average). Calculate $\langle(n_{\nu})^3\rangle$ for noninteracting bosons and fermions. What part of the result survives in the non-degenerate limit?

Part IV

Phase Transitions

Chapter 10

Overview of Phase Transitions

10.1 Thermodynamic Phases

In this chapter, we develop the beginnings of a description of thermodynamic phases and the transitions that occurs as the system changes from one phase to another. Before the beginning of science, people classified the materials in the world about them according to their properties. They saw gases, and liquids, and solids and their distinct behaviors. More recently, scientists have distinguished normal materials from superfluids, and studied a whole variety of magnetic materials, of liquid crystals, of ferroelectrics, and many additional phases of matter. One can make the distinction between the phases in question by observing the qualitative difference among the phases or alternatively by observing the *phase transition* which takes the system from one phase to another. Our prototype system, the Ising model, shows several distinct thermodynamic phases. Some of these are depicted in Fig. 10.1. On the left, we see a paramagnetic phase. There is a considerable randomness to the arrangement of spins and no long-ranged order appears. In contrast, in the right hand panel we see a system with the long-ranged order characteristic of the ferromagnetic phase. Through the entire system the spins tend to point upward with only a few islands of ‘wrong’ behavior, caused by fluctuations. The center panel depicts a situation intermediate between the ferromagnetic and the paramagnetic. In this so-called ‘critical phase’ there are

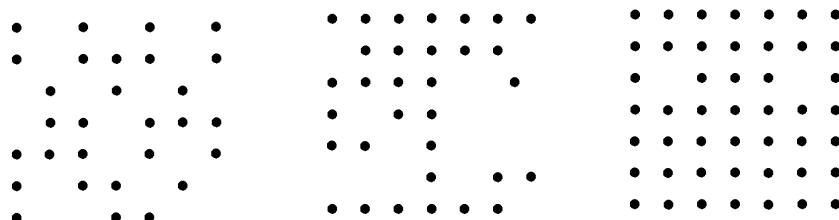


Fig. 10.1. Three different phases for an Ising model. The pictures show spins on a lattice. Spins pointing up are indicated by dots; those pointing down by blanks. The left hand picture shows a paramagnetic phase, the middle one a critical phase, and the right hand picture shows a ferromagnetic phase.

correlations among the different spins. Over large regions of the system, like spins tend to group together. However, one spin direction does not predominate over the other as in the ferromagnetic case. In the following chapters, we shall have much more to say about this critical phase.

10.2 Phase Transitions

The world would indeed be a dull place if there were no distinction among the different phases of matter. No separation of oil and water, no distinction between stream-bed and stream, none between sky and earth, no difference between airy snowflake and sitting water. But it is far from obvious why such distinctions and changes between phases should exist. If a phase transition is to occur, it must be true that two different thermodynamic phases can both exist under the same external thermodynamic conditions. Thus for example a dilute fluid, water vapor, and a dense fluid, liquid water, can be in contact with one another under identical conditions of temperature and pressure. Here the phases are different in character. Each phase of water has its own free energy which depends on number, volume, and temperature. When the free energies of the different phases are different, then the phase with the smaller free energy is the more stable. (This is part of a general rule which states that the relative probability of observing configurations of the system with different free energies is proportional to an exponential of the free energy difference divided by $k_B T$. Thus when two configurations differ by a macroscopic energy difference, in a situation of thermodynamic equilibrium, only the phase with the lower free energy will be observed.)

Thus if two phases are in equilibrium, they must have the same free energy per particle. So coexisting water vapor and liquid water have equal free energy per particle. In fact, the line of coexistence is computed by calculating the free energy as a function of density and temperature in each phase, and then finding the density in which the free energy per particle is equal in the two phases. In this case, the equality of the free energy is viewed as just an accidental occurrence.

But, sometimes there is some symmetry relation which defines the behavior of the system. In that case, there will often be some kind of symmetry connecting the coexisting phases. In a magnetic material, for example, the magnetism is produced by spins and other magnetic moments which can line up spontaneously to produce a natural magnetism. A magnetic moment is a special kind of vector, one which changes sign under the operation of time reversal. (Change the direction of every velocity in a system. The electromagnetic currents will all change sign, and with them all magnetic moments and magnetic fields.) In the absence of a magnetic field applied from outside the material, the system will always have a natural degeneracy: If there is a state in which the average magnetization points in a given direction, then there will be an equivalent state in which it will point in exactly the opposite direction. In the simplest kind of magnetic material there is one ‘easy axis’ and the natural magnetism will occur with the spins lining up parallel or antiparallel to that axis. Call the spin in the direction of that axis σ or σ_z . Then phase transition involves a magnetization density, m , proportional to the average of this spin $\langle \sigma \rangle$. Notice that at the

first order phase transition, the system thus has to choose between two thermodynamically equivalent states, with different values of the magnetization density, m . The two phases have values of m 's which differ by a sign. Furthermore, the value of the magnetization density is same throughout a very large region of the sample, one containing many, many spins.¹ The system spontaneously chooses a particular phase, based upon its history or some weak residual magnetic fields. And after this choice is made and the system has a single thermodynamic phase, then $\langle \sigma \rangle$ will have the same sign and the same value throughout the material. One of the most interesting question about this situation is: How can a huge number of atoms, perhaps 10^{23} of them, can chooses one of the possible phases, and apply the choice across the entire system?

10.3 Two Kinds of Transitions

In nature there are two different kinds of phase transitions. The first kind, observed when we boil water at home, involves a discontinuous change in some intensive thermodynamic quantity. This discontinuity is observed, for example, in the density expressed as a function of pressure and temperature. In a magnet, the direction of magnetization might suddenly change so that the magnetization density vector will change discontinuously. These changes are called *discontinuous* phase transition or *first order* phase transitions. Thermodynamic variables, like this density or magnetization, which exhibit the discontinuity, are called *order parameters*, since their value reflects the strength and kind of ordering in the system. Our two examples of first order transitions are the boiling of water or having a domain of iron jump from one direction of magnetization to another. In either case, if we increase the temperature the jump or discontinuity will become smaller. In the fluid, the vapor density will approach the liquid density. In the magnet, the magnitude of the magnetization will get closer to zero. In both cases, at some critical temperature, T_c , the discontinuity will vanish and the phase transition will change its character. At this special point, we say there is a *continuous* or *second order* phase transition.

All of this is illustrated in Figs. 10.2 and 10.3. These figures plot the magnetization density as it is determined by an approximate theory of the ferromagnetic behavior, called mean field theory. We describe this theory in this chapter and the next. For now, we wish to look at results. Figure 10.2 plots dimensionless magnetization, $\langle \sigma \rangle$ versus dimensionless magnetic field, h , for various values of the temperature. Notice how there is a discontinuity in $\langle \sigma \rangle$ at zero values of the field for $T < T_c$ — reflecting a first-order transition. This $h = 0$ discontinuity disappears at $T = T_c$ — producing a second order transition at that point. This discontinuity in m as we pass through vanishing values of h reflects one kind

¹In what is called a single-domain ferromagnet, the magnetization is uniform throughout the same. But most ferromagnets actually have a tendency to split up into different domains, each with its own direction of the magnetization. This splitting occurs because of weak but long ranged magnetic forces. Magnetic energies are minimized by the splitting into different domains. The domains are usually quite large, containing many atoms. So the ferromagnet is well-represented as a system with long-ranged order over wide regions. In other kinds of ordered phases, the domains can be even larger — extending sometimes over microns or even centimeters.

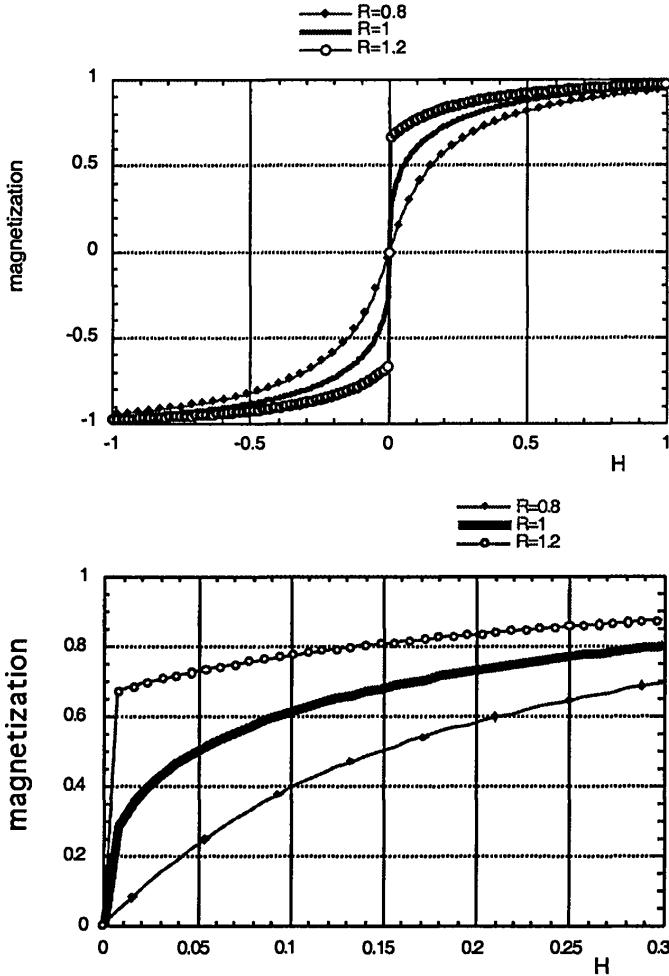


Fig. 10.2. Magnetization plotted as a function of magnetic field. The curves are plotted for three values of $R = T_c/T$, corresponding to above, at, and below the critical temperature. Notice how the curve for $T > T_c$ appears smooth while the one for $T < T_c$ shows a discontinuity at zero field. For $T = T_c$, the discontinuity disappears and is replaced by an infinite slope in the magnetization versus field curve. The upper part shows a larger region of field, the lower is a blowup for small values of the magnetic field.

of singularity in this system. This singularity disappears if $T > T_c$, where magnetization is a smooth function of field. Exactly at the critical temperature, we see an infinite slope of m versus h , showing us that the mathematical singularity remains present at this second order transition.

This same data is plotted in a different way in Fig. 10.3. Here we look at m as a function of T . This figure contains several curves each for a different value of the applied magnetic field. The most interesting is the curve marked ‘ $h = 0$ ’ which shows a magnetization which is zero for $T > T_c$. In contrast, for $T < T_c$, m has two branches, one positive-one negative.

There is an exact symmetry which involves flipping the sign of both m and h . Thus if the function $m(h, T)$ gives the magnetization as a function of temperature and magnetic field,

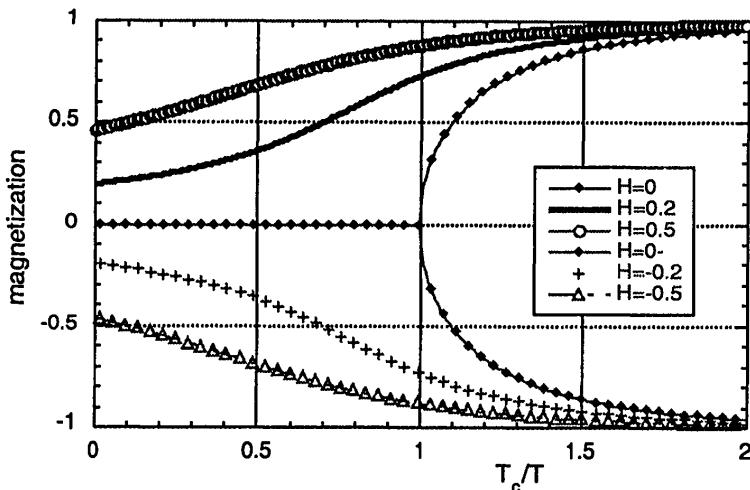


Fig. 10.3. Magnetization plotted as a function of the ratio, R of critical temperature to actual temperature for different values of the magnetic field. Notice the jump in the zero field magnetization for temperatures below the critical temperature.

another equally good solution is $-m(-h, T)$. Each curve with $h > 0$ has a corresponding curve — with oppositely signed m — that applies for the magnetic field with flipped sign. The symmetry is also realized at zero field. At high temperatures, the magnetization is zero for $h = 0$. Then the symmetry is trivially realized since changing the sign of the magnetization changes nothing. However, at low temperatures, for each value of the temperature, the magnetization can take on either of two possible values. The symmetry under flipping the sign of the magnetic field is here reflected in the equality of the magnitude of $\langle \sigma \rangle$ in each of these zero-field phases.

Sometimes we see phase transitions which do not easily fit into the framework given above. There is an interesting phase transition which involves the dissociation of uncharged atoms into charged components. When the charges are tightly bound together we call the material a dielectric. It is an insulator, which may polarize in an electric field but certainly does not conduct electricity. When the atoms dissociate, the charged components may move in opposite directions in response to an electric field. This kind of matter is called a plasma, and can conduct electricity. In general, one does not know whether this *metal to insulator* transition is first order or higher. There is a realization of this transition in three-dimensional condensed matter systems.² A very similar transition occurs in the early universe in which quarks bind together to form the hadrons and mesons we see today. In the Chapters 15 and 16, we shall discuss the two-dimensional version of this phase transition. Of course this transition also occurs in three-dimensional systems.

Transitions into and out of the glassy state, provides other examples in which the basic nature of the transition is unknown. A ordinary glass is a liquid in which some of the molecular motions are very substantially slowed down. The phase transitions become hard

²For a discussion of this transition see the several papers in P. W. Anderson *A Career in Theoretical Physics* (World Scientific, Singapore, 1994).

to see because one has to wait too long. We would like to extrapolate to the phase transition. But we are not quite sure how that might work.

10.4 Back to the Ising Model

We have already discussed in Chapter 4 the setup of an Ising problem which describes the simplest ferromagnets. Recall the previous discussion. We can set up a Hamiltonian which contains a set of spins σ_r , where r is the lattice site defining the location of the spin. Each σ_r takes on two values: plus one and minus one. As in Chapters 2 and 3, we work with a simple hypercubic lattice

$$\mathbf{r} = a(n_1, n_2, \dots, n_\mu, \dots, n_d), \quad (10.1)$$

where a is the lattice constant and each of the n 's is an integer. To produce a ferromagnetic phase transition there must be an interaction between neighboring spins which gives a lower energy to spin configurations in which spins are aligned. An external magnetic field is taken into account by saying that there is a lower energy when a spin is aligned along the magnetic field than opposite to it. This kind of situation can be represented by a Hamiltonian with two terms

$$\mathcal{H} = - \sum_{\mathbf{r}} \sigma_{\mathbf{r}} B(\mathbf{r}) \mu - J \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \sigma_{\mathbf{r}} \sigma_{\mathbf{r}'}. \quad (10.2)$$

Here $2J$ is the energy cost for moving a pair of neighboring spins from an aligned configuration to an anti-aligned one while $2B(\mathbf{r})\mu$ is the energy cost of moving the spin at \mathbf{r} from being lined up with the field to the opposite. The first sum says that the latter energy applies to all spins. The notation $\langle \mathbf{r}, \mathbf{r}' \rangle$ means include all pairs of nearest neighboring spins. The number of nearest neighbors of a given lattice site is generally denoted by z . For the simple hypercubic lattice, $z = 2d$. We take both J and $B\mu$ to be positive. The partition function is obtained by summing an exponential of $-\beta \mathcal{H}$, which we write as

$$W[\sigma] = -\beta \mathcal{H} = \sum_{\mathbf{r}} h(\mathbf{r}) \sigma_{\mathbf{r}} + K \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \sigma_{\mathbf{r}} \sigma_{\mathbf{r}'}. \quad (10.3)$$

Here $h(\mathbf{r})$ is a dimensionless rendition of the magnetic field and K is a dimensionless version of the coupling strength. Both of these go to zero at infinite temperature and to infinity at zero temperature. In most of our calculations we shall let the field $h(\mathbf{r})$ be independent of position. In that case, we shall write it as simply h .

Notice that the Hamiltonian is left invariant if we change the sign of both the magnetic field, h , and also of each of the spins, σ_r .

We have already talked about the possibility (and difficulties) of calculating the consequences of the Hamiltonian (10.3) for statistical systems. The calculation can be carried out for one dimension and at zero field for two dimensions. (See Chapter 4.) Beyond that, little can be done exactly; it is just too hard. However there is one special case which is

quite easy: the one in which the coupling among the spins is zero. Then, as we have already seen, the spin is determined by a single particle Hamiltonian, ϵ , with

$$-\beta H = h\sigma_r, \quad (10.4)$$

a simple calculation gives the average magnetization as

$$\langle \sigma_r \rangle = \tanh h. \quad (10.5)$$

But Eq. (10.5) tells us nothing very direct about the phase transition.

10.5 Mean Field Theory of Magnets

But we can get some of the qualitative properties of the phase transition by examining an approximate theory called ‘mean field theory’. The many variants of this theory work reasonably well and, in fact, often provide a qualitatively correct theory of phase transitions and other physical properties. The idea behind this theory is to make the approximation that each spin behaves as if it were an independent spin sitting in the mean field produced by all the other spins. To reflect this idea we focus upon the particular spin at r and consider how the Hamiltonian depends upon that spin alone. We see that

$$-\beta \mathcal{H} = h\sigma_r + K\sigma_r \sum_{r' \text{ nn to } r} \sigma_{r'} + \text{constant}. \quad (10.6)$$

The last sum is over all r' which are nearest neighbors to r . The ‘constant’ represents all terms which do not depend upon the spin σ_r . Now here comes the approximation. Assume that one can replace the fluctuating sum in Eq. (10.6) by a sum of the averages values of all the neighboring spins. Thus, Eq. (10.6) becomes

$$-\beta H = \sigma_r \left(h + K \sum_{r' \text{ nn to } r} \langle \sigma_{r'} \rangle \right) + \text{constant} \quad (10.7a)$$

which can be equally well represented as

$$-\beta H = \sigma_r h_{\text{eff}}(r) + \text{const}, \quad (10.7b)$$

where the effective field has the value

$$h_{\text{eff}}(r) = h(r) + K \sum_{r' \text{ nn to } r} \langle \sigma_{r'} \rangle. \quad (10.8)$$

As we see, the mean field, h_{eff} , is composed of two parts, first the externally applied field h , and second the internally generated field. Since the spin at r has its probabilities determined by this effective field, its average is given by equation in this approximation the

average is given by Eq. (10.5) with h replaced by h_{eff} . Thus, the mean field theory implies that

$$\langle \sigma_r \rangle = \tanh h_{\text{eff}}(r). \quad (10.9)$$

In the special case in which the system is translationally invariant, we write $\langle \sigma \rangle$ for $\langle \sigma_r \rangle$ and find that Eq. (10.9) is the statement:

$$\langle \sigma \rangle = \tanh h_{\text{eff}} \quad (10.10)$$

where h_{eff} is given by Eq. (10.8) as

$$h_{\text{eff}} = h + Kz\langle \sigma \rangle. \quad (10.11)$$

In this expression, z is, as we have mentioned, the number of nearest neighbors of a given site. In the hypercubic lattice, $z = 2d$, where d is the dimension of the system.

We might expect Eq. (10.10) to be accurate in the limit as z becomes very large. For, when z is large, we have an effective field which is a sum of many terms. The fluctuation in this field gets smaller and smaller as z gets larger and larger. In the limit, the spin in question sees the summed effects of many, many different spins and one might expect to replace the sum by its average. Thus, in particular, we might expect the mean field theory to be particularly accurate for systems in very high dimensions. Notice that K is inversely proportional to the temperature. Therefore, Kz can be thought of as T_c/T , which T_c is some kind of characteristic temperature for the problem. As we shall see that temperature is, in fact, the critical temperature at which we have a continuous transition. We thus can write the effective field for the problem as

$$h_{\text{eff}} = h + \langle \sigma \rangle \frac{T_c}{T}. \quad (10.12)$$

10.6 The Phases

Equations (10.10) and (10.11) constitute the mean field theory for the equilibrium properties of this Ising model. Now we are ready to get the thermodynamic properties of the system by solving Eq. (10.10). Take first the case in which h and $\langle \sigma \rangle$ are both quite small. Then we can expand Eq. (10.10) in a series in both. To first order we find

$$\langle \sigma \rangle = h_{\text{eff}} = h + \langle \sigma \rangle Kz. \quad (10.13)$$

Here z is a symbol for the number of nearest neighbors, which is $2d$ for a hypercubic lattice. Since Kz is inversely proportional to the temperature, we can write it as T_c/T and solve Eq. (10.13) to find

$$\langle \sigma \rangle = \frac{h}{1 - T_c/T}. \quad (10.14)$$

Equation (10.14) shows a singularity at $T = T_c$. Therefore we interpret $T_c = TKz$ as the critical temperature.

From Eq. (10.14), so long as the temperature is above T_c , $\langle \sigma \rangle$ and h point in the same direction while, according to Eq. (10.14), when the temperature is below the critical temperature, $\langle \sigma \rangle$ and h are antiparallel. However the latter is an impossible result. To see its impossibility use Eq. (10.14) to find that the magnetic susceptibility, which is the derivative of magnetization with respect to field, has the value

$$\chi = \frac{\partial \langle \sigma \rangle}{\partial h} \Big|_T = \frac{1}{1 - T_c/T}. \quad (10.15)$$

Equation (10.15) was derived from the mean field theory (10.10) using as the sole assumption that $\langle \sigma \rangle$ and h were both sufficiently small so that one can do an expansion in them.

However for $T < T_c$ Eq. (10.15) must be nonsense. Recall our discussion of operators and field in Chapter 7. The total magnetization operator $M = \sum_r \sigma_r$ is the operator conjugate to the field h . As a result, we know that

$$\langle M \rangle = \frac{\partial}{\partial h} \ln Z = N \langle \sigma_r \rangle. \quad (10.16a)$$

Here the derivative is to be calculated at fixed coupling, K and constant number of sites, N . A higher order calculation is done in which the same way. We see that the derivative of the average spin is exactly the susceptibility

$$\chi = \frac{\partial}{\partial h} \langle \sigma_r \rangle = \frac{\langle (M - \langle M \rangle)^2 \rangle}{N}.$$

Since the last expression is certainly positive, so is the susceptibility. Equation (10.15), then, must fail as soon as T falls below the critical temperature, T_c — since it then gives the wrong sign of the susceptibility. We thus derive a wrong result in this region.

This incorrectness should not be a great surprise to us. If T is far enough below T_c , the magnetization and $\langle \sigma \rangle$ are never very small. Hence one can never expand in them. To see the difficulty, let us try to solve Eq. (10.10) for $\langle \sigma \rangle$ at $h = 0$. To do this, we use a graphical method. We generate graphs for two functions of $\langle \sigma \rangle = x$. The first is just $f(x) = x$. This will represent the left hand side of Eq. (10.10). The second is $g(x) = \tanh(xT_c/T)$. This will be the right hand side. When f crosses g we have a solution for the magnetization. Figures 10.4 and 10.5 show this graphical calculation. The first one, Fig. 10.4, is for $T > T_c$ and shows the one expected root at $x = \langle \sigma \rangle = 0$. The second panel, Fig. 10.5, is for $T < T_c$ and shows three roots! One of these is $\langle \sigma \rangle = 0$ — which has given us trouble. We might suspect that this root is not physically realized. There are two additional roots at nonzero values of the spontaneous magnetization. Because the problem is symmetric under the operation of changing the sign of both σ and h , the two roots are equal in magnitude and opposite in sign.

Somehow the system must choose one of these roots. Which one? We shall see.

A graphical understanding is a beginning. But analytical work often gives us a richer understanding than can be obtained from pure numerics. Therefore, we now turn to obtaining an analytical understanding of the mean field theory for low temperatures.

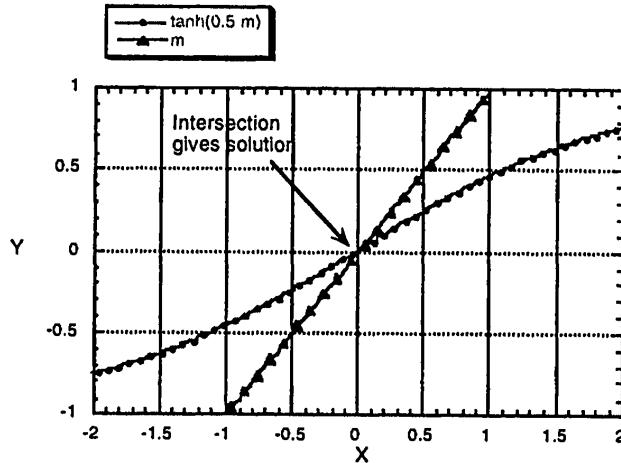


Fig. 10.4. Graphical method of equation solving. Two curves give respectively the left and right hand sides of Eq. (10.9). We calculate the magnetization for zero magnetic field and $T_c/T = 0.5$, using Eq. (10.9). The X -value is $\langle \sigma \rangle$. We draw two curves as a function of X . In one curve, the Y -value is the right hand side of Eq. (10.9) expressed as a function of $\langle \sigma \rangle$ for fixed values of K . For the other it is $\langle \sigma \rangle$ itself. Where these cross we have solutions to Eq. (10.9).

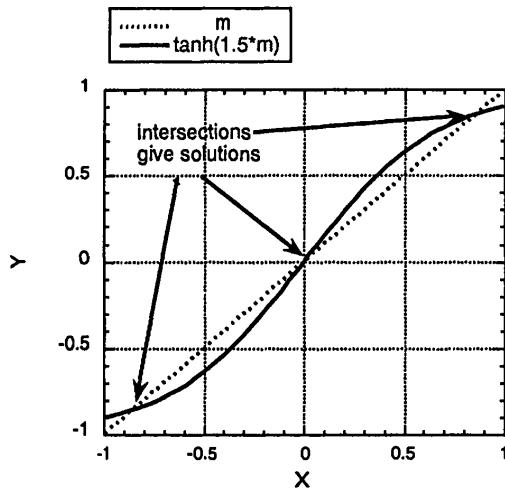


Fig. 10.5. Another graphical calculation of magnetization. Just like Fig. 10.4, except that T is one half of T_c . We follow the same method of equation solving. As in the last figure, the X -axis represents $\langle \sigma \rangle$ while the Y -axis plots $\langle \sigma \rangle$ and the mean field approximation to that quantity. Now there are three solutions: zero magnetization, and the two values of the spontaneous magnetization.

10.7 Low Temperature Result

The quantity $\langle \sigma \rangle T_c/T$ as the interpretation of being the portion of the effective magnetic field induced by the interaction among the spins. For low temperatures, this induced field tends to be very large in magnitude. Let us assume that both this field and the usual magnetic field h , are positive. Thus the induced field is lined up with the applied field. In

this case, the argument of the hyperbolic tangent in Eq. (10.10) is very large and one can use the expression:

$$\tanh x = 1 - 2e^{-2x}, \quad (10.17)$$

which is true for large x . Then Eq. (10.10) becomes:

$$\langle\sigma\rangle = 1 - 2 \exp \left[-2 \left(h + \frac{\langle\sigma\rangle T_c}{T} \right) \right].$$

To lowest order in an expansion appropriate for low temperatures, one can replace the $\langle\sigma\rangle$ on the right hand side of this expression by unity and find:

$$\langle\sigma\rangle = 1 - 2 \exp \left[-2 \left(h + \frac{T_c}{T} \right) \right], \quad (\text{phase } +). \quad (10.18a)$$

When one calculates the susceptibility from this expression one finds a perfectly positive (and small) value consistent with everything we know from thermodynamics and statistical mechanics. We label this phase as $+$ since it has a positive value of the magnetization. Equation (10.18a) looks like a perfectly acceptable solution even for negative values of h . There is another solution which is constructed from the approximation $\langle\sigma\rangle \approx -1$, which we call phase $-$. Its magnetization has the form:

$$\langle\sigma\rangle \approx -1 + 2 \exp \left[-2 \left(-h + \frac{T_c}{T} \right) \right], \quad (\text{phase } -), \quad (10.18b)$$

and yet a third solution, which we obtained before as Eq. (10.14)

$$\langle\sigma\rangle = \frac{-hT}{T_c - T}, \quad (\text{phase } 0). \quad (10.18c)$$

All three solutions look OK. In the next section, we shall argue that only one solution at a time is acceptable. The conclusion as the temperature goes to zero (10.18a) is an acceptable solution only for $h \geq 0$, while (10.18b) is acceptable only for $h \leq 0$, and (10.18c) is never true for low temperatures. This last phase is labeled phase zero since it will have zero magnetization at zero field.

10.8 Free Energy Selection Argument

Equation (10.18) give us three presumably possible thermodynamic states for the system when h is small and the temperature is low. Which one(s) of these situation represents a possible behavior of the real system? To make the right selection we follow a principle that whatever the thermodynamic state achieved by the system is the one which produces the minimum of the free energy, F , or the maximum of the quantity

$$\exp(-\beta F) = \text{Tr } \exp(-\beta H). \quad (10.19)$$

In writing this expression, we use our convention that the quantum sum over states and the classical sum over phase space will be represented by the symbol Tr . To find the free energy we notice that the derivative of the free energy with respect to β is given in terms of the average value of the energy:

$$-\frac{\partial \beta F}{\partial \beta} = \langle H \rangle. \quad (10.20)$$

In mean field theory, to calculate the average energy we start with H and replace each spin in the Hamiltonian by its average. Thus, Eq. (10.20) becomes

$$-\beta \frac{\partial(\beta F)}{\partial \beta} = h \sum_{\mathbf{r}} \langle \sigma \rangle + K \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \langle \sigma \rangle^2 = N \langle \sigma \rangle \left[h + \frac{Kz \langle \sigma \rangle}{2} \right]. \quad (10.21)$$

Here, N is the number of lattice sites while Kz has the physical interpretation of being the ratio T_c/T . Now consider the case $h = 0$. We wish to know how the free energy depends upon our choice of state. For $T > T_c$, there is no choice. For $T < T_c$, in the unmagnetized state $\langle \sigma \rangle$ is and remains zero. Then if F_c is the value of the free energy at the critical point, Eq. (10.21) reads

$$F = F_c \quad \text{for } h = 0 \text{ and all } T \quad (\text{phase 0}). \quad (10.22)$$

Then the free energy is F_c for this configuration. In the magnetized configuration, Eq. (10.21) reads

$$T \left(\frac{\partial(\beta F)}{\partial T} \right)_h = N \frac{T_c}{T} \frac{\langle \sigma \rangle^2}{2}. \quad (10.23)$$

All factors in this expression are non-negative.

Notice that Eq. (10.23) describes all three phases at once. To get the actual free energy at $T < T_c$, one integrates this equation downward in temperature starting at T_c , using the boundary condition that $\beta F = \beta_c F_c$ at the critical temperature. One visualizes doing the integral separately in each of the three phases, in each case stopping the integration at some temperature, T , below the critical temperature. Then one finds that in phase zero the right hand side is zero so that βF remains at the critical value $\beta_c F_c$. On the other hand, in the other two phases, the right hand side of Eq. (10.23) is positive and thus gives a negative contribution to the downward integral, so that

$$\beta F < \beta_c F_c \quad \text{for } h = 0 \text{ and } T < T_c \quad (\text{phase + and phase -}). \quad (10.24)$$

The general rule is that configurations of lower free energy are more likely. In big systems, in which the number of degrees of freedom is approaching infinity, a small difference in free energy per site can result in vastly different probabilities. Here, for $T < T_c$, we have a lower free energy for the two magnetized phases. The system will pick one of these two, and not the unmagnetized phase. A similar argument shows that in a system with a very

large number of lattice sites, N , if h is positive only the positive magnetization phase will be realized. Conversely for negative h only phase — will be achieved. There two phases will be cleanly separated for sufficiently large values of $|h|$. In homework Problem 10.3 we ask you to show that the condition ‘ $|h|$ is sufficiently large’ gets weaker and weaker as the number of sites gets larger. Thus, in an infinite system all nonzero values of $|h|$ give us only one thermodynamically stable phase.

So far, we have not emphasized one essential fact about all these phase transitions. *Phase transitions only occur in infinitely large systems.* Phase transitions are signaled by qualitative differences between two phases of a thermodynamic system. They occur when there is some kind of mathematical discontinuity in the behavior of the system as a function of parameters like K and h . For example, in our Ising example as N goes to infinity the magnetization jumps discontinuously as a function of h . However, it is easy enough to prove mathematically that such a jump cannot occur for a finite system.³ Thus, somehow, phase transitions must be linked to the fact that there are an effectively infinite number of particles in the system. So they are not just a result of mechanics. They are reflections of the mechanics of large systems.

10.9 Behaviors of Different Phases

It is tautological to say that different phases behave differently. A crystalline solid is different from a liquid, which is different from a superfluid, and that is different from a ferromagnet. There is a direct, but deep, reason for the difference. In many, but not all phase transitions, one or more of the phases has a nontrivial set of symmetry properties. In this case ‘nontrivial’ means that the configuration of the system has less than the full symmetry of the Hamiltonian. For example, a crystalline solid has a Hamiltonian which displays both a rotational and a translational invariance. However, the produced lattice shows neither symmetry. Each lattice picks out a set of directions for its crystalline axes. A rotation of the crystal produces another, equivalent, but different configuration. Similarly every lattice picks out preferred positions, which are the equilibrium position of the constituents. Displace the entire lattice a little, and you have other equilibrium positions. Thus, the full translational symmetry is broken. One can often see the broken rotational order. Crystalline solids produce *crystals*, that is pieces of material with surfaces arranged in facets along directions set by the crystal axes. The translational order cannot be seen with the naked eye. Nonetheless these ordering priorities have consequences which are immediately apparent. In contrast to a fluid, a solid is resistant to a shear. It holds its shape. The difference between the disorder of a fluid and the order of a solid is particularly evident in its dynamical behavior. A fluid will propagate only one kind of sound, a longitudinal wave.

³The magnetization is the logarithmic derivative of the partition function. Such a derivative can never show a discontinuity in any region in which Z is analytic in h . But, for a finite system, Z is a finite sum of exponentials of h . It is analytic. Therefore no discontinuities. Indeed, finite-but-large systems can show changes which appear quite abrupt. But, in each case, a close examination of the ‘jump’ region will show a continuous behavior. The abrupt jumps only occur for infinite N .

Typically, a solid will respond to a transient shear by producing a transverse sound wave. This kind of excitation is directly produced because the shear tries to break the produced order and then the system responds dynamically to restore the order. It is generically true that interesting phases show some kind of broken symmetry, by producing a kind of ordering. It is further true that when this ordering is locally disturbed, the system will produce a dynamical response characteristic of the phase in question.

The Bose condensed system provides another example. The superfluid ordering is achieved by having a macroscopic number of particles fall into a single quantum state. This state is defined by a complex wave function. The ordering determines the wave function of this state, defining its magnitude but not its phase angle.⁴ In the Bose condensed system, the condensate wave function has a phase angle, which defines the thermodynamic phase, and takes on all possible values between 0 and 2π . Thus the thermodynamic phase has a symmetry under the rotation of the phase angle. This symmetry is called a ‘U(1)’ symmetry.

In equilibrium the phase angle does not vary in space. The system responds to variations in the phase angle in two different ways. If there is a fixed spatial variation produced by external forces, then the system will produce a ‘supercurrent’ in which there is a mass-flow along the gradient of the phase. This current is entirely different from ordinary mass flow in that this kind of flow can occur without friction, and without energy losses from heating. In contrast, if we apply no forces, but start the system in a situation with a spatially varying phase angle, then it will produce a new characteristic form of sound wave called ‘second sound’. We should not be surprised if a U(1) symmetry can produce waves, after all photons are produced in much the same fashion.

One almost always finds that a broken symmetry produces an ordering and that disturbing that ordering produces some characteristic type of dynamical response. This response is called a ‘Goldstone–Nambu Boson’. Jeffrey Goldstone, now at MIT, and Yoshiro Nambu from Chicago first made this general argument. The word ‘boson’ appears in the argument because one important application of the argument is to broken symmetry states in particle physics. The reader has been prepared, specifically in Chapter 4, for the fact that there is an intimate connection between statistical physics and particle physics. We shall see more of this connection in the next few chapters. We start here. The particle physicist is often interested in understanding the connection between the more ‘fundamental’ short-ranged and high energy interactions and the more accessible lower energy and longer-ranged behavior. The statistical physicist is also interested in relating microscopic interactions to macroscopic behavior. Most of the richness provided by microscopic interactions are really present only at the micro scale. However a few effects persist out to the macro scale. These are:

- (1) The effects of inherently long-ranged forces like electromagnetic interactions or gravity.

⁴Notice that we are in the process of using two different meanings of the word ‘phase’. There is a phase of a thermodynamic system, e.g. liquid or gaseous. To be more precise, we use the words ‘thermodynamic phase’ to specify this meaning. But, there is also the phase of a complex number. We refer to the latter as a ‘phase angle’.

(2) The special effects of long-ranged correlation produced near the critical point. The theory of critical behavior, which develops this class of application is the subject of succeeding chapters.

(3) Long-ranged interaction which occur in broken symmetry states.⁵

The treatment of long-ranged forces are almost identical in particle physics and statistical physics. Thus, in recent years, the paths of statistical theory and particle theory have often run parallel. The discussion of the Higgs particle in high energy physics followed the lines of the treatment of the Anderson mode in superconductors.⁶ The critical state has formed the basis for the calculation of the masses and interactions which occur in particle physics.

This chapter has been concerned with the mean field theory of first order phase transitions. This theory neglects fluctuations in the ordering which drives the phase transition. Of course, in an finite-range, finite-system the fluctuations are always there. Thus, our analysis has left something out. The neglected fluctuations are important. Sometimes the system is in the ‘wrong’ phase — that is it is a liquid when, by free energy considerations, it should be a solid. In another case, its magnetization points opposite to the magnetic field. In these situations the real system will undergo a dynamical process which will bring it to the ‘right’ phase. The process starts with a fluctuation. In a transitory process, the system produces a region within the ‘wrong’ phase that is essentially a small piece of the ‘right’ phase. If that region is large enough it will tend to grow and bring the entire system into the equilibrium phase. Naturally, in order to understand, the process, we must understand fluctuations and it is precisely these fluctuations which are left out in mean field theory. One must go beyond mean field theory to understand some of the most interesting problems in first order phase transitions: the long-lived existence of states of the wrong phase (termed *metastability*), the particularly long-lived metastable states called glasses, and the dynamical processes by which equilibrium is restored. These issues are not fully understood to this day. So we go on, to the somewhat easier problem of second order phase transitions.

Homework

Problem 10.1 (Magnetization versus T_c/T). Draw plots of the solutions to the mean field equation for the magnetization as a function of T_c/T for $h = 0$, $h = 0.1$, $h = 0.2$, and $h = 1.0$.

Problem 10.2 (Anti-ferromagnetism). An anti-ferromagnetic has spins at different sites lined up in opposite directions, so that the total magnetization is zero. Mean field theory gives a description of anti-ferromagnetism directly analogous to the ferromagnetism we discussed. It arises for negative values of the coupling J and hence negative values of K .

⁵Particle physics is much concerned with showing that long-ranged forces can always be understood in terms of microscopic mechanism like #2 and #3. The first point is that there are some inherently long-ranged forces in nature. Statistical physics uses these forces; particle physics must try to explain them, perhaps in terms of #2 and #3.

⁶P. W. Anderson, Phys. Rev. 130, 62 (1962).

- (1) Find the appropriate mean field theory for antiferromagnetism.
- (2) Calculate the magnetic susceptibility for this system.

Problem 10.3 (Phase Probabilities). Below Eq. (10.24) we discussed a free energy evaluation for the relative probabilities for the different phases of the system. Imagine a system with N particles, at $h = 0$ with a temperature a little below the critical temperature. Using mean field theory, estimate the probability that the system will be in the unmagnetized phase for $N = 100$ and $N = 10^{20}$.

Now apply a small positive magnetic field. For $T < T_c$, what is the condition that makes the phase with negative magnetization have a probability of being observed greater than one part in 10^5 .

Problem 10.4 (Magnetic Susceptibility for $T < T_c$). Calculate an expression for the magnetic susceptibility in mean field theory for $T < T_c$ and $h = 0$. Evaluate this expression more explicitly for low temperatures and for temperatures close to the critical temperature.

Chapter 11

Mean Field Theory of Critical Behavior

This chapter is devoted to describing the theory of critical behavior, based upon mean field theory.¹ In this in the next few chapters, we shall devote a considerable attention to the critical point. I should explain to the reader why all this attention is appropriate.

For me, the reason is simple and compelling. I played some role in constructing the modern theory of critical phenomena. I found and find the subject to be fascinating and full of deep connections between physics and mathematics.

I hope that the reader, too, will become convinced of the beauty and depth of the subject. Another reason for studying this subject is that the behavior of systems near the critical point serves as a very good way of getting into some topics which have become very important in modern condensed matter physics, field theory, plasma physics, and hydrodynamics. These topics are described by the following ‘buzz words’.

- (1) Universality: Many physically different systems show the same behavior. For example very many of the observed second order phase transitions have a behavior which only depends on the dimension of the system and the symmetry of the order parameter.
- (2) Scaling: Near the critical point the system is invariant under the symmetry $r \rightarrow \lambda r$, even though the Hamiltonian has no such symmetry. In particle physics this symmetry, when exact, produces massless particles. If there is a weak breaking of the symmetry, one gets low mass particles. The exact and approximate forms of this symmetry are important in connecting physical phenomena which occur at quite different length scales.

¹There are several excellent books on *Critical behavior*, including C. Domb, *The critical point* (Taylor & Francis, London, 1996). S. K. Ma, *Modern Theory of Critical Phenomena* (Benjamin, 1976). H. E. Stanley, *Introduction to Phase Transitions and Critical Phenomena* (Oxford University Press, 1971). Nigel Goldenfeld, *Lectures on Phase Transitions and the Renormalization Group* (Benjamin, 1992) and D. Amit, *Field Theory, the Renormalization Group and Critical Phenomena* (McGraw Hill, 1978).

- (3) Conformal invariance: A symmetry under $\mathbf{r} \rightarrow \mathbf{r}/r^2$. It is a consequence of a underlying field theoretic formulation and of the scale invariance. Conformal invariance was discovered and exploited by A. Polyakov.² In his hands, and others³ this symmetry produced many deep and unexpected consequences.
- (4) Renormalization Group Theory: A calculational method for establishing of the above properties and for a full description of many problems in field theory, statistical physics, dynamical systems theory and many other parts of physics and related subjects. It was first developed by Kenneth Wilson⁴ in the context of critical phenomena.

Thus, in brief, critical phenomena provide a window to look in on modern topics in theoretical physics and to understand these topics in a context closely related to experiment.

11.1 The Infinite Range Model

We now return to mean field theory. We have seen that the mean field approximation gives a qualitatively correct picture of the phase transition in a ferromagnetic system. However, the approach we have given is somewhat unsatisfactory: In replacing the sum of neighboring spins by their average, we used a quite uncontrolled approximation. In other words, we know neither the range of validity nor the size of corrections to this mean field theory. Fortunately, there is another, more controlled, way of generating this same approximation. What we do is define a problem for which the mean field theory is exact.

Instead of putting our spins on a lattice, let us imagine a collection of N spins, each one equally coupled to all the others. Thus the Hamiltonian might read:

$$-\beta\mathcal{H} = h \sum_{j=1}^N \sigma_j + \frac{K}{2N} \sum_{j,k=1}^N \sigma_j \sigma_k, \quad (11.1)$$

instead of (10.3). The problem represented by the Hamiltonian (11.1) is called the infinite-range model. Notice the factor of $1/N$. This factor is designed to make the coupling between any two spins quite weak. However, if there are many many spins then the net effect of the many couplings might be significant. As we shall see in a moment, in the limit as N goes to infinity, the solution to the infinite range model is exactly same as the one we have developed for the thermodynamic behavior of the mean field model.

To derive this fact, look at the partition function of the infinite range model:

$$Z = \text{Tr} \exp \left[hS + \frac{KS^2}{(2N)} \right] \quad \text{where } S = \sum_{j=1}^N \sigma_j \quad (11.2)$$

²A. M. Polyakov, Sov. Phys. JETP 39, 10 (1970).

³A summary of the relation between conformal invariance and statistical physics problems can be found in DGL: J. L. Cardy Volume 11, 55 (1987).

⁴See K. Wilson and J. Kogut, Phys. Reports 12C page 75 (1974) for a review.

and the Tr represents a sum over all of the σ_j 's being plus and minus one. One can use a Gaussian integral to represent the quadratic term:

$$\exp\left[\frac{KS^2}{(2N)}\right] = \sqrt{\frac{K}{2\pi}} \int dt \exp\left[-\frac{Nt^2}{(2K)}\right] \exp(tS),$$

so that the partition function may be rewritten as

$$Z = \sqrt{\frac{K}{2\pi N}} \int dt \exp\left[-\frac{Nt^2}{(2K)}\right] \text{Tr } e^{(h+t)S}.$$

The last trace is easy to compute because of its form as a product of terms referring to different j 's. Since the sum over a single σ is

$$\sum_{\sigma=\pm 1} e^{(h+t)\sigma} = 2 \cosh(h+t).$$

The net result is the single integral

$$Z = \sqrt{\frac{K}{2\pi N}} \int dt \exp\left[-\frac{Nt^2}{(2K)}\right] (2 \cosh(h+t))^N. \quad (11.3)$$

So far, everything we have done is exact. Now we make an assumption which applies only when the number of particles, N , goes to infinity. The integral is now approximated by a steepest descent calculation. This calculation finds a maximum contribution at $t = t^*$ with t^* obeying:

$$\frac{t^*}{K} = \tanh(h + t^*). \quad (11.4)$$

We recognize this result. It is just the same as our previous equation for the average spin, with t^*/K serving in place of $\langle \sigma \rangle$ and K serving in the place of our previous T_c/T .

11.2 Mean Field Theory Near the Critical Point

We write down once again the equations for the mean field theory. The mean field is

$$h_{\text{eff}}(\mathbf{r}) = h(\mathbf{r}) + K \sum_{\mathbf{r}' \text{ nn to } \mathbf{r}} \langle \sigma_{\mathbf{r}'} \rangle, \quad (11.5)$$

which reduces to

$$h_{\text{eff}} = h + \langle \sigma \rangle \frac{T_c}{T}, \quad (11.6)$$

in the special case in which the fields and the average magnetization are independent of position. (As discussed in the last chapter, T_c/T is Kz , with z being the number of nearest neighbors.) The magnetization itself is given in terms of h_{eff} as

$$\langle \sigma_{\mathbf{r}} \rangle = \tanh h_{\text{eff}}(\mathbf{r}). \quad (11.7)$$

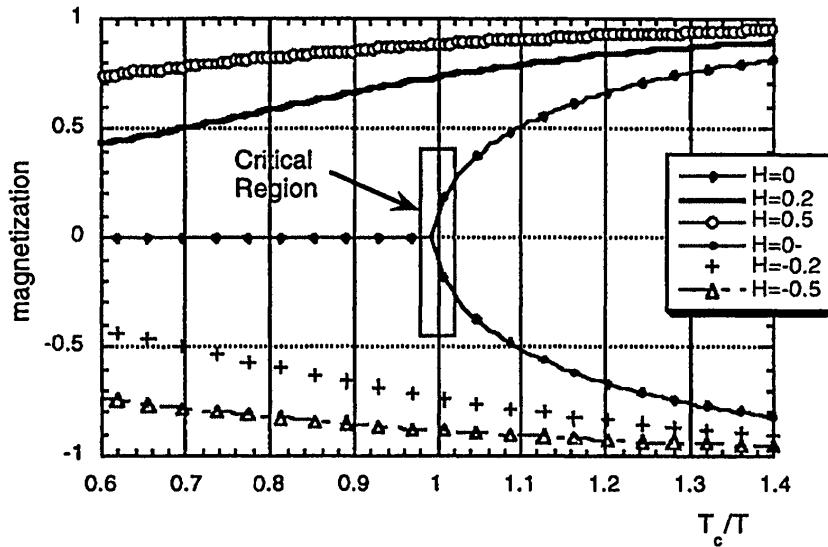


Fig. 11.1. Region of the $T - \langle \sigma \rangle$ plane in which the critical point theory applies. The critical region is outlined.

Now we are ready to get the thermodynamic properties of the system by solving Eq. (11.7). Our goal is to get a useful theory by expanding in parameters which are small near the critical point. We would like to get a consistent expansion so we keep everything that is important for the critical behavior and nothing else.

When we assumed that h and $\langle \sigma \rangle$ were both quite small and expanded to first order in both we found:

$$\langle \sigma \rangle = h + \langle \sigma \rangle \frac{T_c}{T}.$$

One can rearrange this expression as

$$\epsilon \langle \sigma \rangle = h, \quad (11.8)$$

where ϵ is a number measuring the temperature deviation from criticality,

$$\epsilon = 1 - \frac{T_c}{T} \quad (11.9)$$

which we assume to be small, at least in this chapter.

However, we know that as T goes to zero the theory gives three different solutions for $\langle \sigma \rangle$, which we can get by holding on a third order term in $\langle \sigma \rangle$. For this reason, we expand (11.7) to third order in h_{eff} . Notice that for small x , $\tanh x$ expands as $x - x^3/3 + \dots$. Therefore the expansion gives:

$$\epsilon \langle \sigma \rangle = h - \frac{1}{3} [h + (1 - \epsilon) \langle \sigma \rangle]^3. \quad (11.10)$$

Since ϵ is assumed to be small in comparison to unity it is permissible to neglect the ϵ in the cubic term. Furthermore, according to Eq. (11.8), near $T = T_c$ a tiny applied field

produces a huge response in $\langle\sigma\rangle$, making $\langle\sigma\rangle$ much bigger than h . Even though Eq. (11.8) is not right, the order of magnitude statement that $\langle\sigma\rangle$ is much bigger than h is correct. Consequently we can analyze the cubic correction term in Eq. (11.10) by neglecting h in this term. With these simplifications, Eq. (11.10) becomes:

$$\epsilon\langle\sigma\rangle = h - \frac{1}{3}\langle\sigma\rangle^3. \quad (11.11)$$

Now we can *a posteriori* justify the approximations we have made. The mean field analysis is concerned with the region in which three terms in Eq. (11.11) are equally important. This relation will hold if the magnetic field is of the order of cube of the magnetization, while ϵ is of the order of the square of the magnetization. In symbols

$$h \sim \langle\sigma\rangle^3 \quad \text{and} \quad \epsilon \sim \langle\sigma\rangle^2. \quad (11.12)$$

We read Eq. (11.12) by saying that h scales as the magnetization cubed, while ϵ scales as the magnetization squared. As we shall see, scaling laws like these are very useful.

Equation (11.11) is our statement of the mean field equations in the critical region. This equation is a consistent consequence of Eq. (11.7) based upon the assumption that we should keep all terms of order $\langle\sigma\rangle^3$ or lower. Now we are in a position to do an analysis of the behavior in the critical region.

Start out by looking for the spontaneous magnetization. Set $h = 0$ in Eq. (11.11) and find

$$\epsilon\langle\sigma\rangle = -\frac{1}{3}\langle\sigma\rangle^3. \quad (11.13)$$

One solution is $\langle\sigma\rangle = 0$. But since we have a cubic equation, there are three solutions. By factoring out the common factor of $\langle\sigma\rangle$ we find that

$$\epsilon = -\frac{1}{3}\langle\sigma\rangle^2. \quad (11.14)$$

For $T > T_c$ (that is $\epsilon > 0$) this equation has no real solutions. So the only possibility is that the magnetization is zero when the field is zero. Thus we have a disordered state for $T > T_c$. However, for $T < T_c$, $\epsilon < 0$, Eq. (11.14) has two solutions:

$$\langle\sigma\rangle = \pm\sqrt{-3\epsilon}, \quad (11.15)$$

which show that there are two different states of spontaneous magnetization and that in each one the magnitude of the magnetization goes to zero as $\sqrt{T_c - T}$, as T goes to T_c . Next consider the magnetic susceptibility defined as the derivative of magnetization with respect to magnetic field. When T is greater than T_c $\langle\sigma\rangle$ vanishes at zero magnetic field therefore from Eq. (11.11) the susceptibility has the value

$$\chi = \left. \frac{\partial\langle\sigma\rangle}{\partial h} \right|_T = \frac{1}{1 - T_c/T}. \quad (11.16)$$

Physical quantity	Name of index	Formula	Region	Value of index
specific heat	α	$C = A > \epsilon^\alpha$	$h = 0, \epsilon > 0$	0
specific heat	α'	$C = A < (-\epsilon)^{-\alpha}$	$h = 0, \epsilon < 0$	0 (discontinuity)
susceptibility	γ	$\chi = C > \epsilon^{-\gamma}$	$h = 0, \epsilon > 0$	1
susceptibility	γ'	$\chi = C < (-\epsilon)^{-\gamma'}$	$h = 0, \epsilon < 0$	1
magnetization	β	$\langle \sigma \rangle = \pm B(-\epsilon)^\beta$	$h = 0, \epsilon = 0$	1/2
magnetization	δ	$\langle \sigma \rangle \sim h^{1/\delta}$	$\epsilon = 0$	3
correlation length	ν	$\xi \sim \epsilon^{-\nu}$	$h = 0, \epsilon > 0$	1/2
correlation length	ν'	$\xi \sim (-\epsilon)^{-\nu'}$	$h = 0, \epsilon < 0$	1/2
correlation function	η	$G(\mathbf{R}) \sim \mathbf{R} ^{-(d-2)-\eta}$	$h = 0, \epsilon = 0$	0

Table 11.1. Definitions and mean field theory values of critical indices. The word ‘discontinuity’ indicates that in mean field theory the specific heat has a discontinuity at $T = T_c$.

11.3 Critical Indices

A wide variety of systems can be described by mean field theories. All these theories are different in that they have different physical quantities playing the roles we have given to the magnetic field, or $T - T_c$, or serving as the order parameters. Usually there is some operator which undergoes a discontinuous jump, or labels the different states which arise at the same physical conditions. The average of this operator is called the order parameter. Then there are fields which serve to break a symmetry (as h does in our example) or to move one away from criticality in coupling strength (as does our $T - T_c$ or ϵ). These different problems do share many common features. For example many different mean field theories have the very same dependence of the order parameter on the appropriate fields, except for some multiplicative constants. To have results which we can compare with experiments and other theories, we would like to extract from the mean field theory some numbers which do not depend upon these multiplicative constants. We seek to gain the further advantage that the numbers which we shall use to characterize the theory will not change as one changes dimensional quantities (like temperature). We achieve this goal by noticing that typically physical quantities behave as powers of one another near the critical point. We have already realized this power law behavior when we were talking about scaling laws and said that h behaved as $\langle \sigma \rangle^3$ and ϵ behaved as $\langle \sigma \rangle^2$. The powers in expressions like this are called *critical indices*.

To represent the result we have developed so far is to make a list of the so-called critical indices which describe this mean field behavior. This listing is done in Table 11.1. One index in question describes the behavior of the magnetization as $T_c - T$ goes to zero from above. The result is that the magnetization is proportional to the square root of $T_c - T$. More generally, one might imagine that in a class of models of this type the magnetization

might go to zero as the critical temperature is approached as a power of $T_c - T$. This statement is usually written as

$$\langle \sigma \rangle = \text{constant} \times (-\epsilon)^\beta. \quad (11.17a)$$

Equation (11.17a) defines the critical index, β . Notice that the symbol, β , used for this index is the same as the one which is also used in these notes for the inverse temperature, in energy units. Both notations are conventional and we shall try to stay away from the latter use of β in this chapter. In Eq. (11.17a), β is a pure number, which takes on the value 1/2 in the mean field theory developed here. Similarly, another index, γ , can be defined by saying that the susceptibility at zero field goes to infinity as $(T - T_c)^{-\gamma}$ as the temperature approaches the critical temperature from above. Correspondingly, we define γ' as determining the singularity as T goes to T_c from below in the form $(T_c - T)^{-\gamma'}$. According to our analysis, these indices both have the value 1 in mean field theory. These values are noted down in the table. In the first line of our table, we have made use of another quantity called α , which is defined in terms of the specific heat, $C = (\partial^2 F / \partial^2 T)$ at zero magnetic field. The general definition of α is that the specific heat has a singular part which behaves as

$$C = \begin{cases} A_>\epsilon^\alpha & \text{for } T > T_c, \\ A_<(-\epsilon)^{-\alpha} & \text{for } T < T_c. \end{cases} \quad (11.17b)$$

In mean field theory both α and α' are zero. However, a singularity remains because the two coefficients $A_>$ and $A_<$ are not equal to one another so that there is a discontinuity in the specific heat at the critical point.

11.4 Scaling Function for Magnetization

In addition to the critical index values the mean field theory provides an equation for the functional dependence of magnetization upon field and $T - T_c$. As one can see from Eq. (11.11) this relation is cubic in form and relates the small quantities $\langle \sigma \rangle$, h , and ϵ . We would like to factor out the small values and be left with an intrinsic equation connecting these quantities. To achieve this, divide Eq. (11.11) by $|\epsilon|^{3/2}$. This particular power is picked because, according to Eq. (11.8) all three terms in (11.11) scale with this power of ϵ . Let us write

$$\frac{\epsilon}{|\epsilon|} = \pm 1,$$

so that the upper sign refers to $T > T_c$ and the lower to the opposite case. Then we can rewrite Eq. (11.11) as

$$\pm \frac{\langle \sigma \rangle}{|\epsilon|^{1/2}} = \frac{h}{|\epsilon|^{3/2}} - \frac{1}{3} \left(\frac{\langle \sigma \rangle}{|\epsilon|^{1/2}} \right)^3. \quad (11.18)$$

From this form, one can see that the entire result can be rewritten in terms of two variables, which are ratios of quantities which go to zero at the critical point. These *scaling variables*,

M and H are scale-invariant form of the magnetization and magnetic field derived from the original magnetization and field by division of suitable powers of ϵ . Thus we find the rescaled magnetization

$$M = \frac{\langle \sigma \rangle}{|\epsilon|^{1/2}}, \quad (11.19a)$$

and also the rescaled magnetic field

$$H = \frac{h}{|\epsilon|^{3/2}}. \quad (11.19b)$$

The relation between M and H is then obtained from Eq. (11.18) as

$$\pm M = H - \frac{1}{3}M^3. \quad (11.20)$$

The point of this equation is that ϵ has dropped out completely.

The transformation we have just done constructs the *scaling function* $M(H)$ which enables us to express the near-critical magnetization by giving a function of a single variable. Away from the critical point, the magnetization is instead a function of two variables, h and ϵ . Thus a substantial simplification is possible in the near-critical region. The simplified theory enables us to understand the m, h, T data near the critical point in terms of one curve. To see how this is done, we plot, in Figs. 11.2 and 11.3, M versus H . One curve is the scaling theory given by Eq. (11.20). The various points are the ‘experimental data’ obtained from the full solution of the full mean field equations (11.6) and (11.7) for different values of ϵ . Notice how the points cleave to the scaling function curve for small values of ϵ and h , but fall away for larger values. This kind of scaling curve is much used to correlate and understand experimental data. However, as we shall see the actual critical theory has different indices and a different curve because the mean field theory is not quantitatively accurate for two- and three-dimensional systems.

11.5 Spatial Correlations

Now go back to Table 11.1. That table has two lines which describe the coherence length. This length measures the distance over which information is transferred in the near-critical situation. It requires some discussion. Let us put spatial variation back into the problem. We cannot do this with the infinite range model, because the infinite range model does not describe distance at all. So we have to use the form of the mean field theory set out by Eqs. (10.8) and (10.9). In Chapter 7 we discussed how the correlation functions could be computed from the field dependence of the statistical averages. In particular because $h(\mathbf{r})$ and $\sigma_{\mathbf{r}}$ are a conjugate field-operator pair, we can define the spin-spin correlation function as

$$g(\mathbf{r}, \mathbf{r}') = \frac{\partial}{\partial h(\mathbf{r}')} \langle \sigma_{\mathbf{r}} \rangle = \langle (\sigma_{\mathbf{r}} - \langle \sigma_{\mathbf{r}} \rangle)(\sigma_{\mathbf{r}'} - \langle \sigma_{\mathbf{r}'} \rangle) \rangle. \quad (11.21)$$

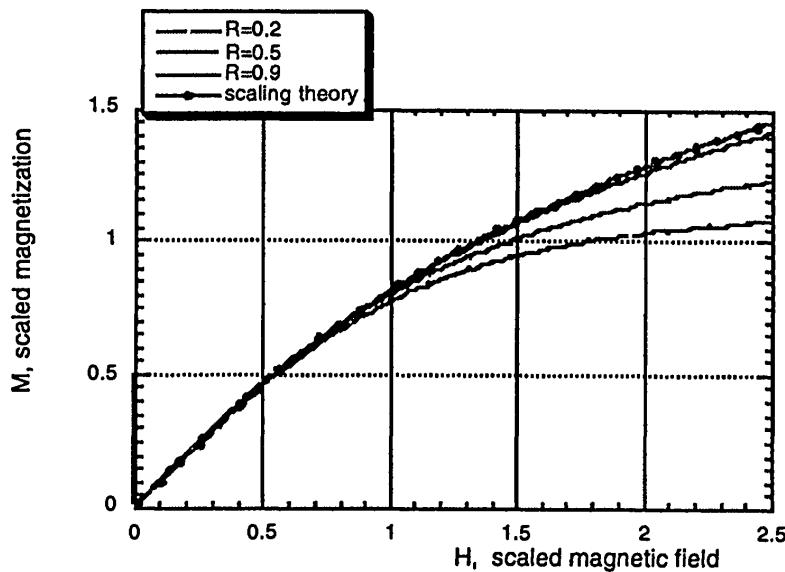


Fig. 11.2. Plot of M versus H showing for different values of the ratio $R = T_c/T$. This plot applies for $T > T_c$. As R gets closer and closer to unity these rescaled curves approach a limiting value. The limiting form is called a scaling function.

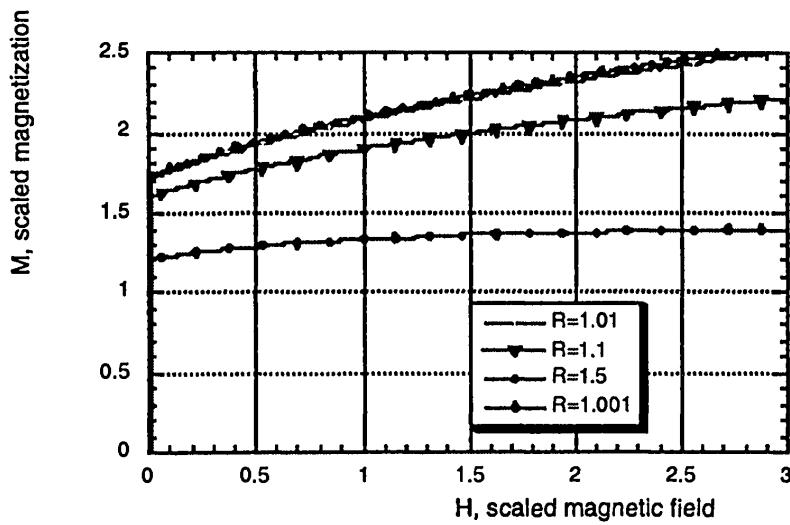


Fig. 11.3. Plot of M versus H showing for different values of the ratio $R = T_c/T$. This plot shows temperatures lower than the critical temperature. Thus these pictures show a discontinuity at zero field. As R gets closer and closer to unity these rescaled curves approach a limiting value — different from the one in the previous figure.

So let us now calculate the correlation function $g(\mathbf{r}, \mathbf{r}')$ using mean field theory as given by Eqs. (10.8) and (10.9). Start from $\langle \sigma_{\mathbf{r}} \rangle = \tanh h_{\text{eff}}(\mathbf{r})$, and just as before simplify this expression by expanding the right hand side in the argument of the hyperbolic tangent. Assume that the system is near the critical point so that one can neglect $h(\mathbf{r})$, and $K - K_c$ in the cubic term. (As in the discussion around Eq. (10.14), the critical coupling is $K_c = 1/z$, where z is the number of nearest neighbors.) We then find:

$$\langle \sigma_{\mathbf{r}} \rangle = h(\mathbf{r}) + K \sum_{\mathbf{s} \text{ nn to } \mathbf{r}} \langle \sigma_{\mathbf{s}} \rangle - \frac{1}{3} \left[K_c \sum_{\mathbf{s} \text{ nn to } \mathbf{r}} \langle \sigma_{\mathbf{s}} \rangle \right]^3.$$

Further simplify this expression by neglecting the difference between $\sigma_{\mathbf{r}}$ and $\sigma_{\mathbf{s}}$ in the cubic term to obtain

$$\langle \sigma_{\mathbf{r}} \rangle = h(\mathbf{r}) + K \sum_{\mathbf{s} \text{ nn to } \mathbf{r}} \langle \sigma_{\mathbf{s}} \rangle - \frac{1}{3} [z K_c \langle \sigma_{\mathbf{r}} \rangle]^3.$$

Recall that $K_c z = 1$, so that our final mean field equation reads

$$\langle \sigma_{\mathbf{r}} \rangle = h(\mathbf{r}) + K \sum_{\mathbf{s} \text{ nn to } \mathbf{r}} \langle \sigma_{\mathbf{s}} \rangle - \frac{1}{3} [z K_c \langle \sigma_{\mathbf{r}} \rangle]^3. \quad (11.22)$$

Equation (11.22) is a consistent statement, within mean field theory, for calculating the response of the magnetization to a varying magnetic field. To get the correlation function differentiate $\langle \sigma_{\mathbf{r}} \rangle$ with respect to $h(\mathbf{r}')$ and find

$$g(\mathbf{r}, \mathbf{r}') = \delta_{\mathbf{r}, \mathbf{r}'} + K \sum_{\mathbf{s} \text{ nn to } \mathbf{r}} g(\mathbf{s}, \mathbf{r}') - [\langle \sigma_{\mathbf{r}} \rangle]^2 g(\mathbf{r}, \mathbf{r}'). \quad (11.23)$$

We wish to calculate the correlation function in a situation in which h does not depend upon \mathbf{r} . (We just used the \mathbf{r} -dependence to form $g(\mathbf{r}, \mathbf{r}')$ by differentiation. However, when the differentiation is all over, we can set $h(\mathbf{r})$ equal to anything we wish, including zero.) Since we take $h(\mathbf{r}) = h$, independent of \mathbf{r} , in Eq. (11.23) we should also set $\langle \sigma_{\mathbf{s}} \rangle = \langle \sigma \rangle$, independent of \mathbf{s} . The resulting equation for $g(\mathbf{r}, \mathbf{r}')$ is

$$g(\mathbf{r}, \mathbf{r}') = \delta_{\mathbf{r}, \mathbf{r}'} + K \sum_{\mathbf{s} \text{ nn to } \mathbf{r}} g(\mathbf{s}, \mathbf{r}') - \langle \sigma \rangle^2 g(\mathbf{r}, \mathbf{r}'). \quad (11.24)$$

Note that Eq. (11.24) describes a translationally invariant situation so that $g(\mathbf{r}, \mathbf{r}')$ will depend only upon the difference between \mathbf{r} and \mathbf{r}' . Equation (11.24) may be solved by Fourier transformation. Both g and the δ symbol may be represented by d -dimensional Fourier integrals as:

$$g(\mathbf{r}, \mathbf{r}') = a^d \int_{-\pi/a}^{\pi/a} \frac{d\mathbf{k}}{(2\pi)^d} g(\mathbf{k}) e^{i\mathbf{k} \cdot (\mathbf{r}-\mathbf{r}')}$$

$$\delta_{\mathbf{r}, \mathbf{r}'} = a^d \int_{-\pi/a}^{\pi/a} \frac{d\mathbf{k}}{(2\pi)^d} e^{i\mathbf{k} \cdot (\mathbf{r}-\mathbf{r}')}.$$

Here there are d components of \mathbf{k} . The integral over each component goes from $-\pi/a$ to π/a .

Thus if we take the transform of Eq. (11.24), we find

$$g(\mathbf{k}) = 1 + 2K \sum_{\alpha=1}^d \cos(k_\alpha a) g(\mathbf{k}) - \langle \sigma \rangle^2 g(\mathbf{k}). \quad (11.25)$$

The reason that the middle term in Eq. (11.25) is relatively simple is that the corresponding term in Eq. (11.24) is in the form of a convolution, and the Fourier transform of a convolution is the product of the corresponding individual transforms. We want to simplify this expression so as to pick out the singularities which are important in the near-critical region. To do this, we recognize that $\langle \sigma \rangle$ is small and that Kz is very close to one. After some rearrangement, the expression becomes:

$$g(\mathbf{k}) = \left\{ \frac{\kappa^2}{2d} + \frac{1}{d} \left(1 - \sum_{\alpha=1}^d \cos(k_\alpha a) \right) \right\}^{-1}, \quad (11.26)$$

with κ^2 having the value

$$\frac{\kappa^2}{2d} = \epsilon + \langle \sigma \rangle^2. \quad (11.27)$$

Notice that the inverse of g has exactly the same form as the Gaussian model correlation function of Eq. (3.19). There is an intimate connection between the Gaussian model and mean field theory.

In a little bit, we shall see that the κ introduced in Eq. (11.27) is related to the coherence length by $\xi = a/\kappa$. We expect the coherence length to go to infinity or κ to go to zero as criticality is approached. At zero field, above the critical point, $\langle \sigma \rangle$ is zero and $\kappa = \sqrt{2d\epsilon}$. Below the critical point, the first term in (11.27) is negative. But the second term is always large enough to make the entire right hand side greater than zero. In this limit, the result is $\kappa = \sqrt{-4d\epsilon}$.

In this way, we reduce the problem of calculating the correlation function to the problem of doing the inverse Fourier integral for $g(\mathbf{k})$. We describe the integration for the simplest case, zero magnetic field and T above T_c . In that case, $\langle \sigma \rangle$ is zero, and (11.27) can be simplified as:

$$g(\mathbf{k}) = \frac{d}{(\kappa^2/2) + \sum_{\alpha=1}^d [1 - \cos(k_\alpha a)]}, \quad (11.28)$$

when T is close to T_c . Here, d is the dimension of space. Thus for $h = 0$ and ϵ small but positive, the correlation function takes the form:

$$g(\mathbf{r}, \mathbf{r}') = da^d \int_{-\pi/a}^{\pi/a} \frac{d\mathbf{k}}{(2\pi)^d} \frac{e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{(\kappa^2/2) + \sum_{\alpha=1}^d [1 - \cos(k_\alpha a)]}. \quad (11.29)$$

We are looking especially for the part of the integral which is singular as κ goes to zero. The singularity will manifest itself when then denominator gets sufficiently small. This will in turn happen if κ is small. We are also looking for long ranged correlation which will be seen when the separation $|\mathbf{r} - \mathbf{r}'|$ is large compared to the lattice separation, a . The contributions for large $|\mathbf{r} - \mathbf{r}'|/a$ will mostly arise for small ka . For both reasons, we expand the denominator in a power series in $k_a a$ and find to lowest order that our integral has the form

$$g(\mathbf{r}, \mathbf{r}') = a^d \int \frac{d\mathbf{k}}{(2\pi)^d} \frac{2d}{\kappa^2 + a^2 k^2} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}. \quad (11.30)$$

The problem was originally set up so that the integral over each component of k would extend from π/a to π/a . But we are now saying that the contributions which interest us all come for small k . If the remaining contributions are small we can safely extend the ka integrations to go from minus infinity to infinity.

The integral (11.30) looks rather formidable. Should we calculate it separately for two dimensions and three and four? There is a trick which enables us to do the problem for all dimensions at once. One uses an integral expression, which puts the denominator in Eq. (11.30) up into an exponential, where the \mathbf{k} integral can be done as a Gaussian integral. The integral expression is:

$$\frac{1}{D} = \int_0^\infty dx e^{-xD}$$

which is just fine if the denominator, D , is positive as it is in Eq. (11.30). Then that integral can be expressed as

$$g(\mathbf{r}, \mathbf{r}') = da^d \int \frac{d\mathbf{k}}{(2\pi)^d} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \int_0^\infty dx \exp[-x(\kappa^2 + a^2 \mathbf{k}^2)/2].$$

The d -dimensional Gaussian integral can be done immediately with the result

$$g(\mathbf{r}, \mathbf{r}') = d \int_0^\infty dx \left(\frac{1}{2\pi x} \right)^{d/2} \exp \left(-\frac{x\kappa^2}{2} - \frac{|\mathbf{r} - \mathbf{r}'|^2}{2a^2} \frac{1}{x} \right). \quad (11.31)$$

This integral converges whenever κ and the distance, $|\mathbf{r} - \mathbf{r}'|$, are greater than zero.

We can further simplify the expression for the correlation function by converting it into a kind of scaling form. We want to analyze this expression in the limit of small values of ϵ and large values of distance. There is one characteristic combination of these two quantities which appears in Eq. (11.31) namely

$$R = \frac{|\mathbf{r} - \mathbf{r}'|}{\xi}, \quad (11.32)$$

where the coherence length, ξ , is given by

$$\xi = \frac{a}{\kappa}. \quad (11.33)$$

This length is the distance over which appreciable spin correlations occur. Notice that it diverges at the critical point. A comparison back to Eq. (11.27) shows that in the mean field ξ goes to infinity as the inverse square root of $(T - T_c)$. This result is included in Table 11.1.

To generate a scaling function change the variable of integration from x to $X = x\kappa$. After that change (11.31) reads

$$g(\mathbf{r}, \mathbf{r}') = \kappa^{d-2} G(R) \quad (11.34a)$$

with

$$G(R) = 2d \int_0^\infty dX \left(\frac{1}{\pi X} \right)^{d/2} \exp \left(-X - R^2 \frac{1}{4X} \right). \quad (11.34b)$$

Here $G(R)$ depends only upon the ratio of the distance to the correlation length, and not explicitly on the magnetic field or upon the temperature deviation from criticality. This function measures the transfer of information within the system. This transfer can occur over very long distances. Consider the limit in which R is large. As one can see by doing a saddle point integral (Homework exercise 11.4) the leading behavior of the correlation function in this large- R limit is

$$G(R) \sim e^{-R} = e^{-|\mathbf{r}-\mathbf{r}'|/\xi}.$$

Thus information transfer dies off exponentially in R . But, as criticality is approached, ξ goes to infinity, so that the fall-off gets slower and slower and information is transferred over an increasingly large distance.

The opposite limit result is also interesting. If R is small, one finds that the maximum contribution to the integral comes from X of the order of R^2 . One can then neglect the first term in the exponent of Eq. (11.31) and find that the resulting integral has the form:

$$g(\mathbf{r}, \mathbf{r}') = \left(\frac{2a}{|\mathbf{r} - \mathbf{r}'|} \right)^{(d-2)} d \int_0^\infty dx \left(\frac{1}{2\pi x} \right)^{(d/2)} \exp \left(-\frac{1}{2x} \right). \quad (11.35)$$

For d greater than two, the integral in Eq. (11.35) is finite. The first factor on the right gives all the r -dependence. Thus Eq. (11.35) implies that when R is small in comparison to one, the correlation function behaves as an inverse power of the distance, so that it gets larger and larger as the distance gets smaller and smaller. This growth is shown in Fig. 11.4. The usual way of writing the critical index associated with the correlation function is to say that

$$g(\mathbf{r}, \mathbf{r}') \sim \left(\frac{a}{|\mathbf{r} - \mathbf{r}'|} \right)^{(d-2)+\eta}. \quad (11.36)$$

The new index, η , has the value zero in mean field theory. For completeness, we include this result in Table 11.1.

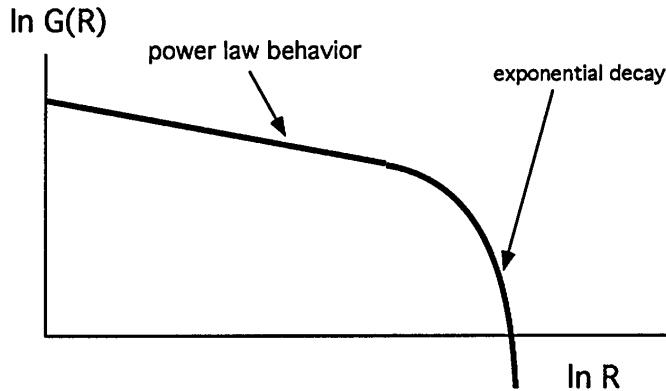


Fig. 11.4. Sketch log-log plot of correlation function showing scaling region and region of exponential decay.

11.6 Analyticity

The divergence of the coherence length gives an important hint about the nature of the singularities which occur at the critical point. Recall the behavior of the magnetization, $\langle \sigma \rangle$, at $h = 0$. For $T > T_c$, the magnetization takes on the value zero. For $T < T_c$, the magnetization takes on nonzero values. As h approaches zero from above, $\langle \sigma \rangle$ takes on a nonzero positive value for $T < T_c$. This qualitative change in behavior is represented mathematically by the statement that $\langle \sigma \rangle$ is not an analytic function of T at the point⁵ $T = T_c$.

There is a spurious argument which suggests that this non-analyticity is impossible. Look at the partition function, Z . This is a sum of $2N$ terms each one positive, representing the different spin configurations possible on a lattice with N sites. Each term is an exponential of the form $\exp(aK + bh)$. There is a theorem which states that such a finite sum of exponentials must be a positive analytic function. Then, the magnetization, the derivative of $\ln Z$ with respect to h , must also be an analytic function of h and K . This argument implies that the magnetization is analytic. But as we have just described, the very existence of the phase transition implies a non-analytic behavior of $\langle \sigma \rangle$. We seem to have reached a contradiction. Is the theorem wrong?

Of course not. It is merely inapplicable. If the system is infinite in size, so that N is infinite, then the theorem about the sum of exponentials being analytic does not apply. The theorem only works for a sum of a finite number of exponential terms. We reach the important conclusion:

The existence of a phase transition requires an infinite system. No phase transitions occur in systems with a finite number of degrees of freedom.

⁵Non-analyticity may take several forms. If any derivative of a function is infinite at some point, the function is non-analytic at the point. The derivative of magnetization with respect to temperature diverges at T_c in mean field theory, so that this theory demands a non-analytical $\langle \sigma \rangle$ at that point. More generally, if a function is zero in one interval of T and nonzero in other adjoining interval, the function must be non-analytic at the point which separates the two regions.

We might expect to see some hint of this conclusion in our mean field theory calculations. The infinite range model uses an integration technique which only applies when N goes to infinity. Even the short ranged mean-field-theory involves an infinite number of particles. In the actual situation, each particle only interacts with $z = 2d$ other particles, but each of these have z interactions. In sufficiently high dimension, this chain of interactions carries through the entire system so that in the end there really are an infinite number of particles involved.

To see the actual number of lattice sites which contribute at once to mean field theory, look at the spin correlation function. Each spin has strong correlations with all the spins within the distance ξ . Thus the number of interacting partners is of order $(\xi/a)^d$. And as $T \rightarrow T_c$, ξ diverges. Thus the number of effectively interacting particles goes to infinity at the critical point.

11.7 Mean Field Theory for the Free Energy

Lev Landau⁶ suggested a most fruitful and general way of looking at mean field theory. He knew that the ferromagnetic transition just discussed can be thought of as containing two types of phase transitions:

- (1) As we vary the magnetic field, we find a discontinuous jump in the magnetization at zero field. This jump occurs for all temperatures below the critical temperature, and reflects what is called a *first order phase transition*.
- (2) At the critical point, where the magnetic field is zero and the temperature is equal to the critical temperature, the jump in magnetization becomes zero. There is some singularity at this point since this is the place where the zero-field magnetization changes its behavior. This point in the phase diagram is termed a second order phase transition (in old-fashioned language) or a critical point (in more modern nomenclature).

This description can be generalized to describe many different situations. Each phase transition is said to have an ‘order parameter’ which can jump discontinuously. In the ferromagnetic case, the order parameter is the magnetization. In a liquid gas phase transition, the density jumps discontinuously so the order parameter is the number of particles per unit volume. In the superfluid, the wave function which describes the macroscopically ordered state can discontinuously change sign or vary its phase. Thus, in this case, the order parameter is the condensate wave function. One can multiply examples. But there is no point in doing so. Each and every phase transition has a quantity, which we call $m(\mathbf{r})$ (m for magnetization) which jumps discontinuously at a first order transition and goes to zero at the critical point. One of the major properties of this order parameter is the symmetry laws it obeys. In the single axis case, the magnetization has two possibilities: being positive or negative. In the group theoretic notation this discrete symmetry is denoted as $Z(2)$. If there were three possibilities (as there are in some kinds of surface ordering) then the symmetry

⁶L. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon, London, 1958).

is $Z(3)$. If there is a symmetry related to a phase which can go between 0 degrees and 360 degrees, this symmetry is indicated as $U(1)$. Every phase transition is thus connected to an underlying symmetry group.

In (almost) every case, the approach to the critical point is controlled by two parameters one like magnetic field, which breaks the basic symmetry of the order parameter and the other like T which controls the amount of ordering. In our discussion we can denote the first kind of external field by the symbol h and the second kind by ϵ . At the critical point, we shall require both h and ϵ to be zero.

Following Landau, we imagine that there is a free energy F which depends upon the fields h and ϵ . As before, we shall consider the situation in which h may depend upon position \mathbf{r} . Now, imagine that the free energy may be expanded in a power series in the relevant physical quantities. Since the quantity varies from place to place, we must allow the free energy — an extensive quantity — to be of the form of a sum (or rather integral) of contributions from all over space. We imagine that the magnetization and the fields are small so that one can do an expansion in them. Following Landau, we write:

$$-\beta F = -\beta F_0 + \int d\mathbf{r} [h(\mathbf{r})m(\mathbf{r}) - a\epsilon m^2(\mathbf{r}) - b m^4(\mathbf{r}) - c(\nabla m(\mathbf{r})) \cdot (\nabla m(\mathbf{r}))] \quad (11.37)$$

assuming also that the gradient of the magnetization is small. Here, once again, β is $1/k_B T$. In the free energy (11.37) b and c are necessarily positive quantities. If b were negative, there would be nothing to prevent the development of arbitrarily large values of the magnetization at each point. If c were negative, there would be nothing to prevent huge gradients in the magnetization. We also take a to be positive. This choice of sign makes the region $\epsilon > 0$ behave as a disordered system and the region $h(\mathbf{r}) = 0, \epsilon < 0$ have two coexisting stable phases.

The lowest order term in Eq. (11.37), F_0 , is independent of the magnetization and is of no interest to us. Since we shall assume that all singularities depend upon the behavior of the magnetization, we must assume that F_0 is a smoothly expandable function of the two small parameters ϵ and h^2 . The square appears in the latter because we assume a symmetry between $+h$ and $-h$. When one flips the sign of h , the sign of m must change also. Thus the lowest order term with the right symmetry is $h(\mathbf{r})m(\mathbf{r})$. The next term with the appropriate symmetry is $m^2(\mathbf{r})$. However, we would like to have $m(\mathbf{r})$ fluctuate a lot. As we shall see this large fluctuation will arise if $m(r)$ can change without changing the free energy very much. A term with the right symmetry which is very small as the critical point is approached is $\epsilon m^2(\mathbf{r})$. Since $m(\mathbf{r})$ is small, the next term in m^4 is also small. The simplest expression involving gradients which is even under $m \rightarrow -m$ and under spatial rotation is the quantity $(\nabla m(\mathbf{r})) \cdot (\nabla m(\mathbf{r}))$ used in the free energy. That is why we use it. Now, we have Landau's free energy. Now what do we do with it?

Landau argued that in any statistical system one could know how the free energy depended upon some macroscopic parameter. For example we might take the system, divide it into two halves, let the energy in the left half be E_L and the temperature in the right half be E_R , with the total energy being fixed to be E , so that we have the constraint $E_L + E_R = E$.

Then we could ask about how these two macroscopic parameters adjust themselves in the real system. As we know, the answer is simple. The system chooses the parameter-values which minimize the free energy under the constraints we have imposed. Thus for example, in our energy case, the system chooses the energy values which equalizes the temperature in the two parts and thus minimizes the free energy. Landau argued that basically the same considerations applied to the magnetization in the example free energy of Eq. (11.37). He demanded that this free energy would be a minimum at the ‘right’, i.e. physically realized, value of the magnetization.

Thus to implement Landau’s calculation scheme, we imagine what happens as we vary the magnetization by a small amount. According to Eq. (11.37)

$$-\beta\delta F = + \int d\mathbf{r} \delta m(\mathbf{r}) [h(\mathbf{r}) - 2a\epsilon m(\mathbf{r}) - 4bm^3(\mathbf{r})] - 2c \int d\mathbf{r} [\nabla \delta m(\mathbf{r})] \nabla m(\mathbf{r}),$$

after an integration by parts,⁷ to get the gradient operation off of $\delta m(\mathbf{r})$, this expression simplifies to

$$-\beta\delta F = + \int d\mathbf{r} \delta m(\mathbf{r}) [h(\mathbf{r}) - 2a\epsilon m(\mathbf{r}) - 4bm^3(\mathbf{r}) + 2c\nabla^2 m(\mathbf{r})]. \quad (11.38)$$

Then, we make the usual statement that if F is to be an extremum, its variation must be zero. This statement requires that the coefficient of magnetization-variation in Eq. (11.38) must vanish. Thus the magnetization obeys

$$h(\mathbf{r}) = 2a\epsilon m(\mathbf{r}) + 4bm^3(\mathbf{r}) - 2c\nabla^2 m(\mathbf{r}). \quad (11.39)$$

Notice that Eq. (11.39) has exactly the same structure as our mean field equations. Therefore, everything we have said about the mean field theory directly carries over to this Landau analysis of the free energy. In fact, the words ‘mean field theory’ are now used to refer to the Landau analysis.

To repay ourselves for this hard work, we should get some new physical result from our Landau-style analysis. To do this look at the free energy itself at zero magnetic field. There are, as we know, three solutions to the mean field theory Eq. (11.39). The field gives zero magnetization and then the free energy is

$$F = F_0, \quad \text{if } m(\mathbf{r}) = 0. \quad (11.40a)$$

On the other hand, Eq. (11.39) has two additional solutions for $\epsilon < 0$, which are

$$m(\mathbf{r}) = \pm \sqrt{\frac{-a\epsilon}{2b}}, \quad (11.40b)$$

with these nontrivial solutions the free energy takes the form

$$F = F_0 - k_B T \int d\mathbf{r} \left(\frac{a^2 \epsilon^2}{4b} \right). \quad (11.40c)$$

⁷We implicitly assume periodic boundary conditions to eliminate any possible contribution from the boundaries of the region of integration.

Since the nontrivial solution has a smaller free energy than the trivial one, the latter is the stable solution for $\epsilon < 0$.

The specific heat at fixed magnetic field is the second derivative of the $-\beta F$ with respect to T (or ϵ). The results are

$$C = T \frac{d^2 F}{dT^2} = \begin{cases} T \frac{d^2 F_0}{dT^2} & \text{for } \epsilon > 0 \\ T \frac{d^2 F_0}{dT^2} + T\Omega \frac{a^2}{2b} & \text{for } \epsilon < 0 \end{cases} \quad (11.41)$$

for T close to its critical value. This result shows that in mean field theory there is a discontinuity in the specific heat at the critical point. The specific heat is higher in the ordered state than in the disordered one because the ordering can absorb some energy. Thus our Table 11.1 should show that the behavior of the specific heat at the critical point is a discontinuity. A discontinuity corresponds to a zero-value of the index, which is then what we list in the table.

11.8 When Mean Field Theory Fails

V. L. Ginzburg derived a very pleasing argument to show when mean field theory would fail.⁸ He argues that mean field theory is correct when fluctuations in the order parameter are much smaller its mean value. Conversely if fluctuations dominate the mean value, then mean field theory will become unreliable and potentially quite wrong. Now use mean field theory to predict its own demise. According to Eq. (11.35)

$$g(\mathbf{r}, \mathbf{r}') \sim \langle \sigma_{\mathbf{r}} \sigma_{\mathbf{r}'} \rangle - \langle \sigma_{\mathbf{r}} \rangle \langle \sigma_{\mathbf{r}'} \rangle \sim \exp\left(-\frac{|\mathbf{r} - \mathbf{r}'|}{\xi}\right) \frac{a^{d-2}}{|\mathbf{r} - \mathbf{r}'|^{d-2}}, \quad (11.42)$$

whenever the separation $|\mathbf{r} - \mathbf{r}'|$ is of order of

$$\xi = \frac{a}{\sqrt{2d|\epsilon|}}.$$

We derived this equation for $T > T_c$ but an essentially similar argument shows that it also holds when $T < T_c$ is one replaces ϵ by $|\epsilon|$ in all order of magnitude statements. Now assume that the crucial fluctuations occur at the characteristic distance for the problem, ξ . Then, according to mean field theory, the characteristic size of the fluctuation is

$$\langle \sigma_{\mathbf{r}} \sigma_{\mathbf{r}'} \rangle - \langle \sigma_{\mathbf{r}} \rangle \langle \sigma_{\mathbf{r}'} \rangle \sim |\epsilon|^{d/2-1}. \quad (11.43a)$$

This fluctuation should be compared with the average value

$$\langle \sigma_{\mathbf{r}} \rangle \langle \sigma'_{\mathbf{r}} \rangle \sim |\epsilon|^{1/2}.$$

⁸V. L. Ginzburg, Sov. Phys., Solid State **2**, 1824 (1960).

The question is which of these is bigger? The fluctuation divided by the squared average has the order of magnitude

$$\frac{\langle \sigma_r \sigma_{r'} \rangle - \langle \sigma_r \rangle \langle \sigma_{r'} \rangle}{\langle \sigma_r \rangle \langle \sigma_{r'} \rangle} \sim |\epsilon|^{d/2-2}. \quad (11.43b)$$

Since ϵ goes to zero, the relative size of the two terms will depend upon whether the exponent in Eq. (11.43b) is positive or negative. If it is positive, as T goes to T_c the relative size of the fluctuation goes to zero and mean field theory is reliable. If the exponent is negative, the relative size of the fluctuations diverge and mean field theory is suspect. We conclude from all this that *near the critical point mean field theory is only reliable for dimensions greater than four.*

We thus expect fluctuations to be of considerable potential importance near the critical point for all two- and three-dimensional systems. One way of seeing this point is to look at the available information about the value of critical indices, as given in Table 11.2. Neither the two-dimensional data nor the three-dimensional data support mean field theory. The disagreement with mean field theory has been known as far back as the 1890s when J. D. van der Waals and J. E. Verschaffelt noted the failure of the van der Waals theory — a mean field theory — to fit experimental data on fluids near their critical points.⁹ This non-classical behavior was later emphasized by E. Guggenheim.¹⁰ By 1966, it became quite evident that the disagreement was always present.^{11,12} In the few years following 1966 mean field theory would become mostly discredited as a descriptor of behavior near phase transitions in two or three dimensions. It was replaced by a fluctuation theory of critical behavior.

Look at Table 11.2. This table focuses upon data for critical indices. Before we look at the values of the indices we should spend a moment on a prior issue. Why do systems have critical indices? Or, better yet, why should they show power law behavior? As the critical point is approached, various physical quantities settle down to a near-critical asymptotic behavior. It is not surprising that this behavior shows power laws and for example that the order parameter goes to zero as a power of $\epsilon = (T_c - T)/T_c$. After all we want to see what happens when this parameter becomes really small. In that limit, there is no other quantity to set the scale for ϵ . Thus we cannot have functions like $\sin(\epsilon)$ because as ϵ goes to zero this will become simply ϵ . The simplest functions without a characteristic scale are powers. Thus, we should not be surprised if experiments and theories gave good support to a power law analysis near the critical point. In fact they do so, and all analysis of near-critical behavior is conducted in terms of power laws and critical indices.

⁹J. M. H. Levelt Sengers, *Physica* **82A**, 319 (1976).

¹⁰E. A. Guggenheim, *J. Chem. Phys.* **13**, 253 (1945).

¹¹See the experimental summary of A. Voronel, DGL: Vol. 5b, 343 (1976).

¹²The experimental situation, and the failure of mean field theory, is summarized in a review paper, L. Kadanoff, W. Götze, D. Hamblen, R. Hecht, E. A. S. Lewis, V. Palciauskas, M. Rayl, J. Swift, D. Aspnes, and J. Kane, *Rev. Mod. Phys.* **39**, 395 (1967) and LPK Essays.

Physical quantity	Name of index	Mean field theory	Index value $d = 3$	Index value $d = 2$
specific heat	α	0 (discontinuity)	0.104 ± 0.003	0 (log singularity)
susceptibility	γ	1	1.2385 ± 0.0015	$7/4$
susceptibility	γ'	1	1.23	$7/4$
magnetization	β	$1/2$	0.325	$1/8$
magnetization	δ	3	5.2 ± 0.15	15
correlation length	ν	$1/2$	$0.632 \pm 0.001 \pm 0.025$	1
correlation functions	η	0	0.039 ± 0.004	$1/8$

Table 11.2. Data for critical indices. Some of the data were taken from C. Domb, *The Critical Point*: p. 354. Other values come from Kadanoff *et al.*, op. cit.

There are three sources of data in the Table 11.2. Most of the two-dimensional results are obtained from Onsager's exact solution of the two-dimensional Ising model.¹³ The implications of this exact solution were worked up by other people including Yang¹⁴ and myself.¹⁵ Experiment provides an excellent source of critical index data for three-dimensional problems. Later developments, based upon universality concepts, would show that one could equally well use data from ferromagnetic transitions, liquid-gas phase transitions, and transitions within critical mixtures (i.e. ones in which different fluids began to separate from one another), as information about the very same type of phase transition. If we use this idea we can include all of these experimental systems in constructing a table like (11.2). (To make the analysis we must identify the order parameters in each of the experimental transitions. For the liquid-gas phase transition, the order parameter is the density. For the fluid mixing transition, the order parameter is the concentration of one of the constituents.)

The final source of data for this table comes from the analysis of power series for thermodynamic quantities. Books¹⁶ have been written about the generation and analysis of power series. Here I can just give the basic idea. Consider a quantity like the susceptibility in the (say) three-dimensional Ising model. Imagine that we can construct the first 20 coefficients of an expansion of logarithm of this susceptibility in a power series in the coupling K , the series being of the form

$$\ln \chi = \sum_{n=0}^{\infty} A_n K^n. \quad (11.44)$$

¹³L. Onsager's solution is described, for example, in index K. Huang, *Statistical Mechanics* (Wiley (1987)) second edition Chapter 15 and also in C. Itzykson and J.-M. Drouffe, *Statistical Field Theory*, Volume I, Sec. 2.2 (Cambridge University Press, Cambridge 1992).

¹⁴C. N. Yang, Phys. Rev. **85**, 808 (1952).

¹⁵LPK ESSAYS: Leo Kadanoff, Nuovo Cimento **44B**, 296 (1966).

¹⁶DGL: Volume 3 is devoted to methods of series expansion.

Here we work at zero magnetic field so that there is a singularity in the susceptibility at the critical value of K which we call K_c . We use the logarithm of χ since we can then say that near the singularity

$$\ln \chi = \gamma \ln(K_c - K). \quad (11.45)$$

Now imagine it were true that this physical singularity is in fact the singularity which is nearest the origin in the K -plane. (If this nearest-singularity condition is not true, one can often do a change of variables which makes it so.) Then one can estimate the critical value of K as:

$$K_c = \lim_{n \rightarrow \infty} \frac{A_{n-1}}{A_n}. \quad (11.46)$$

If one has ten or twenty nonzero terms in the expansion, one can usually get a rather good estimate of K_c by using Eq. (11.46). To find the critical index, one then forms a series for

$$R = (K - K_c) \left(\frac{d}{dK} \right) \ln \chi. \quad (11.47)$$

As K approaches K_c from below, this ratio goes to a constant, which has the value:

$$R^* = (K - K_c) \left(\frac{d}{dK} \right) \ln(K_c - K)^{-\gamma} = \gamma.$$

The series for R usually converges reasonably well at K_c , so that one can get a pretty good estimate of γ by this series analysis method. Much of the data in Table 11.2 is obtained from this, or similar, series method.

The table contains three columns of data. The first data column gives results from mean field theory. We have derived these results in some detail above. The second column gives results on three-dimensional systems both determined by experiments and by series expansions. Notice that the three-dimensional index values are fairly close to the mean field values, but they are certainly different. The last data column refers to the two-dimensional Ising model, which was solved by Onsager. In this lower dimension the index values are quite substantially different from the mean field theory values.

Thus the mean field theory seems wrong for dimensions less than four. However, one can put together a very incisive phenomenological theory from the data and ideas we have presented.¹⁷

We shall develop this point further in the next chapter.

¹⁷In the old Ellery Queen Detective stories, the stories would stop someplace near the end while the authors (there were two of them) asked the reader to solve the mystery. They would say that at this point you have all the facts you need. One might say that here as well. You have all the facts you need to construct a theory with but two independent critical indices. Can you see how to do it?

Homework

Problem 11.1 (Susceptibilities Near the Critical Point). Using the mean field Eq. (11.8), find the form of the magnetic susceptibility for $T = T_c$ and h not equal to zero. Find it also in the magnetized state which arises when $T < T_c$ and $h = 0$. Is the susceptibility positive? How could you derive the form of these results by using the scaling behavior?

Problem 11.2 (Specific Heat). In this chapter, we used the fact that the specific heat at fixed magnetic field is the second derivative of the $-\beta F$ with respect to T (or ϵ). Show that this is true.

Problem 11.3 (Free Energy Near a Critical Point). Use Eq. (11.20) to calculate an analytic expression for the near-critical free energy at $h = 0$ and $T < T_c$. Use this expression to calculate the near-critical specific heat at $h = 0$, for T both above and below T_c .

Problem 11.4 (Spin Correlation Function). Calculate the mean field theory correlation function in r -space in one dimension starting from Eq. (11.29) for $T < T_c$, $h = 0$ and small $|\epsilon|$. Make graphs which compare this result with the estimates derived in this chapter. Describe the different regions of R which can be used to describe this function.

Problem 11.5 (Spin Correlation Function; Continued). For three dimensions, calculate the resulting integral (for $T < T_c$) numerically. What is the form of $G(R)$ for R much smaller than unity. Please include both the leading behavior and the first order correction.

Problem 11.6 (Correlations in the Infinite Range Model). Calculate the correlation function for two spins in the infinite range model.

Problem 11.7 (Mean Field Theory and Infinite Range Model). Calculate the spin–spin correlation function in the infinite range model.

Chapter 12

Continuous Phase Transitions

12.1 Historical Background

As scientists working in this subject gained more experience, they more and more accepted the idea that power laws were the correct description of systems near their critical points. In previous work in physics power law behavior often accompanied situations which could be analyzed by dimensional considerations. Such dimensional estimates were called ‘scaling laws’¹ in fluid mechanics, but were not used very extensively in statistical physics.

By the 1960s the idea of using power laws became generally accepted. Their use was made current by the King’s College School² who analyzed critical behavior in terms of power laws and found that the power laws certainly worked, but that the observed values of the critical indices were quite different from those accepted within mean field theory.

The King’s College school worked only in small part from experimental data. They mostly inferred the forms of singularities in physical quantities by using power series expansions. However, by the middle of the 1960s there was considerable experimental data which clearly pointed away from the correctness of mean field consideration for the observed critical phenomena. For example, the measured values of β in fluid transitions, mostly had β being roughly one third³ — in contrast to the one half predicted by mean field theory. Kellers⁴ had measured the specific heat near the superfluid transition of helium and found it to be apparently diverging — while mean field theory predicted a finite result with a discontinuity. Voronel had measured the specific heat of ordinary non-quantum fluids near

¹In hindsight, one might conclude that some of the ideas discussed here were already well-developed in A. N. Kolmogorov’s 1941 work on turbulence and the independent, but similar, work on the same topic by W. Heisenberg and L. Onsager. Uriel Frisch, in a recent expository work (U. Frisch, *Turbulence*, Cambridge University Press, Cambridge, 1995) argues that concepts of scaling and universality were all to be found in essentially their modern form in the Kolmogorov work. However, the original papers are brief and cryptic, so one cannot be quite sure.

²C. Domb, M. Fisher, M. Sykes and G. Ruskbrooke see C. Domb, *The Critical Point*: page 149 ff.

³E. A. Guggenheim, J. Chem. Phys. 13, 253 (1945).

⁴C. Kellers, Ph.D. thesis, Duke University, 1960. This work was reported in M. J. Buckingham, and W. M. Fairbank, *Progress in Low Temperature Physics*, Vol. III (North Holland, Amsterdam, 1961).

their liquid gas critical point and found, once more, an apparent divergence.⁵ The mean field paradigm was clearly facing a crisis.⁶

The ideas of power laws and scaling were clearly going to form a part of any new theory which was going to emerge. Another very attractive empirical idea also arose from all three sources of data: exact solutions, series expansions, and experiment. Quite different systems seemed to show very similar behavior, with essentially identical values of critical indices. For example one could analyze the Ising model on different lattices. The Onsager solution worked for square and triangular and hexagonal lattices. On all lattices the critical indices were identical. In experimental situations similar phase transitions had closely similar critical indices. For example, the β -values was not only close to $1/3$ for liquids, it also had that value in real magnets and in series expansions of three-dimensional theoretical models. Further T. D. Lee and C. N. Yang⁷ carried out an analysis which suggested an identical behavior for two very different phase transitions: the liquid-gas critical point and the Ising critical magnetic transition so that both transitions (and maybe many others) could be described by a single theory. All these transitions would then have the same values of critical indices.

The word *universality*⁸ expresses the fact that many different systems show the very same critical behavior. The set of all systems which have a given critical behavior is call a *universality class*. By an extension of the same idea, regions of the phase diagram of a single system are said to belong in the same universality class when their long-ranged correlations are identical, and in different universality classes when the behavior is different.

12.2 Widom Scaling Theory

The ideas of scaling and universality would, taken together, produce a theory of critical behavior. The first developments were based upon scaling. Ben Widom, a chemist at Cornell, was studying critical behavior in fluids. I shall translate his ideas into magnetic language because we have used that language in this book. Take the Ising model. One can express the statistical thermodynamics of the Ising problem in terms of the free energy per unit volume, f , which would depend upon the two small parameters, ϵ and h . In detail, the specific heat is

$$C = \left(\frac{\partial^2 f}{\partial \epsilon^2} \right)_h , \quad (12.1)$$

the magnetization is

$$m = \left(\frac{\partial f}{\partial h} \right)_\epsilon , \quad (12.2)$$

⁵A. Voronel *et al.*, Sov. Phys. JETP **18**, 568 (1964).

⁶Thomas Kuhn, *The Structure of Scientific Revolutions* (University of Chicago Press, Chicago, 1970).

⁷T. D. Lee and C. N. Yang, Phys. Rev. **87**, 410 (1952).

⁸The concept of universality has many parents including R. B. Griffiths, Phys. Rev. Lett. **24**, 1479 (1970).

while the susceptibility has the form

$$\chi = \left(\frac{\partial^2 f}{\partial h^2} \right)_\epsilon . \quad (12.3)$$

How could these quantities be related to one another? To answer this question, Widom⁹ asked ‘What sets the scale of f or ϵ or of h ?’. If h and ϵ are simultaneously present some power of ϵ might set the scale of h and vice versa. In addition, some other power of ϵ might set the scale of f . These ideas could be expressed in the form that the critical part of the free energy per site can be written as¹⁰

$$f(\epsilon, h) = \begin{cases} \epsilon^{2-\alpha} f_>(h/\epsilon^\Delta) & \text{for } \epsilon > 0 \\ (-\epsilon)^{2-\alpha} f_<(h/(-\epsilon)^\Delta) & \text{for } \epsilon < 0 \end{cases} . \quad (12.4)$$

In addition to this critical part of the free energy there is a non-singular part which produces no very interesting behavior.¹¹ The Widom scaling theory, as represented by Eq. (12.4), leaves undetermined the two parameters, α and Δ , as well as the function, $f_>$. (Because the free energy is analytic in ϵ at fixed h , $f_<$ can be determined from $f_>$ by an analytic continuation in ϵ .) Equation (12.4) is satisfied by mean field theory with the particular values $\alpha = 0$, $\Delta = 2/3$ and a particular form of the scaling functions $f_>$ and $f_<$. In his thinking, Widom carried over just the right amount from mean field theory. He accepted Eq. (12.4) but put aside the particular determination of α , Δ , and f made by that theory.

In writing Eq. (12.4), we have used Widom’s scaling argument to reduce the number of variables which play a part in our result. Of course this reduction, is only approximately true. It becomes asymptotically correct near the critical point. The functions, like our $f_>$ and $f_<$ which are used in this analysis are called *scaling functions*. Characteristically, scaling functions are used to describe and simplify the near-critical behavior, by saying what combinations of variables are important in this region.

The scaling functions for the free energy do determine all the singular thermodynamic behavior arising at the critical point. For example, look at the specific heat for $T > T_c$. We know that for $T > T_c$ the free energy has no singularities as a function of magnetic field. Then it is correct to assume that $f_>(x)$ is expandable in a power series in x for small x , so that one finds that for $T > T_c$ the specific heat has the form:

$$C = \frac{d^2}{d\epsilon^2} \epsilon^{2-\alpha} f_>(0) = (2 - \alpha)(1 - \alpha)\epsilon^{-\alpha} f_>(0) . \quad (12.5)$$

⁹The two crucial papers are B. Widom, J. Chem. Phys. **43**, 3892 (1965) and *ibid.* page 3896.

¹⁰What I have said here is slightly a-historical. Widom was dealing with fluids not magnets. He was using temperature and chemical potential as his independent variables. The dependent variable was not the free energy but the order parameter. But although my example is different from his, the conclusions have the same character.

¹¹The reader will recognize that I have might have made a mistake here. This year’s dull thing can become the source of next year’s deep insight.

Equation (12.4) is consistent with our previous definitions of α in Eq. (11.17b). The next step is to find the magnetization

$$m = \frac{\partial}{\partial h} (-\epsilon)^{2-\alpha} f'_<(h/(-\epsilon)^\Delta) = (-\epsilon)^{2-\alpha-\Delta} f'_<(h/(-\epsilon)^\Delta).$$

The first order phase transition is a discontinuous jump in magnetization obtained when one crosses the half-line $h = 0$, $T < T_c$. We demand that $f'_<(x)$ be approach a non-vanishing (and in fact positive) limit as x approaches zero from above. It approaches a negative limit as x approaches zero from below. This discontinuity gives us a nonzero value of the spontaneous magnetization. In contrast $f'_>(0)$ is zero, so there is no discontinuity above the transition. A comparison with our previous definition of β in Table 11.1 then tells us that β has the value

$$\beta = 2 - \alpha - \Delta. \quad (12.6)$$

Thus, if we measure the magnetization jump and the specific heat when the magnetic field is zero, we will have determined our two unknowns. The theory then predicts all other possible measurements of critical indices. A comparison of theory with experiment can show whether the scaling idea is right. To start this process, look at the susceptibility when $T > T_c$. We find:

$$\chi = \frac{\partial^2}{\partial h^2} \epsilon^{2-\alpha} f'_>(h/\epsilon^\Delta) = \epsilon^{2-\alpha-2\Delta} f''_>(h/\epsilon^\Delta). \quad (12.7)$$

Now set h equal to zero. Demand that $f''_>$ goes to a constant as h goes to zero and find that the critical index γ obeys

$$\gamma = 2 - \alpha - 2\Delta. \quad (12.8)$$

The unknown, Δ , can be eliminated from the pair (12.6) and (12.8) and one finds that

$$\gamma + 2\beta = 2 - \alpha. \quad (12.9)$$

Equation (12.9) agrees with all the data, even the mean field theory data. It is very pleasing to know that all the thermodynamic critical indices can be expressed in terms of the two unknowns: α and Δ . A similar argument determines the index δ in terms of the already-known indices. Similar arguments give the additional scaling relations $\gamma = \gamma'$ and $\alpha = \alpha'$.

The coherence length index, ν , can be understood by an extension of this same argument. Imagine that the free energy were produced by a large number N_{eff} of classical excitations. These excitations would have a whole range of sizes with the largest size being of the order of the coherence length, ξ . It is these largest excitation which would be most characteristic of the critical behavior and most susceptible to variation in the region near the critical point. Thus the free energy's critical part is best estimated from these excitations. Since each excitation takes up a volume of order ξ^d and the total number of these should be $N_{\text{eff}} \sim (L/\xi)^d$, and the critically fluctuating term in the free energy will be of the order of

$(L/\xi)^d k_B T$. Since there are L^d sites, the free energy per site is of then order of $k_B T \xi^{-d}$. A comparison back to previous estimates [see Eq. (12.4)] indicates that the coherence length's index, ν , is determined by¹²:

$$d\nu = 2 - \alpha. \quad (12.10)$$

Equation (12.10) is most certainly not satisfied by the mean field theory except at the special dimension, $d = 4$. However, it is obeyed by the other data shown in Table 11.2.

The difference between the mean field theory and the scaling estimates, first appear in the derivation of Eq. (12.10). Mean field theory assumes, naturally enough, that the mean field dominates all physical quantities. It assumes, in addition, that expansions of the free energy in these quantities can be performed near criticality. In contrast, the scaling theory drops the idea that the free energy can be expanded. Instead the scaling theory assumes that mean field and fluctuation effects are of equal importance. For this reason, the scaling theory produces quite different estimates of all kinds of critical behavior, particularly in the estimate for the correlation length for fluctuations.

The description of critical phenomena provided by Widom's theory is essentially correct. It does give some insight into how the behavior near the critical point does work. And that in turn gets us closer to another big question, involving length scales: We all know that the world around us shows an amazing variety of length scales: There is the Hubble radius of the universe, 10^{10} light years or so and the radius of our own solar system, 10^{11} meters roughly, and us-two meters perhaps, and an atom- 10^{-10} meters in radius, and a proton 10^{-16} meters, and the characteristic length of quantum gravity — which involves another factor of about 10^{20} .

How these vastly different lengths arise is a very interesting and fundamental question. We cannot say much about this question here. (Not much is known.) However, we can think about how one describes the region between these lengths. If one is looking at scales between two fundamental lengths, there are no nearby characteristic lengths. Similarly in critical phenomena, whenever one looks any event which take place between the scale of the lattice constant and the much larger scale of the coherence length, one is in a situation in which there are no nearby characteristic lengths.

Thus, from one point of view, critical phenomena look vastly special. To find them one must adjust the temperature and perhaps the magnetic field to special values. This fine adjustment makes these behaviors very artificial and delicate. On the other hand, the universe does give us vast ranges of distances and the phenomena which lie between characteristic distances seem to be explicable in the same terms as critical phenomena. Thus from this point of view the underlying stuff of critical phenomena appear to be very robust and worthy of study.¹³

¹²This relation has been named by M. E. Fisher the *hyperscaling* relation.

¹³This conundrum has been particularly pointed out by P. Bak, C. Tang and K. Wiesenfeld. (See the reprints at the end of Chapter 6.) These authors pointed out many cases of non-equilibrium behavior in which the system showed what they called *self-organized criticality*. That is the system organized itself so that its internal dynamics produced critical behavior over a very wide range of length scales. It might be

Widom's point of view provided a partial understanding of this situation. It certainly seemed to be correct. However, it left many questions unanswered. Why should there be precisely two unknown indices? How could one predict their values? Did the indices have simple, rational values as the two-dimensional Ising example suggested? Was the whole problem solvable?

In the years immediately following Widom's work, we saw excellent progress toward answering these questions. Widom's work was understood as a result of invariance under a scale transform.¹⁴ In work done even before Widom's, the scaling structure of all correlation functions were understood by Patashinskii and Pokrovskii.¹⁵ Theory and experiment were incisively compared.¹⁶ Then in 1971 a full theory (a theory of the renormalization group) was developed by Kenneth Wilson.¹⁷ This theory was quite extensively applied. The most remarkable application of this theory was to the development of an expansion about four dimensions.¹⁸ At this point, I shall drop the historical perspective and begin to describe the renormalization theory, not as it was actually invented but instead as it was later understood.

12.3 The Ising Model: Rescaled

In this section, I shall introduce a scale transformation which can be performed on any lattice model in statistical mechanics. In order to see what is going on it is very nice to have a concrete example. For this purpose let us choose our old friend the two-dimensional Ising model.

The basic variables are $\sigma_{j,k}$ with $j = 1, 2, \dots, L$ and $k = 1, 2, \dots, L$. Use periodic boundary conditions so that $\sigma_{j,k} = \sigma_{j+L,k} = \sigma_{j,k+L}$ and take the partition function to be a sum of the form:

$$Z = \text{Tr } e^{W[\sigma]}, \quad (12.11)$$

where the action, $W = -\beta H$, has the specific form

$$W = \sum_{jk} (K_0 + K_x \sigma_{j,k} \sigma_{j+1,k} + K_y \sigma_{j,k} \sigma_{j,k+1} + h \sigma_{j,k}). \quad (12.12)$$

that their suggestion has a deep connection with the existence of many length scales in the observed universe. This possibility is under intense investigation.

¹⁴LPK essays, L. Kadanoff, Physics **2**, 263 (1966).

¹⁵A. Z. Patashinskii and V. L. Pokrovskii, Soviet Phys. JETP **19**, 667 (1964).

¹⁶The experimental situation, and the failure of mean field theory, is summarized in a review paper in LPK Essays:, L. Kadanoff, W. Götze, D. Hamblen, R. Hecht, E. A. S. Lewis, V. Palciauskas, M. Rayl, J. Swift, D. Aspnes and J. Kane, Rev. Mod. Phys. **39**, 395 (1967). Parallel review which shows the failure of mean field theory critical indices are: M. E. Fisher *Reports of Progress in Physics* **30**, 615 (1967) and P. Heller, *ibid.* page 731.

¹⁷K. Wilson, Phys. Rev. B. **4**, 3171 (1971).

¹⁸K. Wilson and M. E. Fisher, Phys. Rev. Lett. **28**, 240 (1972).

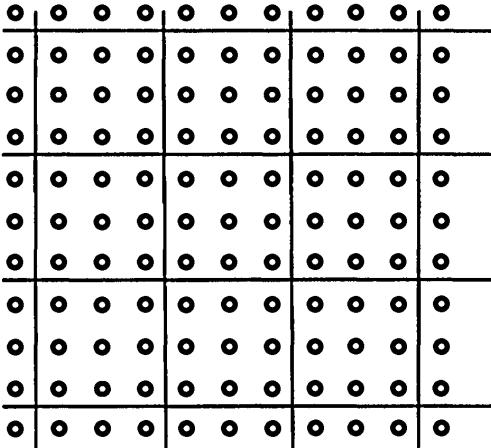


Fig. 12.1. Renormalization of cell-size in a lattice. The lines mark off blocks, and each block is represented by a new spin variable.

For most of our purposes, we shall set $K_x = K_y = K$ so that the couplings in the two directions are identical. When we do this, we write

$$Z = Z(K_0, h, K, \dots, L^d) = e^{L^d f(K_0, h, K, \dots)} . \quad (12.13)$$

Here the \dots stand for all the other couplings which might be in the problem. All our pictures and coordinate indices will be set up to describe two-dimensional systems. However, most of the arguments and the renormalization formulae will be more general. We shall almost always think about a large system so that L will be a very large number.

We shall often simplify our notation by writing instead of a list of coupling constants (like K_0, h, K) a vector $\mathbf{K} = (K_0, h, K, \dots)$. In this notation Eq. (12.13) would read

$$Z = Z(\mathbf{K}, L^d) = e^{L^d f(\mathbf{K})} . \quad (12.14)$$

We want to think about the ferromagnetic transition of the Ising model. (See Fig. 10.1.) Then, the system organizes itself so that for K near K_c there is a substantial correlation even among spins separated by a large distance. This is a reflection of the basic phase transition in which the system is lining itself up to produce, at low temperatures, an infinite range spin correlation. We use this correlation to organize our thinking about how to study the phase transition problem.¹⁹

Figure 12.1 shows the basic idea of our calculation. The lattice is divided into cells, each cell with side λ times the original lattice spacing and $\lambda \gg 1$. We introduce a new label \mathbf{R} for each cell and a new statistical variable $\mu_{\mathbf{R}}$ (which takes on values ± 1), one such variable for each cell. In this setup, the probability that $\mu_{\mathbf{R}}$ takes on one or the other of its values is determined by the distribution of neighboring $\sigma_{j,k}$ values. In the simplest case, the sign

¹⁹The structure of correlations among two far-separated spins is given in: Leo Kadanoff, Spin-Spin Correlation in the Two-Dimensional Ising Model, *Nuovo Cimento* 44, 276 (1966), See LPK: Essays.

of the new variable is determined by the sign of the total magnetization in the cell,

$$m_{\mathbf{R}} = \sum_{j,k \text{ in } \mathbf{R}} \sigma_{j,k}, \quad (12.15)$$

so that the probability distribution for $\mu_{\mathbf{R}}$ would be

$$t(\mu_{\mathbf{R}}, \{\sigma\}) = \delta(\mu_{\mathbf{R}}, \text{sign}(m_{\mathbf{R}})). \quad (12.16a)$$

Alternatively one might choose an exponential probability distribution for the new spin, perhaps something of the form:

$$t(\mu_{\mathbf{R}}, \{\sigma\}) = \frac{e^{K_t \mu_{\mathbf{R}} m_{\mathbf{R}}}}{2 \cosh(K_t m_{\mathbf{R}})}. \quad (12.16b)$$

Here K_t is an adjustable parameter which is used to set the renormalization transformation. In the limit as K_t goes to infinity, the distribution (12.16b) reduces to (12.16a). One can use these definitions of the distributions for μ or many others. The scheme is very flexible and can be modified to fit the needs of a particular calculation. We shall describe some particular examples below.

With either of these two definitions or a wide variety of other ones one can define a probability distribution for all the μ 's according to

$$T[\mu, \sigma] = \prod_{\mathbf{R}} t(\mu_{\mathbf{R}}, [\sigma]_{\mathbf{R}}). \quad (12.17)$$

Here $T[\mu, \sigma]$ is the probability that the ‘new’ spins will have the set of values $\{\mu\}$ given that the old spins have the set of values $\{\sigma\}$. To fit this interpretation, we demand that the probability sum to unity, that is

$$\text{Tr}_{\mu} T[\mu, \sigma] = 1. \quad (12.18)$$

In fact, (12.18) will be our principal demand upon the renormalization function probability function, T . Our only other demand on T , beyond (12.18), is the μ 's each have values determined by the σ 's in their spatial neighborhood. The simplest way of realizing this condition is to demand that in the product form of Eq. (12.17), $t[\mu_{\mathbf{R}}, \sigma_{\mathbf{R}}]$ depend only upon a set of σ 's in the neighborhood of the point \mathbf{R} . The normalization condition of Eq. (12.18) is then satisfied if we have a simple normalization for each component:

$$\text{tr}_{\mu} t[\mu, \sigma] = 1. \quad (12.19)$$

Now we are ready to start. As we go through the transformation, we use Table 12.1 to record and keep track of the various renormalizations. There are lots of them. To start out, we take our basic Ising model and perform a renormalization transformation upon it according to the scheme

$$e^{W'[\mu]} = \text{Tr}_{\sigma} T[\mu, \sigma] e^{W[\sigma]}. \quad (12.20)$$

Quantity	Renormalization	Comment
lattice spacing	$a \rightarrow a' = \lambda a$	
number of lattice sites	$N \rightarrow N' = \lambda^d N$	
physical distance	$\mathbf{r} \rightarrow \mathbf{R} = \mathbf{r}$	invariant
coherence length	$\xi \rightarrow \xi' = \xi$	invariant
$\kappa = a/\xi$	$\kappa \rightarrow \kappa' = \lambda \kappa$	
action	$W[\sigma] \rightarrow W'[\mu] = \ln\{\text{Tr}_\sigma T[\mu, \sigma] \exp W[\sigma]\}$	
couplings, \mathbf{K}	$\mathbf{K} \rightarrow \mathbf{K}' = \mathbf{R}(\mathbf{K})$	
Partition function hence free energy	$Z \rightarrow Z' = Z(\mathbf{K}', N') = Z(\mathbf{K}, N)$	invariant
fixed point	$\mathbf{K}^* = \mathbf{R}(\mathbf{K}^*)$	invariant
scaling field	$h^\alpha \rightarrow h'^\alpha = \lambda^{y_\alpha} h^\alpha$	
magnetic field	$h \rightarrow h' = \lambda^{y_h} h$	
temperature deviation	$\epsilon \rightarrow \epsilon' = \lambda^{y_T} \epsilon$	
scaling operator	$X^\alpha[\mu] \cong \lambda^{-y_\alpha} X^\alpha[\sigma]$	
operator density	$O^\alpha(\mathbf{R})[\mu] \cong \lambda^{x_\alpha} O^\alpha(\mathbf{r})[\sigma]$	note $x_\alpha + y_\alpha = d$

Table 12.1. Scaling properties under renormalization group transforms. In this table, the wiggly equal sign in the last two lines means equality in averages near the critical point. This equality for the density operators, $O^\alpha(\mathbf{R})$, implies that these local operators have equal long-distance correlations.

Now we have generated a new action W' from the old one, W . The crucial fact here is that the new action $W'[\mu]$ describes the very same problem that we had at the beginning. But it is described in a new representation. The transformation from σ to μ and from \mathbf{r} to \mathbf{R} has changed the lattice constant by a factor of λ so that the number of lattice sites is not at its original value, N , but now there is a new number of sites:

$$N' = N \lambda^{-d}. \quad (12.21)$$

If the old $W[\sigma]$ were described by a set of couplings \mathbf{K} , then the new weight factor, $W'[\mu]$ is described by a set of new couplings \mathbf{K}' . Since the old couplings determine the new ones, the couplings are related by:

$$\mathbf{K}' = \mathbf{R}(\mathbf{K}), \quad (12.22)$$

so the a th new coupling is given by $K'_a = \mathbf{R}_a(\mathbf{K})$. Notice that there is no reason to believe that our original list of couplings, K_0, h , and K , is at all sufficient. The renormalization transform (12.20) might well generate all kinds of new couplings: between pairs of next-nearest neighbors, among quartets of particles arranged around the corners of a square, couplings of three and six Ising spins, and so on and so forth. Be that as it may, the renormalization transform which we have described here gives an alternative description of the very same statistical system in terms of two sets of variables, $\{\sigma\}$ and $\{\mu\}$, two different lattices with spacings a and $a' = \lambda a$, and two sets of couplings, \mathbf{K} and \mathbf{K}' .

It is hard to think about a infinite set of coupling constants and a correspondingly infinite set of couplings. However, we know that the most relevant properties of the near-critical Ising system can be described in terms of $T - T_c$ and the magnetic field, h . Universality states that all the remaining possible couplings do not change the structure of the result. Thus, one might expect that one can get away with thinking about just two fields, K and h —and their corresponding conjugate operators: the local magnetization $\sigma_{j,k}$ and the local energy density:

$$\mathcal{E}_{j,k} = \sigma_{j,k} \{\sigma_{j+1,k} + \sigma_{j-1,k} + \sigma_{j,k+1} + \sigma_{j,k-1}\}. \quad (12.23)$$

We shall see that we can learn all about Widom scaling by thinking about the transformation properties of the fields ϵ and h and also the ‘trivial’ field K_0 .

Before discussing things which change under renormalization transformations, we should think about quantities which are not changed under the renormalization transformation. The first such quantity is the free energy. Calculate the partition function after the transformation. It has the value:

$$Z(\mathbf{K}', N') = \text{Tr}_\mu e^{W'[\mu]} = \text{Tr}_\mu \text{Tr}_\sigma T[\mu, \sigma] e^{W[\sigma]}. \quad (12.24)$$

But, because the transformation function obeys the sum rule (12.18), we can calculate the trace over μ on the right hand side of Eq. (12.24). It gives unity and we find

$$Z(\mathbf{K}', N') = \text{Tr}_\sigma e^{W[\sigma]} = Z(\mathbf{K}, N). \quad (12.25)$$

Thus, the free energy is unchanged under the transformation. Since the number of sites changes by a factor of λ^{-d} , the free energy per site, $f(\mathbf{K})$, obeys:

$$f(\mathbf{K}') = \lambda^{-d} f(\mathbf{K}). \quad (12.26)$$

The coherence length is an additional invariant quantity. To see the reason for its invariance, imagine that we calculate the correlation function of two μ 's which are very far separated. Then the leading behavior of the correlation function is an exponential fall-off. In symbols,

$$\langle (\mu_{\mathbf{R}} - \langle \mu \rangle)(\mu_{\mathbf{S}} - \langle \mu \rangle) \rangle \sim \exp\left(-\frac{|\mathbf{R} - \mathbf{S}|}{\xi'}\right). \quad (12.27a)$$

In writing this expression we have left out some prefactors which vary more slowly than exponentially with the distance. In the neighborhood of the critical point, the coherence length ξ' is independent of \mathbf{R} and \mathbf{S} but away from that point the isotropy is lost and ξ' depends upon the angle that $\mathbf{R} - \mathbf{S}$ makes with the crystal axes. Of course, there is an identical expression for correlations of σ

$$\langle (\sigma_{\mathbf{r}} - \langle \sigma \rangle)(\sigma_{\mathbf{s}} - \langle \sigma \rangle) \rangle \sim \exp\left(-\frac{|\mathbf{r} - \mathbf{s}|}{\xi}\right). \quad (12.27b)$$

Once again, we have left out some non-exponential prefactors. Now let \mathbf{r} and \mathbf{s} be respectively positions which lie within or close to the sets defined by the cells of \mathbf{R} and \mathbf{S} . In that case, since the renormalization transform determines the μ 's in terms of σ 's within their cell, $\sigma_{\mathbf{r}}$ is going to be proportional to $\mu_{\mathbf{r}}$ with some nonzero constant of proportionality. Therefore, to exponential order, the right hand sides of (12.27a) and (12.27b) are going to be equal. Since the distances $|\mathbf{R} - \mathbf{S}|$ and $|\mathbf{r} - \mathbf{s}|$ are also closely equal, the coherence lengths must be identical. We thus conclude $\xi = \xi'$ or more precisely

$$\xi(\mathbf{K}', a') = \xi(\mathbf{K}, a). \quad (12.28)$$

Notice that ξ is a dimensional quantity, with dimensions of a length. For this reason, we have written $\xi = a/\kappa$, where a carries the dimensions and κ , which is dimensionless, depends upon coupling constants. Since a is changed by a factor of λ in the transformation:

$$\kappa(\mathbf{K}') = \lambda\kappa(\mathbf{K}). \quad (12.29)$$

Thus κ increases in every step of the renormalization.

12.4 Fixed Points

There are four important ideas in the construction of the renormalization group theory. The first is that scale transformations are important. The second is that because of universality, different sets of couplings may really describe the same physical situation. The third is that you can describe any system by an infinite string of coupling constants, \mathbf{K} , and that the scale transformation may be considered to be change in the values of these couplings. We say that the renormalization transform *renormalizes* the coupling constants. Now we come to the fourth big idea: Each phase of the system, including and especially the critical phase, can be described by a special set of couplings, \mathbf{K}^* , which are invariant under the renormalization group transform. In symbols

$$\mathbf{K}^* = \mathbf{R}(\mathbf{K}^*) \quad \text{criticality condition.} \quad (12.30)$$

A set of couplings which satisfies Eq. (12.30) is said to be a fixed point of the renormalization group transformation.

Any critical point has the property that the system has a behavior which is independent of the length scale. The fixed point condition, (12.28), will ensure scale-invariant behavior. Alternatively, we might note that, in virtue of Eq. (12.30), any fixed point has $\kappa(\mathbf{K}^*) = \lambda\kappa(\mathbf{K}^*)$. This condition, in turn, has two solutions $\kappa = 0$ and $\kappa = \infty$. These two kinds of solutions may be found in the different kinds of fixed point solutions present in the Ising model:

- (1) $\kappa = 0$, which is characteristic of the infinite correlation length of the critical fixed point, and

- (2) $\kappa = \infty$, which is the zero correlation length, of a fixed point corresponding to independent and uncoupled spins. This is usually called the weak coupling fixed point.
- (3) In addition there is a third fixed point corresponding to points on the phase coexistence curve, called the strong coupling fixed point. In the Ising case, this fixed point has zero correlation length.

For now, we would like to focus upon what happens near the critical fixed point.

12.5 Phenomenology of Scaling Fields

Before getting to detailed and exact renormalization calculations, let us do another phenomenological calculation: Imagine that we develop an analysis of an Ising model on a two-dimensional lattice as shown in Fig. 12.1. Instead of using the coupling constant \mathbf{K} we describe the system by a deviation from the critical temperature, $\epsilon = (T - T_c)T_c$. We also employ the usual dimensionless magnetic field, h . This pair is the essential set of fields. They work together with \mathbf{K}_0 to provide most of the description of the relevant portion of the problem. So we continue to work with the reduced coupling vector $\mathbf{K} = (\mathbf{K}_0, h, \epsilon)$.

Now imagine that we went through the whole renormalization scheme described by Fig. 12.1 and by the discussion of the previous section. We would derive from a whole new problem described in terms of the μ -variables. The new problem would be described by some set of coupling including probably nearest neighbor interactions, more distant interactions, and a whole mess of couplings among many spins. But ignore the mess. Think of universality. Any problem involving a near critical behavior with an appropriate symmetry is supposed to be describable in the same terms as the two-dimensional Ising model. Since our new problem in the μ -variables is then also a near-critical Ising model, we should express its thermodynamic state by giving the values of two effective interactions, a new value of the magnetic field, h' , and a new value of the effective temperature distance from criticality, ϵ' . Using Eq. (12.26), we find an identity which relates the free energy per site before and after the scale transformation

$$f(h', \epsilon') = f(h, \epsilon)\lambda^d. \quad (12.31)$$

This scaling formula must be supplemented by equations for the new parameters, ϵ', h' which express the deviation from criticality in terms of the old ones, ϵ, h . Since the new problem is not really a new one but merely the re-expression of the old one, the two problems should approach criticality together. We express this by saying that, for small values of these so-called scaling fields the new ones must be proportional to the old ones. Thus we expect that ϵ' and h' are linear combinations of ϵ and h . But, because these quantities have different symmetries under spin flip operations, the linear relations among these quantities cannot mix ϵ and h , so that the relations become $\epsilon' = \lambda_T \epsilon$ and $h' = \lambda_h h$. It will be more convenient for our purposes to rewrite the two multipliers λ_T and λ_h in terms of the scaling multiplier for the lattice constant, by saying

$$\epsilon' = \epsilon \lambda^{y_T} \quad \text{and} \quad h' = h \lambda^{y_h}. \quad (12.32)$$

Here the two numbers, y_T and y_h describe the Widom scaling in the system. If the theory is right, their values are independent of λ .

Equations (12.31) and (12.32) combine to give the scaling equation for the free energy per site, namely

$$f(\epsilon, h) = \lambda^{-d} f(\epsilon \lambda^{y_T}, h \lambda^{y_h}). \quad (12.33)$$

The Widom scaling solution is a consequence of Eq. (12.33). We demand that the right hand side of (12.33) be independent of λ . After all, λ , is only a parameter which defines two different ways of looking at the very same problem. There are two scale invariant ratios which we can form of the quantities on the right hand side of Eq. (12.33). The first is ϵ^{y_h}/h^{y_T} . The second is $f^{1/y_T} \epsilon^{1/d}$. These scalars must be the only combination which appear in the free energy per site. We previously wrote this as

$$f(\epsilon, h) = \epsilon^{2-\alpha} f(h/\epsilon^\Delta). \quad (12.34)$$

Now y_T and y_h are determined in terms of the previously defined α and Δ as

$$\frac{d}{y_T} = 2 - \alpha \quad \text{and} \quad y_h = \Delta y_T. \quad (12.35)$$

Thus, the demand for universality — when applied to changing the length-scale of our system — gives Widom's form of scaling.

Another part of Widom's scaling, the index ν for the coherence length, can also be evaluated from in terms of y_T . At $h = 0$ and $T > T_c$, $\xi = a/\kappa(\epsilon)$, with κ being proportional to ϵ^ν . As we have already said, see Eq. (12.29), $\kappa' = \lambda\kappa$. Under renormalization ϵ changes to ϵ' with the ratio being a factor of $\lambda_T = \lambda^{y_T}$. Since κ renormalizes precisely because ϵ does so, it follows that

$$(\lambda_T \epsilon)^\nu = \lambda \epsilon^\nu$$

and consequently

$$\nu = \frac{1}{y_T}. \quad (12.36)$$

To keep track of the various relation among critical indices, we express all indices in terms of y_h and y_T and store the result in Table 12.2.

12.6 Theory of Scaling Fields

We have dealt with the near-critical behavior of two fields. We can now do them all without much additional work. The fixed point is the special value of \mathbf{K} , namely \mathbf{K}^* , which obeys

$$\mathbf{K}^* = \mathbf{R}(\mathbf{K}^*). \quad (12.37)$$

Quantity	Index	Value
specific heat	$\alpha = \alpha'$	$2 - d/y_T$
magnetization	β	$(d - y_h)/y_T$
magnetization	δ	$1/(d - y_h)$
susceptibility	$\gamma = \gamma'$	$(d - 2y_h)/y_T$
coherence length	$\nu = \nu'$	$1/y_T$
spin correlation	η	$(d - 2) + \eta = 2(d - y_h)$

Table 12.2. Relations among critical indices.

Now imagine that \mathbf{K} differs from the fixed point value: $\mathbf{K}_a = \mathbf{K}_a^* + \delta\mathbf{K}_a$. The renormalization equation becomes:

$$\mathbf{K}_a^* + \delta\mathbf{K}'_a = \mathbf{R}_a(\mathbf{K}^* + \delta\mathbf{K}). \quad (12.38)$$

To zeroth order in the deviation, \mathbf{R} reproduces \mathbf{K}^* . We do a first order expansion in the coupling about their fixed point value and find

$$\delta\mathbf{K}'_a = \mathbf{R}_a(\mathbf{K}) - \mathbf{K}_a^* = \mathbf{R}_a(\mathbf{K}^*) - \mathbf{K}_a^* + \sum_b M_{ab} \delta\mathbf{K}_b = \sum_b M_{ab} \delta\mathbf{K}_b.$$

Equation (12.39) is the generalization of Eq. (12.32) to include all possible fields. The previous equation was derived by looking at the linear response and arguing that it was effectively diagonal. To analyze Eq. (12.39) imagine picking a linear combination of $\delta\mathbf{K}_a$'s, which diagonalizes M . Call the various linear combinations which do the job h^α 's. (Note that we use superscripts instead of subscripts and a Greek-letter-index rather than a Latin one.) We write the combination as

$$h^\alpha = \sum_a C_a^\alpha h_a. \quad (12.39)$$

The eigenvalue equation is that this linear combination of deviations obeys:

$$h'^\alpha = \lambda^{y_\alpha} h^\alpha. \quad (12.40)$$

In detail this becomes the statement that

$$h'^\alpha = \sum_a C_a^\alpha \delta K'_a = \sum_{ab} C_a^\alpha M_{ab} \delta K_b = \lambda^{y_\alpha} h^\alpha = \lambda^{y_\alpha} \sum_b C_b^\alpha \delta K_b.$$

Thus the eigenvalue condition is that

$$\lambda^{y_\alpha} C_b^\alpha = \sum_a C_a^\alpha M_{ab}, \quad (12.41)$$

which then determines the eigenvalue λ^{y_α} . Notice then that the C 's and the h 's are essentially determined as left eigenvalues of the deviation matrix, M .

Naturally we describe Eq. (12.40) by saying that under the renormalization transformation in which distances transform according to $r \rightarrow R = r/\lambda$ the fields transform according to

$$h^\alpha \rightarrow (h')^\alpha = \lambda^{y_\alpha} h^\alpha, \quad (12.42a)$$

we express this result in words by saying that h^α scales like r^{-y_α} , or that

$$h^\alpha \sim r^{-y_\alpha}. \quad (12.42b)$$

These h^α 's with simple scaling properties are called *scaling fields*.

The scaling fields are classified according to their values of the eigenvalue determined in Eq. (12.40). The different cases are described as²⁰ for a more complete classification.

$$\text{if } y_\alpha \text{ is } \begin{cases} > 0 & \text{then the field is called } \textit{relevant}, \\ = 0 & \text{then it is called } \textit{marginal}, \\ < 0 & \text{the field is termed } \textit{irrelevant}. \end{cases} \quad (12.43)$$

This naming follows from the behavior of these fields under the scale changes of the renormalization group. Since $\lambda > 1$, the fields with $y_\alpha > 0$ tend to grow under renormalization group transformations and become more and more important as larger distance scales are reached. The larger the value of y_α , the quicker the growth, and the more important is the field. This then gives us a means of classifying fields by their importance.

In the standard critical phenomena problem there are precisely three relevant fields: There is a field which break the underlying symmetry in the system — the magnetic field in the Ising example. The next relevant field is the temperature deviation — the sign of this field determining whether the system is ordered. The last is the constant field K_0 — which scales as λ^d . These are the only field we need to watch really carefully.

The fields with $y_\alpha < 0$ tend to diminish with successive renormalization group transforms and hence become effectively zero when we are examining effects at large scales. Thus they are unimportant to critical behavior. These are exactly the fields which make most changes be quite irrelevant to criticality, and hence produce universality. These are then called irrelevant fields.

The relevant fields grow under renormalization and thus must be set to zero in order to have the system be at its critical point. Because they are set to zero, they do not ruin universality either. However, the marginal fields, if they exist, do not change as the scale changes. The behavior at the critical point can vary as these fields are changed. If they are present they ruin universality. Usually they are not present.

We can also make the converse statement: If we see a situation in which behavior is both critical and non-universal, we can expect to find marginal fields someplace.

²⁰See F. Wegner DGL: Volume 6 page 8 (1976).

There is yet another class of fields: Ones that do not have any effect on the critical correlations. The operators defined by these field have only short ranged correlations. These are called redundant fields, and usually totally ignored. Leaving these out, we can write a scaling relation for the free energy density

$$f(h^0, h^1, \dots, h^\alpha, \dots) = \lambda^{-d} f(\lambda^d h^0, \lambda^{y_1} h^1, \dots, \lambda^{y_\alpha} h^\alpha, \dots). \quad (12.44)$$

Notice that the theory is making a very striking claim. There are many different ways of constructing valid renormalization transforms. For example Eq. (12.16b) gives a whole family of such transforms, continuously parametrized by K_t . The claim is that (except for the redundant operators) the sets of y_α 's constructed from each of these schemes are identical, one to the next. Remarkable, unlikely, but apparently true. Equation (12.44) was derived to work for a particular value of λ , and by extension to positive integer power of that λ . However, if it is equally true for all transforms, it effectively applies to all value of λ in the range that the unrenormalized and renormalized fields (h^α and $\lambda^{y_\alpha} h^\alpha$ for $\alpha = 1, 2, \dots$) are small.

Notice that the scaling fields are given as linear combination of the physical fields K_a . Thus, unless there is some symmetry consideration, every physical field should appear in every scaling field. Thus, it is to be expected that the magnetic field should appear in the ordering scaling field h^1 and that ϵ should appear in the ‘temperature changing’ scaling field. Thus, derivatives with respect to the physical fields have, to lowest order, the same behavior as derivatives with respect to the corresponding scaling fields.

12.7 Scaling Relations for Operators

Now, we are in a position to extend what we have said to include all couplings and all operators. Any action can be written in terms of the couplings K_a . Specifically, the deviation of the action from the fixed point is

$$\delta W[\sigma] = \sum_a \delta K_a X_a[\sigma]. \quad (12.45)$$

Here, $X_a[\sigma]$ are the fluctuating operator conjugate to K_a . Because the system is translationally invariant, this operator is extensive. Each operator depends, of course, on the basic set of spins σ_r . Each extensive operator, X_a , can be expressed as a sum of densities which depend upon spins in the neighborhood of r . Thus,

$$X_a[\sigma] = \sum_r O_a(r). \quad (12.46)$$

Here, r are the lattice sites and $O_a(r)$ are the densities of the various fluctuating operators at the lattice site, r . These densities can also be written as $O_a(r, [\sigma])$ to emphasize their dependence on the σ . Each density is defined so that it only depends on the spins in the immediate neighborhood of the point r . One of the simplest such density is the magnetization density, $O_1(r, [\sigma]) = \sigma_r$. (The very simplest one is the unit operator: $O_0(r) = 1$.) We

Table 12.3. Some of the fluctuating operators in the theory.

Operator	Definition	Conjugate field	Comment
magnetization density	$\sigma_{j,k}$	h	odd under spin flip
energy density	$\mathcal{E}(j, k) = \sigma_{j,k}[\sigma_{j,k+1} + \sigma_{j+1,k} + \sigma_{j,k-1} + \sigma_{j-1,k}]$	K	odd under dual transform
unity	1	K_0	
stress tensor	$T_{xx} - T_{yy} = \sigma_{j,k}[-\sigma_{j,k+1} + \sigma_{j+1,k}]$	$K_x - K_y$	density for component of stress tensor
stress tensor	$T_{xy} \sim \sigma_{j,k}[\sigma_{j+1,k+1} - \sigma_{j-1,k-1}]$		density for another component

list in Table 12.3 the densities which can be found in the Ising action (12.12). Some of the ‘comments’ in that table, such as the meaning of the stress tensor, will be discussed below.

In this section, we aim to describe the scaling properties of the extensive operators and their densities. Since we have already discussed the scaling properties of many physical quantities, we will be relatively sketchy in our discussion of the operators.

Start with the extensive operators. We derive the scaling properties of the operators from those of the fields. By defining X^α as an appropriate linear combination of the physical fields, X_a , we can rewrite the change in the action in term of scaling fields and the newly-defined scaling operators X^α , specifically

$$\delta W = \sum_\alpha X^\alpha h^\alpha, \quad (12.47)$$

with the extensive scaling operator obeying

$$X^\alpha = \sum_a C_a^\alpha X_a,$$

the very same coefficients used to define h^α . In this way, we have defined a scaling operator, X^α , which by construction has the property that the derivative with respect to h_α automatically generates a factor of X^α . In symbols

$$X^\alpha \leftrightarrow \frac{\partial}{\partial h^\alpha}. \quad (12.48)$$

But, Eq. (12.48) says that X^α scales as the inverse of h^α . Since h scales with a factor λ^{y_α} we expect the scaling operator to scale with the inverse factor, λ^{-y_α} . In symbols,

$$X^\alpha\{\mu\} \cong \lambda^{-y_\alpha} X^\alpha\{\sigma\}. \quad (12.49)$$

Here \cong means that the left and right hand side behave the same when used to calculate averages in their respective systems. Let us check (12.49) by applying it to a calculation of the total magnetization: $\langle M \rangle = N \langle \sigma \rangle_{\mathbf{K}}$ and $\langle M' \rangle = N' \langle \mu \rangle'_{\mathbf{K}}$. Equation (12.49) asserts that $\langle M' \rangle = \lambda^{-y_h} \langle M \rangle$. For vanishing h and T below the critical point, $\langle M \rangle = N(-\epsilon)^{\beta}$ and

$$\langle M' \rangle = N'(-\epsilon)^{\beta} = \langle M \rangle \lambda^{-d+\beta y_T}. \quad (12.50)$$

A quick peek back at Table 12.2 shows that $d - \beta y_T = y_h$, as required. After this check, we include the result (12.49) in Table 12.3.

Notice that there were two factors which went to make up the $\lambda^{-d+\beta y_T}$ appearing in Eq. (12.50). The λ^{-d} came from the factor N' and N which counted the number of terms in $\langle M' \rangle$ and $\langle M \rangle$. The other factor, $\lambda^{\beta y_T} = \lambda^{d-y_h}$, was intrinsic to the scaling properties of the magnetization density. The extensive operators all contain this fact of the number of sites, lacking in the density operators. Thus, we argue that the latter have the scaling property:

$$O_R^\alpha \{\mu\} \cong \lambda^{-d+y_\alpha} O_r \{\sigma\}. \quad (12.51)$$

Here, as before, the \cong mean that the quantities on the two sides have the same average when included in near critical averages in their respective systems, assuming that the spatial points are identical. Since we will often have use of the scaling exponent in (12.51) we give it a special name, x_α and then say that x_α and y_α are related by

$$x_\alpha + y_\alpha = d. \quad (12.52)$$

Like Eq. (12.10), Eq. (12.52) is also called a *hyperscaling* relation. Since ‘hyper’ means ‘too much’ as in hyperactive child or hypersensitive adult, the implication of the word was that the theory should not include this kind of relation. However, it has proven to be an essential part of the theoretical development.

Notice that larger values of x_α imply a faster dropoff of the renormalized operator as λ is increased. Thus operators with larger x -values are intrinsically less significant near the critical point. We have already made the same point by saying that smaller y -values produce less important fields.

How could the scaling of Eq. (12.51) show itself? We saw how it worked for $\langle \sigma \rangle$. The next order calculation might involve two σ 's separated by a distance which is large compared to the lattice constant: In that case, the two spin correlation functions would have the form:

$$\langle \sigma_r \sigma_s \rangle = \frac{A}{\left(\frac{|r-s|}{a}\right)^{d-2+\eta}}, \quad (12.53a)$$

where A is some positive constant. The $d-2+\eta$ is the conventional way of writing the index in this expression.²¹ The corresponding correction function for the renormalized quantity

²¹The index, η , defined in this fashion is usually small. It is exactly zero in mean field theory. It must be either zero or positive.

is

$$\langle \mu_{\mathbf{r}} \mu_{\mathbf{s}} \rangle = \frac{A}{\left(\frac{|\mathbf{r}-\mathbf{s}|}{\lambda a} \right)^{d-2+\eta}}. \quad (12.53b)$$

Since μ is $\lambda^{-x_h}\sigma$, Eqs. (12.53) imply:

$$2x_\sigma = d - 2 + \eta. \quad (12.54)$$

The same argument implies more generally that the correlation function

$$\langle O^\alpha(\mathbf{r}) O^\beta(\mathbf{s}) \rangle = \frac{A^\alpha \beta}{\left| \frac{\mathbf{r}-\mathbf{s}}{a} \right|^{x_\alpha+x_\beta}}, \quad (12.55)$$

at the critical point.

We have already seen that scaling fields can be divided into three types. (See Eq. (12.43).) Just the same kind of division applies to the local scaling operators $O_\alpha(\mathbf{r})$. Recall that the two kinds of scaling are related by $x_\alpha + y_\alpha = d$. If x_α is bigger than the dimensionality, d , then the operator is related to an irrelevant variable. If x_α is less than the dimensionality, the corresponding operator is connected with a relevant field and therefore plays an important role in the thermodynamics. In principle, x_α can be smaller than zero so that the average of an operator product like that in Eq. (12.55) will grow when the separation increases. This behavior is uncommon in statistical mechanics, in which the local operators are typically bounded—like the Ising variable. In turbulence,²² however, very large fluctuations in the velocity variable are possible and appear to be connected with the analog of negative x_α 's. For another example, the deviation of a surface from a flat configuration²³ can grow with time, so that in the end it becomes quite unbounded. Correlations among these distances can grow as separations between measuring points increase.

The most interesting case is the marginal one in which x_α is equal to the dimensionality. If the local operator is a scalar under rotation, it will ruin universality. If it is a vector or a tensor (like the stress tensor) it will not destroy universality but may very well distort the system in some fashion. The stress tensor always exists in any critical theory or field theory. If terms proportional to the stress tensor appear in the basic statistical weight, W , it will tend to make the correlations have an ellipsoidal rather than a spherical rotation symmetry. The correlation length in one direction will differ from that in another. That change in the spatial properties of the system is interesting, but in the end quite simple. However, there is a whole theory of the relation between spatial properties and the stress tensor,²⁴ in which the stress tensor is used to simulate the effect of nontrivial topological or metric properties of the surface. So there is deep knowledge to be obtained in the study of the effects of marginal operators.

²²See U. Frisch *Turbulence* (Cambridge University Press, 1995), pages 139–141.

²³See Chapters 3 and 4 in F. Family and T. Vicsek, editors, *Dynamics of Fractal Surfaces* (World Scientific, Singapore 1991). See also A. Barabási and H. E. Stanley, *Fractal Concepts in Surface Growth* (Cambridge University Press, 1995).

²⁴See any text about string theory.

12.8 Transforming Operators

We have derived the main phenomenological results about operator transformation properties without once resorting to actually transforming an operator. It can all be done with coupling constants. However, it is reassuring to know that one can work with the operators if necessary. Imagine that one has some product of local transformed operators:

$$P'[\mu] = O_a(\mathbf{R})[\mu]O_b(\mathbf{S})[\mu]\cdots. \quad (12.56)$$

What σ -operators will transform into these? The answer is quickly reached. Take this product, multiply by the transformation function $T[\mu, \sigma]$ and sum over μ . The result is the operators which transform into P' , namely

$$P[\sigma] = \text{Tr}_\mu P'[\mu]T[\mu, \sigma]. \quad (12.57)$$

If $P'[\mu]$ is composed of operators separated by a large distance, e.g. if \mathbf{R} and \mathbf{S} are far separated, then $P[\sigma]$ will also be composed of separated operators.

It is just as easy to go the other way. To form the image of some product of σ -operators, say $Q[\sigma]$, form the sum

$$\text{Tr}_\sigma T[\mu, \sigma]Q[\sigma]\exp(W[\sigma]) = Q'[\mu]\exp(W'[\mu]). \quad (12.58)$$

As the equation says, the result will be the renormalization image of Q , $Q'[\mu]$ times the exponential of the renormalized action, $W'[\mu]$.

12.9 Universality

Our renormalization arguments suggest that *universality* has a rich meaning for critical systems. The behavior of the *RG* transforms for free energy, fields, and operators are determined by the fixed point. This argument then says that except for some normalization factors all thermodynamic functions and correlation functions are fully determined. Hence all problems which have the same fixed point have precisely the same critical behavior. They will have the very same thermodynamic properties and the same long-ranged correlations. All problems which are attracted into the same fixed point so that they have identical critical properties and are said to belong to the same *universality class*.

Thus, in one sense, the physical problem of critical phenomena reduces to the mathematical problem of enumerating and describing the different universality classes. One can probably not expect to see an evaluation of every correlation function or every free energy function.²⁵ One can expect to see some, and in the next chapters we shall give some examples. One can also expect to see a partial enumeration of the universality classes. We shall develop a little bit of this enumeration.

²⁵However, the string theorists have come close to an understanding of *all* different fixed points in two dimensions. See D. Freidan, Z. Qiu, S. Shenker, Phys. Rev. Let. 52, 1575 (1984).

12.10 Operator Product Expansions

The local scaling operators, $O_\alpha(\mathbf{r})$, can be considered to be the deepest and most fundamental objects defining the scaling and universality theory. We have said that these operators completely describe what is going on in a critical system. If they do provide a complete description, then the system cannot generate anything new or different. Now imagine a product of two or more local operators, perhaps,

$$P_{\alpha\beta}(\mathbf{R}) = O_\alpha \left(\mathbf{R} + \frac{\mathbf{r}}{2} \right) O_\beta \left(\mathbf{R} - \frac{\mathbf{r}}{2} \right). \quad (12.59)$$

When viewed from a point, say \mathbf{S} , far away from the product (i.e. with $|\mathbf{R} - \mathbf{S}|$ much larger than $|\mathbf{r}|$), the operator $P_{\alpha\beta}(\mathbf{R})$ is a local operator defined at the point \mathbf{R} . Thus, it must be expandable in all the other local operators in theory. Specifically, we must have

$$O_\alpha \left(\mathbf{R} + \frac{\mathbf{r}}{2} \right) O_\beta \left(\mathbf{R} - \frac{\mathbf{r}}{2} \right) = \sum_\gamma C_{\alpha\beta\gamma}(\mathbf{r}) O_\gamma(\mathbf{R}). \quad (12.60)$$

The Eq. (12.60) is called an operator product expansion.²⁶ Here, the expansion coefficient $C_{\alpha\beta\gamma}(\mathbf{r})$ is a number which depends upon the distance \mathbf{r} , while the $O_\gamma(\mathbf{R})$ is one of our familiar local operators. Scaling determines \mathbf{r} -dependence of $C_{\alpha\beta\gamma}(\mathbf{r})$ as:

$$C_{\alpha\beta\gamma}(\mathbf{r}) = A_{\alpha\beta\gamma} |\mathbf{r}|^{x_\gamma - x_\alpha - x_\beta} \quad (12.61)$$

if all the local operators are rotational scalars. The coefficients $A_{\alpha\beta\gamma}$ encode the algebraic properties of the critical system.

The reader may wonder whether Eq. (12.60) has any objective content. Can it really be verified. Equations (12.62) and (12.63) below are nontrivial consequences of Eq. (12.60) which may and has²⁷ been checked against known forms of critical correlations. These relations are:

$$\left\langle O_\alpha \left(\mathbf{R} + \frac{\mathbf{r}}{2} \right) O_\beta \left(\mathbf{R} - \frac{\mathbf{r}}{2} \right) O_\mu(\mathbf{S}) \right\rangle = \sum_\gamma C_{\alpha\beta\gamma}(\mathbf{r}) \langle O_\gamma(\mathbf{R}) O_\mu(\mathbf{S}) \rangle \quad (12.62)$$

$$\left\langle O_\alpha \left(\frac{\mathbf{R}_\mathbf{r}}{2} \right) O_\beta \left(\mathbf{R} - \frac{\mathbf{r}}{2} \right) O_\mu \left(\mathbf{S} + \frac{\mathbf{s}}{2} \right) \right\rangle = \sum_\gamma C_{\alpha\beta\gamma}(\mathbf{r}) \sum_\lambda C_{\mu\nu\lambda}(\mathbf{s}) \langle O_\gamma(\mathbf{R}) O_\lambda(\mathbf{S}) \rangle. \quad (12.63)$$

In these relations, the sums over operators converge more quickly as the distance $|\mathbf{R} - \mathbf{S}|$ becomes larger.

²⁶K. Wilson, Phys. Rev. **179**, 1699 (1969); L. P. Kadanoff, ‘Operator Algebra and the Determination of Critical Indices’, Phys. Rev. Letts. **23**, 1430 (1969).

²⁷See for example, L. Kadanoff, Phys. Rev. **188**, 859 (1969) and L. Kadanoff and A. Brown, Ann. Phys. **121**, 319 (1979).

Homework

Problem 12.1 (One More Critical Index Relation). Use the Widom form of the free energy, Eq. (12.4), to determine δ in terms of α and β .

Problem 12.2 (The Free Energy). Find the free energy scaling functions $f_>$ and $f_<$ of Eq. (12.4) using mean field theory.

Problem 12.3 (Different Scaling Forms). Another way of writing the scaling form (Eq. (12.4)) for the near-critical free energies is to write

$$f = h^a g^*(\epsilon/h^b).$$

Find a , b and g^* in term so the quantities defined in Eq. (12.4).

12.11 Reprints on Critical Correlations

12.11.1 Kadanoff: Correlations Along a Line

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Correlations along a Line in the Two-Dimensional Ising Model*

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The $2n$ -spin correlation function for the two-dimensional Ising model at $T=T_c$ is evaluated for the special case in which all the spins lie along a straight line, separated by many lattice constants. The resulting $2n$ -spin function is simply a quotient of products of two-spin correlations. A hypothesis of reducibility of fluctuations in the critical state is introduced. This hypothesis asserts that the product of any two local fluctuating quantities in the same neighborhood of space may be effectively replaced by a finite sum of local fluctuating quantities in this neighborhood. As a result, the previously found form for the $2n$ -spin function may be used to evaluate the correlation function of n energy densities when all n points lie on a line. The n -energy correlation function is simply a sum of products of two-energy correlations. The quotient form for the spin correlation plus scaling is shown to immediately imply the logarithmic specific heat.

I. INTRODUCTION

SINCE Onsager's original work,¹ many authors have discussed thermodynamic properties^{2,3} and correlations⁴⁻¹¹ in the two-dimensional Ising model. Much of this work has concentrated on using the Onsager solution to learn about the behavior near the critical point. The concept of scaling,¹²⁻¹⁵ for example, has arisen in part from information gained from this model. According to the scaling idea, there are two indices, described¹² as x and y , which together determine the nature of all the critical singularities.

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⁵ T. T. Wu, Phys. Rev. 149, 380 (1966).

⁶ E. W. Montroll, R. B. Potts, and J. C. Ward, J. Math. Phys. 4, 308 (1963).

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¹² L. Kadanoff, Physics 2, 263 (1966).

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¹⁴ A. Z. Patashinskii and V. L. Pokrovskii, Zh. Eksperim. i Teor. Fiz. 50, 439 (1966) [English transl.: Soviet Phys.—JETP 23, 292 (1966)].

¹⁵ M. E. Fisher, Physics 3, 255 (1967).

In the two-dimensional Ising model, x and y each have simple values: $x=15/8$, $y=1$. However, even though the Onsager solution exists as a guide, no fully satisfactory physical argument is known to be available for understanding the values of x and y . These values are only obtained by very detailed and rather untransparent calculations. One can hope, however, that such simple values of x and y can be seen as the result of some structural property of critical correlations. In this paper, I argue that the result $y=1$, which implies the logarithmic specific heat, is a natural result of a simple structure of the n -spin correlation function.

This argument is based upon an evaluation of the $2n$ -spin correlation function under the conditions: (a) that the Ising model is at the critical point; (b) that all the spins lie on a single straight line; and (c) that the spins are all separated from one another by many lattice constants. Then, if the spins are ordered along the line as $\sigma_1, \sigma_{1'}, \sigma_2, \sigma_{2'}, \dots, \sigma_n, \sigma_{n'}$, the correlation function is calculated to have the form

$$\langle \prod_{i=1}^n \langle \sigma_i \sigma_{i'} \rangle \rangle = \prod_{i=1}^n \prod_{j=1}^n \frac{\langle \sigma_i \sigma_j \rangle}{(\langle \sigma_i \sigma_j \rangle \langle \sigma_i \sigma_j \rangle)^{1/2}}. \quad (1.1)$$

At first sight, it does not appear that the result (1.1) defines any critical indices. Further progress comes from the introduction of an extra idea, of the *reducibility of critical fluctuations*. Reducibility arises from the idea that there are only a limited number of independent fluctuating local variables in any phase-transition problem. Say there are s of these, $O_\nu(r)$ for $\nu=1, 2, \dots, s$. A product of two O_ν 's at neighboring positions is

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again a local fluctuating quantity, which then must be a linear combination of the O_i 's. In symbols, whenever \mathbf{r} and \mathbf{r}' are sufficiently close together,

$$O_{\nu}(\mathbf{r})O_{\nu'}(\mathbf{r}') = A_{\nu\nu'}(\mathbf{r}-\mathbf{r}') + \sum_{\nu''} A_{\nu\nu''\nu'}(\mathbf{r}-\mathbf{r}')O_{\nu''}\left(\frac{\mathbf{r}+\mathbf{r}'}{2}\right). \quad (1.2)$$

Here the A 's are simply numbers and the O 's are fluctuating operators.

Equation (1.2) permits us to reduce to simpler forms correlations of $2n$ spins whenever pairs of spins lie very close together. If the reducibility equation (1.2) is applied to a product of two spins, the main term in the sum involves the operator $\mathcal{E}(r)$, which is physically the energy density minus its critical value. Thus Eqs. (1.1) and (1.2) may be combined to yield expressions for energy-energy correlations. This analysis yields two notable results. First, the energy-energy correlation function is evaluated just from (1.1) and (1.2) with the result that at the critical point

$$\langle \mathcal{E}(1)\mathcal{E}(2) \rangle \sim 1/|\mathbf{r}_1 - \mathbf{r}_2|^2. \quad (1.3)$$

Equation (1.3) implies $y=1$ and a logarithmic singularity in the specific heat for this two-dimensional system. The other result is that whenever the points $1, 2, \dots, 2n$ lie many lattice constants from one another along a single straight line, we have

$$\begin{aligned} \langle \mathcal{E}(1)\mathcal{E}(2)\cdots\mathcal{E}(2n) \rangle &= \sum_{\text{perm}} \langle \mathcal{E}(1)\mathcal{E}(2) \rangle \\ &\times \langle \mathcal{E}(3)\mathcal{E}(4) \rangle \cdots \langle \mathcal{E}(2n-1)\mathcal{E}(2n) \rangle \end{aligned} \quad (1.4)$$

at the critical point.

Section II is devoted to the derivation of Eq. (1.1). Since this derivation is highly technical, many readers will wish to skip this part. Section III discusses reducibility [Eq. (1.2)] and its application to the two-dimensional Ising model. Section IV includes information about energy correlations and includes the deviations of the results (1.3) and (1.4).

II. EVALUATION OF MULTIPLE-SPIN CORRELATIONS

Consider $2n$ spins on the x axis at the points $1=(0,k_1)$, $1'=(0,k_1')$, \dots , $n'=(0,k_n')$ arranged so that

$$k_1 \leq k_1' \leq k_2 \leq \cdots \leq k_n'. \quad (2.1)$$

The condition $k \in \{i\}$ means that k lies between k_i and k_i' , or, more precisely, that we have

$$k \in \{i\} \quad \text{when} \quad k_i < k \leq k_i'. \quad (2.2)$$

An evaluation of the $2n$ -spin correlation function is most easily obtained via the Toeplitz determinant method⁶ as applied by Wu.⁵ For completeness, we mention a derivation of our beginning formula starting from the work of Ref. 4. The $2n$ -spin case can be

handled by the method described in Sec. 3.1 of Ref. 4. In direct analogy to Eq. (I.3.13), we find that

$$\begin{aligned} \langle \prod_i \sigma_i \sigma_{i'} \rangle &= \exp \frac{1}{4} \text{tr} \ln (1 - 2\eta g \eta)^2 \\ &= [\det(1 - 2\eta g \eta)]^{1/2}. \end{aligned} \quad (2.3)$$

The last line follows because

$$\text{tr} \ln X = \ln \det X$$

for any X . The quantity g is a matrix in j, k space and a 2×2 "spin" space, while η is diagonal in coordinate space. In fact, we have

$$\begin{aligned} \eta(j, k) &= \delta_{j,0}, \quad \text{if } k \in \{i\} \text{ for any } \{i\} \\ &= 0, \quad \text{otherwise.} \end{aligned} \quad (2.4)$$

The relevant part of g is then diagonal in j and takes the form

$$g(0k; 0k') = \frac{1}{2} \delta_{kk'} + \int_{-\pi}^{\pi} \frac{dp_y}{4\pi} e^{ip_y(k-k')} [\Phi(p_y)]^{\tau_3 \tau_2} \quad (2.5)$$

according to (I.3.21). Here τ_3 and τ_2 are standard Pauli-spin matrices, while $\Phi(p_y)$ is defined by Eq. (I.3.18). In this definition, Φ depends upon two parameters called A and B in the notation of I and of Refs. 2 and 3. At the critical point, $B=1$, and then Φ takes the form

$$\Phi(p_y) = -\left(\frac{A e^{ip_y} - 1}{A - e^{ip_y}}\right)^{1/2}. \quad (2.6)$$

The remaining parameter A is a measure of the asymmetry of the lattice. When $A=1$, the coupling in the y direction is much stronger than the coupling in the x direction; when $A=\infty$, the coupling in the x direction is much stronger. At $A=3+2\sqrt{2}$, the couplings in both directions are equal.

It is difficult to evaluate the trace in Eq. (2.3) exactly for any finite value of the asymmetry parameter A . However, Wu has argued⁵ that the A dependence of the two-spin correlation function is very simple. In the limit of large separations in the y direction, he suggests that the total A dependence of $\langle \sigma_i \sigma_{i'} \rangle$ is a multiplicative factor $[(A+1)/(A-1)]^{1/4}$.

To generalize Wu's conjecture, consider

$$\ln \langle \prod_i \sigma_i \sigma_{i'} \rangle = \frac{1}{4} \text{tr} \ln (1 - 2\eta g \eta)^2. \quad (2.7)$$

In the asymptotic limit of large separations, the main term on the right-hand side of Eq. (2.7) might be expected to come from the large $k-k'$ form of $g(0k, 0k')$, which in turn comes from small p_y . However, at $p_y=0$, Eq. (2.6) implies that $\Phi(p_y)$ is independent of A . Therefore, we might expect the main term in the asymptotic expansion of (2.7) to be independent of A .

We therefore write

$$\ln\langle\prod_i \sigma_i \sigma_{i'}\rangle = \ln\langle\prod_i \sigma_i \sigma_{i'}\rangle_0 + \text{correction term},$$

where the subscript zero indicates a correlation function at a particular value of A , picked to be $A = \infty$.

The correction to g arising from terms which do not vanish as $A \rightarrow \infty$ occurs only for $p_y \neq 0$, and hence is a relatively short-ranged function of $k - k'$. Since this correction is short-ranged, the entire correction term cannot involve correlations between different regions $\{i\}$ and $\{j\}$. Hence, the correction term is of the form of a sum over the different regions:

$$\begin{aligned} \text{correction term} &= \sum_i [\frac{1}{4} \text{tr} \ln(1 - 2\eta_i g \eta_i)^2]_A \\ &\quad - \frac{1}{4} \text{tr} \ln(1 - 2\eta_i g \eta_i)|_{A=\infty}. \end{aligned}$$

However, Wu⁵ has already argued that if $k_i - k_j \gg 1$, the correction term for two spins is $\frac{1}{4} \ln(A+1)/(A-1)$. Consequently, the correction for $2n$ spins is n times as large. As a final result, we find that

$$\langle\prod_i \sigma_i \sigma_{i'}\rangle = [(A+1)/(A-1)]^{n/4} \langle\prod_i \sigma_i \sigma_{i'}\rangle_0. \quad (2.8)$$

Here the subscript zero denotes the average at $A = \infty$. In this limit, the average can be computed, since⁶ at $A = \infty$, we have

$$\begin{aligned} [1 - 2g(0k; 0k')] &= -\frac{1}{\pi} \frac{\tau_3}{k - k' + \frac{1}{2}\tau_3} \tau_2 \\ &= h_{kk'}, \end{aligned} \quad (2.9a)$$

and

$$\langle\prod_i \sigma_i \sigma_{i'}\rangle_0 = [\det_q(-h_{kk'})]^{1/2}, \quad (2.9b)$$

where \det_q covers the part of k space in which η is different from zero. Wu has, in fact, evaluated a determinant precisely like this one. The result is [see Wu⁵ Eqs. (4.7) and (4.8)]

$$\langle\prod_i \sigma_i \sigma_{i'}\rangle_0 = \prod_k \left(\frac{2}{\pi} \prod_{k' < k} \frac{1}{1 - [2(k-k')]^{-2}} \right). \quad (2.10)$$

In Eq. (2.10) the products cover the region in which $\eta \neq 0$.

To simplify Eq. (2.10), the products are grouped according to the different regions $\{i\}$ denoted by Eq. (2.1). Then, we have

$$\langle\prod_i \sigma_i \sigma_{i'}\rangle_0 = \prod_i F_i \prod_{j < i} F_{ij}, \quad (2.11)$$

with

$$F_i = \prod_{k \in \{i\}} \frac{2}{\pi} \prod_{k' \in \{i\}, k' < k} \frac{1}{1 - [2(k-k')]^{-2}}, \quad (2.12)$$

$$F_{ij} = \prod_{k \in \{i\}} \prod_{k' \in \{j\}} \frac{1}{1 - [2(k-k')]^{-2}}. \quad (2.13)$$

The F 's can be expressed in more physical terms. By considering the case of only two spins, we see that

$$F_i = \langle\sigma_i \sigma_{i'}\rangle_0, \quad (2.14)$$

while the four-spin case gives

$$F_{ij} = \frac{\langle\sigma_i \sigma_{i'} \sigma_j \sigma_{j'}\rangle_0}{\langle\sigma_i \sigma_{i'}\rangle_0 \langle\sigma_j \sigma_{j'}\rangle_0}. \quad (2.15)$$

Therefore, Eq. (2.11) reduces to

$$\langle\prod_i \sigma_i \sigma_{i'}\rangle_0 = \prod_i \langle\sigma_i \sigma_{i'}\rangle_0 \prod_{j < i} \frac{\langle\sigma_i \sigma_{i'} \sigma_j \sigma_{j'}\rangle_0}{\langle\sigma_i \sigma_{i'}\rangle_0 \langle\sigma_j \sigma_{j'}\rangle_0}. \quad (2.16)$$

Therefore, for example, we obtain

$$\begin{aligned} &\langle\sigma_1 \sigma_1' \sigma_2 \sigma_2' \sigma_3 \sigma_3'\rangle_0 \\ &= \frac{\langle\sigma_1 \sigma_1' \sigma_2 \sigma_2'\rangle_0 \langle\sigma_1 \sigma_1' \sigma_3 \sigma_3'\rangle_0 \langle\sigma_2 \sigma_2' \sigma_3 \sigma_3'\rangle_0}{\langle\sigma_1 \sigma_1'\rangle_0 \langle\sigma_2 \sigma_2'\rangle_0 \langle\sigma_3 \sigma_3'\rangle_0}. \end{aligned} \quad (2.17)$$

Nevertheless, the four-spin correlation function can be further simplified. In Eq. (2.17) we set $2 = 1'$ and $2' = 3$. Then, since the case $A = \infty$ is still an Ising model, we get $\sigma_i^2 = \sigma_i'^2 = 1$ and Eq. (2.17) becomes

$$\langle\sigma_1 \sigma_2\rangle_0 = \frac{\langle\sigma_1 \sigma_3\rangle_0 \langle\sigma_1 \sigma_1' \sigma_2 \sigma_2'\rangle_0 \langle\sigma_1' \sigma_3'\rangle_0}{\langle\sigma_1 \sigma_1'\rangle_0 \langle\sigma_1 \sigma_3\rangle_0 \langle\sigma_2 \sigma_2'\rangle_0}. \quad (2.18)$$

Consequently, we obtain

$$\frac{\langle\sigma_i \sigma_{i'} \sigma_j \sigma_{j'}\rangle_0}{\langle\sigma_i \sigma_{i'}\rangle_0 \langle\sigma_j \sigma_{j'}\rangle_0} = \frac{\langle\sigma_i \sigma_{i'}\rangle_0 \langle\sigma_j \sigma_{j'}\rangle_0}{\langle\sigma_i \sigma_j\rangle_0 \langle\sigma_i \sigma_{i'}\rangle_0}, \quad (2.18)$$

and Eq. (2.16) reads

$$\langle\prod_i \sigma_i \sigma_{i'}\rangle_0 = \prod_i \langle\sigma_i \sigma_{i'}\rangle_0 \prod_{j < i} \frac{\langle\sigma_i \sigma_{i'}\rangle_0 \langle\sigma_j \sigma_{j'}\rangle_0}{\langle\sigma_i \sigma_j\rangle_0 \langle\sigma_i \sigma_{i'}\rangle_0}. \quad (2.19)$$

Equation (2.19) is an exact result for correlations when $A = \infty$ and all the spins lie on the x axis. However, Eq. (2.8) enables us to relate each correlation function with finite A to a correlation with $A = \infty$ for the special case in which all the spins are separated by a distance much larger than a lattice constant. By applying Eqs. (2.19) and (2.8) we see that Eq. (2.19) remains true for correlations with finite A . After a rearrangement of terms, we derive Eq. (1.1):

$$\langle\prod_i (\sigma_i \sigma_{i'})\rangle = \prod_i \prod_j \frac{\langle\sigma_i \sigma_{i'}\rangle}{(\langle\sigma_i \sigma_j\rangle \langle\sigma_{i'} \sigma_{j'}\rangle)^{1/2}}. \quad (1.1)$$

The derivation of Eq. (1.1) requires that the spins all lie on the x axis. However, because of the rotational invariance of the critical state,⁴ one can expect that

Eq. (1.1) will hold true whenever the spins are widely separated on *any* line in the lattice, even when that line is not parallel to one of the principal axes.

III. REDUCIBILITY OF FLUCTUATIONS

To use Eq. (1.1) to derive other types of critical correlations, we introduce the concepts of local critical variables and of the reducibility of fluctuations in products of these variables.

It is possible to define several thermodynamic variables which have anomalously large fluctuations near the critical point. For example, in the Ising model the magnetization M and the energy \mathcal{H} each have divergent fluctuations at the critical point. To see this divergence, we need only note that the constant- H specific heat and magnetic susceptibility, each divergent quantities, are proportional, respectively, to the mean-squared fluctuations in \mathcal{H} and M .¹⁶

Both of these extensive fluctuating variables can be expressed as a sum over all coordinates of local fluctuating variables. The magnetization is proportional to the sum of spins at the different sites and the energy is proportional to a sum of a local energy density. We find it convenient to use an energy density which has zero expectation value at the critical point, so we write for the case of equal couplings in the two directions

$$\begin{aligned} \mathcal{E}(j,k) = & -\frac{1}{2}J\sigma_{j,k}(\sigma_{j+1,k} + \sigma_{j-1,k} + \sigma_{j,k+1} + \sigma_{j,k-1}) \\ & + \frac{1}{2}J\langle\sigma_{j,k}(\sigma_{j+1,k} + \sigma_{j-1,k} + \sigma_{j,k+1} + \sigma_{j,k-1})\rangle, \end{aligned} \quad (3.1)$$

where angular brackets denote an expectation value at the critical point. These densities of critical fluctuating quantities σ_1 and $\mathcal{E}(1)$ are local variables in the sense that they depend only upon spins in the neighborhood of point 1. In general, we write a density of a fluctuating quantity as $O_\nu(r)$, with ν being an index which defines which quantity we have under consideration.

We wish to assert that there are effectively only a finite number—say, s —of independent fluctuating quantities. This assertion is an unproved hypothesis whose consequences we wish to develop. First, we must state quite precisely what we mean. Let $O(R)$ be a local variable at R which depends only upon spins in the neighborhood of R . That is,

$$O(R) \text{ depends upon } \sigma_r, \text{ only if } |R-r'| \lesssim R_0 \quad (3.2)$$

for some fixed R_0 . Let X be an operator which depends only upon spins far from R , i.e.,

$$X \text{ depends upon } \sigma_r, \text{ only if } |R-r| > R_0 \lambda \quad \text{with } \lambda \gg 1. \quad (3.3)$$

Then all averages of the form $\langle O(R)X \rangle$ may be eval-

¹⁶ L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon Publishing Corp., New York, 1958), pp. 350–357.

uated as

$$\begin{aligned} \langle O(R)X \rangle = & A_0 \langle X \rangle + \sum_{\nu=1}^s A_\nu \langle O_\nu(R)X \rangle \\ & + \text{terms which go to zero as } \lambda \rightarrow \infty, \end{aligned} \quad (3.4)$$

where the A 's are the same for all X 's. In this sense, any $O(R)$ is expandable in our basic operators as

$$O(R) = A_0 + \sum_{\nu=1}^s A_\nu O_\nu(R), \quad (3.5)$$

with constant coefficients A_ν .

But now consider a product of basic variables of the form

$$O_\nu(R + \frac{1}{2}r)O_\nu(R - \frac{1}{2}r). \quad (3.6)$$

If $r \lesssim R_0$, this is a local variable in the sense of Eqs. (3.2)–(3.4). Hence, it must be expandable in the form (3.5). We conclude that the product variable (3.6) is reducible in the form of a sum of basic variables.

$$\begin{aligned} O_\nu(R + \frac{1}{2}r)O_\nu(R - \frac{1}{2}r) = & A_{\nu\nu,0}(r) + \sum_{\nu'} A_{\nu\nu',\nu''}(r)O_{\nu''}(R), \end{aligned} \quad (3.7)$$

where the A 's are constants, not fluctuating variables.¹⁷ Equation (3.7) is our basic assertion of reducibility.

In our applications, we shall always choose the $O_\nu(R)$ such that the average of $O_\nu(R)$ at the critical point will vanish. Then, we obtain

$$A_{\nu\nu,0}(r) = \langle O_\nu(R + \frac{1}{2}r)O_\nu(R - \frac{1}{2}r) \rangle_c. \quad (3.8)$$

In this paper, we apply Eq. (3.7) to the reduction of a product of two spins. We assume that the two most singular local variables that can appear in a product of two σ 's are σ_r and $\mathcal{E}(r)$, so that Eq. (3.7) reads

$$\begin{aligned} \sigma_{R+r/2}\sigma_{R-r/2} = & \langle \sigma_{R+r/2}\sigma_{R-r/2} \rangle_c [1 + B(r)\sigma_R + C(r)\mathcal{E}(R) \\ & + \text{less singular operators}]. \end{aligned} \quad (3.9)$$

A further simplification arises because of the necessity for symmetry of all critical-point correlations under the change of sign of all spins. The left-hand side of (3.9) is even under this symmetry operation; the right-hand side can only be even if $B(r)$ vanishes.

Our conclusion is that

$$\begin{aligned} \sigma_{R+r/2}\sigma_{R-r/2} = & \langle \sigma_0\sigma_r \rangle [1 + C(r)\mathcal{E}(R) \\ & + \text{less singular terms}]. \end{aligned} \quad (3.10)$$

This conclusion is not new. It has been used by several previous authors.^{9,11,18,19} Furthermore, parts of the general idea of reducibility have been previously stated by Green.²⁰

¹⁷ Examples of this reducibility are contained in Hecht's thesis (Ref. 9).

¹⁸ M. E. Fisher and R. J. Burford, Phys. Rev. 156, 583 (1967).

¹⁹ M. Ferer, M. A. Moore, and M. Wortis, Phys. Rev. Letters 22, 1382 (1969).

²⁰ M. Green, J. Phys. Soc. Japan Suppl. 26, 84 (1969).

IV. ENERGY CORRELATIONS

According to Eq. (1.1), at the critical point

$$F_{12} = \frac{\langle \sigma_1 \sigma_{1'} \sigma_2 \sigma_{2'} \rangle}{\langle \sigma_1 \sigma_{1'} \rangle \langle \sigma_2 \sigma_{2'} \rangle} = \frac{\langle \sigma_1 \sigma_{2'} \rangle \langle \sigma_2 \sigma_{1'} \rangle}{\langle \sigma_1 \sigma_2 \rangle \langle \sigma_{1'} \sigma_{2'} \rangle}, \quad (4.1)$$

when all the points are far separated along a line. Now let the pair of points 1 and 1' as well as the pair 2 and 2' be much closer to one another than the separation between these pairs:

$$R_{12} = |\frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_{1'}) - \frac{1}{2}(\mathbf{r}_2 + \mathbf{r}_{2'})|. \quad (4.2)$$

In that case, we can reduce the product of neighboring spins according to Eq. (3.10) and find that

$$F_{12} \approx 1 + C(|\mathbf{r}_1 - \mathbf{r}_{1'}|)C(|\mathbf{r}_2 - \mathbf{r}_{2'}|)\langle \mathcal{E}(\mathbf{R}_1) \mathcal{E}(\mathbf{R}_2) \rangle, \quad (4.3)$$

with

$$\mathbf{R}_1 = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_{1'}), \quad \mathbf{R}_2 = \frac{1}{2}(\mathbf{r}_2 + \mathbf{r}_{2'}). \quad (4.4)$$

The right-hand side of (4.1) is expandable in a power series in $|\mathbf{r}_1 - \mathbf{r}_{1'}|/R_{12}$ and $|\mathbf{r}_2 - \mathbf{r}_{2'}|/R_{12}$. To second order in these variables, we find that

$$F_{12} \approx 1 + |\mathbf{r}_1 - \mathbf{r}_{1'}| |\mathbf{r}_2 - \mathbf{r}_{2'}| (d^2/dR_{12}^2) \times \ln\langle \sigma(\mathbf{R}_1) \sigma(\mathbf{R}_2) \rangle. \quad (4.5)$$

A comparison of (4.3) with (4.5) now yields the relations

$$C(|\mathbf{r}_1 - \mathbf{r}_{1'}|) = |\mathbf{r}_1 - \mathbf{r}_{1'}| c, \quad (4.6)$$

$$\langle \mathcal{E}(\mathbf{R}_1) \mathcal{E}(\mathbf{R}_2) \rangle = (1/c^2) (d^2/dR_{12}^2) \ln\langle \sigma(\mathbf{R}_1) \sigma(\mathbf{R}_2) \rangle. \quad (4.7)$$

Since the spin-spin correlation function obeys a power law at the critical point,

$$\langle \sigma(\mathbf{R}_1) \sigma(\mathbf{R}_2) \rangle \sim 1/R_{12}^y, \quad (4.8)$$

we find that

$$\langle \mathcal{E}(\mathbf{R}_1) \mathcal{E}(\mathbf{R}_2) \rangle = (\eta/c^2) 1/R_{12}^y. \quad (4.9)$$

According to scaling,¹² the energy-energy correlation function $\sim R_{12}^{-2(d-y)}$ at the critical point. Hence $y=1$ follows as a consequence of the structure of spin correlations on a line, Eq. (1.1), and the reduction equation (3.10).

Multiple energy correlations can be evaluated by the same technique. According to Eq. (1.1),

$$\langle \prod_i \sigma_i \sigma_{i'} \rangle / \prod_i \langle \sigma_i \sigma_{i'} \rangle = \prod_{i < j} F_{ij}, \quad (4.10)$$

where F_{ij} is of the form (4.1). As each i and i' approach one another, the left-hand side of (4.10) can be reduced with the aid of (3.10) and the right-hand side evaluated with the aid of (4.3). We find

$$\langle \prod_i [1 + C(|\mathbf{r}_i - \mathbf{r}_{i'}|) \mathcal{E}(\mathbf{R}_i)] \rangle = \prod_{i < j} [1 + C(|\mathbf{r}_i - \mathbf{r}_{i'}|) \times C(|\mathbf{r}_j - \mathbf{r}_{j'}|) \langle \mathcal{E}(\mathbf{R}_i) \mathcal{E}(\mathbf{R}_j) \rangle]. \quad (4.11)$$

From equating the coefficients of $\prod_i C(|\mathbf{r}_i - \mathbf{r}_{i'}|)$ in Eq. (4.11) we find that

$$\begin{aligned} \langle \prod_{i=1}^n \mathcal{E}(\mathbf{R}_i) \rangle &= 0, \quad \text{for } n \text{ odd} \\ &= \sum_{\text{perm}} \langle \mathcal{E}(\mathbf{R}_1) \mathcal{E}(\mathbf{R}_2) \rangle \langle \mathcal{E}(\mathbf{R}_3) \mathcal{E}(\mathbf{R}_4) \rangle \dots \\ &\quad \langle \mathcal{E}(\mathbf{R}_{n-1}) \mathcal{E}(\mathbf{R}_n) \rangle, \quad \text{for } n \text{ even,} \end{aligned} \quad (4.12)$$

which is the result (1.4). This result holds at the critical point whenever the \mathbf{R}_i lie well separated along a single line.

12.11.2 Kadanoff–Wegner: Marginal Behavior

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Some Critical Properties of the Eight-Vertex Model*

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The eight-vertex model solved by Baxter is shown to be equivalent to two Ising models with nearest-neighbor coupling interacting with one another via a four-spin coupling term. The critical properties of the model in the weak-coupling limit are in agreement with the scaling hypothesis. In this limit where $\alpha \rightarrow 0$, the critical indices obey $\gamma/\gamma_0 = \beta/\beta_0 = \nu/\nu_0 = 1 - \frac{1}{2}\alpha$, $\delta/\delta_0 = \eta/\eta_0 = 1$, with the subscripts zero denoting the index values for the ordinary two-dimensional Ising model.

In a recent publication, Baxter¹ has found the free energy for the eight-vertex problem and shown that α is a continuous function of the interaction constants. This continuous variation of a critical index contradicts the hypothesis of smoothness² or universality³ often postulated for near-critical problems.

One way of seeing the source of this behavior is to rephrase the eight-vertex problem as an Ising model.⁴ Imagine a spin placed at the interstitial points of the lattice as in Fig. 1. An arrow to the right (or upward) corresponds to the case in which the adjacent spins are parallel; a leftward or downward arrow makes the adjacent spins antiparallel. Then, the four combinatorical factors a , b , c , and d corresponding to the vertices shown can all be represented by a factor in the partition function

$$A e^{K \sigma_1 \sigma_4 + K^* \sigma_2 \sigma_3 + \lambda \sigma_1 \sigma_2 \sigma_3 \sigma_4},$$

and we obtain the complete partition function

$$\sum_{\{\sigma_r=\pm 1\}} \prod_{j,k} A \exp(K \sigma_{j,k} \sigma_{j+1,k+1} + K^* \sigma_{j+1,k} \sigma_{j,k+1} + \lambda \sigma_{j,k} \sigma_{j+1,k+1} \sigma_{j+1,k} \sigma_{j,k+1}), \quad (1)$$

in which next-nearest-neighbor spins are coupled by interaction constants K^* depending upon the direction of the diagonal. The factor λ couples all four spins. The precise connection is that

$$a = A e^{K^* + K - \lambda},$$

$$b = A e^{-(K^* + K) + \lambda},$$

$$c = A e^{K^* - K - \lambda},$$

$$d = A e^{-(K^* - K) - \lambda}. \quad (2)$$

The constant A does not, of course, enter into the critical properties.

The Baxter solution shows that this Ising-type problem has a very new kind of singularity at the critical point, namely, one in which the singularity in the specific heat as $\epsilon \sim (b+c+d-a)/a$ goes to zero is of the form $\epsilon^{-\alpha}$ with α being a function of the parameters, namely,⁵

$$\sin \frac{\pi \alpha}{4(1 - \frac{1}{2}\alpha)} = \tanh 2\lambda. \quad (3)$$

This result seems at first to contradict the smoothness hypothesis² which suggests that critical indices should not change their value unless there is a symmetry change. However, this eight-vertex model certainly has a different set of symmetries than the usual two-dimensional Ising model. Notice that at $\lambda=0$, the lattice with $j+k$ = (even integer) does not interact with the lattice with $j+k$ = (odd integer). Even at $\lambda \neq 0$ for $T > T_c$, i.e., $\epsilon > 0$, the spins on these two sublattices are uncorrelated. Therefore, the Ising form of the eight-vertex model can be viewed as having two lattices with "independent" ferromagnetic transitions which occur at exactly the same temperature. The coupling between these two lattices is of the form

$$\lambda \sum_r u_r; \quad u_r = \mathcal{E}_r^{(1)} \mathcal{E}_r^{(2)}, \quad (4)$$

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$$\begin{aligned}
 a &= \begin{array}{|c|c|} \hline \uparrow & \uparrow \\ \uparrow & \uparrow \\ \downarrow & \downarrow \\ \downarrow & \downarrow \\ \hline \end{array} = \begin{array}{|c|c|} \hline \downarrow & \downarrow \\ \downarrow & \downarrow \\ \uparrow & \uparrow \\ \uparrow & \uparrow \\ \hline \end{array} = \begin{array}{|c|c|} \hline \uparrow & \downarrow \\ \downarrow & \uparrow \\ \uparrow & \downarrow \\ \downarrow & \uparrow \\ \hline \end{array} = \begin{array}{|c|c|} \hline \downarrow & \uparrow \\ \uparrow & \downarrow \\ \downarrow & \uparrow \\ \uparrow & \downarrow \\ \hline \end{array} \\
 b &= \begin{array}{|c|c|} \hline \uparrow & \downarrow \\ \uparrow & \downarrow \\ \downarrow & \uparrow \\ \downarrow & \uparrow \\ \hline \end{array} = \begin{array}{|c|c|} \hline \downarrow & \uparrow \\ \downarrow & \uparrow \\ \uparrow & \downarrow \\ \uparrow & \downarrow \\ \hline \end{array} = \begin{array}{|c|c|} \hline \uparrow & \uparrow \\ \downarrow & \downarrow \\ \uparrow & \uparrow \\ \downarrow & \downarrow \\ \hline \end{array} = \begin{array}{|c|c|} \hline \downarrow & \downarrow \\ \uparrow & \uparrow \\ \uparrow & \uparrow \\ \downarrow & \downarrow \\ \hline \end{array} \\
 c &= \begin{array}{|c|c|} \hline \uparrow & \uparrow \\ \uparrow & \downarrow \\ \downarrow & \uparrow \\ \downarrow & \downarrow \\ \hline \end{array} = \begin{array}{|c|c|} \hline \downarrow & \downarrow \\ \downarrow & \uparrow \\ \uparrow & \downarrow \\ \uparrow & \uparrow \\ \hline \end{array} = \begin{array}{|c|c|} \hline \uparrow & \downarrow \\ \downarrow & \uparrow \\ \uparrow & \downarrow \\ \downarrow & \uparrow \\ \hline \end{array} = \begin{array}{|c|c|} \hline \downarrow & \uparrow \\ \uparrow & \downarrow \\ \uparrow & \downarrow \\ \downarrow & \uparrow \\ \hline \end{array} \\
 d &= \begin{array}{|c|c|} \hline \uparrow & \downarrow \\ \uparrow & \downarrow \\ \downarrow & \uparrow \\ \downarrow & \uparrow \\ \hline \end{array} = \begin{array}{|c|c|} \hline \downarrow & \uparrow \\ \downarrow & \uparrow \\ \uparrow & \downarrow \\ \uparrow & \downarrow \\ \hline \end{array} = \begin{array}{|c|c|} \hline \uparrow & \uparrow \\ \downarrow & \downarrow \\ \uparrow & \uparrow \\ \downarrow & \downarrow \\ \hline \end{array} = \begin{array}{|c|c|} \hline \downarrow & \downarrow \\ \uparrow & \uparrow \\ \uparrow & \uparrow \\ \downarrow & \downarrow \\ \hline \end{array}
 \end{aligned}$$

FIG. 1. The correspondence between the Ising-spin configurations, the eight-vertex configurations, and the Boltzmann factors a, b, c, d .

where $\mathcal{E}_\alpha^{(1)}$ and $\mathcal{E}_\beta^{(2)}$ are the energy densities on the two sublattices. This kind of coupling leaves the spontaneous magnetizations on the two lattices free to point in either the same or in opposite directions. Since this two-sublattice symmetry is very different from that of the usual Ising model, it is not surprising that the critical indices of the Baxter solution are, in general, different from those of the Onsager solution.

A second unexpected feature of the solution is that α varies continuously with λ . The scaling hypothesis usually rules out this idea as is shown in the discussion of Ref. 3. However, there is one special case in which the scaling idea does permit the continuous variation of critical indices—if there is a term in the Hamiltonian of the form of $\lambda \sum \bar{u}_r$, and \bar{u} , scales as $1/r^d$ (d denotes the dimension of the lattice).

To see why this particular scaling is so significant, recall the definition of scaling: In the critical region, the phase transition is supposed to be described by fluctuating local quantities, e.g., the magnetization density and the energy density, which we can write as $O_\alpha(r)$. The α distinguishes among different quantities. Let O be a product of n different quantities of this type,

$$O = \prod_{i=1}^n O_{\alpha_i}(r_i), \quad (5a)$$

and take each pair of operators in the product to be separated by a distance $|\vec{r}_i - \vec{r}_j|$ of the order of magnitude of R , with R much greater than a lattice constant and much smaller than a coherence length. Then the statement $O_\alpha(r)$ scales as $1/r^{\alpha}$ means precisely⁶ that

$$\langle O \rangle_{K,\lambda} \sim \frac{1}{R^x}, \quad x = \sum_{j=1}^n x_{\alpha_j} \quad (5b)$$

for $n \geq 2$.

Here the x_α 's are critical indices which describe the behavior of the fluctuating variables. For the

ordinary two-dimensional Ising model, the magnetization has an index $x_\alpha = \frac{1}{8}$, and the energy density $x_\beta = 1$.

If these indices vary with λ , then the derivative of $\langle O \rangle_{K,\lambda}$ contains a term like $R^{-x} \ln R$, in particular,

$$\frac{\partial \langle O \rangle_{K,\lambda}}{\partial \lambda} = - \langle O \rangle_{K,\lambda} \sum_{j=1}^n \left(\frac{\partial x_{\alpha_j}}{\partial \lambda} \right) \ln R + \dots, \quad (6)$$

where the \dots represents terms which are not logarithmic in R . Therefore, these logarithmic terms are signals of continuously varying critical indices.

To see how this logarithm can arise, notice that if λ is conjugate to u_r , which contains a term \bar{u}_r , then

$$\frac{\partial}{\partial \lambda} \langle O \rangle_{K,\lambda} = \sum_r \langle O \bar{u}_r \rangle_{K,\lambda} + \dots \quad (7)$$

According to the operator algebra concept, when a product of two operators which are relatively close to one another appears inside a correlation function, their product may be approximately replaced according to

$$O_\alpha(r_1) O_\beta(r_2) = \sum_y A_{\alpha\beta,y} (\vec{r}_1 - \vec{r}_2) O_y(\frac{1}{2}(r_1 + r_2)), \quad (8)$$

where, according to scaling,

$$A_{\alpha\beta,y} = \frac{a_{\alpha\beta,y} [(\vec{r}_1 - \vec{r}_2)/(|r_1 - r_2|)]}{|r_1 - r_2|^{\alpha+y_\beta-y_\alpha}} \quad (9)$$

for separations $|r_1 - r_2|$ large in comparison to the lattice constant. In the particular case in which $O_\beta = \bar{u}$, which scales as $1/r^d$, then the product in (8) contains a term of the form

$$O_\alpha(r_1) u(r) = \frac{a_\alpha O_\alpha(\frac{1}{2}(r_1 + r))}{|r_1 - r|^d} + \dots, \quad (10)$$

when O_α and \bar{u} are scalars under rotation. Here a_α is, of course, the particular coefficient which appears in the reduction formula (9) when $\alpha = \gamma$ and $O_\beta = \bar{u}$.

As a result, the sum in (7) contains a succession of terms

$$\frac{\partial}{\partial \lambda} \langle O \rangle_{K,\lambda} = \sum_{j=1}^n \sum_{|r_i - r_j| \ll R} \frac{a_j}{|r_i - r_j|^x} \langle O \rangle_{K,\lambda} + \dots \quad (11)$$

which corresponds to $|r_i - r_j|$ being much smaller than the average separation distance $|r_i - r_j| \sim R$. Here the $+ \dots$ include all terms in which all separations are at least of order R . The logarithms then appear in \sum_r . In two dimensions one obtains

$$\sum_{r \in R} 1/r^2 \approx 2\pi \ln(R/a_0). \quad (12)$$

When Eqs. (11) and (12) are combined, a set of logarithms appears in the derivative. A comparison with Eq. (6) then shows that

$$\frac{\partial x_\alpha}{\partial \lambda} = -2\pi a_\alpha. \quad (13)$$

We apply this result to the model solved by Baxter

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SOME CRITICAL PROPERTIES OF THE EIGHT-VERTEX MODEL

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for the particular case $\lambda=0$. At $\lambda=0$, the operator

$$\bar{u}_r = \delta \mathcal{E}_r^{(1)} \delta \mathcal{E}_r^{(2)} \quad (14)$$

does indeed scale as $1/r^2$ if $\delta \mathcal{E}_r^{(1)}$ and $\delta \mathcal{E}_r^{(2)}$ are the deviations of the energy on the two sublattices from their critical values. To see this, calculate $\langle \bar{u}_r \bar{u}_0 \rangle$ at $\lambda=0$ and at the critical point. At $\lambda=0$, the two sublattices are independent so that

$$\langle \bar{u}_r \bar{u}_0 \rangle = \langle \delta \mathcal{E}_r^{(1)} \delta \mathcal{E}_0^{(1)} \rangle^2. \quad (15)$$

However, the statement that $x_s=1$ at $\lambda=0$ implies that at criticality for large r

$$\langle \delta \mathcal{E}_r^{(1)} \delta \mathcal{E}_0^{(1)} \rangle = q/2\pi r^2. \quad (16)$$

From Ref. 7 we obtain $q=4/\pi$. (Note that nearest neighbors in the sublattices are separated by $\sqrt{2}$.) The correlation function on the left-hand side of (15) is then $(q/2\pi r^2)^2$ and, consequently, \bar{u}_r scales as $1/r^2$.

Because \bar{u}_r has this special value of the scaling index, the critical phenomena theory indicates that the critical indices can vary continuously in λ . Conversely, if there is no operator with index d , then there can be no continuous variation of the critical indices.

To find the first variation in the critical index for the energy, calculate

$$\delta \mathcal{E}_{r_1}^{(1)} \bar{u}(r_2) \approx \delta \mathcal{E}_{r_1}^{(1)} \delta \mathcal{E}_{r_2}^{(1)} \delta \mathcal{E}_{r_2}^{(2)}. \quad (17)$$

According to Eq. (17), as r_1 approaches r_2 at $\lambda=0$, the product of the energy fluctuations on lattice (1) can be replaced by a constant divided by $|r_1 - r_2|^2$. In particular,

$$\delta \mathcal{E}_{r_1}^{(1)} \bar{u}(r_2) \approx \frac{q}{2\pi |r_1 - r_2|^2} \delta \mathcal{E}_{r_2}^{(2)}. \quad (18)$$

Note, however, that this result is not of the form (10), needed to reach Eq. (13). To achieve the form (10), we consider the combinations

$$\delta \mathcal{E}_r^{\pm} = \delta \mathcal{E}_r^{(1)} \pm \delta \mathcal{E}_r^{(2)}, \quad (19)$$

which have a simple symmetry under the interchange of the two lattices. Equations (18) and (19) give

$$\delta \mathcal{E}_{r_1}^{\pm} \bar{u}(r_2) = \pm \frac{q}{2\pi |r_1 - r_2|^2} \delta \mathcal{E}_{r_2}^{\pm}$$

when r_1 and r_2 are relatively close together compared to all other distances but $|r_1 - r_2|$ is large compared to a lattice constant. It now follows that δ_r^{\pm} scales as $1/r^{\pm}$ with Eq. (10) giving

$$\frac{dx_{\pm}}{d\lambda} = \mp q.$$

Since the scaling index is 1 at $\lambda=0$, we find that for small λ

$$x_s = 1 \mp \lambda q. \quad (20a)$$

A similar argument applied to $\sigma_r^{(1)}$ indicates that

at $\lambda=0$, $dx_s/d\lambda=0$ so that to first order in λ

$$x_s = \frac{1}{8}. \quad (20b)$$

To derive this result, notice that for r_1 close to r_2 ,

$$\sigma_{r_1}^{(1)} u_{r_2} = \sigma_{r_1}^{(1)} \delta \mathcal{E}_{r_2}^{(1)} \delta \mathcal{E}_{r_2}^{(2)}$$

contains no term which is like $\sigma_r^{(1)}$ since this expression contains a reference to fluctuations on lattice 2. Hence the coefficient a in Eq. (13) vanishes. It follows that $\eta=2x_s$ does not change to first order in λ .

From these results and scaling theory, we can predict all critical indices to first order in λ . For example, the deviation of energy from criticality contains a singular term of the form

$$\delta \mathcal{E} \sim \xi^{-x_s},$$

where ξ is the correlation length, since x_s is the index which goes with the energy. Also the free energy contains a singular term like

$$\delta F \sim \xi^{-2}.$$

Since $\xi \sim \epsilon^{-\nu}$, $\delta F \sim \epsilon^{2-\alpha}$, and $\delta \mathcal{E} \sim \epsilon^{1-\alpha}$, we find

$$(2 - x_s) \nu = 1$$

or

$$\nu = 1 - q\lambda, \quad (21a)$$

$$\alpha = 2\lambda q. \quad (21b)$$

Equation (21b) is in agreement with Baxter's result, Eq. (3). Similarly, scaling theory implies that

$$\langle \sigma \rangle \sim \xi^{-x_s} = (-\epsilon)^{\nu x_s}$$

on the coexistence curve. Thus, $\beta = \nu x_s$ yields

$$\beta = \frac{1}{8} (1 - q\lambda) \quad (21c)$$

to first order in λ . Thus, we find all the critical indices by using the assumption that scaling holds.

To check this assumption we use first-order perturbation theory. There is a term $\lambda \sum_r \delta_r^{(1)} \delta_r^{(2)}$ in $-\beta H$. This term may be written as

$$\begin{aligned} \lambda (\langle \delta_r^{(1)} \rangle \langle \delta_r^{(2)} \rangle + \Delta \delta_r^{(1)} \langle \delta_r^{(2)} \rangle \\ + \Delta \delta_r^{(2)} \langle \delta_r^{(1)} \rangle + \Delta \delta_r^{(1)} \Delta \delta_r^{(2)}) . \end{aligned} \quad (22)$$

For simplicity, set $K^+ = K^- = K$. Now consider any expectation value $\langle O \rangle_{K,\lambda}$ where O is a product of terms $O^{(1)} O^{(2)}$ with $O^{(1)}$ containing spins on the first sublattice and $O^{(2)}$ containing spins on the second sublattice. To zeroth order, we may write

$$\langle O \rangle_{K,\lambda} = \langle O^{(1)} \rangle \langle \epsilon^0 \rangle \langle O^{(2)} \rangle \langle \epsilon^0 \rangle + \text{order } \lambda. \quad (23)$$

Here $\epsilon^0 = K_s^0 - K$, with K_s^0 being the critical value of K at $\lambda=0$.

In first-order perturbation theory,

$$\frac{d}{d\lambda} \langle O \rangle_{K,\lambda} = \langle \delta^{(1)} \rangle \langle O^{(2)} \rangle \langle \epsilon^0 \rangle \sum_r \langle \Delta \delta_r^{(1)} O^{(1)} \rangle_{K,\lambda=0}$$

$$+\langle \mathcal{E}^{(1)} \rangle \langle O^{(1)} \rangle (\epsilon^0) \sum_r \langle \Delta \mathcal{E}_r^{(2)} O^{(2)} \rangle_{K, \lambda=0} \\ + \sum_r \langle O^{(1)} \Delta \mathcal{E}_r^{(1)} \rangle_{K, \lambda=0} \langle O^{(2)} \Delta \mathcal{E}_r^{(2)} \rangle_{K, \lambda=0}. \quad (24)$$

Since \mathcal{E} is conjugate to K , the first two terms in (24) generate derivatives with respect to K of $\langle O^{(1)} \rangle_{K, \lambda=0}$ and $\langle O^{(2)} \rangle_{K, \lambda=0}$. To first order in λ , we may replace Eq. (24) by

$$\langle O^{(1)} O^{(2)} \rangle_{K, \lambda} \approx \langle O^{(1)} \rangle (\epsilon^*) \langle O^{(2)} \rangle (\epsilon^*) \\ + \lambda \sum_r \langle O^{(1)} \Delta \mathcal{E}_r^{(1)} \rangle \langle O^{(2)} \Delta \mathcal{E}_r^{(2)} \rangle, \quad (25)$$

with

$$\epsilon^* = \epsilon^0 - \lambda \langle \mathcal{E} \rangle_{\lambda=0}. \quad (26)$$

Equation (26) gives a renormalized $T - T_c$. Near T_c , $\langle \mathcal{E} \rangle$ is given by

$$\langle \mathcal{E} \rangle = \frac{1}{2} \sqrt{Z} - p \epsilon^0 + q \epsilon^0 \ln |\epsilon^0|, \quad (27)$$

with p being a new constant and q being the same as the constant defined by Eq. (16). [Eq. (27) can be obtained, e.g., from Eq. (97) of Ref. 8. Note that $2K_c(0) = \ln \operatorname{ctg}(\frac{1}{8}\pi)$.] To first order in λ , we can write

$$\epsilon^* = (\epsilon^0 - \lambda \frac{1}{2} \sqrt{Z} + p \lambda \epsilon^0) (1 - \lambda q \ln |\epsilon^0|) \\ = \epsilon (1 - \lambda q \ln |\epsilon|) = \epsilon e^{-\lambda q \ln |\epsilon|} = \epsilon |\epsilon|^{-\lambda q}, \quad (28)$$

with

$$\epsilon = \epsilon^0 - \lambda \frac{1}{2} \sqrt{Z} + p \lambda \epsilon^0 \quad (29)$$

being essentially $K_c(\lambda) - K$. The shift in K_c given by Eq. (29) checks directly against the value given by Baxter's solution.

Equations (25) and (28) may now be used to evaluate critical indices directly. When $O = \sigma_r^{(1)}$ and $T < T_c$, we find, to first order in λ ,

$$\langle \sigma_r^{(1)} \rangle_{K, \lambda} = \pm (-\epsilon^*)^{\beta_0} = \pm (-\epsilon)^{\beta_0(1-\alpha)},$$

where β_0 is the magnetization index for the Onsager solution. This direct solution then recovers the scaling result (21c). Similarly, the two-spin correlation functions which have the form

$$\langle \sigma_0^{(1)} \sigma_r^{(1)} \rangle_{K, \lambda=0} = \frac{1}{r^{1/\Delta}} f(r/\xi_0)$$

when $\xi_0 \sim |\epsilon^0|^{-1}$ become, to first order,

$$\langle \sigma_0^{(1)} \sigma_r^{(1)} \rangle_{K, \lambda} = \frac{1}{r^{1/\Delta}} f(r/\xi) + \text{order } \lambda^2 \quad (30)$$

when $\xi \sim |\epsilon|^{-1+\lambda q}$. It follows that the two-spin correlation function has a scaling form to first order in λ , and that the coherence length index is correctly given by Eq. (21a). Also, an integration of Eq. (30) over all r gives

$$\gamma = \frac{1}{4} (1 - q\lambda), \quad (31)$$

as would be predicted by scaling.

In fact, we can see that scaling holds quite generally to first order in λ . Consider the behavior of a product of n spins on the first sublattice at positions $r_1^{(1)}, \dots, r_n^{(1)}$ and m spins on the second at $r_1^{(2)}, \dots, r_m^{(2)}$. If they are far enough separated so that scaling holds at $\lambda=0$, then

$$\langle \sigma_{r_1} \cdots \sigma_{r_n} \rangle_{K, \lambda=0} = |\epsilon^0|^{n\beta} f_n \left(\left\{ \frac{r_i}{\xi_0} \right\} \right) \quad (32a)$$

while the correlation with an energy density at R takes the form

$$\langle \sigma_{r_1} \cdots \sigma_{r_n} \delta \mathcal{E}_R \rangle_{K, \lambda=0} = \frac{|\epsilon^0|^{n\beta}}{\xi_0} f_{n,1} \left(\left\{ \frac{r_i}{\xi_0} \right\}, \frac{R}{\xi_0} \right). \quad (32b)$$

Then, Eq. (25) implies that to first order in λ ,

$$\langle \sigma_{r_1} \cdots \sigma_{r_n} \sigma_{r_1'} \sigma_{r_2'} \cdots \sigma_{r_m'} \rangle \\ = |\epsilon|^{(n+m)\beta} \left[f_n \left(\left\{ \frac{r_i^{(1)}}{\xi} \right\} \right) f_m \left(\left\{ \frac{r_i^{(2)}}{\xi} \right\} \right) \right. \\ \left. + \lambda \int \frac{d^2 R}{\xi^2} f_{n,1} \left(\left\{ \frac{r_i^{(1)}}{\xi} \right\}, \frac{R}{\xi} \right) f_{m,1} \left(\left\{ \frac{r_i^{(2)}}{\xi} \right\}, \frac{R}{\xi} \right) \right], \quad (33)$$

which indicates that for large separations among all the spins their correlation functions obey all the scaling laws, at least to first order in λ .

It now follows that thermodynamic derivatives with respect to magnetic fields inserted in $-\beta H$ as $h_1 \sum_r \sigma_r^{(1)} + h_2 \sum_r \sigma_r^{(2)}$ must obey scaling in the form

$$\frac{\partial^n}{\partial h_1^n} \frac{\partial^m}{\partial h_2^m} \ln Z \Big|_{h_1=h_2=0} \sim |\epsilon|^{(n+m)\beta - [\Gamma(n+m)-1]2\nu}. \quad (34)$$

In this way, we see that the free energy in the presence of magnetic fields contains a scaling term of the form

$$\epsilon^{2\nu} g \left(\frac{h_1}{\epsilon^\Delta}, \frac{h_2}{\epsilon^\Delta} \right), \quad (35)$$

with $\Delta = 2\nu - \beta$, and that this scaling term dominates all derivatives with respect to magnetic fields. Therefore the critical exponent $\delta = \Delta/\beta$ does not change to first order in λ .

To check the critical index α in first-order perturbation theory, we consider the free-energy density

$$-\beta f_\lambda = -\beta f_0 + \lambda \langle \mathcal{E}^{(1)} \rangle \langle \mathcal{E}^{(2)} \rangle. \quad (36)$$

From Eqs. (27) and (29) we find that the nonanalytic contributions are

$$-\beta f_{\text{sing}} = -q \epsilon^2 \ln |\epsilon| + \lambda q^2 \epsilon^2 (\ln |\epsilon|)^2, \quad (37)$$

which in first order in λ can be written

$$(|\epsilon|^{2-2q\lambda} - \epsilon^2)/2\lambda,$$

which again checks against Eq. (21b).

From Eq. (20a) we obtain the ratio $(2-x_+)/2-x_-$ = $1+2\lambda q$ to first order in λ . To check this ratio we consider the model with an interaction constant

K_1 for the two-spin interactions in the first sublattice and an interaction constant K_2 in the second sublattice. In first order in λ we obtain similarly to Eq. (25)

$$\langle O^{(1)} O^{(2)} \rangle_{K_1 K_2 \lambda} \approx \langle O^{(1)} \rangle (\epsilon_1^*) \langle O^{(2)} \rangle (\epsilon_2^*) + \lambda \sum_r \langle O^{(1)} \Delta \delta_r^{(1)} \rangle \langle O^{(2)} \Delta \delta_r^{(2)} \rangle, \quad (38)$$

with

$$\epsilon_1^* = \epsilon_1^0 - \lambda \langle \delta_2 \rangle_{\lambda=0}. \quad (39)$$

In first order in λ we can write

$$\epsilon_1^* = \epsilon_1 - \lambda q \epsilon_2 \ln |\epsilon_2|, \quad (40)$$

$$\epsilon_1 = \epsilon_1^0 - \lambda \frac{1}{2} \sqrt{2} + p \lambda \epsilon_2^0, \quad (41)$$

and similar equations hold for ϵ_2 and ϵ_2^* . Therefore the critical line $\epsilon_1 = 0$ for $\lambda = 0$ moves to $\epsilon_1^* = 0$ at λ , that is,

$$\epsilon_1 = \lambda q \epsilon_2 \ln |\epsilon_2| \quad (42a)$$

in first-order perturbation theory. This equation as well as

$$\epsilon_2 = \lambda q \epsilon_1 \ln |\epsilon_1| \quad (42b)$$

can be written, in first order in λ ,

$$|\epsilon_1 + \epsilon_2| = |\epsilon_1 - \epsilon_2|^{1+2\lambda q}. \quad (43)$$

Since $\epsilon_1 + \epsilon_2$ and $\epsilon_1 - \epsilon_2$ are conjugate to the energy

densities δ_* , the exponent in Eq. (43) is expected to be $(2 - x_*)/(2 - x_)$, in agreement with Eq. (20a).

APPENDIX

When shown the results of this paper, Wilson drew our attention to a similar problem in field theory which was studied by Wilson,⁹ Callen,¹⁰ and Symanzik.¹¹ In field theory the operator Φ^4 corresponds to the operator \tilde{u}_r . In the free-field limit Φ^4 has the critical index (dimension) d , but in first-order perturbation theory its critical index changes. This leads to a breakdown of scaling.

According to Baxter's solution, the critical index α changes continuously with λ , Eq. (3). Therefore we expect \tilde{u}_r to scale like $1/r^2$ for any λ . Wilson and Fisher urged us to show this in first-order perturbation theory.

To see this, note that for $r_1 \neq r$ the operator

$$O_\alpha(r_1) \tilde{u}(r) = \tilde{u}(r_1) \tilde{u}(r)$$

is even under the Kramers-Wannier (KW) transformation of one sublattice only. (Under the KW transformation of sublattice $1 \delta \delta_r^{(1)}$ is odd and $\delta \delta_r^{(2)}$ is even.) Since $\tilde{u}(r)$ is odd under this transformation, α_α vanishes. Thus, according to Eq. (13), the critical exponent x_* does not change in first order in λ .

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[†]On leave from the Institut für Festkörperforschung of the Kernforschungsanlage Jülich, Germany.

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⁵For positive interaction constants K^* and small λ the phase transition takes place for $a = b + c + d$. To obtain $\epsilon \sim (b + c + d - a)/a$ and Eq. (3) we use the symmetry property $Z(a, b, c, d) = Z(c, d, a, b)$, Eq. (11) of C. Fan and F. Y. Wu, Phys. Rev. B 2, 723 (1970).

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Chapter 13

Renormalization in One Dimension

13.1 Introduction

This chapter is concerned with exploring the relation between renormalization calculations and the physics of the statistical systems. We do this by developing recursion relations for the particularly simple physical system which occur in one dimension. We then study the phase diagram and the coherence length using the recursion relation. Finally, we reach for an approximate recursion relation for a two-dimensional system, which is brought in to exemplify a more complicated physical situation.

13.2 Decimation

Since the partition function for all nearest-neighbor $d = 1$ problems may be computed exactly (See Chapter 4), it should serve as no surprise that one can also do an exact renormalization calculation on them. The technique is very simple. We imagine summing over all variables at odd-numbered lattice sites while holding all variable at even numbered sites unchanged. Specifically, let the original variables, σ , sit on lattice sites at positions, r equal to ja , with integer j . Define new statistical variables for even numbered sites with

$$\mu(r) = \sigma(r) \quad \text{for } r = 2ka \text{ with } k \text{ being an integer.} \quad (13.1)$$

Here μ or σ are the names for any kind of statistical variable, not just an Ising variable. Now, if the problem involves nearest neighbor couplings, the statistical weight factor is

$$e^{W[\sigma]} = \prod_{j=1}^N e^{w(\sigma(r), \sigma(r+a))}, \quad (13.2)$$

with periodic boundary conditions $\sigma(r) = \sigma(r + Na)$. The summation to be performed is:

$$e^{w'(\mu(r), \mu(r+a'))} = \text{tr}_\sigma e^{w(\mu(r), \sigma)} e^{w(\sigma, \mu(r+a'))}, \quad (13.3)$$

with $a' = 2a$. If w contains the old couplings, \mathbf{K} , then w' will contain the new couplings $\mathbf{K}' = R(\mathbf{K})$. In the decimation just described, $\lambda = 2$, but a generalization to other λ -values is quite direct.

Our transfer matrix analysis of one-dimensional systems shows that whenever the two largest eigenvalues of the transfer matrix are non-degenerate, correlation functions in space have a very simple large-distance behavior. The highest eigenstate lends the system a behavior in which there is no fall-off of correlations; the next eigenstate produces an exponential die off with a correlation length $\xi = a/\kappa(\mathbf{K})$. We argued in the previous chapter that renormalizations change κ by a factor of λ (See Eq. (12.29)). For this reason,

$$\kappa(\mathbf{R}(\mathbf{K})) = \lambda\kappa(\mathbf{K}). \quad (13.4)$$

13.3 The Ising Example

The simplest situation is the one in which σ is an Ising variable. We take the most general $w(\sigma, \sigma')$ which obeys the spin flip symmetry

$$w(-\sigma, -\sigma') = w(\sigma, \sigma'). \quad (13.5)$$

This eliminates the possibility of a magnetic field coupling of the form $h(\sigma + \sigma')$, and leaves us with:

$$w(\sigma, \sigma') = K_0 + K\sigma\sigma'. \quad (13.6)$$

The computation is simple and direct. Plug (13.6) into (13.3), perform the sum and find that

$$e^{K'_0 + K'\mu\mu'} = [(1 + \mu\mu') \cosh 2K + (1 - \mu\mu')]e^{2K_0},$$

so that the new couplings obey

$$K' = \frac{1}{2} \ln \cosh 2K, \quad (13.7a)$$

$$K'_0 = 2K_0 + \ln 2 + K'. \quad (13.7b)$$

It is instructive to express Eq. (13.7a) in terms of the dual coupling $\tilde{K} = D(K)$ defined in Eq. (4.23b) as

$$\tilde{K} = D(K) = -\frac{\ln \tanh K}{2}.$$

After a little algebra, we see that we can reexpress Eq. (13.7a) in very simple form by using the dual coupling, namely

$$D(K') = 2D(K) \quad \text{or} \quad \tilde{K}' = 2\tilde{K}. \quad (13.8)$$

We should have expected this simple result. Recall that the transfer matrix for the Ising model, \mathcal{T} , is proportional to $\exp(\tilde{K}\tau_1)$. This matrix moves the system from one site to the

neighboring site. If we wish to move two sites we apply \mathcal{T} twice. Since everything perfectly well commutes, we get a two-site transfer matrix proportional to $\exp(2\tilde{K}\tau_1)$. This nice result enables us to calculate the effect of any renormalization upon K . A renormalization which multiplies the lattice constant by a factor of λ takes the transfer matrix into $(\mathcal{T})^\lambda$, \tilde{K} into $\lambda\tilde{K}$, and thence takes K into $K' = D(\lambda D(K))$.

13.4 Phase Diagrams, Flow Diagrams, and the Coherence Length

We already noted, in passing, the phase diagram of the one-dimensional Ising model. The system has the very same qualitative behavior for all finite values of K , including $K = 0$: it has only short-ranged correlations among its spins, and never shows any signs of a phase transition at any finite value of K . The infinite values of the coupling, $K = \pm\infty$ are different. At these points there is long-ranged order, ferromagnetic for positive K and antiferromagnetic for negative K , and a non-analytic behavior of many different physical quantities. Hence the phase diagram has the structure depicted in Fig. 13.1.

A *phase diagram* is a picture drawn in the space defined by some coupling constants or fields showing where the different thermodynamic phases occur. Most often, a properly defined renormalization transformation will not change the thermodynamic phase of the system.¹ Then the renormalization transformation will connect points in the coupling space which are in the very same thermodynamic phase. Thus, we can figure out the phase diagram by working out another kind a diagram, a flow diagram, in which we look to see how each point in phase space is connected to the others by renormalization transforms.

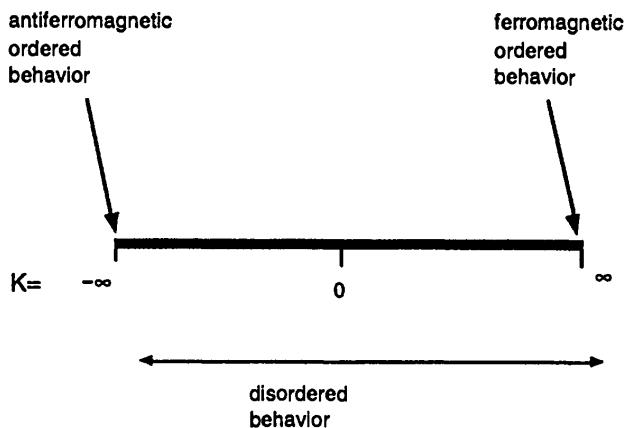


Fig. 13.1. Phase diagram for an Ising Model. The model is disordered for all values of K except the extreme cases $K = -\infty$ and $K = \infty$.

¹There are exceptions to this rule. In Ising antiferromagnets, neighboring spins point in opposite directions. Then $\lambda = 2$ transformations can often focus upon one sublattice or the other. They can thus average half the spins and convert an antiferromagnetic problem into a ferromagnetic one. But this kind of exception is rare.

The flow diagram may be understood in terms of the inverse correlation length, $\kappa(K)$. We noted in the previous chapter that, in a renormalization in which the lattice constant increases by a factor of λ , κ will increase by a factor of λ also. Weak coupling fixed points have $\kappa = \infty$; critical ones have $\kappa = 0$. Finite κ points in the phase diagram cannot be fixed points.

Now let us return to the one-dimensional Ising model. We have just finished saying that κ increases by a factor of λ in the RG transform. So does the dual coupling, $D(K)$. Since these two function behave the same, they must be proportional to one another. We thus conclude that κ is proportional to \tilde{K} . In fact, our calculation gave $\kappa = \tilde{K}$, see Eq. (4.47b).

To see what the renormalization means, let us focus our attention upon Eq. (13.7a), which describes how the coupling constant varies. For large K , one can express the hyperbolic cosine in (13.7a) as approximately $\exp(2K)/2$ and find then that this equation reduces to

$$K' = K - \frac{\ln 2}{2}. \quad (13.9)$$

Thus if the coupling is initially very strong renormalization makes it weaker. In fact successive renormalizations make it weaker and weaker and weaker still until after enough renormalizations the potential becomes so weak that we can solve the problem with perturbation theory.

This kind of result is usually described by a picture like the one shown in Fig. 13.2. Here the dots show the values of K 's after successive renormalizations and the arrows show the progression. As stated the progression is always toward weaker values of the coupling.² By following the arrows, one sees that this picture shows that the flow goes in the direction from order ($K = \infty$) to disorder ($K = 0$).

Figure 13.3 shows a more elegant representation of the same information. The weak coupling fixed point is shown by the circle; the strong coupling fixed point by the cross. All the points to the left of the cross flow into the weak coupling fixed point and below to the weak coupling phase. The point at infinity, belongs to the infinite coupling phase. These two different phases show qualitatively different behavior in, for example, the behavior of their spin correlations at very large separation, and thus belong to different thermodynamic phases. Equally well, we may say that different regions of the phase diagram fall into different universality classes.

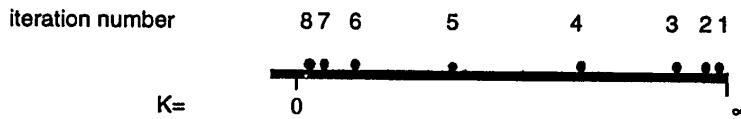


Fig. 13.2. Successive renormalizations for a one-dimensional Ising model. This figure shows the values of the coupling at the different stages of the renormalization. Note that the coupling gets weaker step by step.

²We know this because the renormalization always increases the dual coupling. But the dual coupling always increases as the direct coupling decreases. Q.E.D.

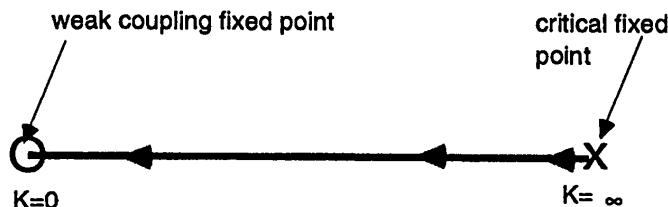


Fig. 13.3. Flow diagram for a Ising Model.

13.5 The Gaussian Model

The same basic renormalization technique that we applied to the Ising model also works for the Gaussian model. This model has a action on a single bond of the form

$$w(q, p) = -\frac{1}{4}(q^2 + p^2) + Kqp + K_0, \quad (13.10)$$

where q is a variable which is to be integrated from minus infinity to infinity. In Eq. (13.10), K_0 is a constant terms which we shall eventually adjust to produce a fixed point.

Then the decimation, that is the sum over every second variable, is represented by the process:

$$\begin{aligned} e^{v'(q,p)} &= \int_{-\infty}^{\infty} dx \exp[w(q, x) + w(x, p)] \\ &= \int_{-\infty}^{\infty} dx \exp \left[-\frac{q^2 + p^2}{4} - \frac{x^2}{2} + Kx(p + q) + 2K_0 \right]. \end{aligned} \quad (13.11)$$

The integral over x is easily performed. It gives

$$e^{v'(q,p)} = \sqrt{2\pi} \exp \left[-\frac{q^2 + p^2}{4} (1 - 2K^2) - pqK^2 + 2K_0 \right]. \quad (13.12)$$

Notice that this expression is not in the normal form which we are using to describe Gaussian behavior. In the normal form of Eq. (13.10) q^2 is multiplied by $1/4$ and not by the extra factor of $1 - 2K^2$ as in Eq. (13.12). This ‘difficulty’ may be cured by using as our new, ‘renormalized’, variables³

$$q' = q\sqrt{1 - 2K^2}, \quad p' = p\sqrt{1 - 2K^2}. \quad (13.13)$$

Notice that, because of the ‘extra’ variable transformation of Eq. (13.13) what we are doing is not precisely a decimation transformation. But, whatever one calls it, one can write the new bond in terms of the new variables as

$$w'(q\sqrt{1 - 2K^2}, p\sqrt{1 - 2K^2}) = v'(q, p) - 0.5 \ln(1 - 2K^2). \quad (13.14)$$

³This kind of multiplication is what gave the name ‘renormalization’ to the entire process.

The second term on the right is the result of our going from dq to dq' as the differential element in our integrations. Then we have made w' have the same form (13.10) as we had before the renormalization. After the transform, the two constants K and K_0 are replaced by renormalized constants. The new coupling is

$$K' = \frac{K^2}{1 - 2K^2}, \quad (13.15)$$

while the new constant term has the form:

$$K'_0 = 2K_0 + 0.5 \ln \frac{2\pi}{1 - 2K^2}. \quad (13.16)$$

13.6 Analysis of Recursion Relation

The recursion relation for the coupling would look simpler if we use as our variable $J = 1/K$ and wrote instead of Eq. (13.15)

$$J' = J^2 - 2. \quad (13.17)$$

In fact, we can solve this recursion equation exactly. Try to make the further change of variables

$$J = 2 \cosh Z.$$

Then the two sides of the equation become:

$$2 \cosh Z' = (e^Z + e^{-Z})^2 - 2 = 2 \cosh 2Z.$$

Then the recursion relation becomes the very simple statement

$$Z' = 2Z \quad (13.18)$$

which means that we can as before understand out that the result of changing the lattice constant by a factor of λ will be to change the coupling variable, $Z(\lambda)$, which gives the value of Z after a renormalization through λ as

$$Z(\lambda) = \lambda Z(1). \quad (13.19)$$

When we look back at the transformations, we find that Z is related to the original coupling by

$$\cosh Z = \frac{J}{2} = \frac{1}{2K}. \quad (13.20)$$

If K is close to but smaller than one half, Z is just a hair bigger than zero. After n renormalization transforms, each with $\lambda = 2$, then the new Z will be $Z_n = 2^n Z$. For large enough n , Z_n will become very large. Large Z will translates into large J which implies

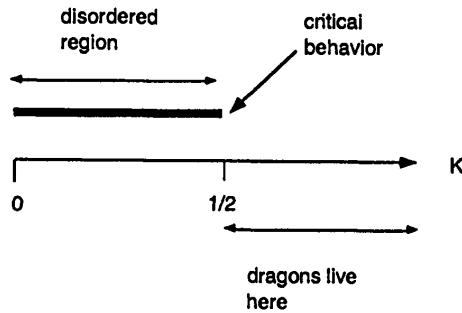


Fig. 13.4. Phase diagram for a Gaussian model.

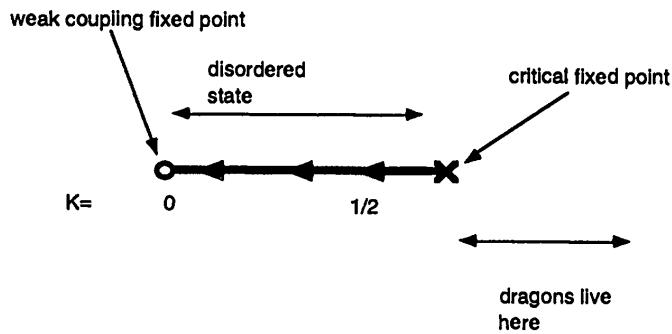


Fig. 13.5. Flow diagram for a Gaussian model.

small K . So after many renormalizations K will go toward zero. The flow diagram looks like the one in Fig. 13.4.

But what about the region where dragons dwell? Here, the Gaussian integral actually diverges so that the renormalization calculation is not required to make sense. On the other hand it does make sense of a sort. In this region J is smaller than 2 so Z is pure imaginary, $Z = i\theta$ and hence $J = 2 \cos \theta$. The recursion relation gives θ_n as $2^n \theta$ so that $J_n = 2 \cos \theta_n = 2 \cos 2^n \theta$. If we are close to the critical point, at the start, θ is small. Then after many renormalizations, J_n will start varying in a chaotic fashion and K_n will similarly vary, while keeping in the range between $1/2$ and infinity. Thus, in the region where the dragons dwell, the renormalization will produce a chaotic sequence of K_n , with the result depending in a very sensitive manner upon the initial data.

The flow diagram for the Gaussian model is shown in Fig. 13.5. Once again the flow is from stronger couplings to weaker, but in this case the strongest possible coupling is $1/2$.

13.7 Fixed Point Analysis for the Gaussian Model

The critical fixed point sits at $K = K_c = 1/2$. To analyze this critical point, look at the renormalization transform in its neighborhood. The recursion relation is

$$K' = R(K) \quad \text{with} \quad R(K) = \frac{K^2}{1 - 2K^2}. \quad (13.21)$$

Near the fixed point, we have $K = K^* + \delta K$, where δK is small and negative. The new coupling is obtained to linear order by expanding $R(K)$ in a series expansion in δK as

$$K' = K^* + \delta K' = R(K) = R(K^*) + \frac{dR}{dK} \Big|_K^* \delta K = K^* + 4\delta K.$$

In this way, we obtain the the linearized recursion relation

$$\delta K' = 4\delta K. \quad (13.22)$$

The recursion relation (13.22) describes the case $\lambda = 2$.

Now we can determine the behavior of the correlation length in the neighborhood of the critical point. In this region of couplings we might expect that the correlation length should diverge. Hence, we can write

$$\kappa(K) \approx (-\delta K)^\nu, \quad (13.23)$$

where the critical index for the correlation length, ν , is to be determined. Notice that since κ must increase by a factor of $\lambda = 2$ on each iteration, in virtue of (13.22), κ must be proportional to $\sqrt{\delta K}$. Thus, we make the determination

$$\nu = 1/2 \quad (13.24)$$

for this one-dimensional Gaussian model.

We can follow an entirely similar argument for the order variable q_j . First, I would like to argue that at $K = K_c$, the fluctuations in q_j are so large that $\langle q_j^2 \rangle$ diverges. To see this consider the renormalization equation for the field. According to Eq. (13.13), the renormalized theory involves a new Gaussian variable, q' , defined by

$$q'_{j/2} = q_j \sqrt{1 - 2K^2}. \quad (13.25)$$

Specialize this result to the critical point. Look at the point, $j = 0$, which is not special, but is left invariant under the renormalization transformation. Now Eq. (13.25) gives

$$q'_0 = q_0 \sqrt{1 - 2K^2} = \frac{q_0}{\sqrt{2}}. \quad (13.26)$$

Since the statistical weight, W , is exactly the same before and after the transformation it must be true that

$$\langle q'_0^2 \rangle = \langle q_0^2 \rangle. \quad (13.27)$$

Equations (13.26) and (13.27) cannot possible be consistent unless the average is very special. It can be either zero or infinity. A little calculation shows that the average is nonzero for $K = 0$ and grows as K grows. Thus, zero is out, and consequently:

$$\langle q_0^2 \rangle = \infty \quad \text{for } K = K_c. \quad (13.28)$$

We can even calculate the strength of the divergence. Let K be a little different from K_c . If there is a divergence at $K = K_c$, we might expect that near the critical point the average would grow large, perhaps with the algebraic form:

$$\langle q_0^2 \rangle = A(K_c - K)^{-\mu}, \quad (13.29)$$

where A is a constant of order unity. Using the renormalization transformation (13.26) we find that very close to K_c

$$\langle q_0'^2 \rangle_{K'} = A(K_c - K')^{-\mu} = \frac{1}{2} \langle q_0^2 \rangle_K = \frac{1}{2} A(K_c - K)^{-\mu}.$$

The factor of $1/2$ arises from the $\sqrt{1 - 2K^2}$ in Eq. (13.13) which describes the renormalization of the q -variables. Near criticality $(K_c - K') = 4(K_c - K)$, it follows that

$$4^\mu = 2 \quad \text{so that} \quad \mu = 1/2. \quad (13.30)$$

A little more argumentation shows that the result (13.29) generalizes to the statement

$$\langle q_j q_{j+\Delta} \rangle = A(K_c - K)^{-\mu}, \quad (13.31)$$

for any Δ . The idea is basically that the infinity is driven by long wave-length fluctuations in q_j . These long-wavelength fluctuations are then the same for all positions. Consequently the divergences are identical for all values of position — and A does not depend upon Δ .

From Eq. (13.31), we see that the leading order infinity cancels out when one calculates $\langle (q_j - q_{j+\Delta})^2 \rangle$. We might then expect that at the critical point, this correlation function might behave as a power of the separation, with the behavior

$$\langle (q_0 - q_\Delta)^2 \rangle = B\Delta^{-2x_q}, \quad (13.32)$$

where B is a constant of order unity. Now after the renormalization, the correlation remains the same. However, the distance Δ has been replaced by $\Delta/2$ while according to Eq. (13.26) q has been replaced by $q' = q/\sqrt{2}$.

Thus the renormalization equation reads:

$$\langle (q_0' - q'_{\Delta/2})^2 \rangle = B(\Delta/2)^{2x_q} = \frac{\langle (q_0 - q_\Delta)^2 \rangle}{2} = \frac{B}{2}\Delta^{-2x_q}.$$

so that $x_q = -1/2$ and that the correlation equation yields

$$\langle (q_0 - q_\Delta)^2 \rangle = B\Delta. \quad (13.33)$$

Correlation functions like (13.33) composed of powers of spatial differences are called structure functions. The correlations between the two order variables grows as the distance between them increases. This result is somewhat unexpected but it is not illogical. It is merely the statement that q becomes unbounded under the Gaussian integral as the critical point is approached. However if j and j' are close together q_j and $q_{j'}$ remain close to one another, and their difference remains small. Thus as the distance, Δ , decreases, the structure function (13.33) gets smaller. Conversely, for large Δ the unbounded fluctuations in q can make the result very large indeed.

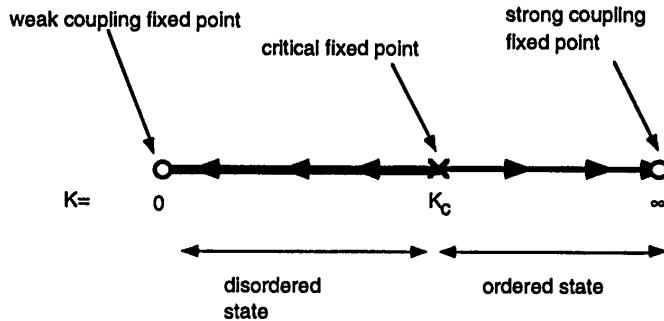


Fig. 13.6. Flow diagram for an Ising Model in two dimensions.

13.8 Two-Dimensional Ising Model

Both of the examples we have just given are quite typical of phase transition that occur in the real world. They both have a phase diagram in which the disordered phase ends in a special point which terminates the whole line. In contrast, the two-dimensional Ising model has a more typical behavior. The disordered phase ends in a critical point which is followed by an ordered phase. (See Fig. 13.6.) Each of these three phases is in a different universality class.

As a part of our study of phase and flow diagrams, we would like to study a recursion relation which produces the result shown in Fig. 13.6. Unfortunately no exact recursion relation is known for this problem. Instead, we borrow a result from what is known as the Migdal approximation. This is a flexible but somewhat inaccurate approach. It is discussed in detail in the next chapter. For the d -dimensional Ising model with nearest neighbor interaction K , we can write a recursion relation

$$K' = R_\lambda(K) \quad (13.34)$$

and the Migdal approach gives the recursion function

$$R_\lambda(K) = \lambda^{d-1} D(\lambda D(K)). \quad (13.35)$$

Here D is the familiar dual function given by Eq. (4.62)

$$D(K) = -\frac{\ln \tanh K}{2}.$$

We could find the consequences of Eq. (13.34) at any value of λ . We specialize to the case in which λ is very close to one.

To find the way K changes under the renormalization, one differentiates Eq. (13.34) with respect to λ and then evaluates the result at $\lambda = 1$, to obtain the β -function:

$$\beta(K) = \left. \frac{d}{d\lambda} R_\lambda(K) \right|_{\lambda=1}. \quad (13.36)$$

Notice that if β is positive the coupling increases with renormalization, if it is negative the coupling decreases. These signs then define the sense of the arrows in the flow diagram. If β is zero, then we are at a fixed point. Within the Migdal approximation, the β -value is

$$\beta(K) = (d - 1)K + D(K)D'(K).$$

In this first line of the calculation, we have used the fact that $\lambda = 1$. Next we simplify the expression by using the ‘dual’ property that $D(D(K)) = K$ to obtain

$$\beta(K) = (d - 1)K + D(K)D'(K) = (d - 1)K - \frac{1}{2}D(K) \cosh^2 D(K). \quad (13.37)$$

One can see the nature of the flow diagram by looking at Eq. (13.37). For very large K , and d greater than one, the first term on the right hand side of Eq. (13.37) dominates so that β is positive. Thus, for large K the renormalization group flow points toward even larger K . We depict this in Fig. 13.6 by the rightward pointing arrows for large K . The story is just the opposite for K positive but very close to zero. Then the dual coupling, $D(K)$, is very large, the second term on the right of (13.37) dominates, and the flow goes toward weaker couplings. Thus there are flows that move toward stable fixed points at very weak and very strong coupling. These two fixed points describe respectively the weak coupling and the ordered phases.

These two phase are separated by a critical point which occurs when $\beta = 0$. In one of the homework exercises, you are asked to calculate the value of this fixed point coupling. The result is particularly simple when $d = 2$. A brief calculation shows that the vanishing occurs when the direct and the dual couplings are identical. This answer is exactly correct.

Homework

Problem 13.1 (The Potts Model). Consider a variable s which takes on q possible values: $s = 1, 2, \dots, q$. These variables form the substance of what is called the q state Potts Model. Consider a situation in which the classical statistical system has the potential

$$w(s, t) = K\delta_{s,t}.$$

Now consider

$$Z = \text{Tr} \exp \sum_{j=1}^N w(s_j, s_{j+1}),$$

where each of the s_j takes on q possible values.

- (a) How does the renormalization work in this case?
- (b) What is the value of the coherence length?
- (c) Use the renormalization approach to check the value of the coherence length you calculated.

Problem 13.2. If we have a situation in which

$$\langle s|M|t\rangle = \exp[w(s,t)]$$

with $w(s,t) = K\delta_{s,t} + h(\delta_{s,1} + \delta_{1,t})/2$.

Here s and t take on higher values between 1 and q . When K is big and h is small this problems represents some sort of exponential of a Hamiltonian. What is the Hamiltonian?

Problem 13.3 (Anti-ferromagnetic Gaussian Model). Discuss the $d = 1$ Gaussian renormalization for negative K . In what region of K will the integral converge? How will the value of the integral for negative K be related to its value for positive K ?

Problem 13.4. For $K = 1/4$ calculate numerically the free energy for the Gaussian chain. How does your numerical result compare with the exact answer?

Problem 13.5 (Ising Fixed Point). Calculate the fixed point coupling for the d -dimensional Ising model by using the Migdal approximation in the limit λ to unity. Draw a picture of your result. What is the form of the answer as d approaches very close to 1? What is the form as d approaches infinity?

Chapter 14

Real Space Renormalization Techniques

14.1 Introduction

Renormalization provides a theoretical framework for critical phenomena (and many other things), but it is not quite a calculational method. In Chapter 11, we emphasized that renormalization ideas make it possible to relate the critical behavior of many different physical quantities. However, without a specific calculation the theory provides only relations — it does not provide a single value for a critical index. In the last chapter, we showed how to do calculations for one-dimensional problems. Now we wish to carry out calculations beyond one-dimensional situations.

A wide variety of different methods have been developed for doing renormalization calculations. Several methods use diagrammatic expansion techniques partially borrowed from field theory. Since these are widely discussed in the literature,¹ I will not go into them here. Instead I will describe a set of approximate methods which go under the name of the *real space renormalization group*. These techniques have the advantage that they are relatively simple and direct. Their disadvantage is that they each use a physically motivated (but mathematically uncontrolled) approximation.

The methods which will be described in this chapter work, with varying degrees of success on any problem. We will apply them here only to Ising models, since these models will provide the simplest calculation.

¹See Domb, The critical Point: Secs. 7.5–7.7 and C. Itzykson and J.-M. Drouffe, *Statistical Field Theory*, Volume II, Chapter 7. (Cambridge University Press, Cambridge (1992)).

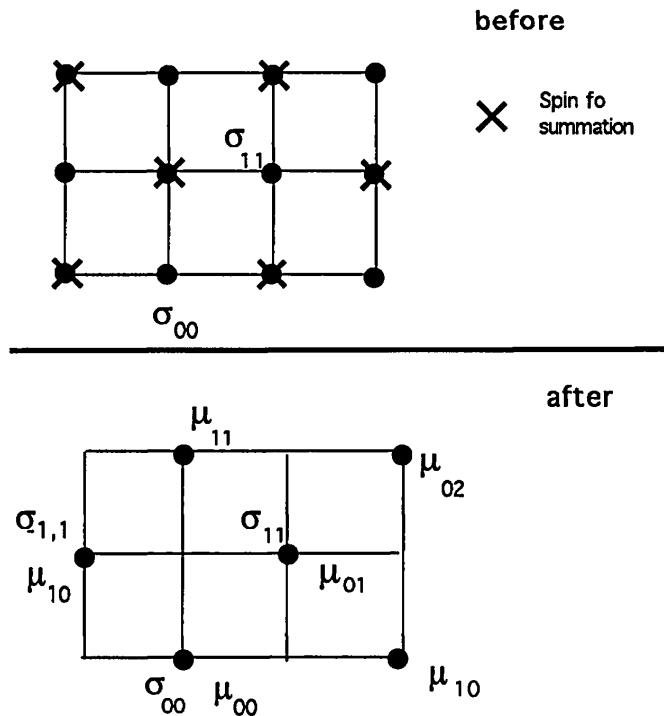


Fig. 14.1. Decimation on a two-dimensional Ising lattice. The original spins, σ , are shown in the first frame. The crosses mark spins which will disappear because they have been summed over. The second frame shows the new lattice produced after the summation.

14.2 Decimation: An Exact Calculation

Consider² a two-dimensional Ising model on a simple square lattice with a constant coupling term K_0 and a nearest neighbor coupling K_{nn} . (See Fig. 14.1.) The model is described by variables $\sigma_{j,k}$, where the subscripts are integers and by an action

$$\mathcal{W} = -\beta \mathcal{H} = \sum_{jk} [K_0 + K_{nn}\sigma_{j,k}(\sigma_{j+1,k} + \sigma_{j,k+1})]. \quad (14.1)$$

To do a renormalization calculation, imagine that we sum over every other spin variable in the lattice. That is we sum over all $\sigma_{j,k}$ for which the sum $j+k$ is odd. The remaining variables, with $j+k$ even are merely renamed, and called μ 's. The basic sum to be performed is a sum over one spin, σ , coupled to four fixed spins called $\mu_1, \mu_2, \mu_3, \mu_4$. (These four spins might be the ones called $\mu_{10}, \mu_{00}, \mu_{01}$, and μ_{11} in Fig. 14.1.) If there are $N\sigma$ -spins at the beginning, then the new partition function is a product of $N/2$ terms which each look like

$$z(\mu_1, \mu_2, \mu_3, \mu_4) = \sum_{\sigma=-1}^1 \exp[2K_0 + K_{nn}\sigma(\mu_1 + \mu_2 + \mu_3 + \mu_4)].$$

²I here follow the argument of a paper which Humphrey Maris and I wrote together. H. Maris and L. Kadanoff, Am. J. Phys. 46(6), 652 (1978). It can also be found in LPK: Essays.

The factor of 2 in front of K_0 arises because there are twice as many initial sites $\sigma_{j,k}$ as summation sites. The sum gives

$$z(\mu_1, \mu_2, \mu_3, \mu_4) = 2 \exp(2K_0) \cosh K_{nn}(\mu_1 + \mu_2 + \mu_3 + \mu_4). \quad (14.2)$$

Notice that the right hand side of Eq. (14.2) is an expression in the four μ 's which is unchanged if any two μ 's are interchanged or if they are all flipped in sign. Given that the four μ 's have values plus one or minus one, there are only three such expressions we can make:

$$S_0 = 1, \quad S_2 = (\mu_1\mu_2 + \mu_1\mu_3 + \mu_1\mu_4 + \mu_3\mu_2 + \mu_4\mu_3 + \mu_2\mu_4), \quad S_4 = \mu_1\mu_2\mu_3\mu_4. \quad (14.3)$$

Thus z must be of the form

$$z(\mu_1, \mu_2, \mu_3, \mu_4) = \exp[L_0 S_0 + L_2 S_2 + L_4 S_4]. \quad (14.4)$$

Here L_0 , L_2 , and L_4 will determine new coupling constants. The first of these depends upon K_0 and the old coupling constant K_{nn} , the second and third depend upon K_{nn} . A brief calculation gives

$$\begin{aligned} L_0 &= 2K_0 + \ln 2 + \frac{1}{8} \ln \cosh(4K_{nn}) + \frac{1}{2} \ln \cosh(2K_{nn}), \\ L_2 &= \frac{1}{8} \ln \cosh(4K_{nn}), \\ L_4 &= \frac{1}{8} \ln \cosh(4K_{nn}) - \frac{1}{2} \ln \cosh(2K_{nn}). \end{aligned} \quad (14.5)$$

Now we see that the decimation has generated a new nearest neighbor coupling and a new constant term

$$K'_{nn} = 2L_2, \quad (14.6a)$$

$$K'_0 = L_0. \quad (14.6b)$$

The factor of two arises because there are two summations which border on a new nearest neighbor site and hence contribute to the new nearest neighbor coupling. In addition, the sum has generated two new kinds of couplings not in the original problem: a new four spin interaction

$$K'_4 = L_4, \quad (14.6c)$$

coupled to all four of the μ 's, and a next nearest neighbor coupling

$$K'_{nnn} = L_2. \quad (14.6d)$$

Now we are faced with a substantial problem. We started with one kind of coupling and ended up with several kinds. But we want to apply the recursion method again and again. Therefore, we must do something about the new kinds of coupling generated. There are several possible things which might be done:

- (a) Do some kind of expansion in the new kinds of couplings, getting yet more kinds. Then try to solve the approximate problem involving many couplings as well as possible. Wilson³ carried out this kind of calculation in one of his first applications of the renormalization group method. This method was also employed, in parallel, by A. Houghton and myself.⁴ Th. Niemeijer and J. M. van Leeuwen worked in parallel on this kind of calculation and actually derived the first good answers.⁵
- (b) Neglect the couplings we do not like. This approach might be called the method of neglect. We show below how to carry out this kind of calculation.
- (c) Try to do something approximate to the sum so as not to generate unwanted terms. One method for producing this desired effect is called ‘potential moving’. We also show example of this approach below.

14.3 The Method of Neglect

In professional applications of renormalization group methods, one sometimes applies a method of neglect. However, one should be very careful to neglect only small things. To see the danger, let us brutally apply the decimation method by making the approximation of neglecting the generated couplings K'_4 and K'_{nnn} in Eq. (14.6a). With these terms neglected, the decimation generates a problem precisely like the starting point. The new coupling has the value:

$$K'_{nn} = \frac{1}{4} \ln \cosh(4K_{nn}). \quad (14.7)$$

In this case, the approximation is too brutal. The recursion relation of Eq. (14.7) has as its fixed points zero and infinity. All points in between flow into the weak coupling critical point at $K = 0$. There is no critical fixed point and hence no description of critical behavior.

Better calculations, in which one makes an effort to throw away only weaker couplings give useful results.

We should not be too surprised that the decimation method has failed.⁶ It has a major problem connected with it. The problem is connected with the calculation of the correlation function $\langle \sigma_{0,0}, \sigma_{0,0+\Delta} \rangle$ when Δ has the value 2^n . If we are at any fixed point, this correlation function should not change under a renormalization. The names of the variables change, σ gets replaced by μ , and n gets replaced by $n - 1$, but the problem and the coupling remain quite the same. Because there is a direct translation of σ into μ , the actual value of the correlation changes not at all. Therefore it is true that at the critical point

$$\langle \sigma_{0,0}, \sigma_{0,0+\Delta} \rangle = \langle \sigma_{0,0}, \sigma_{0,0+\Delta/2} \rangle.$$

³K. Wilson, Rev. Mod. Phys. **47**, 733 (1975).

⁴A. Houghton and L. Kadanoff, Phys. Rev. **B11**, 377 (1975).

⁵See Th. Niemeijer and J. M. van Leeuwen, Phys. Rev. Lett. **31**, 1411 (1973). A reprint of this work is included at the end of this chapter.

⁶The argument of this paragraph was originally formulated by K. Wilson.

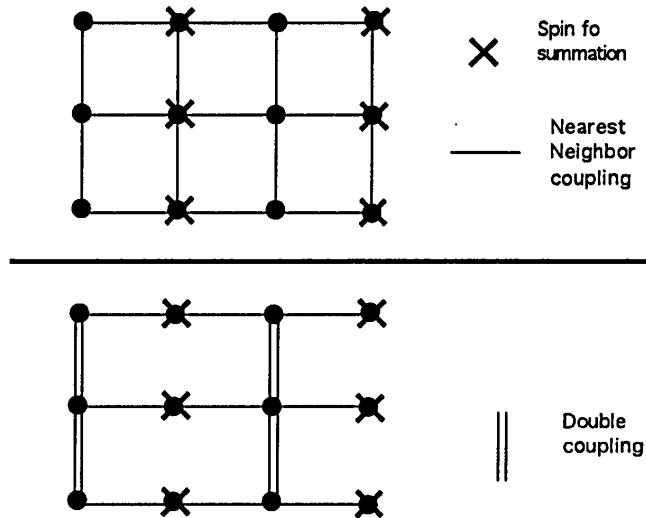


Fig. 14.2. A lattice with nearest neighbor interactions. First part: The coupling between the summation variables makes it impossible to calculate the sums. Second part: The offending coupling terms are moved onto a neighboring bond so that the summation can be performed.

But this result is quite inconsistent with the correct statement that at criticality, the two-dimensional Ising model is,

$$\langle \sigma_{0,0}, \sigma_{0,0+\Delta} \rangle \sim \Delta^{-1/4}.$$

The only possibility is that the renormalization scheme that we are using is itself flawed in that it never gets one to the fixed point. That is the right answer.⁷ Thus, one must use a better scheme than decimation to describe the critical fixed point in dimensions higher than one.

14.4 Potential Moving

Despite what was just said, we now follow up on another decimation calculation. This calculation, originally due to A. A. Migdal,⁸ provides a beautiful and simple renormalization method which seems to give pretty decent answers for a very wide variety of problems. In addition, this discussion gives us a chance to introduce potential moving in a particularly simple context.

Imagine that one wished to do the necessary sums for a renormalization calculation. For example let us imagine removing every second spin in the configuration shown in Fig. 14.2. The success of our previous decimation depended upon the fact that the system could be grouped into two sublattices, A and B and that there was no coupling between different spins in A. Then we could easily sum over all the spins in subset A. But, in the case depicted in Fig. 14.2, the next neighbor interactions make it impossible to divide the system into

⁷K. W. Wilson, private communication.

⁸See the reprints by A. A. Migdal in Sec. 14.6.5 and L. P. Kadanoff in Sec. 14.6.4 at the end of this chapter.

sublattices, with no interaction within a sublattice. Thus all the summations are coupled and they cannot be performed in an explicit fashion.

The analogous couplings connecting the unsummed spins are harmless and can be taken into account exactly. Thus the K_y couplings come in two kinds, ‘good’ and ‘bad’.

We want to take the ‘bad’ couplings and handle them in an approximate fashion. We know that because of the symmetry of the system these ‘bad’ y -directional couplings have exactly the same effect as their ‘good’ siblings. Imagine a free energy calculation, if the good couplings were increased by a small amount, say λ , and the bad couplings were to be decreased by the same amount, then — to first order in λ — the partition function will be unchanged. The change is of second order or higher. Thus, we make a much smaller error by this combined process of increase and decrease than we would make by just decreasing the bad couplings. This more accurate process is equivalent to moving a portion of the bad couplings from where they are unwanted to where they are harmless.

Let me restate the same argument in symbols. Imagine that we have a partition function which is given by $Z = \text{Tr } \exp(\mathcal{W})$, where \mathcal{W} is some action which has a some kind of symmetry property. Let \mathcal{V} be some kind of perturbation term anti-symmetrical under the symmetry property so that the trace, $\text{Tr } \mathcal{V} \exp(\mathcal{W})$, must vanish. Now for the argument. Define

$$Z(\lambda) = \text{Tr } e^{\mathcal{W} + \lambda \mathcal{V}}. \quad (14.8)$$

The exact free energy is $Z(0)$. By the symmetry property, the first derivative of Z with respect to λ vanishes at $\lambda = 0$. The second derivative is

$$\frac{d^2}{d\lambda^2} \ln Z(\lambda) = \langle (\mathcal{V} - \langle \mathcal{V} \rangle_\lambda)^2 \rangle_\lambda. \quad (14.9)$$

Here the average, $\langle \cdot \rangle_\lambda$ is defined with respect to the weight given in Eq. (14.8). The average on the right hand side of Eq. (14.9) is manifestly positive. Therefore, it follows that

$$Z(\lambda) \geq Z(0). \quad (14.10)$$

The right hand side is the exact answer. The potential moving must have the effect of raising the calculated value of the partition function compared to the exact one. It also gives a correlation which is second order in the parameter λ .

Variational methods are widely used through mathematical physics. A statement of the form of Eq. (14.10) enables one to compare different approximation schemes, with the best one having the highest free energy. Further this statement is an assurance that errors in the free energy are quadratic functions of the approximation errors.

We carry this potential moving process to an extreme. The sum is performed by not moving just a little of the unwanted couplings. On the contrary, we move all the unwanted coupling from the bad y -direction bond to the good one.⁹ After the move, the new coupling

⁹In essence we set λ equal to one of the coupling values. Thus we do not really have a free parameter left in the problem and we do not know how large our error might be. However, we do know that the approximate free energy is certainly less than the correct one.

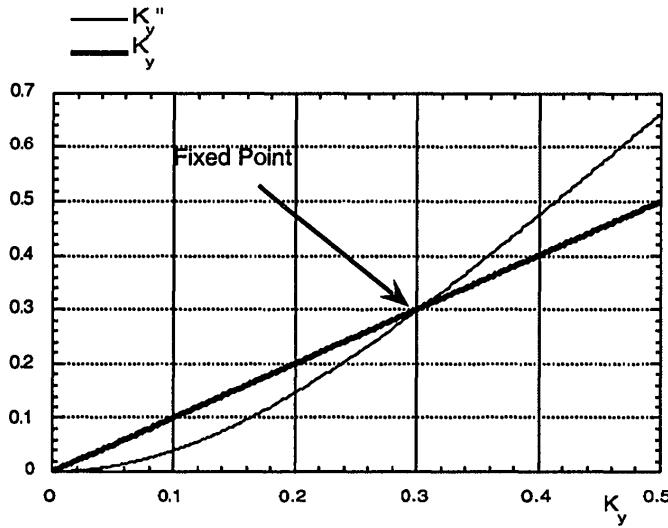


Fig. 14.3. Graphical method for finding the fixed point of the Migdal recursion relations.

in the y -direction is then just double the old coupling

$$K'_y = 2K_y . \quad (14.11a)$$

This value of the new coupling survives the summation. The summation process is exactly the same as in the one-dimensional Ising model, involving two spins coupled to a summation variable and giving, as before

$$K'_x = \frac{1}{2} \ln \cosh(2K_x) . \quad (14.11b)$$

To complete the recursion process, one interchanges x and y and sums again, giving a second recursion of the form:

$$K''_x = 2K'_x = \ln \cosh(2K_x) , \quad (14.12a)$$

$$K''_y = \frac{1}{2} \ln \cosh(2K'_y) = \frac{1}{2} \ln \cosh(4K_y) . \quad (14.12b)$$

These recursion equations give a fixed point. After two iterations we come back to our starting point so that the fixed points obey:

$$K^*_x = \ln \cosh(2K^*_x) . \quad (14.13a)$$

$$K^*_y = \frac{1}{2} \ln \cosh(4K^*_y) . \quad (14.13b)$$

The fixed couplings are indicated by stars. Notice that the two fixed couplings are different and that they are related by $K^*_x = 2K^*_y$.

Figure 14.3 shows the graphical solution of the recursion relation (14.13a). The fixed point values are $K^*_x = 0.61$, $K^*_y = 0.31$. These fixed points enable one to calculate the critical

index associated with the temperature variable as

$$\left(\frac{\partial K_x''}{\partial K_x} \right)_{K_x=K_x^*} = 2 \tanh 2K_x^* = 2^{x_T}, \quad (14.14)$$

leaving us with the numerical value of x_T which is roughly 0.75. (See homework problem.) This index is known exactly for the two-dimensional Ising model. It has the value $x_T = 1$. The approximate result is far from wonderfully accurate. However, the approximation is very simple. It has the advantage that it can be applied effectively to a wide variety of situations. For example, Eq. (14.13a) can be extended to a situation of a hypercubic lattice in d dimensions giving a recursion relation

$$K' = \ln \cosh(2^{d-1} K). \quad (14.15)$$

14.5 Further Work

There has been a very considerable amount of work using real-space techniques to establish the phase diagram and critical properties of various models. Much of this work is slightly controversial in that it is hard to assess the accuracy of any given real-space calculation. However, the method does provide a quick method for gathering indicative data about even quite complex problems. The interested student might wish to look at some of my own papers in which real space methods and potential moving techniques are developed and analyzed.¹⁰

The most interesting single application of the real space method is to the XY model. See the final chapter of this book.

Homework

Problem 14.1 (Numerics of Migdal's Approximation). Use Migdal's approximation to find critical couplings and x_T values for the Ising model in dimension d .

14.6 Reprints on Real Space RG

¹⁰See LPK: Essays.

14.6.1 Niemeijer and van Leeuwen: Triangular Lattice R.G.

Wilson Theory for Spin Systems on a Triangular Lattice

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(Received 21 September 1973)

A special renormalization transformation is constructed for one-component spin systems on a two-dimensional triangular lattice. Fixed point, eigenvalues, and eigenvectors are determined in various approximations, which converge well to known Ising data.

Most of the specific results of the renormalization approach to critical phenomena have been obtained by the ϵ expansion for continuous spin systems interacting through a Landau-Ginzburg Hamiltonian¹ (with $\epsilon = 4 - d$, and d the dimensionality of the spin lattice). This Letter concerns an application of Wilson's² ideas to a general class of

discrete spin Hamiltonians which comes closer to Kadanoff's¹ original derivation of the scaling laws and which avoids the ϵ expansion (which is presumably asymptotic rather than convergent).

The method is best illustrated³ for a two-dimensional (2D) triangular lattice. In Fig. 1 the lattice is divided into cells (triangles) having an *odd*

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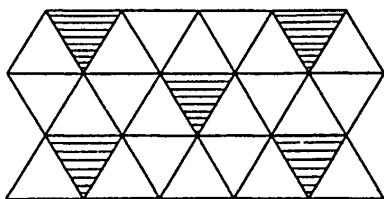


FIG. 1. Triangular lattice with cells shaded.

number (three) of sites such that the lattice of cells is again *triangular*. Other cell divisions are possible but this choice has the additional advantage that the cells are as small as possible (three sites) and that the cells fully occupy the lattice. Each of the N sites i has a spin $s_i = \pm 1$ which interacts through a general Hamiltonian $H(s)$ ($-\beta = -1/k_B T$ included). $H(s)$ is decomposed into its various types of interactions, viz., nearest-neighbor (nn) pair interactions $K_{nn} s_i s_j$, longer-ranged pair interactions, triple-spin interactions $K_{tr} s_i s_j s_k$, etc. Formally we write, where the sum over b runs over all subsets of sites,

$$H(s) = \sum_b K_b s_b, \quad s_b = \prod_{i \in b} s_i. \quad (1a)$$

The strength parameters K_b can be obtained from $H(s)$ as

$$K_b = 2^{-N} \sum_{\{s\}} s_b H(s), \quad (1b)$$

where the sum over $\{s\}$ runs over all possible spin configurations. $H(s)$ is taken to have short-range interactions and to be invariant under the symmetries of the lattice. So the sum in (1) includes no sets with sites far apart, and the K_b of sets b of the same type β (e.g., nearest-neighbor pairs) have the same value K_β .

We associate with a cell i' a spin $s_{i'}$ defined as the signature of the sum over all spins in cell i' :

$$s_{i'} = \text{sgn} \left(\sum_{i \in i'} s_i \right). \quad (2)$$

Since a cell has an odd number of sites, $s_{i'}$ is unambiguously ± 1 . For a given value of $s_{i'}$ there are a number (viz., four) of internal configurations $\sigma_{i'}$ for the spins of cell i' . Thus $H(s)$ can also be written as $H(s', \sigma)$. Then define a renormalization transformation from a site-spin Hamiltonian $H(s)$ to a cell-spin Hamiltonian $H'(s')$ as

$$\sum_{\sigma} \exp H(s', \sigma) \approx \exp H'(s'). \quad (3)$$

Here it should be noted that even if one starts out with only simple interactions (e.g., only nearest-

neighbor interactions) on the site lattice, (3) generates in principle all types of interactions on the cell lattice. The main point of this Letter is to show, by studying various approximations, that (3) exhibits a fixed point with properties to be expected for 2D spin systems. We view (3) as a map of the original interaction constants K_α to renormalized K'_α [belonging to $H'(s')$]:

$$K'_\alpha = K_\alpha'(K). \quad (4)$$

A fixed point is a set of values K_α^* such that $K'_\alpha(K^*) = K_\alpha^*$. The critical properties (exponents) can be expressed in terms of the eigenvalues and eigenvectors of the matrix

$$T_{\alpha\beta} = (\partial K'_\alpha / \partial K_\beta)_{K=K^*}. \quad (5)$$

From the known results for the 2D triangular Ising system, one expects two eigenvalues λ_T and λ_H to be

$$\begin{aligned} \lambda_T &= l = \sqrt{3} = 1.732\ 05, \\ \lambda_H &= l^{15/8} = 3^{15/16} = 2.800\ 92 \end{aligned} \quad (6)$$

(l being the cell spacing measured in units of the site spacing), and all others < 1 in absolute value.

A fixed point is located in the surface of critical systems. The tangent plane in this fixed point is (for vanishing odd interactions) determined by the (left) eigenvector φ_α^T belonging to λ_T . Since the fixed point has no special physical significance, the critical surface will not be anomalous there. We found, in fact, very little curvature around the fixed point. So the tangent plane gives a good measure for the variation of the critical temperature $T_c(J)$ with the (even) interaction constants $J_\alpha = (k_B T) K_\alpha$. One may write the equation for the tangent plane in the form

$$T_c(J) = T_c [1 + \sum_{\alpha=nn} (\varphi_\alpha^T / \varphi_{nn}^T) (J_\alpha / J_{nn})], \quad (7)$$

where T_c is the Ising critical temperature (with only nearest-neighbor interactions present). We used the intercept of the Ising axis ($K_\alpha = 0$ except $\alpha = nn$) with this tangent plane as an estimate for the Ising critical parameter K_c (Table I, third column).

In order to study (3) we must approximate the sum over the internal configurations σ . Most naively one separates $H(s)$ into a piece H^0 containing the intracell interactions and a perturbation V containing the intercell interactions. The results of first-order perturbation theory for λ_T , λ_H , and K_c are listed in the first line of Table I.

A more promising approximation uses the fact that the transformation (3) can be studied in any

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TABLE I. Values of the "thermal" and "magnetic" eigenvalues λ_T and λ_H and the value K_c for an Ising system as deduced from the fixed-point tangent plane.

Approximation	λ_T	λ_H	K_c
1 st order perturbation	1.634	3.036	0.336
cluster	1.544	3.036	0.365
	1.501	2.501	0.255
	1.567	2.497	0.253
	1.782	3.186	0.281
	1.7590	2.8024	0.27416
exact (Ising)	1.73205	2.80092	0.27465

detail on a small system. If c is a (specific) cluster of cells with Hamiltonian $H_c(s)$, we write

$$\sum_{\{\sigma\}} \exp H_c(s', \sigma) = \exp H_c'(s') = \exp \sum_{b \in c} K_b' s_b', \quad (8)$$

TABLE II. Fixed-point values for the interaction parameters K_α^* and components $r_\alpha = \varphi_\alpha^T / \varphi_m^T$ of the left eigenvector belonging to λ_T . Here, as in Eq. (4), α corresponds to the particular geometrical arrangement of interacting spins or cells as shown in Fig. 1.

Approximation												
1 st order part	K_a^*	0.3356	—	—	—	—	—	—	—	—	—	—
cluster	K_a^*	0.365	—	—	—	—	—	—	—	—	—	—
-	K_a^*	0.255	—	—	—	—	—	—	—	—	—	—
-	K_a^*	0.257	-0.0022	—	-0.00065	—	—	—	—	—	—	—
-	K_a^*	0.331	-0.0275	-0.0267	0.0086	0.0080	—	-0.0037	—	—	—	—
-	K_a^*	0.3069	-0.0183	-0.0214	0.0034	0.0066	0.0036	-0.0022	-0.0016	-0.0009	0.0003	0.0004
-	r_α	1	1.205	—	2.990	—	—	—	—	—	—	—
-	r_α	1	1.708	1.917	1.237	5.978	—	2.742	—	—	—	—
-	r_α	1	1.607	1.811	1.248	5.782	1.083	2.808	1.372	3.081	0.452	2.777

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to be important because, e.g., pair interactions are partially compensated at the fixed point by quadruple interactions of the same range.

In Table II we have listed the locus K_α^* of the fixed point in the various approximations together with the left eigenvector $r_\alpha = \varphi_\alpha^T / \varphi_{nn}^T$ belonging to λ_T . From this table one observes which interaction parameters are included and also that among the K_α^* the nearest-neighbor interaction stands out by a factor 15 over the other (negative) pair interactions, which again are a factor 4 larger than the four-spin interactions and many times larger than the six-spin interactions. Although the fixed point shifts notably, a lower approximation could very well be used as a guess for the fixed point of a higher approximation, indicating that the transformation does not develop singularities for larger and larger clusters at the fixed point (which is a basic assumption in the renormalization approach).

In Table I the values for λ_T , λ_H , and K_c are given and compared with the values for a triangular Ising system.⁴ The last approximation (seven cells symmetrically arranged) gives particularly accurate values, in our opinion, not only because it is the largest basic figure but also because its symmetry is the same as that of the lattice. On the basis of these λ_T and λ_H we find, e.g., the

critical exponents

$$\nu = \ln l / \ln \lambda_T = 0.973, \quad (10)$$

$$\delta = \ln \lambda_H / (2 \ln l - \ln \lambda_T) = 15.017,$$

which should be compared with the exact values $\nu = 1$ and $\delta = 15$. The value of r_α may be compared with the coefficients giving the variation of $T_c(J)$ with J around the Ising system ($J_\alpha = 0$, $\alpha \neq nn$) obtained either analytically⁵ or numerically.⁶ Dalton and Wood⁶ find $r_{nn} = 1.35$. Our rather high value of 1.607 could be lowered only a few hundredths by accounting for the curvature of the surface of criticality. One must conclude that longer-range forces than fit in our largest cluster play a role in determining r_α .

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14.6.2 David Nelson's Early Summary

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review article

Recent developments in phase transitions and critical phenomena

David R. Nelson*

Universal dimensionless numbers characterise singularities at the critical point in magnets, binary mixtures and alloys, superfluids, and in a variety of other systems. A desire to understand these numbers has stimulated a significant breakthrough in the analysis of statistical mechanical partition sums. Critical phenomena can now be understood in terms of universality, Hamiltonian flows, and renormalisation group recursion relations.

PHASE changes of matter in thermodynamic equilibrium are often accompanied by sharp discontinuities in quantities such as the magnetisation in a ferromagnet, the density in a liquid-vapour system, or the concentration in a binary mixture. Usually, these phase transitions can be made continuous by adjusting some external parameter such as the temperature. The point at which the discontinuity vanishes is called a critical point. At temperatures above the critical point, the spontaneous magnetisation of a ferromagnet is zero, the liquid and vapour phases of a fluid become indistinguishable, and the chemical species present in a binary fluid mixture are completely miscible. One usually associates the discontinuities below the critical temperature with some sort of broken symmetry¹⁻³.

Although critical points were discovered in the nineteenth century, they have been the focus of particularly intense scientific investigation during the past few decades¹⁻³. A rather precise characterisation of critical point singularities by experiments⁴ and perturbation techniques such as high temperature series expansions⁵ was followed by a detailed theory due to Wilson⁶. In this review, I shall describe Wilson's renormalisation group approach to critical phenomena, and illustrate its utility with examples chosen from the recent literature.

The spontaneous magnetisation and susceptibility of a ferromagnet are plotted schematically in Fig. 1. Below the Curie temperature, a substance such as iron or nickel will support a spontaneous magnetisation $M_0(T)$, which accounts for the well known magnetic properties of these substances. As the temperature is raised, however, the magnetisation drops to zero at T_c , as shown in the figure. The magnetic susceptibility in zero field, $\chi_0(T)$, which is a measure of the response of the magnetisation to a small magnetic field, actually diverges to infinity as one approaches the Curie temperature from above or below.

The extraordinary thing about the anomalies shown in Fig. 1 is that they seem to be universal. That is, a wide variety of ferromagnets displays spontaneous magnetisations which tend to zero and susceptibilities which apparently diverge in precisely the same way. Despite differing chemical compositions, lattice structures, and Curie temperatures, one finds that $M_0(T)$ behaves as

$$M_0(T) \sim |T - T_c|^\beta \quad (1)$$

near T_c , while $\chi_0(T)$ diverges according to

$$\chi_0(T) \sim |T - T_c|^{-\gamma} \quad (2)$$

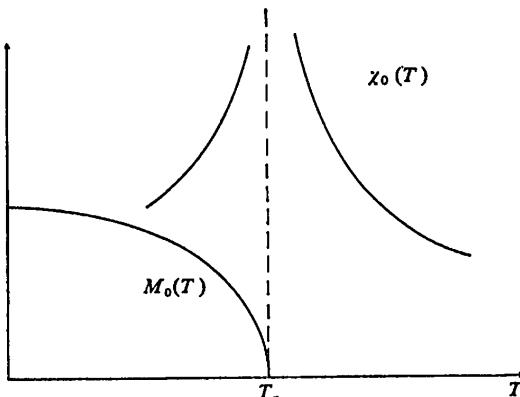
where the critical exponents β and γ are essentially the same for all magnets. A second curious fact is that the universal numbers β and γ are not simply one-half or unity, although most simple theories lead inevitably to these values¹⁻³. In fact, experiments⁴ and evidence from high-temperature series expansions⁵ suggest that β and γ lie in the ranges,

$$0.31 \leq \beta \leq 0.38 \quad 1.25 \leq \gamma \leq 1.38 \quad (3)$$

in most substances. Although equation (3) indicates some variation in the observed values of β and γ , it now seems that magnets with the same symmetry should have precisely the same exponents: that is, if we imagine that a magnetic crystal is described by a lattice of classical spin vectors (see Fig. 2a), there is a weak dependence of critical exponents on the number of spin components n which actively participates in the phase transition. The number of such spin components is related to the symmetry group of the crystal.

The universality of critical phenomena is not limited to ferromagnetism. Analogous quantities to the magnetisation and

Fig. 1 The magnetisation $M_0(T)$ and zero field susceptibility $\chi_0(T)$ of a ferromagnet. The magnetisation goes to zero at the Curie temperature T_c , while $\chi_0(T)$ diverges as this temperature is approached from above or below.



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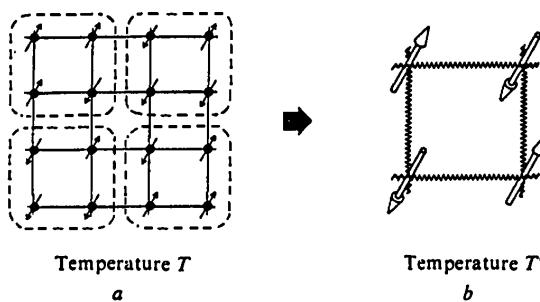


Fig. 2 Kadanoff block scheme. Dashed lines enclose groups of spins on lattice (a), which is at temperature T . Out of each block, we construct a collective spin variable by integrating over the internal degrees of freedom. The new spin degrees of freedom populate a lattice (b) with twice the old lattice spacing, and interact as if they were at temperature T' .

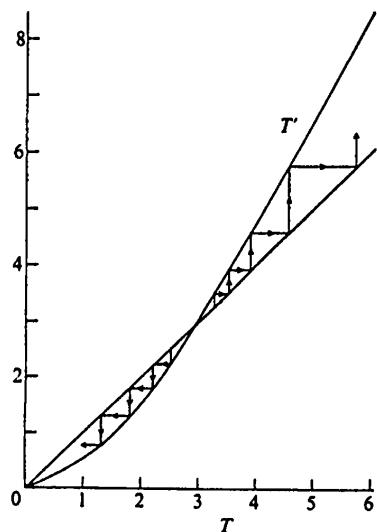
susceptibility exhibit singularities at the critical point of liquid-gas systems, binary mixtures, and alloys, at the λ -transition in superfluid helium, and at the Néel temperature in antiferromagnets¹⁻³. Exponents such as β and γ which characterise the anomalous behaviour are very close to the numbers found for ferromagnets. A variety of other exponents can be defined for systems near a critical point, and they, too, seem to be universal.

The behaviour of a liquid-gas system near its critical point is particularly striking. The fluid suddenly becomes milky and opaque, and scatters laser light intensely in the forward direction. It seems clear that some sort of cooperative phenomenon is taking place, and that the particles of fluid are strongly correlated over distances comparable with the wavelength of the laser light. The correlation length $\xi(T)$ of the fluid, which is a measure of the cooperativity, is expected to diverge strongly at T_c

$$\xi(T) \sim |T - T_c|^{-\nu} \quad (4)$$

The exponent ν is in the range

Fig. 3 Approximate recursion relation for $n = 1$ or Ising spins, with a fixed point at $T^* = T_c = 2.98$. The 'ladder' construction shows successive temperatures produced by repeated iterations of the transformation. The slope of the function $T'(T)$ through its fixed point is related to the critical exponent ν .



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$$0.64 \leq \nu \leq 0.70 \quad (5)$$

in most substances.

Where do the universal exponents β , γ , and ν come from? What is their precise numerical value? Can we account for slight variations, if any, in β , γ , and ν from system to system? A desire to answer these puzzling questions culminated in a major breakthrough in 1971. Wilson's renormalisation group theory of critical phenomena⁴. Building on work by Kadanoff⁷, Wilson showed why the exponents were universal and how to calculate them. In doing so, he placed at the disposal of condensed matter physicists a powerful mathematical tool, the renormalisation group.

Kadanoff blocks and lattice renormalisations

If critical exponents are indeed universal, one might hope to understand them using only a very simple model of magnetism. Consider for concreteness a d -dimensional hypercubical lattice populated with fixed length, classical spin vectors S_i (see Fig. 2). To each configuration $\{S_i\}$ of spins we assign an energy,

$$H[\{S_i\}] = -J \sum_{\langle i,j \rangle} S_i \cdot S_j \quad (6)$$

where i and j label the sites of the lattice, and the sum is restricted to nearest-neighbour pairs of spins. Each spin has n components, where n can be different from d , the dimensionality of space. According to the rules of statistical mechanics, the macroscopic properties of such a system follow from a calculation of the partition function,

$$Z = \frac{\text{Tr}}{\{S_i\}} \exp(-\beta H[\{S_i\}]) \quad (7a)$$

$$= \frac{\text{Tr}}{\{S_i\}} \exp\left(-\frac{1}{T} \sum_{\langle i,j \rangle} S_i \cdot S_j\right) \quad (7b)$$

In passing from (7a) to (7b), we have combined β (not to be confused with a critical exponent!) and the coupling constant J into a dimensionless 'temperature', $T \equiv 1/\beta J$. The trace operation (Tr) means an integration over all spin configurations $\{S_i\}$ consistent with the fixed length requirement, namely

$$|S_i| = 1, \text{ all } i \quad (8)$$

The partition sum (7) can be computed exactly in one dimension for all values of n (ref. 8) but does not exhibit a finite temperature phase transition. Onsager obtained the partition function in two dimensions⁹ for the special case of the Ising model, or $n = 1$. Onsager's work, which remains today a true mathematical *tour de force*, eventually led to the exponent predictions¹⁻³

$$\beta = \frac{1}{8}, \quad \gamma = \frac{7}{4}, \quad \nu = 1 \quad (9)$$

An analytical evaluation of (7) for other values of n and d seems to be a hopeless task.

Rather than attempting to evaluate (7) exactly, we can, in fact, make progress by merely thinning out the spin degrees of freedom slightly. To do this, we follow the original suggestion of Kadanoff⁷ and group the spins on the original lattice (which is at temperature T) into blocks as shown in Fig. 2. With some ingenuity, it turns out to be possible to integrate approximately over the internal degrees of freedom within each block. We are then left with a new statistical mechanical problem with twice the lattice spacing. Provided the interactions between spins in the new lattice are of the same form as in the old, couplings in the new lattice can be characterised simply by a new temperature T' .

This sort of program was first carried successfully for Ising ($n = 1$) spins on a triangular lattice by Niemeyer and van Leeuwen¹⁰. A very primitive version of their transformation gives a relationship between the new and old temperatures, namely¹⁰

$$T' = \frac{1}{2} T (e^{3/T} + 3e^{-1/T})^2 / (e^{3/T} + e^{-1/T})^2 \quad (10)$$

Equation (10) is depicted graphically in Fig. 3, together with a

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'ladder' construction which shows how the temperature changes with repeated iterations of the transformation. The recursion formula (10) has a fixed point at $T^* \approx 2.98$, and it seems natural to identify this isolated point with the Curie temperature T_c of the spin system.

We can see the utility of this procedure of 'thinning out' spins as follows: even an approximate calculation of partition function (7) is difficult near T_c because of the large correlation length $\xi(T)$ in this region. Note from Fig. 3, however, that the renormalisation transformation increase temperatures which, initially, are slightly above T_c . By repeatedly applying the transformation (10), we can relate a difficult calculation near T_c to a more tractable high temperature problem. A very accurate calculation of the partition sum (7) is possible at high temperatures by expanding in powers of $1/T$. No information about Z is lost during the thinning out procedure, because there is a very precise relationship between the partition function calculated at temperature T , and the corresponding quantity calculated at temperature T' (refs 6 and 10-12). In a similar fashion, we see that the transformation (10) decreases temperatures initially slightly below T_c , and eventually produces a more manageable (low temperature) problem.

As emphasised by Wilson¹⁴, the physics behind a renormalisation transformation is in the reduction of the correlation length. If the lattice spacing is changed by a factor b by the thinning out process, it follows the correlation length transforms according to¹⁴

$$\xi(T') = \xi(T)/b \quad (11)$$

For the square lattice spin system shown in Fig. 2, $b = 2$, while for the triangular lattice of Niemeyer and van Leeuwen (it turns out that)¹⁰ $b = \sqrt{3}$. Equation (11) can be used in conjunction with (10) to produce a critical exponent. Near the fixed point $T^* = T_c = 2.98$, equation (10) can be written in the approximate form,

$$T - T_c = b^{0.89} (T - T_c) \quad (12)$$

which when combined with (11) gives a functional equation for $\xi(T - T_c)$,

$$\xi(T - T_c) = b \xi[b^{0.89} (T - T_c)] \quad (13)$$

It is easy to check that the solution of this functional equation is $\xi(T) \sim |T - T_c|^{-\nu}$ with $\nu \approx 1.12$, which is not too different from the exact result $\nu = 1.0$.

In more sophisticated calculations^{10,15-18}, it is not possible to describe a renormalisation transformation in terms of a single coupling constant. More complicated couplings such as next-nearest-neighbour and multispin interactions are generated after one iteration. When these extra couplings are taken into account^{10,15-18}, they not only produce more accurate estimates of critical exponents, but also provide a qualitative explanation of universality: if several couplings are included in the calculation, the renormalisation transformation can be viewed as a mapping of one Hamiltonian to another in a multidimensional coupling-constant space. As T is adjusted towards T_c , it turns out that any initial set of couplings 'flows' toward a unique fixed point under repeated applications of the transformation. Just as in the one-interaction-constant example, critical exponents are related to eigenvalues of the transformation about this fixed point. We are led to the conclusion that the exponents are independent of the precise values of the initial couplings, and depend instead on the 'universal' properties of the fixed point.

Calculations by the Kadanoff block method for Ising spins have now become quite refined. Niemeyer and Van Leeuwen¹⁰ presented a series of cluster approximations to an exact transformation which seems to converge to the exact results of Onsager. Wilson¹⁵ carried out renormalisations on a square lattice keeping track of 217 different interaction constants, and obtained critical exponents accurate to better than 1%. Kadanoff has proposed a variational principle^{17,18} which, when coupled with a simple block

spin transformation, gives exponents accurate to 0.1% in two dimensions, and results competitive with high temperature series expansions in three dimensions!

Despite some initial success, this field is still in its infancy. The principal achievement of the block spin analysis so far (beyond providing an intuitive understanding of universality) has been to reproduce the results of Onsager and high temperature series expansions. Nevertheless, lattice renormalisation groups may eventually become a powerful computational tool, similar to various methods used to evaluate integrals numerically in ordinary calculus. The partition sum (7) can be viewed as a complicated functional integral which until now could only be computed in a few fortuitous cases. Renormalisation theory suggests that such sums can be evaluated routinely and very accurately at any temperature, without relying on a mathematical *tour de force* such as Onsager's solution⁹ of the two-dimensional Ising model.

Continuation in dimensionality

Wilson has characterised developments in the theory of critical phenomena as a "search for analyticity". The idea is to find a mathematical framework in which critical point singularities are described by smooth, analytic functions. Landau¹⁹ proposed that critical phenomena could be understood in terms of an analytic expansion of the free energy in powers of a local magnetisation variable. Although Landau's theory has led to a qualitative understanding of a wide variety of critical points, the exponent predictions disagree with experiments¹⁻³.

The proposal that critical points can be understood in terms of analytical recursion relations⁶ seems to be the correct modification of Landau's theory. The method of construction ('thinning out' degrees of freedom) virtually guarantees that the recursion relations will be analytic at finite temperatures. Wegner¹⁹ has shown that a wide variety of critical point singularities follow from the analyticity of recursion relations about a fixed point.

Perhaps the most useful analyticity property of recursion relations is that they are remarkably easy to continue in dimensionality. The original continuation of Wilson and Fisher into $4-\varepsilon$ dimensions (Landau's theory turns out to be correct above $d = 4$) led to quantitatively accurate estimates of exponents in three dimensions, and to a detailed understanding of a wide variety of complicated critical point phenomena. The formulas for β and γ as a function of n and d ($d < 4$) are^{21,22}

$$\beta = \frac{1}{2} - \frac{3}{2(n+8)}(4-d) + \frac{(n+2)(2n+1)}{2(n+8)^3}(4-d)^2 + \dots \quad (14a)$$

$$\gamma = 1 + \frac{n+2}{2(n+8)}(4-d) + \frac{(n+2)(n^2+22n+52)}{4(n+8)^3}(4-d)^2 + \dots \quad (14b)$$

Although expansions like these in $\varepsilon = 4-d$ (and, to a lesser degree, expansions in $1/n$)²³⁻²⁵ probably represent the most powerful and versatile application of Wilson's theory, this work has been extensively reviewed elsewhere^{14,26-28}. We shall turn instead to more recent investigations of critical points in $2+\varepsilon$ dimensions.

Critical phenomena in $(2+\varepsilon)$ dimensions

To a first approximation, the action of a renormalisation group on a Hamiltonian can be compared with the motion of a ball rolling down a hill⁶. One assumes that the differential change in temperature $dT \equiv T' - T$ associated with a block spin transformation that changes the lattice spacing by a factor $d \equiv db/b$ is described by a potential function $V(T)$ (ref. 6)

$$\frac{dT(l)}{dl} = - \frac{dV[T(l)]}{dT(l)} \quad (15)$$

Here, dl is an infinitesimal change in the logarithm of the Kadanoff block size, and $T = T(l)$ is the effective temperature produced by

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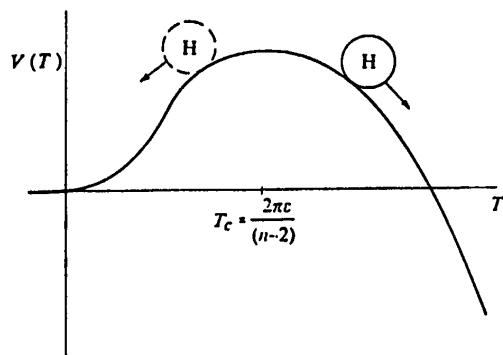


Fig. 4 Potential function $V(T)$ for fixed length spins in $2 + \epsilon$ dimensions, with ϵ small and $n \geq 3$. Hamiltonians initially to the right of T_c 'roll' toward higher temperatures, while systems with temperatures less than T_c roll toward a zero temperature fixed point.

blocks of size $b = e^l$. Although a differential change in the block size is hard to visualise, it turns out to be fairly easy to effect this transformation mathematically.

Recent studies of the fixed length spin Hamiltonian (7) near two dimensions²⁹⁻³⁴ provide a particularly simple realisation of these ideas. The potential $V(T)$ has now been calculated by using a low-temperature spin-wave theory, with the result^{29,31}

$$V(T) = \frac{1}{2}(d-2)T^2 - \frac{n-2}{6\pi}T^3 + \dots \quad (16)$$

As shown in Fig. 4, Hamiltonians at temperatures initially to the right of the crest in this potential roll toward high temperatures, while Hamiltonians at lower temperatures roll toward the minimum at $T = 0$. There is no oscillatory motion about this minimum because the 'equation of motion' (15) contains only one derivative in the time-like parameter, t .

This is precisely the behaviour we found using the discrete recursion formula (10), and it is natural to associate the crest of the potential hill with the critical temperature,

$$T_c = 2\pi(d-2)/(n-2) \quad (17)$$

In contrast to the $n = 1$ or Ising model, T_c tends to zero as d approaches two from above for $n \geq 3$. Linearisation of the equation (15) about the maximum in the potential leads to the correlation length exponent prediction²⁹⁻³¹

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$$\nu = \frac{1}{(d-2)}[1 + O(\epsilon)] \quad (18)$$

Higher order corrections to this result are determined in ref. 31.

Note that for the interesting case of an XY model ($n = 2$) in precisely two dimensions, the potential (16) is perfectly flat. This result (which holds to all orders in T) suggests that such a system would exhibit a line of critical points with continuously variable critical exponents³⁵⁻³⁶. Work by Berezinskii³⁷ and by Kosterlitz and Thouless^{38,39} gives convincing evidence that this line actually ends at some finite temperature. Renormalisation group flow patterns for the XY model obtained using a more sophisticated theory by Kosterlitz³⁹ and later by José *et al.*⁴⁰ are plotted in Fig. 5, which shows the motion of the temperature coupling $T(t)$ together with the motion of a new parameter $y(t)$, which gives the probability of a vortex pair excitation in the system. These flows suggest that vortices become unimportant at low temperatures, so that spin-wave theory (which neglects vortices) should be qualitatively correct in region I. The instability in the flows in regions II and III, however, suggests a finite temperature transition into a phase not describable by spin-wave theory. It is possible that this bizarre phase transition may actually be observable in superfluid ${}^4\text{He}$ films.

Concluding remarks

We have seen that the renormalisation group is a rather powerful and sophisticated tool for understanding the behaviour of matter near a critical point. Much of the progress in this area resulted from a rather fertile interaction of statistical mechanics with quantum field theory, where the renormalisation group was first developed⁴¹. Renormalisation groups constructed for problems in statistical mechanics may eventually be of some use in understanding certain lattice quantum field theories⁴².

Modern renormalisation theory may also be useful in other areas of condensed matter physics. Anderson⁴³ and Wilson¹⁸ have applied renormalisation group ideas to the Kondo problem, while Licciardello and Thouless⁴⁴ and Wegner⁴⁵ have used these techniques to study localisation in metals. Equilibrium time-dependent critical phenomena have been successfully treated⁴⁶ using Wilson's ideas, and there is now some effort to extend these techniques to non-equilibrium problems. One might hope that they would be of some utility in understanding, for example, properties of turbulent fluids at high Reynold's number.

Much of my understanding of static critical phenomena is the result of stimulating interactions with Michael Fisher, Kenneth Wilson, and Leo Kadanoff.

This research was supported in part by the National Science Foundation.

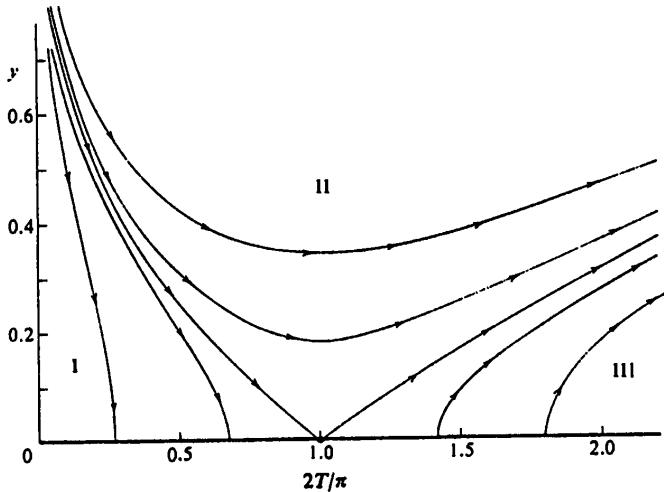


Fig. 5 Hamiltonian flows for the two-dimensional XY model. The flowlines show the motion of the coupling constants T and y under repeated iterations of a renormalisation group transformation. The parameter y measures the probability of exciting a vortex pair in the system. The flowlines are both attracted and repelled by a line of fixed points at $y = 0$. Two separating trajectories divide the plane of possible Hamiltonians into three distinct regions. Vortices are unimportant to the critical properties in region I, but become increasingly important in regions II and III.

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14.6.3 Kadanoff: Bond-moving, and a Variational Method

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Variational Principles and Approximate Renormalization Group Calculations*

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Approximate recursion relations which give upper and lower bounds on the free energy are described. "Optimal" calculations of the free energy can then be obtained by treating parameters within the renormalization equations variationally. As an example, simple lower-bound relations are defined for the two- and three-dimensional Ising models. At the fixed point, a parameter is set variationally, and then critical indices are calculated.

Several recent papers¹ have followed up on the pioneering work of Wilson² in using the renormalization group to perform approximate calculations of the free energy. In general, the problem is to calculate a free energy $F_N(\bar{K})$ for a system with N degrees of freedom and a set of coupling constants \bar{K} , starting from a Hamiltonian $\mathcal{H}_{\bar{K}}(\sigma)$, in which the σ represents some set of statistical variables.³ A renormalization transformation $\bar{K}' = R(\bar{K})$ defines a new set of coupling parameters as a function of the old parameters.

The \bar{K}' defines couplings in a system with fewer degrees of freedom, $N' < N$, described by a new set of variables which we call μ . The special property of this transformation is that it leaves the total free energy invariant, i.e.,

$$F_N(\bar{K}) = F_{N'}(R(\bar{K})). \quad (1)$$

To realize such a transformation, define $F_N(\bar{K}) = -\ln \text{Tr}_\sigma \exp[-\beta \mathcal{H}_{\bar{K}}(\sigma)]$ and construct a new Hamiltonian as

$$\mathcal{H}'(\mu) = -\ln \text{Tr}_\sigma \exp[S(\mu, \sigma) - \mathcal{H}_{\bar{K}}(\sigma)]. \quad (2)$$

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If $S(\mu, \sigma)$ obeys the restriction $\text{Tr}_\mu \exp S(\mu, \sigma) = 1$, then \mathcal{K}' and $\mathcal{K}_{\bar{K}}$ have exactly the same free energy. If the set of parameters \bar{K} is sufficiently inclusive so that all conceivable Hamiltonians which obey a given symmetry⁴ can be represented as $\mathcal{K}_{\bar{K}}(\sigma)$, and if in addition $S(\mu, \sigma)$ obeys this symmetry, then $\mathcal{K}'(\mu)$ must also be expressible as $\mathcal{K}_{\bar{K}'}(\mu)$ for some value of \bar{K}' . In this way, one realizes the renormalization group mappings.

A most important part of the Hamiltonian $\mathcal{K}_{\bar{K}}(\sigma)$ is a constant term, which I define to be $-NK_0$. In the evaluation of the free energy, one visualizes an infinite number of renormalizations

$$\bar{K}^\alpha = R(\bar{K}^{\alpha-1}), \quad \bar{K}^0 = \bar{K}. \quad (3)$$

After many renormalizations, the trivial term K_0^α will grow in magnitude, and, dominating all else, will provide an evaluation of the free energy as

$$F_N(\bar{K}) = -\lim_{\alpha \rightarrow \infty} N_\alpha K_0^\alpha. \quad (4)$$

Thus, if R is known, F can be computed.^{1,2}

But R is not known. Instead, I seek a prescription for constructing upper and lower "bounding" approximations to R denoted as R^U and R^L , which respectively have the properties

$$F_N(R^U(\bar{K})) \geq F_N(R(\bar{K})) \geq F_N(R^L(\bar{K})). \quad (5)$$

Note that if one uses upper (lower) boundary recursion relations in the sequence of calculations described by Eqs. (3), the resulting limit (4) will be an upper (lower) bound to the true free energy. Furthermore, any parameters in R^U or R^L (including parameters in S) can be varied so as to obtain optimum bounds on $F_N(\bar{K})$.

The standard variational principles in statistical mechanics⁵ define appropriate R^U and R^L . Define a variational function $H_0(\mu, \sigma)$ which includes the basic symmetries and obeys $\text{Tr}_\sigma \times \exp H_0(\mu, \sigma) = 1$. Then notice that⁶

$$\begin{aligned} \mathcal{K}^U(\mu) &= -\text{Tr}_\sigma \exp[H_0(\mu, \sigma)] \\ &\times [S(\mu, \sigma) - \mathcal{K}_{\bar{K}}(\sigma) - \mathcal{K}_0(\mu, \sigma)] \end{aligned} \quad (6)$$

must equal or exceed $\mathcal{K}'(\mu)$ for all values of μ —if \bar{K} and S are held fixed. When \mathcal{K}^U is parameterized in terms of \bar{K}' , Eq. (6) generates a recursion $\bar{K}' = R^U(\bar{K})$, which certainly obeys Eq. (5). Similarly define

$$\begin{aligned} \mathcal{K}^L(\mu) &= -\ln \text{Tr}_\sigma \\ &\times \exp[S(\mu, \sigma) - \mathcal{K}_{\bar{K}}(\sigma) + V(\mu, \sigma)]. \end{aligned} \quad (7)$$

If we demand that $V(\mu, \sigma)$ is a sum of terms which

are each odd under a lattice symmetry operation and that \mathcal{K}^L obeys all the symmetries, then $\mathcal{K}^L(\mu) \leq \mathcal{K}'(\mu)$ for all values of μ . (This statement is easily proved.⁷) We can then once more parameterize in terms of \bar{K}' and say that Eq. (7) generates a recursion relation $\bar{K}' = R^L(\bar{K})$ which obeys Eq. (5).

It is relatively easy to see how to derive upper bounds via Eq. (6). The transforms used in Kadanoff and Houghton³ can easily be modified to fit into the form (6). It is harder to see that the form (7) is also usable. To write an odd representation of V , take $V(\mu, \sigma) = V_1(\sigma) + V_2(\mu)$. Define a set of functions $s_{i,j}(\sigma)$ in which the index i defines different kinds of terms—e.g., nearest-neighbor products or products of four spins in a square. Then j is essentially a position variable which distinguishes among different—but equivalent—terms. Now a suitable V_1 can be written as

$$V_1(\sigma) + \sum_{i,j} v_1(i, j) s_{i,j}(\sigma), \quad (8)$$

with $\sum_{i,j} v_1(i, j) = 0$. Also, V_2 can be written in exactly the same form.

Notice that in Eq. (7) $V_1(\sigma)$ is added to $\mathcal{K}_{\bar{K}}(\sigma)$. Then we may say that V_1 changes $\mathcal{K}_{\bar{K}}$ by moving⁸ equivalent interaction bonds to different portions of the lattice. A suitable choice of V_1 will break the bonds which connect spins in different regions of the lattice. Then the entire sum in Eq. (7) factorizes into a product of independent terms which each can be summed exactly.

Once the sum is calculated, in general $\mathcal{K}^L(\mu)$ will not obey the lattice symmetries. But since $V_2(\mu)$ is antisymmetric, a suitable choice of V_2 can always be found which will force $\mathcal{K}^L(\mu)$ to obey the symmetries. This $\mathcal{K}^L(\mu)$ is then used to calculate the new couplings $\bar{K}' = R^L(\bar{K})$.

For illustrative purposes, in this paper I carry through a simple example of this calculation on the square lattice as shown in Fig. 1. Within each square, I can define spin operators, s_0 , s_1 , s_{nn} , s_{nnn} , s_3 , and s_4 . Here s_0 is 1; s_1 , s_3 , and s_4 are respectively the sums of all possible products of 1, 3, and 4 spins in the square; while s_{nn} and s_{nnn} are respectively sums of products of all nearest-neighbor and next-nearest-neighbor pairs of spins. I write

$$\mathcal{K}_{\bar{K}} = - \sum_{\text{square } i} \sum_j K_i s_i. \quad (9)$$

Every fourth square contains a new spin $-\mu$. I call these red squares. I choose (see Kadanoff and Houghton³) an S which depends upon a varia-

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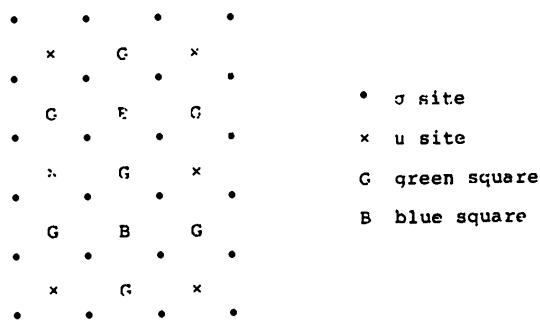


FIG. 1. Recursion setup on the $d=2$ lattice. The "red squares" are those with μ sites at their centers.

tional parameter, p :

$$S(\mu, \sigma) = \sum_{\text{red squares}} (\mu s_i - \sum_i u_i s_i). \quad (10)$$

Here, the u 's are functions of p chosen so that $\sum_i u_i s_i = \ln(2 \cosh p s_i)$. Then, these terms in S insure that the sum over μ of e^s is exactly 1 so that the transformation preserves the value of F . Moreover, when p is well chosen, these terms will tend to subtract away some of the strongest terms in K_R , leaving a weaker and more tractable interaction.

However, some interactions must still be moved in order to make the sum in Eq. (7) tractable. To eliminate all the interaction terms in the red and green squares, choose

$$v_1(i, j) = \begin{cases} -K_i + u_i & \text{in red squares,} \\ -K_i & \text{in the green,} \\ 3K_i - u_i & \text{in the blue.} \end{cases} \quad (11)$$

Since all interactions now lie in the blue squares, the sum (7) can be split into a product of sums over blue squares. Each such sum contains only sixteen terms and can easily be calculated on the computer. These partial sums produce new cou-

plings of up to four spins of exactly the form (9). [Since the resulting $K^L(\mu)$ obeys the lattice symmetries, $V_2(\mu)$ is zero.] Therefore, by calculating some rather simple sums, I have found a lower-bound recursion relation.

Exactly the same approach may be applied to the simple cubic lattice. If the lattice sites are $r = j, k, l$, the red cubes are centered at $r = 2(j, k, l) + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ and the blue at $r = 2(j, k, l) - (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. Here there are 22 basic interactions within the cube instead of the six which occur in the square. Everything else is the same as for $d = 2$.

I use the approximate recursion relation to discuss critical behavior by considering the neighborhood of the fixed point. For each p , there is a fixed point $\bar{K}^*(p)$ defined by $\bar{K}^*(p) = R_p^{-L}(\bar{K}^*(p))$. To fix p , I use the condition that the best p should make the free energy an extremum for fixed \bar{K} . In particular, I write the recursion relations

$$\bar{K}^\alpha = [R_{p+\Delta p}^{-L}]^\alpha(K^*(p)).$$

In general $K_0^\alpha - K_0(p)$ will grow as $2^{d\alpha} g(p) \Delta p$ for large α and small Δp . (See Wegner's¹ eigenvalue analysis of deviations from criticality.) The extremum condition for the approximation is that $g(p) = 0$. In two dimensions this is satisfied at $p = p^* = 0.76$.

Now fix p at p^* . Calculate the remaining eigenvalues of the approximate recursion relation. Use the standard^{1,2} formulas to calculate the critical indices δ and α from these eigenvalues. The resulting calculated indices are shown in Table I. In the three-dimensional case, the errors in my estimated indices are totally unknown. In two dimensions, I have achieved comparable accuracy with previous work³ by using a recursion calculation which is very much simpler than that used heretofore.

The procedure outlined in this paper gives better numerical results than one might have expected *a priori*. Why? I am not sure. To investigate this point further, I have applied the varia-

TABLE I. Calculated values of critical indices. The exact values come from the Onsager solution of the two-dimensional Ising model.

Parameter	$d=2$		$d=3$	
	Calculated value	Exact value	Calculated value	"Accepted" value
δ	15.04	15.0	4.818	5.0 ± 0.2
$2-\alpha$	1.998	2.0	1.887	1.875

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tional technique of this paper to the Gaussian model, using the same recursion method as used by Bell and Wilson.¹⁰ For the Gaussian model, the present method gives a \bar{K}^* which agrees exactly with the critical coupling strengths and gives precisely the right critical indices for all values of dimensionality. Further study will be required to establish why the errors of this procedure are so unexpectedly small.

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²K. G. Wilson, Phys. Rev. B **9**, 3174, 3184 (1971). A review on the renormalization method appears in K. G. Wilson and J. Kogut, to be published.

³The notation in this paper follows reasonably closely upon L. Kadanoff, in *Proceedings of the Cargèse Summer School on Field Theory and Critical Phenomena, 1973*, edited by E. Brézin and J. Charap (Gordon and

Breach, New York, to be published) and also L. Kadanoff and A. Houghton, Phys. Rev. B **11**, 377 (1975).

⁴The symmetries actually considered in this paper are translational invariance plus the point group of the square or cube.

⁵R. P. Feynman, *Statistical Mechanics: A Set of Lectures*. Richard P. Feynman, edited by D. Pines (Benjamin, Reading, Mass., 1972), pp. 66–71.

⁶This equation and others assume that all the variables commute. A generalization to noncommuting cases is easily obtained (see Ref. 5).

⁷Proof that $\mathcal{K}^L(\mu) \leq \mathcal{K}'(\mu)$: Let $\mathcal{K}^L(\mu)$ obey the lattice symmetries and be defined by Eq. (7), in which $V(\mu, \sigma)$ is odd under these symmetries. Then the standard methods (Ref. 5) suffice to prove that

$$\text{Tr}_\mu X(\mu) e^{-X^L(\mu)} \geq \text{Tr}_\mu X(\mu) e^{-X'(\mu)}$$

for any positive semidefinite $X(\mu)$ which obeys the lattice symmetries. Choose $X(\mu)$ to be projection operator onto all configurations of the μ lattice which are equivalent to μ under the symmetry operations. The desired result then follows.

⁸Such motion was actually used by Kadanoff and Houghton (Ref. 3) to get rid of some “hard” terms.

⁹K. Wilson, private communication; Th. Neimeijer and J. M. J. van Leeuwen, Phys. Rev. Lett. **31**, 1412 (1973), and *Physica (Utrecht)* **71**, 1974; M. Nauenberg and B. Nienhuis, Ref. 1; Kadanoff and Houghton, Ref. 3.

¹⁰T. L. Bell and K. G. Wilson, to be published.

14.6.4 Kadanoff: Migdal's Simple and Versatile Method

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Notes on Migdal's Recursion Formulas*

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A set of renormalization group recursion formulas which were proposed by Migdal are rederived, reinterpreted, and critically analyzed. The new derivation shows the connection between these formulas and previous work on renormalization via decimation and block transformations. The new interpretation which arises from these derivations indicates that Migdal's formulas are best understood as referring to systems in which the couplings are anisotropic. A strong indication of the correctness of this reinterpretation comes from the two-dimensional Ising model: The new interpretation gives an exact (!) expression for the critical couplings in this case for all ratios of J_x to J_y . This paper describes the major failings of this approximation which arise from its source as a decimation approximation, in terms of the well-known inadequacy of the fixed points which result from this type of scheme. Some proposals for improvement of the approximation are described. Finally, a new potential-moving scheme is proposed which is used to show that the Migdal approximation is exact when the potentials are strong and ferromagnetic in sign.

I. INTRODUCTION

The renormalization group recursion formulas proposed by Migdal [1, 2] are a very important new contribution to the calculation of near-critical properties in many-particle systems. These formulas are important because

1. They can be applied to systems with all kinds of internal symmetries, including local "gauge" symmetries [3-5].
2. They can be analytically continued in dimensionality (d) with relative ease, and are apparently asymptotically exact
 - a. As $d \rightarrow 1$ for all systems
 - b. As $d \rightarrow 2$ for systems with a set of local internal symmetries (gauge symmetries)

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3. They become exact in the limits of both weak coupling and strong.
4. Because they decouple the different directions of coupling, they hold the promise of being an effective starting point for highly anisotropic problems, including especially those in which one of the axes of the coordinate system is time.
5. Their region of qualitative accuracy apparently includes dimensionalities near those at which the phase transitions first begins to appear. Hence, they offer the possibility of attacking “strong-coupling” phase transitions as, for example, the Heisenberg model at dimensionality $2 + \epsilon$.
6. These approximations apparently include some of the dual symmetries first introduced by Kramers and Wannier [6] and later extended by Wegner [7]. For this reason, they give an exact (!) determination of the critical point of the two-dimensional Ising model. This duality is not really present in Migdal’s interpretation of his formulas, but the reinterpretation of his work given here does agree with this symmetry principle.

The remainder of this section is devoted to defining the notation for the description of the recursion calculations. The next section describes two methods for treating the exactly soluble problems of $d = 1$ systems with ordinary (global) symmetries and $d = 2$ systems with gauge (local) symmetries. The first method is analogous to decimations [8–10], the second to the “block transformations” which has also been very extensively employed in renormalization group work [11–17].

Then, Section III uses these calculations as bases for the rederivation and reinterpretation of Migdal’s formulas. Numerical results are also given in this chapter. From the decimation interpretation, we argue that there is an essential defect in the method, that it is—in some sense—limited to situations in which the critical index, β , is zero. However, the block transformation interpretation permits us to recover a useful formulation of the theory for all cases—except that of the Ising model, where the $\beta = 0$ restriction still seems to be implicit in the method.

Section IV describes a new potential-moving method based upon the group theoretic generalization of the Fourier transform of the exponential of the coupling. This new version of potential-moving gives, once again, the same Migdal-style results as derived in Section III. The new derivation shows that these results are accurate when the potential is very strong.

A. Notation for Description of Renormalizations

Start from a Hamiltonian $H_{\mathbf{K}}(\sigma)$, which depends upon statistical variables σ and a set of coupling constants \mathbf{K} . If Tr_{σ} represents a sum over states, then this Hamiltonian defines a free energy

$$F(\mathbf{K}) = F[H] = -\ln \text{Tr}_{\sigma} e^{-H_{\mathbf{K}}(\sigma)} \quad (1.1)$$

A renormalization transform defines a new Hamiltonian, $H'(\mu)$, depending upon a new set of variables μ according to

$$e^{-H'(\mu)} = \text{Tr}_\sigma e^{T(\mu, \sigma) - H(\sigma)}. \quad (1.2)$$

When the transformation function $T(\mu, \sigma)$ obeys

$$\text{Tr}_\mu e^{T(\mu, \sigma)} = 1. \quad (1.3)$$

Then the transformation leaves the free energy unchanged:

$$F[H'] = F[H] \quad (1.4)$$

The transformation (1.2) is formally expressed as

$$H' = R_T[H] \quad (1.5)$$

since the new Hamiltonian depends upon the old one and upon the transformation function. Alternatively, we can say that $H'(\mu)$ also can be written in terms of new coupling constants K' as $H_{K'}(\mu)$. Then (1.5) can be re-expressed as a relationship between new couplings and old, which depends upon the parameters, p , appearing in $T(\mu, \sigma)$ as

$$K' = R_p(K) \quad (1.6)$$

B. Global Symmetries

Each σ -variable can be labeled by a space index r and an internal index i :

$$\sigma = \{\sigma_i(r)\}. \quad (1.7)$$

In most cases, $H(\sigma)$ is invariant under a set of symmetry operations $\sigma \rightarrow \sigma'$ with

$$\sigma'_i(r) = \sum_j G_{ij}^\alpha \sigma_j(r). \quad (1.8)$$

Here α labels the different elements of the internal symmetry group G_{ij}^α is some matrix (or perhaps Abelian) representation of the group. Equation (1.8) holds for all values of r with the same coefficients G_{ij}^α . The global symmetry is the statement $H(\sigma') = H(\sigma)$.

Thus, for example, the two-dimensional rotation symmetry of the xy model is realized via a two-component $\sigma_i(r)$ and a representation of rotation through the angle α via

$$G_{ij}^\alpha = \begin{pmatrix} \cos \alpha & \sin \alpha \\ -\sin \alpha & \cos \alpha \end{pmatrix}. \quad (1.9)$$

For the symmetry to be realized in the free energy, the sum Tr_σ must also be invariant under the symmetry operations. Of course, this trace is a product of sums over individual spins

$$\text{Tr}_\sigma = \prod_r \text{tr}_{\sigma(r)}. \quad (1.10)$$

We define a “simple” representation of the symmetry to be one in which the sum over the individual spins at each site is just a sum over the results of the basic group operations. In this case, for any function f of the spin $\sigma(r)$, we have

$$\text{tr}_{\sigma(r)} f(\sigma(r)) = \sum_\alpha f(G^\alpha \sigma(r)). \quad (1.11)$$

(In more standard language, Eq. (1.11) is described by saying that the symmetry group has a transitive action upon the variables, σ .) Thus, in the particular case defined by Eq. (1.9), the simple representation of the $X-Y$ symmetry gives an integration over angles, α , at each point in the lattice. In this representation, the magnitude of each $\sigma_i(r)$ is fixed at, say, the value 1. In the most common compound representation, we integrate over magnitudes as well as angles.

The simplicity implies that there is no way of forming any scalar (save unity) from a spin variable at a single point in space. Of course, one can form a scalar from variables at two different spacial positions. If the most general form of such a scalar function is written $K(\sigma(r), \sigma(r'))$, then one can represent nearest-neighbor interactions by writing the Hamiltonian

$$H(\sigma) = - \sum_{\langle rr' \rangle} K_l(\sigma(r), \sigma(r')). \quad (1.12)$$

Here the angular brackets indicate (as usual) a nearest-neighbor sum while the subscript l distinguishes among different directions of the nearest-neighbor bond, K . Consequently we can have all the couplings in the $l = x, y, z, \dots$ directions be different.

C. Local (Gauge) Symmetries

A considerable body of recent work [18–22] has been focused upon systems with a much richer group of symmetries: the “gauge” systems in which there is an independent symmetry operation for every lattice point. In these systems, it is convenient to define the basic spin variables to lie between (for example) nearest-neighbor lattice sites (see Fig. 1), and to carry two internal indices i and j . Thus, we write these variables as $\sigma_{ij}(r, r')$. The Hamiltonian $H(\sigma)$ is taken to be invariant under a simultaneous symmetry transform at all points in the lattice. Now, however, the transformation may differ from point to point. In particular, the symmetry operation is $\sigma \rightarrow \sigma'$ with

$$\sigma'_{ij}(r, r') = \sum_{mn} (G^{\alpha(r)})_{im} (G^{\alpha(r')})_{jn}^* \sigma_{mn}(r, r'). \quad (1.13)$$

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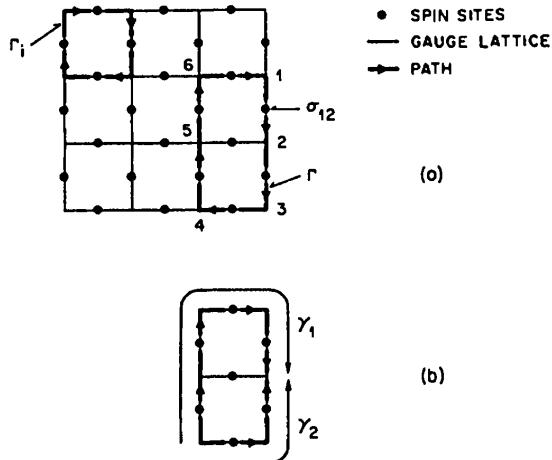


FIG. 1. Paths on a two-dimensional lattice.

The significant new feature is that the symmetry operation, G^α , varies from point to point in space, i.e., $\alpha = \alpha(r)$. For simplicity, we choose a unitary representation of the symmetry, and take

$$(G^\alpha)^\dagger = (G^\alpha)^{-1}. \quad (1.14)$$

Hence Eq. (1.13) can be abbreviated as

$$\sigma'(r, r') = G^{\alpha(r)} \sigma(r, r') [G^{\alpha(r')}]^{-1}. \quad (1.15)$$

To construct a Hamiltonian which obeys $H(\sigma') = H(\sigma)$, we must construct scalars. The conventional technique for this construction is to draw a closed path through the lattice as in Fig. 1. This path, Γ , goes from 1 to 2 to 3... to n and back to 1. Then σ_Γ is defined as

$$\sigma_\Gamma = \sigma(r_1, r_2) \sigma(r_2, r_3) \cdots \sigma(r_{n-1}, r_n) \sigma(r_n, r_1). \quad (1.16)$$

Here matrix multiplication is understood. Note that the traces of powers of the σ_Γ 's are scalars under the operation (1.15). Consequently, the most general gauge-invariant Hamiltonian is a function of these traces, i.e.,

$$-H(\sigma) = \sum_{\Gamma} K(\sigma_\Gamma). \quad (1.17)$$

To get the simplest starting Hamiltonian, we specialize once more to a particular "simple" representation of the symmetry. In this representation, the matrix $\sigma_{tt}(r, r')$ obeys Eq. (1.11) and

$$\sigma(r, r') = [\sigma(r', r)]^{-1} = [\sigma(r', r)]^\dagger.$$

Then, there is no nontrivial scalar which can be formed from one or two spins. Instead, the first invariant is formed from three spins as $(\sigma_1(r_1 r_2) \sigma(r_2 r_3) \sigma(r_3 r_1))$. However, this term cannot exist on a simple hypercubic lattice. On this lattice, the first invariant is formed from four spins arranged in a square—as indicated in Fig. 1. This square is the basic gauge plaquette of Wilson. We then write Eq. (1.17) as

$$-H(\sigma) = \sum_{\text{squares}} K_l(\sigma_l). \quad (1.19)$$

The subscript l indicates that squares oriented in different directions [$l = (x, y)$ or $l = (x, z)$ or \dots] may have different couplings.

We also wish to write the Hamiltonian in a form analogous to Eq. (1.12). To do this we factorize the closed path Γ into open paths γ_1 and γ_2 as shown in Fig. 1. Thus, if Γ goes from 1 to 2 to \dots m to $m + 1 \dots$ to n to 1, we can have γ going from 1 to 2 to 3 to $m - 1$ to m and γ' going from 1 to n to $n - 1$ to \dots $m + 1$ to m and we can write

$$\sigma_\gamma = \sigma(r_1, r_2) \sigma(r_2, r_3) \dots \sigma(r_{m-1}, r_m). \quad (1.20)$$

Here matrix multiplication is understood and σ_γ is itself a matrix. Now if the path Γ factorizes into γ and γ' , we find

$$\sigma_\Gamma = \sigma_\gamma \sigma_{\gamma'}^{-1}. \quad (1.21)$$

Hence Eq. (1.19) may be rewritten in the form:

$$-H(\sigma) = \sum_{\text{squares}} K_l(\sigma_\gamma, \sigma_{\gamma'}) \quad (1.22)$$

Finally, since the representation is simple, we can represent the basic statistical sums in just the same form as Eq. (1.11) by writing

$$\begin{aligned} \text{Tr}_{\sigma(r, r')} f(\sigma(r, r')) &= \sum_{\alpha} f(G^\alpha \sigma(r, r')) \\ &= \sum_{\alpha} f(G^\alpha). \end{aligned} \quad (1.23)$$

II. EXACT RECURSION FORMULAS

Before we attack any complex situations, we shall investigate two trivial examples: one-dimensional systems with ordinary global symmetries and gauge systems in two dimensions. In both cases, we shall employ two different modes of solution:

1. A decimation transform in which one simply sums over some of the old variables σ . The remaining unsummed variables are then the μ 's.

2. A block transformation in which $T(\mu, \sigma)$ couples each new variables, μ , to two of the old variables σ .

The first mode of solution is conceptually simpler. But, in higher dimensions, this type of approach is known [17] to lead to fixed points with long-ranged couplings and unpleasant forms of correlations. The second mode of transformation probably eliminates these difficulties-at least for some systems of physical interest.

A. Decimation in One Dimension

Here we write the coordinate of the spin variable σ as $\sigma(r) = \sigma(kL)$ with $k = 0, 1, 2, \dots$ and also write $\mu(r) = \mu(k\lambda L)$, where λ is an integer greater than 1 which defines the change in length scale. To obtain this change (see Fig. 2), one must sum over $n = \lambda - 1$ σ 's in a row. Thus, the transformation function takes the form:

$$e^{T(\mu, \sigma)} = \prod_k \delta(\mu(k\lambda L) - \sigma(kL)). \quad (2.1)$$

If the Hamiltonian includes only nearest-neighbor interactions

$$-H(\sigma) = \sum_k K[\sigma(kL), \sigma((k+1)L)] \quad (2.2)$$

then the new Hamiltonian is of exactly the same form with

$$e^{K'(\mu, \mu')} = \text{tr}_{\sigma_1} \text{tr}_{\sigma_2} \cdots \text{tr}_{\sigma_n} e^{K(\mu, \sigma_1)} e^{K(\sigma_1, \sigma_2)} \cdots e^{K(\sigma_n, \mu')}. \quad (2.3)$$

Since the sum in Eq. (2.3) is effectively a matrix product, it can be calculated in simple cases.

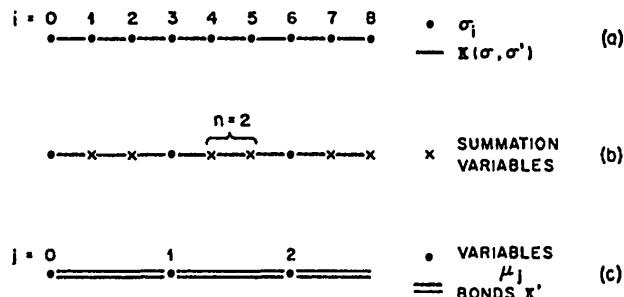


FIG. 2. Decimations in one dimension. Part (a) shows the original couplings; (b), the summations; (c), the result.

Eq. (2.3) expresses the new coupling function $K'(\sigma, \sigma')$. We can abbreviate this functional relation provided by the n summations in Eq. (2.3) as the functional equation

$$K' = R_0^{n+1}[K]. \quad (2.4a)$$

However, any function $K(\sigma, \sigma')$ may be expanded in a set of basis functions $U_i(\sigma, \sigma')$ as

$$K(\sigma, \sigma') = \sum_i K_i U_i(\sigma, \sigma'). \quad (2.5)$$

Thus the function $K(\sigma, \sigma')$ may be specified by giving the vector of coupling constants K , while $K'(\sigma, \sigma')$ may be equivalently specified in terms of its coupling constant vector \mathbf{K}' . In this vector notation Eq. (2.4a) is written

$$\mathbf{K}' = R_0^{n+1}(\mathbf{K}) \quad (2.4b)$$

To actually calculate the sums in Eq. (2.3), it is helpful to construct still another representation of the coupling function. Notice how the sum in Eq. (2.3) is exactly similar to matrix multiplication. Imagine then that we constructed a matrix $Z[K]$ which had matrix elements which were related to the coupling function by

$$\langle \sigma | Z[K] | \sigma' \rangle = e^{\mathbf{K}(\sigma, \sigma')} \quad (2.6a)$$

Then the product of $n + 1$ of these matrices would be

$$\langle \sigma | (Z[K])^{n+1} | \sigma' \rangle = e^{\mathbf{K}'(\sigma, \sigma')} \quad (2.6b)$$

Thus, in this notation, the summations become matrix products. For most purposes, it will prove more convenient for us to deal with an exponentiated version of Eqs. (2.6). Instead of $Z[K]$, we define a matrix $\tilde{K}[K]$ which obeys

$$\langle \sigma | e^{\tilde{K}[K]} | \sigma' \rangle = e^{\mathbf{K}(\sigma, \sigma')} \quad (2.7a)$$

Then, the n matrix multiplications become trivial. After the multiplications are performed, we have a new matrix given by $\exp \tilde{K}' = (Z[K])^{n+1}$. Hence the new matrix is just

$$\tilde{K}' = (n + 1) \tilde{K}[K]. \quad (2.7b)$$

Finally, once \tilde{K}' is determined, the new coupling may be found by taking a matrix element

$$e^{\mathbf{K}'(\sigma, \sigma')} = \langle \sigma | e^{\tilde{K}'} | \sigma' \rangle. \quad (2.7c)$$

Just as it is convenient to replace the function $K(\sigma, \sigma')$ by the set of coupling parameters \mathbf{K} , so it is convenient to replace the matrix $\langle \sigma | \tilde{K} | \sigma' \rangle$ by a vector of

parameters which can fully define the matrix. Write a set of basic matrices $\langle \sigma | V^i | \sigma' \rangle$, and then write

$$\langle \sigma | \tilde{K} | \sigma' \rangle = \sum_i \tilde{K}_i \langle \sigma | V^i | \sigma' \rangle \quad (2.8)$$

so that the vector of parameters \mathbf{K} fully defines the matrix $\langle \sigma | \tilde{K} | \sigma' \rangle$.

Thus, for any set of couplings, we have a pair of vectors \mathbf{K} and $\tilde{\mathbf{K}}$. The two vectors are related by Eq. (2.8) which effectively gives $\tilde{\mathbf{K}}$ as a function of \mathbf{K} . We can then write the result of this equation as

$$\tilde{\mathbf{K}} = D(\mathbf{K}) \quad \text{or} \quad \mathbf{K} = D^{-1}(\tilde{\mathbf{K}}). \quad (2.9)$$

We use the notation D because, as we shall see, $\tilde{\mathbf{K}}$ and \mathbf{K} obey a kind of duality relationship, which is a generalization of the duality used by Kramers and Wannier [7] and by Wegner [6].

In a practical sense, the essential step in this kind of renormalization calculation is the construction of the function $D(\mathbf{K})$. Assume this function and its inverse are known. Before the renormalization, the problem is described by \mathbf{K} and by $\tilde{\mathbf{K}} = D(\mathbf{K})$. After the renormalization, the problem is defined by a new set of couplings \mathbf{K}' or by a new set of dual couplings $\tilde{\mathbf{K}}'$. But in virtue of the matrix multiplication (see Eq. (2.7b)), $\tilde{\mathbf{K}}'$ is exactly $(n + 1)\tilde{\mathbf{K}}$. Hence the new couplings are given as

$$\mathbf{K}' = D^{-1}(\tilde{\mathbf{K}}') = D^{-1}((n + 1)\tilde{\mathbf{K}})$$

or finally as

$$\mathbf{K}' = D^{-1}(\lambda D(\mathbf{K})) \quad (2.10)$$

with

$$\lambda = n + 1. \quad (2.11)$$

Once D is known, then we know the renormalization function (2.4b).

B. Simple Representations

All of this can be worked out very explicitly when σ is a simple representation of the symmetry and therefore obeys Eq. (1.11). Define the class of a pair of variables (σ_1, σ_2) by saying that the pair (σ'_1, σ'_2) will fall into the same class as (σ_1, σ_2) if there is a group element G such that

$$\begin{aligned} \sigma'_1 &= G\sigma_1, \\ \sigma'_2 &= G\sigma_2. \end{aligned}$$

Any scalar like $K(\sigma, \sigma')$ which depends upon two group representation variables cannot really depend upon σ and σ' , but upon the class in which (σ, σ') falls.

A formal representation of this class dependence can be written by defining a delta symbol

$$\begin{aligned}\delta_c(\sigma, \sigma') &= 1 && \text{if } (\sigma, \sigma') \text{ falls in Class } c \\ &= 0 && \text{otherwise.}\end{aligned}\quad (2.11a)$$

Then the statement that $K(\sigma, \sigma')$ depends upon the class can be expressed in the form

$$K(\sigma, \sigma') = \sum_c K_c \delta_c(\sigma, \sigma'). \quad (2.12a)$$

The parameters K_c then define the coupling function and form one way of writing the coupling vector $\mathbf{K} = K_0, K_1, \dots, K_c, \dots$

There is an alternative expression for $K(\sigma, \sigma')$ based upon an expansion into irreducible representations. Let $\phi_{\gamma m}(\sigma)$ and $\phi_{\gamma m}^*(\sigma)$ be the basis functions for the all irreducible representations of the symmetry group which can be formed from products of the σ 's. Here the index γ distinguishes among the different irreducible representations while m distinguishes among the different orthogonal basis functions for a given representation. The index m runs from 1 to $d_\gamma M_\gamma$, where d_γ is the dimensionality of the representation and M_γ is the number of times that it appears. These functions can then serve to give an alternative expansion of any class function in the form

$$K(\sigma, \sigma') = \sum_\gamma K_\gamma \chi_\gamma(\sigma, \sigma'). \quad (2.12b)$$

Here χ_γ is the character function defined by

$$\chi_\gamma(\sigma, \sigma') = \sum_{m=1}^{M_\gamma d_\gamma} \phi_{\gamma m}(\sigma) \phi_{\gamma m}^*(\sigma'). \quad (2.13)$$

The $\phi_{\gamma m}$ are normalized so that

$$\text{tr}_\sigma \phi_{\gamma m}(\sigma) \phi_{\gamma' m'}^*(\sigma) = \delta_{\gamma, \gamma'} \delta_{m, m'} g$$

where g is the number of elements in the basic sum over σ , i.e.,

$$g = \text{tr}_\sigma 1.$$

We describe the two alternative expansion (2.12a) and (2.12b) as, respectively, the class picture and the representation picture of the coupling.

The character table χ_γ^c is defined by expanding the character function in the class picture as

$$\chi_\gamma(\sigma, \sigma') = \sum_c \delta_c(\sigma, \sigma') \chi_\gamma^c M_\gamma \quad (2.14a)$$

or by expanding the delta symbol in the representation picture as

$$\delta_c(\sigma, \sigma') = \sum_{\gamma} \frac{\chi_{\gamma}(\sigma, \sigma')}{d_{\gamma}} (\chi_{\gamma}^c)^* \frac{n_c}{g}. \quad (2.14b)$$

Here n_c is the number of group elements in the class c . The two expansion (2.14a) and (2.14b) are mutually consistent in virtue of the character orthogonality relations

$$\sum_{\gamma} (\chi_{\gamma}^c (\chi_{\gamma}^c)^* M_{\gamma}/d_{\gamma}) = \delta_{c,c'} g/n_c \quad (2.15a)$$

$$\sum_c \chi_{\gamma}^c (\chi_{\gamma}^c)^* n_c = \delta_{\gamma,\gamma'} d_{\gamma} g/M_{\gamma}. \quad (2.15b)$$

Equations (2.14) are very useful in moving up and back between the class picture and the representation picture.

The utility of this point of view is shown if we consider the matrix

$$\langle \sigma | z | \sigma' \rangle = e^{K(\sigma, \sigma')}.$$

On one hand, the class expansion gives

$$\langle \sigma | z | \sigma' \rangle = \sum_c \delta_c(\sigma, \sigma') e^{K_c}. \quad (2.16a)$$

On the other hand, the representation expansion may be used to express this matrix element of z in the form

$$\begin{aligned} \langle \sigma | z | \sigma' \rangle &= \sum_{\gamma} \chi_{\gamma}(\sigma, \sigma') (e^{K_{\gamma}}/g) \\ &= \sum_{\gamma m} (\phi_{\gamma m}(\sigma) \phi_{\gamma m}^*(\sigma')/g) e^{K_{\gamma}}. \end{aligned} \quad (2.16b)$$

From the second form of writing (2.16b), we see that we have diagonalized the matrix z and that $\exp(K_{\gamma})$ is its set of eigenvalues. Hence the parameters K_{γ} are an explicit realization of the matrix parameters of Eq. (2.7a).

Of course, K_{γ} is not at all the same thing as K . The latter is given by combining Eqs. (2.12) and (2.14b) in the form

$$K = \sum_c (K_c n_c / g d_c) (\chi_{\gamma}^c)^*.$$

On the other hand K_{γ} is related to K_c by

$$e^{K_c} = \sum_{\gamma} \chi_{\gamma}^c (e^{K_{\gamma}}/g) M_{\gamma} \quad (2.17a)$$

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and

$$e^{K\gamma} = \sum_c ((\chi_{\gamma}^c)^* n_c / d_c) e^{K_c}. \quad (2.17b)$$

In some sense, K_c and $\tilde{K}\gamma$ may be viewed as "Fourier transformed" descriptions of the interaction. Strong coupling implies that e^{K_c} is by far largest for the class $c = 0$ in which $\sigma = \sigma'$. In that case $\tilde{K}\gamma$ will be almost independent of γ . On the other hand, weak coupling is the limit in which K_c is almost independent of c so that $e^{K\gamma}$ will be by far largest in the identity representation ($\gamma = 0$) for which $\chi_0^c = 1$.

Notice that Eqs. (2.17) are an explicit realization of the functions D and D^{-1} of Eqs. (2.9). These functions then permit us to calculate in a very explicit fashion the renormalizations of any one-dimensional problem involving irreducible representations.

C. An Example: The Potts Model

The N -state Potts model is a generalization of the Ising model in which the spin, σ , can take on the values $1, 2, \dots, N$. The underlying symmetry group is the permutation group for N objects. In describing $K(\sigma, \sigma')$ we say that there are two classes ($c = 0$ and $c = 1$) representing, respectively, the cases $\sigma = \sigma'$ and $\sigma \neq \sigma'$. These two classes have n_c equal to 1 and $N - 1$, respectively. Then the class picture of the coupling has the form $K(\sigma, \sigma') = K_0 \delta_{\sigma, \sigma'} + K_1 (1 - \delta_{\sigma, \sigma'})$. The two relevant irreducible representations of the symmetry have basis functions

$$\begin{aligned} \phi_0(\sigma) &= 1 \\ \phi_{1m}(\sigma) &= (N - 1)^{-1/2} (N \delta_{m, \sigma} - 1) \quad \text{for } m = 1, 2, \dots, N - 1. \end{aligned}$$

These two representations have respectively dimensionality 1 and $N - 1$. In this case, M_γ equals 1. Using these basis functions, one can construct

$$\chi_\gamma(\sigma, \sigma') = \delta_{\gamma, 0} + \delta_{\gamma, 1} (N \delta_{\sigma, \sigma'} - 1).$$

Thus the representation picture of the coupling has the form

$$K(\sigma, \sigma') = K^0 + K^1 (N \delta_{\sigma, \sigma'} - 1).$$

Most commonly, when one speaks of "the" nearest neighbor coupling one means K^1 .

Since the character table is

$$\chi_\gamma^c = \delta_{\gamma, 0} + \delta_{\gamma, 1} [(N - 1) \delta_{c0} - \delta_{c1}]$$

the relationship between K_e and \tilde{K}^v is given by

$$\begin{aligned} e^{K_0} &= (1/N)[e^{\tilde{K}^0} + (N - 1)e^{\tilde{K}^1}], \\ e^{K_1} &= (1/N)[e^{\tilde{K}^0} - e^{\tilde{K}^1}], \end{aligned} \quad (2.18a)$$

and

$$\begin{aligned} e^{\tilde{K}^0} &= e^K + (N - 1)e^K \\ e^{\tilde{K}^1} &= e^K - e^K. \end{aligned} \quad (2.18b)$$

Then, to perform the recursion, we first find \tilde{K}^0 and \tilde{K}^1 as a function of the original coupling constants with the aid of Eq. (2.18b). The recursion then increases \tilde{K}^0 and \tilde{K}^1 by multiplying each by a factor of $\lambda = n + 1$. Finally, Eq. (2.18a) is used to find the new couplings as

$$\begin{aligned} e^{K_0'} &= (1/N)\{[e^{K_0} + (N - 1)e^{K_1}]^\lambda + (N - 1)[e^{K_0} - e^{K_1}]\}^\lambda \\ e^{K_1'} &= (1/N)\{[e^{K_0} + (N - 1)e^{K_1}]^\lambda - [e^{K_0} - e^{K_1}]\}^\lambda. \end{aligned}$$

The Ising model comes from the special case $N = 2$. The standard coupling constant in this case is usually called K and is defined in terms of Potts model variables be

$$K = (K_0 - K_1) \div 2 \quad (2.19a)$$

The standard dual coupling constant in the Ising case is given by

$$\tilde{K} = (\tilde{K}^0 - \tilde{K}^1) \div 2. \quad (2.19b)$$

Then Eq. (2.18b) is expressed by the standard dual relationship

$$\begin{aligned} e^{-2K} &= \tanh K, \text{ or} \\ e^{-2\tilde{K}} &= \tanh \tilde{K}. \end{aligned}$$

Finally, the value of the coupling after the recursion is given by

$$\tanh K' = (\tanh K)^\lambda.$$

D. Block Transformations in One Dimension

To derive the block transformation, choose each μ to be coupled to its two nearest-neighboring σ 's as shown in Fig. 3. In particular, take

$$e^{T(\mu, \sigma)} = \prod t(\mu(X_k), \sigma(X_k + L/2), \sigma(X_k - L/2)) \quad (2.20a)$$

with

$$X_k = k\lambda L$$

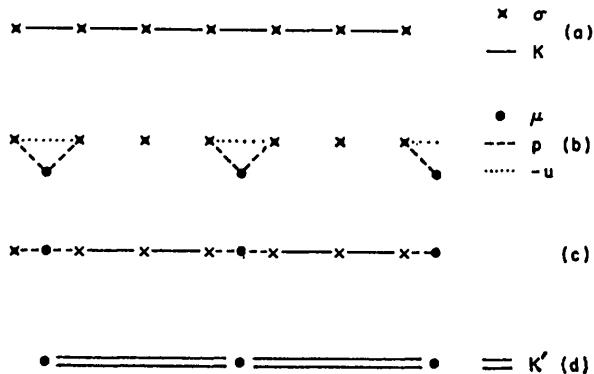


FIG. 3. The block transformation in one dimension. Part (a) shows the original lattice; (b) shows $T(\mu, \sigma)$; (c) puts the two together; and (d) shows the result of the summation.

and

$$t(\mu, \sigma, \sigma') = \exp[p(\mu, \sigma) + p(\sigma', \mu) - u(\sigma, \sigma')] \quad (2.20b)$$

Here u is given by

$$u(\sigma, \sigma') = \ln \text{tr}_\mu e^{p(\sigma', \mu) + p(\mu, \sigma)}. \quad (2.20c)$$

This last condition is required in order that Eq. (1.3) be satisfied, i.e., that the renormalization not change the free energy.

From Fig. 3, we see that the renormalization has introduced new couplings between μ and its neighboring σ 's and changed the coupling between these σ 's from $K(\sigma, \sigma')$ to $K(\sigma, \sigma') - u(\sigma, \sigma')$. The sum over σ 's may be performed if there is no coupling between these σ 's. Hence, choose the undetermined parameters in the renormalization transform, i.e., the function $p(\mu, \sigma)$ such that

$$u(\sigma, \sigma') = K(\sigma, \sigma'). \quad (2.21)$$

In the dual language, this requirement will be satisfied if $\tilde{K}(u) = \tilde{K}(K)$. But, from (2.20c), $\tilde{K}(u) = 2 \times \tilde{K}(p)$. Hence we require that p obey:

$$\tilde{K}(K) = 2 \cdot \tilde{K}(p). \quad (2.22)$$

Now we can perform the sum. In place of Eq. (2.7c) we find

$$e^{K'(\sigma, \sigma')} = \langle \sigma | e^{\tilde{K}(p)} e^{n\tilde{K}(K)} e^{\tilde{K}(p)} | \sigma' \rangle. \quad (2.23)$$

But the matrices $\tilde{K}(p)$ and $\tilde{K}(K)$ are simply proportional. Hence they commute. We add up the right-hand side of Eq. (2.23) and find

$$e^{K'(\sigma, \sigma')} = \langle \sigma | e^{(n+1)\tilde{K}(K)} | \sigma' \rangle. \quad (2.24)$$

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Equation (2.24) is exactly the same as our earlier result (2.7c). As a consequence, when we make the special choice of p demanded by Eq. (2.20c), the block renormalization and the decimation become identical.

Hence Eq. (2.3) equally well expresses the result of the one-dimensional renormalization for both types of renormalization functions.

E. Decimations for the Gauge System

To see how the analogous results emerge in the gauge system, start by summing over the central spin in the 7-spin configuration shown in Fig. 4a. The result of this summation is of the form

$$e^{-H'} = \text{tr}_{\sigma_{11'}} e^{K(\sigma_{1A}\sigma_{AA'}\sigma_{A'1'}\sigma_{11'}^{-1})} e^{K(\sigma_{11'}(\sigma_{1B}\sigma_{BB'}\sigma_{B'1'})^{-1})} \quad (2.25)$$

Here each K depends upon the trace of its matrix argument. For a simple representation, we can always change the integration variable from $\sigma_{11'}$ to $\tilde{\sigma}$ defined by

$$\sigma_{11'} = \sigma_{1B}\tilde{\sigma}\sigma_{BB'}\sigma_{B'1'}.$$

Then, after we perform a cyclic rearrangement of the trace inside each K , we find that

$$e^{-H'} = \text{tr}_{\tilde{\sigma}} e^{K(\sigma_F\tilde{\sigma}^{-1}) + K(\tilde{\sigma})} \quad (2.26)$$

with

$$\sigma_F = \sigma_{B1}\sigma_{1A}\sigma_{AA'}\sigma_{A'1'}\sigma_{1'B'}\sigma_{B'B}. \quad (2.27)$$

The new variables are then defined by

$$\begin{aligned} \mu_{AA'} &= \sigma_{AA'} \\ \mu_{BB'} &= \sigma_{BB'} \\ \mu_{BA} &= \sigma_{B1}\sigma_{1A} \\ \mu_{A'B'} &= \sigma_{A'1'}\sigma_{1'B'} \end{aligned} \quad (2.28)$$

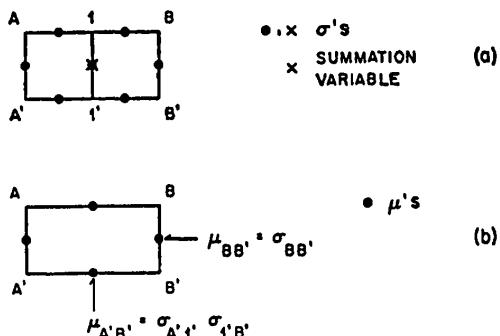


FIG. 4. The simplest gauge system sum. Part (a) shows the configuration before the sum; part (b) shows the configuration afterwards.

so that the σ_R defined by Eq. (2.27) can also be written as

$$\sigma_R = \mu_R = \mu_{BA} \mu_{AA'} \mu_{A'B'} \mu_{B'B}. \quad (2.29)$$

Thus, for this simple renormalization, Eq. (2.25) defines a function of the μ -variables,

$$-H' = K'(\mu_R)$$

which takes the form

$$e^{K'(\mu_R)} = \text{tr}_{\sigma} e^{K(\omega_R \sigma^{-1}) + K(\sigma)}. \quad (2.30)$$

A direct generalization of this argument gives the result of n summations, as shown in Fig. 5, to be

$$e^{K'(\mu_R)} = \text{tr}_{\sigma_1 \sigma_2 \dots \sigma_n} e^{K(\omega_R \sigma_1^{-1})} e^{K(\sigma_1 \sigma_2^{-1})} \dots e^{K(\sigma_{n-1} \sigma_n^{-1})} e^{K(\sigma_n)}. \quad (2.31)$$

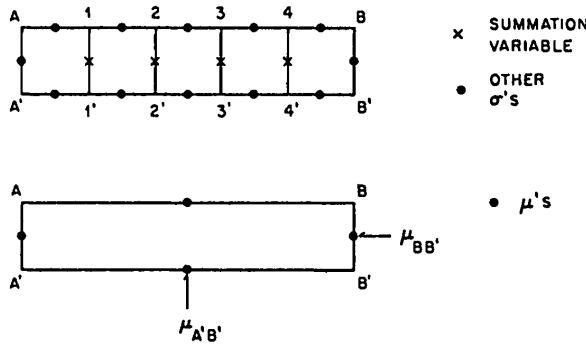


FIG. 5. Like Figure 4, except that there are more spins to be summed.

Here μ_R still appears in the form (2.29), but now μ_{AB} has a more complex structure, i.e.,

$$\mu_{AB} = \sigma_{A1}\sigma_{12} \dots \sigma_{n-1,n}\sigma_{nB}. \quad (2.32)$$

Finally, if we extend to the two-dimensional example shown in Fig. 6, the five summations on each of the different rows are quite independent so that Eq. (2.31) holds in the two-dimensional example as well.

Of course, each of these figures only shows a fragment of the lattice. In particular, only one period in the μ -lattice is shown. However, the recursion equation, (2.31), remains valid as we go to the full, infinite two-dimensional lattice.

Finally, we follow Migdal to notice that the structure of summations is precisely the same in Eqs. (2.31) and (2.3). Thence, in both cases

$$K' = R_0^{n+1}(K).$$

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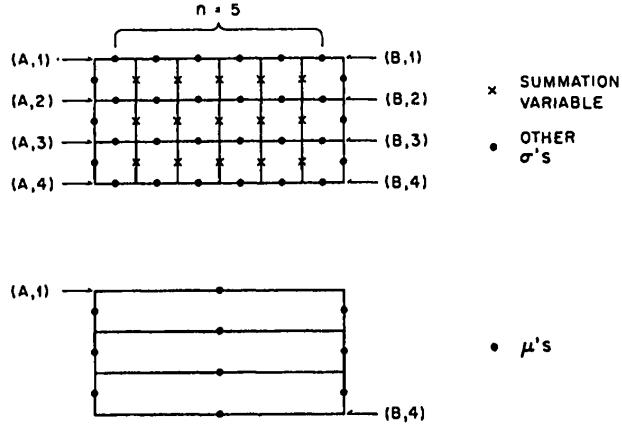


FIG. 6. The gauge system sum in two dimensions.

When $K(\sigma_1, \sigma_2)$ takes the special form $K(\sigma_1\sigma_2^{-1})$, the function R_0 is exactly the same for the local symmetry (at $d = 2$) and the global symmetry (at $d = 1$). The form of this function depends only upon the symmetry group and upon the representation.

F. Block Transformation for the Gauge Case at $d = 2$

These results also can be derived from a special kind of block transformation analogous to the transform of Eq. (2.18). The basic geometry is shown in Fig. 7a for a transformation with $n = 2$. The μ_{AB} variables are defined as in Eq. (2.32). However, $\mu_{AA'}$ appears in a new manner, i.e., in a t function of the form

$$t(\mu_{AA'}, \sigma) = \exp\{p(\sigma_{AA'}, \mu_{AA'}) + p(\mu_{AA'}, \sigma_\gamma) - u(\sigma_{AA'}, \sigma_\gamma)\}. \quad (2.33)$$

Here, in the case shown in Fig. 7b,

$$\sigma_\gamma = \sigma_{A0}\sigma_{00'}\sigma_{0'A'}. \quad (2.34)$$

Together the product $\sigma_{AA'}\sigma_\gamma^{-1}$ forms the σ_Γ for the plaquette containing the μ .

In general, u obeys

$$e^{u(\sigma, \sigma')} = \text{tr}_\mu e^{p(\sigma, \mu) + p(\mu, \sigma')}. \quad (2.35)$$

However, we can once more gain a particularly simple result if we once again adjust p so that $u(\sigma, \sigma')$ equals (and cancels) $K(\sigma, \sigma')$. Then we follow through the same arguments as in the global symmetry situation and conclude that, as in all the other cases

$$\mathbf{K}' = R_0^{n+1}(\mathbf{K}).$$

Thus, all of these approaches lead us back to the very same result.

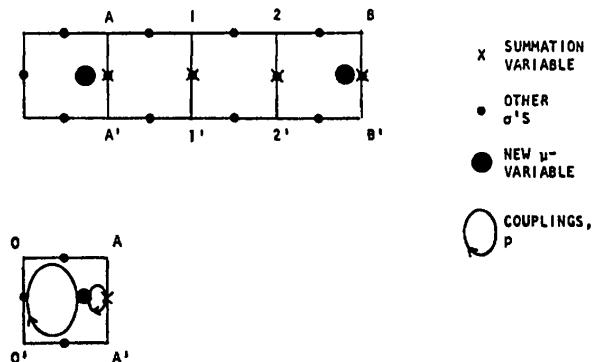


FIG. 7. Block sum for the gauge system. Part (a) shows the lattice; (b) shows the couplings in $T(\mu, \sigma)$.

III. "DERIVATION" AND INTERPRETATION OF MIGDAL'S APPROXIMATION

A. Lower Bound Approximations

In this section, we employ a "variational" method of deriving approximate recursion equations to obtain results similar to Migdal's. The method starts from Eq. (1.2)

$$e^{-H'(\mu)} = \text{Tr}_\sigma e^{T(\mu, \sigma) - H(\sigma)} \quad (3.1)$$

and the resulting invariance principle for the free energy $F[H'] = F[H]$. To derive an approximate recursion equation, one compares Eq. (3.1) with a corresponding approximate equation, namely,

$$e^{-H_{A'}(\mu)} = \text{Tr}_\sigma e^{T(\mu, \sigma) - H(\sigma) - \Delta(\mu, \sigma)}. \quad (3.2)$$

Then, if $\Delta(\mu, \sigma)$ obeys

$$\text{Tr}_\mu \text{Tr}_\sigma e^{T(\mu, \sigma) - H(\sigma)} \Delta(\mu, \sigma) = 0 \quad (3.3)$$

the new approximate Hamiltonian will generate a free energy which is smaller than the exact free energy, i.e.,

$$F[H_A'] \leq F[H'] = F[H].$$

The success of the method depends upon choosing a $\Delta(\mu, \sigma)$ which

1. makes the sum in Eq. (3.2) calculable,
2. obeys (3.3), and
3. is small.

If conditions 1 and 2 are met and if Δ still contains some free parameters, one can obtain a "best" Δ by varying the free parameters to make the approximate free energy a maximum.

The error in the calculated free energy will be of second order in Δ .

It is easy to construct several different kinds of $\Delta(\mu, \sigma)$ which automatically satisfy Eq. (3.3). One kind of representation is to choose a $T_p(\mu, \sigma)$ which depends on a parameter (or set of parameters) p . Let the normalization condition, (1.3), hold for all p . Then a change in p will not change the free energy. As a consequence

$$\Delta_i(\mu, \sigma) = \partial T_p(\mu, \sigma) / \partial p_i$$

will certainly satisfy Eq. (3.3). More generally, we can choose

$$-\Delta(\mu, \sigma) = \sum_i q_i (\partial T_p(\mu, \sigma) / \partial p_i) \quad (3.5)$$

for any value of q_i and still have (3.3) hold true.

Alternatively, imagine any set of local variables $a_r(\mu, \sigma)$. For example, a_r might be just $\sigma_{x,y}, \sigma_{x+1,y}$ in some two-dimensional case. We only require that the symmetry of the problem demand that

$$\text{Tr}_\mu \text{Tr}_\sigma e^{T(\mu, \sigma) - H(\sigma)} a_r(\mu, \sigma) \sim \langle a_r(\mu, \sigma) \rangle$$

be independent of r . Then, if we have m sets of such equivalent variables $a_r^i(\mu, \sigma)$, $i = 1, 2, \dots, m$ we can choose

$$-\Delta(\mu, \sigma) = \sum_i \sum_r q^i(r) a_r^i(\mu, \sigma). \quad (3.6)$$

If we then insist that for all i

$$\sum_r q^i(r) = 0 \quad (3.7)$$

then (3.3) will certainly hold true.

We can give a simple geometrical interpretation to Eqs. (3.6) and (3.7). Consider $a_r^i(\mu, \sigma)$ to be a kind of local coupling term. For example, if it is $\sigma_{x,y}, \sigma_{x+1,y}$ it is just a nearest-neighbor coupling in the x -direction. Then in the expression $T - H - \Delta$, which appears in Eq. (3.2), $q^i(r) a_r^i(\mu, \sigma)$ add some coupling strengths of the form a^i at the point r . The condition (3.7) says that we are allowed to add and subtract such couplings within the variational constraint if we just demand that for every bit of strength we add at one set of points we make sure we subtract an equivalent total strength at other points.

More simply stated: The variational principle allows us to move potential terms from one set of bonds in the lattice to equivalent bonds but not to increase or decrease the total amount of any type of bond.

B. Decimations on the Globally Symmetrical System

To see how this works in practice, let us employ a decimation recursion upon a system in d dimensions. This recursion employs a $T(\mu, \sigma)$ of the form shown in Fig. 8. We sum freely over all σ 's save those with an x -coordinate equal to $k(n + 1)/L$. These σ 's are set equal to the new variables, μ . Thus as in Eq. (2.1), we have

$$e^{T(\mu, \sigma)} = \prod_{k, y, z, \dots} \delta(\mu(k\lambda L, y, z, \dots) - \sigma(k\lambda L, y, z, \dots)). \quad (3.8)$$

We call this kind of decimation, in which the lattice constant in the x direction is changed from L to λL an x -decimation.

We assume a Hamiltonian with nearest-neighbor interactions, i.e., one of the form (1.12). Thus, we have nearest-neighbor bonds K_x, K_y, K_z, \dots . Figure 8 shows the K_x and K_y bonds. Notice that the summation over σ 's cannot be performed because of the K^y, K^z, \dots bonds which connect two summation variables. Within the context of the variational principle, this difficulty is easily cured—if we are willing to accept a (rather large) error in the free energy. We choose a Δ of exactly the form (1.12)

$$-\Delta(\sigma) = \sum_{\langle rr' \rangle} \Delta_{rr'}^l(\sigma(r), \sigma(r')) \quad (3.9)$$

and take Δ^l to be exactly zero if $l = x$. For the remaining bonds, we choose

$$\Delta_{rr'}^l(\sigma, \sigma') = -K_l(\sigma, \sigma') \quad (3.10a)$$

when $\sigma(r)$ and $\sigma(r')$ are summation variables and

$$\Delta_{rr'}^l(\sigma, \sigma') = nK_l(\sigma, \sigma') \quad (3.10b)$$

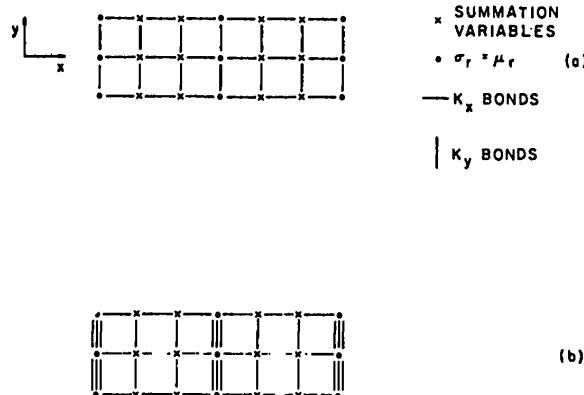


FIG. 8. Decimation geometry. Part (a) shows the situation before bonds are moved; part (b) shows the situation afterwards.

on the bonds which connect two μ -variables. The net effect of (3.10) is to move nK_l bonds ($l = y, z, \dots$) from summation bonds to the bonds between two μ -variables.

Now the summation over σ is easy to perform. We sum as before and find a new x -coupling

$$\mathbf{K}_x' = R_0^\lambda(\mathbf{K}_x). \quad (3.11a)$$

The y, z, \dots bonds are the sum of the bond that was always present and the n bonds that were moved:

$$\mathbf{K}_l' = (n + 1) \mathbf{K}_l. \quad (3.11b)$$

Migdal's result now emerges if we consider the effect of successive x, y, z, \dots , decimations. All these decimations together change the lattice constant from L to $\lambda L = (n + 1)L$. Successive applications of Eqs. (3.11) imply that the x -coupling constant after the change is:

$$\mathbf{K}_x(\lambda L) = \lambda^{d-1} R_0^\lambda(\mathbf{K}_x(L)) \quad (3.12a)$$

while all the other coupling constants obey

$$\mathbf{K}_l(\lambda L) = \lambda^{d-l} R_0^\lambda(\lambda^{l-1} \mathbf{K}_l(L)), \quad (3.12b)$$

Here $l = 2, 3, 4, \dots$ is the index which describes the coupling constant in the y, z, t, \dots direction.

In one sense, Eq. (3.12a) is exactly the same as Migdal's result. Migdal does write this same equation. However, he assumes that it holds for all the couplings in all directions. Thus, our derivations gives a \mathbf{K}_l which depends on \mathbf{K}_i and obeys Eqs. (3.12), while Migdal's argument gives

$$\mathbf{K}_x = \mathbf{K}_y = \dots = \mathbf{K}_t \quad (3.13)$$

and all coupling constants obeying Eq. (3.12a).

To see the different consequences of these assumptions, consider the fixed point of Eqs. (3.12). At the fixed point, we have

$$\begin{aligned} K_x^* &= \lambda^{d-1} R_0^\lambda(K_x^*) \\ K_l^* &= \lambda^{-(l-1)} K_x^*. \end{aligned} \quad (3.14)$$

In two dimensions, this becomes

$$K_x^* = \lambda R_0(K_x^*) \quad (3.15a)$$

$$K_y^* = \lambda^{-1} K_x^*. \quad (3.15b)$$

In contrast, Migdal would have both K_x^* and K_y^* obey Eq. (3.15a).

In the tilde notation of Eq. (2.12), Eqs. (3.15) reduce to

$$\begin{aligned}\widetilde{\mathbf{K}_y}^* &= \lambda \widetilde{\mathbf{K}_x}^* \\ \mathbf{K}_x^* &= \lambda \mathbf{K}_y^*\end{aligned}\quad (3.16)$$

Eqs. (3.16) have a solution with $\mathbf{K}_x^* = \widetilde{\mathbf{K}_y}^*$.

The important coupling term is $K = (K_0 - K_1)/N$ which describes the energy difference between the lined up configuration and one of the others. According to Eq. (2.18a)

$$e^{-NK} = \frac{1 - e^{K^1 - K^0}}{1 + (N - 1) e^{K^1 - K^0}}.$$

Hence, if \tilde{K} is defined as $(\tilde{K}^0 - \tilde{K}^1)/N$,

$$e^{-NK} = \frac{1 - e^{-N\tilde{K}}}{1 + (N - 1) e^{-N\tilde{K}}}.$$

Since $\mathbf{K}_x^* = \mathbf{K}_y^*$, we see that the critical couplings are defined by

$$K_x^* = \widetilde{K}_y^* = \frac{1}{N} \ln \frac{e^{N\mathbf{K}_y^*} + N - 1}{e^{N\mathbf{K}_y^*} - 1}.$$

This is exactly the equation for the critical point of the Potts model. At $N = 2$, the Ising case, this result reduces to the familiar result

$$\sinh 2K_x^* = 1/\sinh 2K_y^*. \quad (3.17)$$

Of course, Eq. (3.17) agrees with Migdal's result in the limit $n \rightarrow 0$, where $K_x \rightarrow K_y$. However, as one can see from Fig. 9, these solutions are quite different for $n \neq 0$. Since Eq. (3.17) is exactly true, Fig. 9 is a strong argument for preferring the present interpretation of the recursion equations over Migdal's.

C. Troubles With the Approximation

The first and most obvious difficulty of the approximation described by Eq. (3.12) is the lack of interaction among the different \mathbf{K}_i . The x -coupling does not affect the recursion equations for the y -coupling and vice versa. Hence the equations are totally senseless in, say, the limit as K_y goes to zero.

A second difficulty is the inaccuracy of the approximation. Figure 10 plots the critical index ν , derived from the approximation in the standard fashion, as a function of n for the two-dimensional Ising model. By any set of reasonable standards, the approximation seems weak.

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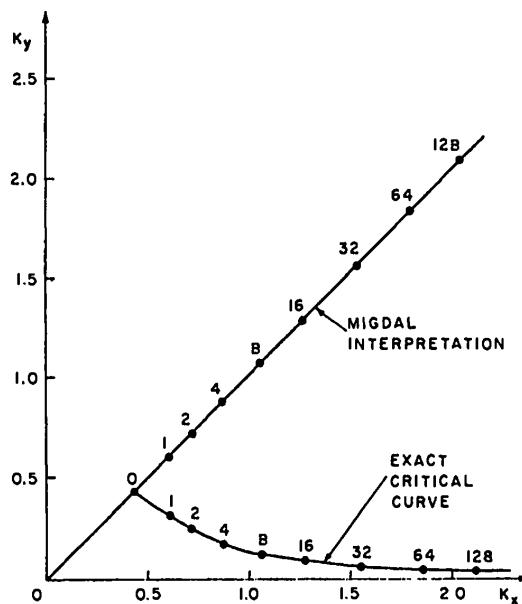


FIG. 9. Critical couplings for the $d = 2$ Ising model. The numbers on the graph give the value of n used in the construction of the Migdal recursions.

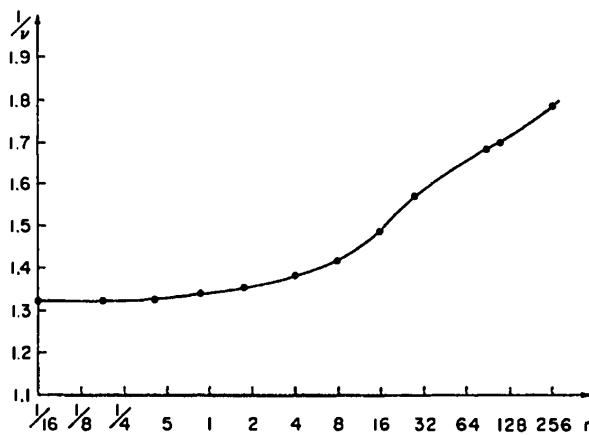


FIG. 10. Plot of $1/v$ versus n . The result compares poorly with the exact value of $v = 1.0$.

A third difficulty is inherent in the decimation form of $e^{T(\mu, \sigma)}$. With this form, there will be some σ 's which will be left unsummed after m recursions. Let $\sigma(r_1)$ and $\sigma(r_{11})$ be two such σ 's. Then we can compute the spin correlation and find

$$\langle \sigma(r_1) \sigma(r_{11}) \rangle_H = \langle \mu(r_1) \mu(r_{11}) \rangle_{H^m}. \quad (3.18)$$

Here μ is the variable after m recursions and H^m is the corresponding Hamiltonian. At the fixed point, $H = H^m = H^*$. But then the correlation function is left unchanged by a change in length scale. Since the scaling index which goes with σ is β/ν , Eq. (3.18) implies that

$$\beta/\nu = 0 \quad (3.19)$$

Thus the decimation form of T only leads to sensible results when $\beta/\nu = 0$.

Fortunately, most of Migdal's most striking results occur for systems in which β/ν might be very small. Hence there might be some asymptotic sense in which the approximation described here is right. To see how this might be true, I would like to refer the reader to the results of a (mostly) unpublished decimation calculation on the $d = 2$ Ising system by A. Houghton and the author [16]. This calculation was for the two-dimensional Ising system, for which Eq. (3.19) was certainly false. Nonetheless, we got reasonable looking answers by expanding in a small parameter, namely, the next-nearest neighbor interaction. The results of our calculation of ν^{-1} should be compared with the exact value $\nu = 1.0$. We got in zeroth order 1.3 (like Migdal), in first order 1.03, in second 1.002, and in third order 1.7 (sic). It would appear that we had our hands on an asymptotic series of some kind. Perhaps the decimation calculation described above is the zeroth order in some asymptotic series.

D. Decimations in the System With Local Symmetries

Just about the same derivation—and the same objections—apply to the gauge system. This system is shown in Fig. 11. Once more a decimation is performed

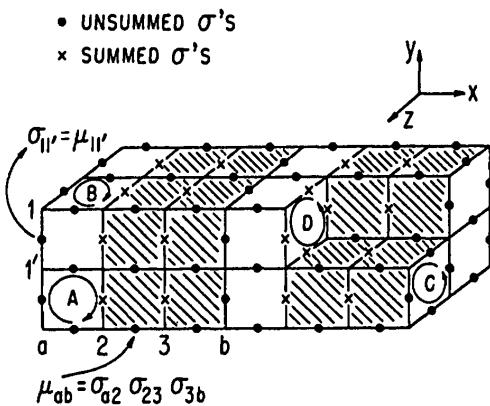


FIG. 11. The geometry for the decimation of the locally symmetric system. A , B , and C represent respectively K_{xy} , K_{xz} , and K_{yz} couplings which can be summed; D represents a K_{yy} coupling which cannot be summed directly.

which changes the lattice constant in the x direction. As shown in the figure, in each plane the μ -variables are related to the σ -variables in exactly the same manner as in the $d = 2$ system. Now we can handle exactly all $K_l(\sigma_R)$, whenever l refers to the xy , xz , xt ,... planes. However some of the $K_l(\sigma_R)$ connect summation variables in different planes. These difficult K_l 's are for l 's referring to the yz , yt , zt ,... planes. Once again, we sum whatever we can handle exactly and move all the couplings which we cannot handle from summation sites to unsummed sites. The net result looks exactly like (3.11) namely

$$\begin{aligned} K'_l &= R_0^\lambda(K_l) \quad \text{for } l = (x, y), (x, z), (x, t), \dots \\ &= \lambda K_l \quad \text{otherwise.} \end{aligned} \quad (3.19)$$

To obtain Migdal's result, imagine that we perform successively an x , y , z , and t decimation on a four-dimensional system. Then we find that after the resulting change in lattice constant

$$L \rightarrow \lambda L \quad (3.20)$$

we find new coupling constants. For each new constant, there are two chain summations (producing a R_0^λ) and two motions (producing a factor λ). Thus, for example

$$K_{xz}(\lambda L) = \lambda R_0^\lambda(\lambda R_0^\lambda(K_{xz}(L))) \quad (3.21a)$$

and

$$K_{xy}(\lambda L) = \lambda^2 R_0^\lambda(R_0(K_{xy}(L))). \quad (3.21b)$$

Equation (3.21a) can be reinterpreted in the following fashion: Imagine that we visualized the change (3.20) to occur in two stages

$$L \rightarrow \lambda^{1/2}L \rightarrow \lambda^{1/2}(\lambda^{1/2}L)$$

and the recursion (3.21) to occur in two stages as well:

$$K_{xz} \rightarrow K'_{xz} = \lambda R_0^\lambda(K_{xz})$$

$$K'_{xz} \rightarrow K''_{xz} = \lambda R_0^\lambda(K'_{xz}).$$

Then in place of (3.21a) we can write the simpler form

$$K_{xz}(\lambda^{1/2}L) = \lambda R_0^\lambda(K_{xz}). \quad (3.22)$$

Migdal asserted that Eq. (3.22)—which is analogous to his equation for the two-dimensional system with global symmetries—held for all K_l .

We would argue instead that, at best, it holds for some of the coupling constants, e.g., K_{xz} , and not others, e.g., K_{xy} .

Once again we can argue that the poor approximation is at fault for the lack of any interactions among the different K_i 's. However, we must again blame the basic decimation approach for the peculiar invariance of some of the correlation functions. Instead of Eq. (3.18), we find an invariance relation:

$$\langle \sigma_{\Gamma_1} \sigma_{\Gamma_2} \rangle_H = \langle \mu_{\Gamma_1} \mu_{\Gamma_2} \rangle_{H^m}. \quad (3.23)$$

Here σ_{Γ_1} and μ_{Γ_1} are identical closed paths on the original lattice and the m -times decimated lattice. Basically, Eq. (3.23) implies that the fixed point produces a correlation between σ_Γ 's which is invariant under the combined operation of

- a. multiplying the distance between two closed loops by a factor λ , and
- b. multiplying the area of each of the loops by a factor λ^2 .

We do not know when the exact critical point has this type of invariance, so we cannot predict when the decimation will lead to a fixed point which has some simple connection with the exact critical point.

E. The Block Transforms for the Globally Symmetric System

Now we have seen that the decimations lead to an apparently unphysical type of fixed point behavior. Thus, we do not wish to base our approach solely upon decimations. Fortunately, we had two alternative methods of attacking the one- and two-dimensional problems. As an alternative to the decimation, we could introduce the new spin via a block transformation—and get exactly the same form of recursion relation as with the decimation.

In this section, we show that the basic “Migdal” recursion relations, Eqs. (3.11) or (3.19), can be rederived via the block transformation scheme. In one sense, we will then have made no progress whatsoever—merely rederived a known set of equations. However, the block transformations do not obey the distressing correlation function identities (3.18) and (3.23). Hence they form a much more suitable starting point for the derivation of more refined approximations.

The globally symmetric case is handled in very much the same manner as in the $d = 1$ case of Section IIB. The σ -lattice is a simple hypercubic lattice. We focus on the chains of coupled spins along lines parallel to the x -axis. Figure 12 shows how we once again introduce new spins, μ , spaced by $n + 1$ links on the chain. Each new spin, μ , is coupled to its immediate neighbors σ and σ' by a coupling of exactly the form (2.20).

Recall that these couplings involved arbitrary function $p(\mu, \sigma)$. In the one-dimensional case, we choose p so that $T(\mu, \sigma)$ removed all couplings between the spins σ and σ' which lie close to the μ . Since, in our case, it is the x direction coupling

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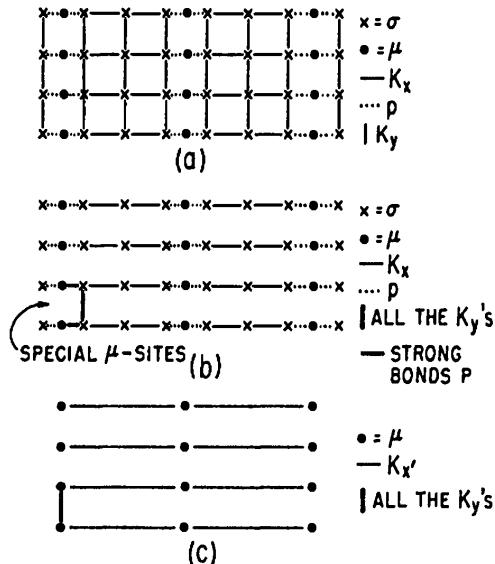


FIG. 12. The block transformation in two dimensions. Part (a) shows the geometry before moving; (b), afterwards; and part (c) shows the result of the summation.

which connects σ and σ' , the corresponding conditions in the present case are $u(\sigma, \sigma') = K_x(\sigma, \sigma')$ (see Eq. (2.21)) and

$$\tilde{K}(K_x) = 2\tilde{K}(p)$$

(see Eq. (2.22)).

Now let us assume that we can, for the moment, forget about K_y, K_z, \dots because they have been “moved away” via the potential moving trick. If so, the same argument as at the end of Section II B implies that we can perform all sums over σ and find

$$K'_x = R_0^{n+1}(K_x). \quad (3.24)$$

Next we must decide what to do with all the other couplings K_y, K_z, \dots . Imagine that we move all the K_y couplings to one special spot on the lattice. Hence, if there are N sites on the original lattice and $N' = N/(n + 1)$ sites on the new lattice, the coupling on this special bond is (see Fig. 12b)

$$K_y(\sigma, \sigma') = NK_y(\sigma, \sigma') = N'(n + 1) K_y(\sigma, \sigma'). \quad (3.25a)$$

To get the Migdal approximation, we move enough $p(\sigma, \mu)$ -type couplings to the other sites to make the coupling of the μ 's nearest the special bond infinitely tightly coupled to their corresponding σ 's, i.e., to make the special bond $P(\sigma, \mu)$ where

$$e^{P(\sigma, \mu)} = \delta(\sigma - \mu). \quad (3.25b)$$

In a moment, we shall argue that we can construct the “strengthened” bond (3.26) with a motion so weak that we can, in effect, not disturb any of the other bonds in the lattice. Figure 12c shows that the couplings (3.25a) and (3.25b) lead to a new bond $\hat{K}_y'(\mu, \mu')$ defined by

$$e^{\hat{K}_y'(\mu, \mu')} = \text{tr}_{\sigma} \text{tr}_{\sigma'} e^{P(\mu, \sigma) + K_y(\sigma, \sigma') + P(\sigma' \mu')}$$

so that

$$\hat{K}_y'(\mu, \mu') = N'(n+1) K_y(\mu, \mu'). \quad (3.26)$$

The potential moving trick allows us to move this new potential to any nearest-neighbor bonds between two μ 's separated by one unit in the y -direction. We in fact distribute the new coupling (3.26) equally among the N' such bonds and then find a new coupling

$$K_y' = (n+1) K_y. \quad (3.27)$$

Equation (3.24) and (3.27) are the two basic pieces of the Migdal approximation, Eqs. (3.11). Hence, we have once more derived this approximation—but now as a result of a block transformation instead of a decimation.

Finally, we must fill one gap in the proof. To gather together the potential $P(\sigma, \mu)$ in Eq. (3.25b) we must decrease the coupling $p(\sigma, \mu)$ at every other place by an amount $P(\sigma, \mu)/N'$. For sufficiently large N' , this change in $p(\sigma, \mu)$ can be made to be infinitesimally small. Hence, the construction of the bond (3.25b) does not interfere with any of our other evaluations, e.g., Eq. (3.24), of any other part of the recursion.

F. The Correlation Function Identity

Thus, the basic Migdal approximation does appear as a lowest-order consequence of a transformation scheme which does not fully share the correlation function problems of the decimation scheme. However, some portion of the correlation function troubles do remain. To see the new troubles, derive an analog of Eq. (3.18) for the block transformation approach.

This derivation starts from Eq. (2.14), which defines the probability function for the new variable, μ , given the values of the neighboring spins σ and σ' . Then, the average of μ , given σ and σ' , can be expressed by the function

$$M(\sigma, \sigma') = \text{tr}_{\mu} \mu t(\mu, \sigma, \sigma'). \quad (3.28)$$

Then the block transformation gives a correlation function identity which is—instead of Eq. (3.28)—the more complex result

$$\langle \mu(r_1) \mu(r_{11}) \rangle_{H'} = \langle M(\sigma_1, \sigma'_1) M(\sigma_{11}, \sigma'_{11}) \rangle_H. \quad (3.29)$$

Here σ_1 is an abbreviation for $\sigma(r_1 + L\hat{e}_x/2)$ and σ_1' means $\sigma(r_1 - L\hat{e}_x/2)$, with \hat{e}_x being a unit vector in the x -direction.

In general, $M(\sigma, \sigma')$ can be a complex function of the invariant $\sigma \cdot \sigma'$. Therefore, in the general case, Eq. (3.29) provides no restriction on the correlation function which is incompatible with the expected form of critical correlations.

Troubles only arise when $p(\mu, \sigma)$ is chosen to make $M(\sigma, \sigma')$ particularly simple. For example, imagine that

$$M(\sigma, \sigma') = (b/2)(\sigma + \sigma') \quad (3.30)$$

where b is some constant. Then Eq. (3.29) has the implication for $|r_1 - r_{11}| \rightarrow \infty$

$$\langle \mu(r_1) \mu(r_{11}) \rangle_{H'} \approx b^2 \langle \sigma(r_1) \sigma(r_{11}) \rangle_H. \quad (3.31)$$

Now imagine that d transforms are performed, changing the lattice constant from L to λL . Since the correlation function at the fixed point is supposed to vary as

$$|r_1 - r_{11}|^{-[d-2+\eta]}$$

we find that Eq. (3.31) implies

$$b^{2d} = \lambda^{d-2+\eta}. \quad (3.32)$$

Thus, if (3.30) is satisfied, the fixed point only really makes sense, at least in a simple way, if b obeys Eq. (3.32).

This restriction can actually be exploited in some favorable situations in which the variational principle is used to choose p (and hence b) to optimize the free energy. Then a value for η automatically comes out of the calculation via Eq. (3.32).

However, if the representation is simple and if Eq. (3.30) is satisfied, troubles do remain. The simple representations obey $\mu\mu^+ = 1$. If $t(\mu, \sigma, \sigma')$ has the interpretation of a probability then the Schwartz inequality implies that $|b|^2 \leq 1$, so that Eq. (3.32) then implies the result

$$d - 2 + \eta \leq 0. \quad (3.33)$$

Equation (3.33) is not expected to hold for any real physical system with dimensionality ≥ 2 . Hence, the simplicity of the representation is incompatible with the simple form (3.30).

In general, by choosing a $p(\mu, \sigma)$ which has some moderately complex behavior, we can get a $M(\sigma, \sigma')$ which is more complex than that given by Eq. (3.30) and avoid the difficulty expressed by the false result (3.33). However, in one special case, the Ising case, Eq. (3.30) necessarily holds because there is no other possible form for an $M(\sigma, \sigma')$ which is odd under $\sigma \rightarrow -\sigma, \sigma' \rightarrow -\sigma'$. Thus, for all cases save the Ising case, the use of the block transformation (2.13)–(2.15) can eliminate

the correlation function difficulty. In the Ising case, a more complex transformation involving more than two σ 's must be used.

F. Block Transforms in the Gauge Case

The block transform scheme may also be extended to the gauge case. The basic geometry for this situation is shown in Fig. 13. The "new" μ -variables are introduced in a transformation function $t(\mu, \sigma, \sigma')$ just like that in Eqs. (2.33) and (2.34). In addition, there are "old" μ -variables which are just products of $(n + 1)$ of the spin variables.

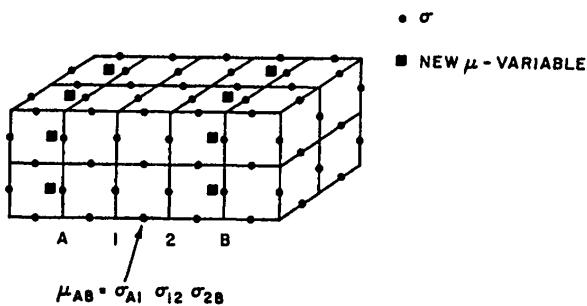


FIG. 13. The block transforms for the gauge system.

To make the x decimation work, we once again adjust p to cancel all interactions in the plaquette containing the new μ -variables. Then all couplings K_{xy}, K_{xz}, \dots can be included in sums exactly as before. Once again we handle the hard couplings (K_{yz}, K_{yt}, \dots) by moving them entirely onto specially strengthened bonds. Nothing new happens. In the end, we simply rederive Eqs. (3.19) via this new scheme.

However, because the new scheme does not lead to the false result (3.23), we may be hopeful that it provides a suitable starting point for further approximations.

IV. FOURIER TRANSFORM POTENTIAL-MOVING

One of the major defects of potential-moving approximations outlined in the previous chapter is that they apparently tend to become worse and worse as the potential gets stronger and stronger. With increasing potential strength, the potentials to be moved get stronger, and the error apparently will grow as the square of the potential strength.

However, it would appear that the Migdal approximation is actually most accurate for strongly coupled systems. Clearly, our arguments so far are incapable of explaining this domain of accuracy. For this reason, we seek another kind of potential-moving; one which might apply to strongly coupled systems. In this

search, we shall utilize a generalization of the "Fourier transform" technique which led to \tilde{K}^ν . Once again, we shall argue that $\tilde{K}^\nu - \tilde{K}^0$ is small for strongly interacting systems and that therefore we can get a good approximation by moving this small potential from place to place.

A. Construction of the Lower Bound Approximation

Start from the expression for the partition function

$$Z = \text{Tr}_\sigma e^{-H(\sigma)}. \quad (4.1)$$

Express the Hamiltonian as a sum of terms of the form

$$-H(\sigma) = \sum_r K(s_r). \quad (4.2)$$

Here s_r is a composite variable which depends upon a small number of different $\sigma(r)$: those lying within a specified neighborhood of the point r . For example, in the case of a two-dimensional system, s_r might be an abbreviation for the four variables $\sigma(r)$ at the corners of a square centered at r .

Now rewrite the partition sum, (4.1), by expanding each term in $\exp -H(\sigma)$ in the form

$$e^{K(s_r)} = \sum_\gamma \chi_\gamma(s_r) e^{\tilde{K}^\nu}. \quad (4.3)$$

In Eq. (4.3), $\chi_\gamma(s)$ form a set of basis functions which, for the moment, we will choose to be any set which is sufficiently complete so that the expansion (4.3) works. The rewritten partition sum now takes the form

$$Z = \text{Tr}_\gamma e^{-H(\gamma)} WT(\gamma). \quad (4.4)$$

In this sum, the Tr_γ stands for a sum over all the γ -variables at all the different points r . In symbols

$$\text{Tr}_\gamma = \prod_r \sum_{\gamma(r)}. \quad (4.5)$$

Then, $H(\gamma)$ represents the sum over the $\tilde{K}^{\nu(r)}$ which appear as factors in Eq. (4.3), i.e.,

$$-H(\gamma) = \sum_r \tilde{K}^{\nu(r)}. \quad (4.6)$$

Finally, the factors of χ_γ and the Tr_σ are subsumed in the weight factor

$$WT(\gamma) = \text{Tr}_\sigma \left[\prod_r \chi_{\gamma(r)}(s_r) \right]. \quad (4.7)$$

In going from Eq. (4.1) to (4.4), we have attained a rewriting of the partition sum in terms of new summation variables $\gamma(r)$ and new potentials \tilde{K}^γ at the cost of introducing the complicated weighting factor (4.7). We are about to engage in potential-moving in which we move the "Fourier transform" potentials $K^{\gamma(r)}$ from point to point in the lattice. Strictly speaking, such potential-moving will result in an approximation to Z which gives a lower bound to the free energy if the following two conditions hold:

1. the potentials \tilde{K}^γ are all real
2. the weight $WT(\gamma)$ is positive semi-definite

$$WT(\gamma) \geq 0 \quad \text{for all } \gamma. \quad (4.8)$$

We shall describe expansions (4.4) which satisfy these conditions as *ferromagnetic expansions* of the partition function.

In general, it is difficult to specify the conditions under which an expansion like (4.4) will indeed be a ferromagnetic expansion. However, one can see some of the conditions which are appropriate to the case in which the underlying variables $\sigma(r)$ are Ising spins. In that case, Eq. (4.8) will indeed be satisfied whenever $\chi_\nu(s)$ is a sum of products of $\sigma(r)$'s with all terms in the sum having positive coefficients. Furthermore, there exists an expansion into such a set $\chi_\nu(s)$ with real potentials \tilde{K}^γ , i.e., positive coefficients e^{K^γ} , whenever all the couplings in the original Hamiltonian $-H(\sigma)$ are ferromagnetic i.e., a sum of positive coefficients times products of $\sigma(r)$'s.

It is possible, but we have not proved, that a ferromagnetic expansion may exist for a whole class of Hamiltonians in which the interactions are (in some sense) all of one sign. If the basic variables $\sigma(r)$ are simple, it is natural to look for such expansions in terms of $\chi_\nu(s)$ which are simple generalizations of the character functions $\chi_\nu(\sigma, \sigma')$ which we considered heretofore.

Now, we can state our basic approach with some precision. Replace the exact calculation (4.4) by an expression for an approximate partition function

$$Z^A(\lambda) = \text{Tr}_\gamma e^{-\tilde{H}(\gamma) + A(\gamma)\lambda} WT(\gamma) \quad (4.9)$$

where the potential-moving term is

$$A(\gamma) = \sum_r \delta(r, \gamma(r)). \quad (4.10)$$

To make the total potential added equal to the total potential subtracted for all γ , we require

$$\sum_r \delta(r, \gamma) = 0 \quad \text{for all } \gamma. \quad (4.11)$$

The exact partition function is $Z(0)$; the approximate partition function is

$$Z^A = Z(\lambda)|_{\lambda=1}.$$

We can now simply prove the following two statements

$$(dZ(\lambda)/d\lambda)|_{\lambda=0} = 0$$

$$(d^2Z(\lambda)/d\lambda^2) \geq 0 \quad \text{for a ferromagnetic expansion.}$$

These two statements imply $Z^A > Z$ or that the approximate free energy is a lower bound on the exact free energy.

B. The Migdal Approximations

We are about to perform once more the Migdal decimation upon a system with two-body nearest neighbor interactions of the form $K_i(\sigma, \sigma')$ with σ and σ' being simple representations of the symmetry of K_i . In particular, the bond structure looks like that in Fig. 14a. We shall not touch the bonds in the directions orthogonal to x , but we shall move the \tilde{K}' 's in the x -bond. These \tilde{K}' 's are defined as before by the statement

$$e^{K_z(\sigma, \sigma')} = \sum_y \chi_y(\sigma, \sigma') (e^{\tilde{K}_y}/g). \quad (4.12)$$

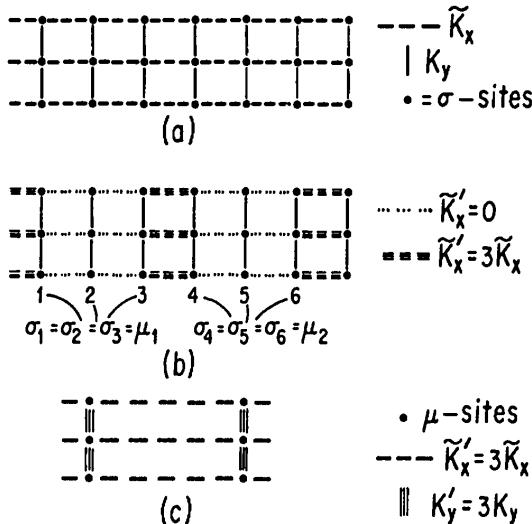


FIG. 14. Fourier transform potential-moving. Part (a) gives the configuration before the move; Part (b) gives the situation afterward. In Part (c), the delta functions are used to introduce the new variables, μ .

Move these bonds to produce the configuration shown in Fig. 14b. The sites connected by the dotted lines have a new bond strength

$$(\tilde{K}_{x''})' = 0 \quad (4.13a)$$

while the remaining x -bonds have the bond strength

$$(\tilde{K}_{x'})' = (N + 1) \tilde{K}_{x'}. \quad (4.13b)$$

Here n is the number of donor bonds for each recipient. The $K_x(\sigma, \sigma')$, $K_z(\sigma, \sigma')$, ... bonds remain untouched.

Now comes the key point. The new “bonds” (4.13a), with $\tilde{K}_x = 0$, have a coupling strength which is, in the conventional representation

$$e^{K_x(\sigma, \sigma')} = \sum_{\nu} (\chi_{\nu}(\sigma, \sigma')/g) = \delta_{\sigma, \sigma'}. \quad (4.14)$$

Therefore in the conventional picture these bonds are infinitely strong. They then force $(n + 1)$ consecutive σ -variables to be equal to one another. Call the common value of these σ -variables μ . Then the derived coupling picture is shown in Fig. 14b, where we have collapsed the equal σ -variables onto one another. Notice that the new y -direction coupling is

$$K_y'(\mu, \mu') = \lambda K_y(\mu, \mu'). \quad (4.15a)$$

The new x direction coupling has \tilde{K} increased by a factor of λ . We have expressed such an increase in terms of K_x as

$$K_x' = R_0(\lambda) K_x \quad (4.15b)$$

Equations (4.15) are; once more, the basic Migdal approximation. But now they have been derived by moving \tilde{K}_x , a motion which can be expected to be particularly accurate in the limit of strong couplings, $K_x(\sigma, \sigma')$.

Precisely the same technique serves to derive the Migdal result in the case of gauge symmetry. For the basic plaquette, shown in Fig. 15, the coupling term can be expanded as

$$e^{K(\sigma_{12}\sigma_{23}\sigma_{34}\sigma_{41})} = \sum_{\beta} e^{\tilde{K}\beta} \chi_{\beta}(\sigma_{\nu}, \sigma_{\nu'})/g. \quad (4.16)$$

We can make a large number of different choices of the pair of conjugate variables $\sigma_{\nu}, \sigma_{\nu'}$ including for example

$$\begin{aligned} \sigma_{\nu} &= \sigma_{12} \sigma_{23} \sigma_{34} \sigma_{41} & \sigma_{\nu'} &= 1 \\ \sigma_{\nu} &= \sigma_{12} \sigma_{23} \sigma_{34} & \sigma_{\nu'} &= \sigma_{14} \\ \sigma_{\nu} &= \sigma_{12} \sigma_{23} & \sigma_{\nu'} &= \sigma_{34} \sigma_{41}. \end{aligned} \quad (4.17)$$

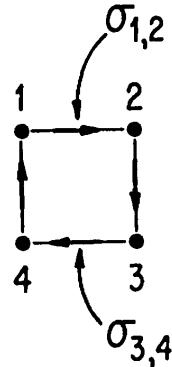


FIG. 15. A basic square.

All these choices give the very same expansion, (4.16). The key point for our further analysis is that if \tilde{K}^g is moved away so that the sum in Eq. (4.16) is replaced by

$$Z_0 = \sum_g \frac{\chi_g(\sigma_y, \sigma_{y'})}{g} \quad (4.18a)$$

then the result of the sum is

$$Z_0 = \delta_{\sigma_y, \sigma_{y'}}. \quad (4.18b)$$

The rest of the calculation is relatively direct. Refer once again to Fig. 11. As before, we take four-spin interactions of the form (4.16) on each of the cube faces. These interactions are labeled as K_{xy} , K_{xz} , and K_{yz} to indicate the orientation of the face. Apply the expansion (4.16) to the K_{xy} and K_{xz} couplings. Move all the interactions \tilde{K}_{xy}^g and \tilde{K}_{xz}^g from the shaded faces into the nearest unshaded plaquette of the same orientation. Thus, an unshaded plaquette like the one labeled "A" ends up with a new interaction

$$(\tilde{K}_{xy}^g)' = (n + 1) \tilde{K}_{xy}^g \quad (4.19a)$$

The shaded faces then attain the trivial, infinitely strong, interaction (4.18).

Because of this trivial interaction, one can do the sums shown in the figure immediately. The σ 's indicated by the crosses are summed; the remaining σ 's define the new variables μ by the scheme shown in the figure. The net result of these sums is very simple. The coupling strengths in unshaded plaquettes like A remain the same but the variables in these couplings are converted into μ 's. Thus, Eq. (4.19a) defines correctly the new xy-plane coupling. For the coupling "D" the delta functions leave K_{yz} unchanged but, in effect, move it two steps to the right,

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into a position adjacent to C . Thus, the new $y-z$ couplings are the sum if these "moved" potentials are

$$K'_{y*} = (n + 1) K_{y*}. \quad (4.19b)$$

Equations (4.19) may be recognized to be once more the Migdal approximation—now derived for the case in which K_{xz} and K_{xy} are very strong potentials.

C. Extensions of Method

The Fourier transform version of potential moving seems to have a very broad range of applications. I have looked at Ising problems in the range of dimensionalities between $d = 1$ and $d = 3$ and applied this type of potential moving to coupling clusters $K(s)$ involving 2, 3, 4, ..., 8 spins at a time. The results look quite reasonable for all the fixed points and eigenvalues which appear in the cases $1 < d \leq 2$. In these cases, the coupling does appear strong enough to make the basic method work. Details will be reported in future publications.

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14.6.5 Migdal's Original Papers

Recursion equations in gauge field theories

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 (Submitted April 28, 1975)
 Zh. Eksp. Teor. Fiz. 69, 810-822 (September 1975)*

An approximate recursion equation is formulated, describing the scale transformation of the effective action of a gauge field. In two-dimensional space-time the equation becomes exact. In four-dimensional theories it reproduces asymptotic freedom to an accuracy of 30% in the coefficients of the β -function. In the strong-coupling region the β -function remains negative and this results in an asymptotic prison in the infrared region. Possible generalizations and applications to the quark-gluon gauge theory are discussed.

PACS numbers: 11.10.Np

INTRODUCTION

Many experiments favor the model of confined quarks. According to this model the quarks are relatively light and are almost free inside the hadrons. The forces between the quarks must increase with the distance, as if they were connected by strings. Recently a hypothesis was put forward^[1] according to which such strings are formed from the non-Abelian gauge fields called gluons which interact with the color of the quarks.

As was stressed by Wilson,^[2] it is essential for this that the vacuum be gauge-invariant. Then there arise local selection rules which interdict the decay of gauge-invariant excitations such as

$$\hat{V}(r) \hat{T} \exp\left\{i \int B_i dr_i\right\} \psi(0) |0\rangle, \quad (0)$$

into free quarks ψ and gluons B , or into other colored objects. The local selection rules follow directly from the transformation laws of the fields

$$\begin{aligned} \Omega \psi_s(r) \Omega^+ &= S(r) \psi_s(r), \\ \Omega B_i \Omega^+ &= S^{-1}(r) B_i S(r) - i S^{-1}(r) \partial_i S(r) \end{aligned}$$

and the invariance of the vacuum $\Omega |0\rangle = |0\rangle$.

The usual vacuum of quantum electrodynamics which is realized in perturbation theory is not gauge-invariant. It is filled with the longitudinal field which participates in the gauge transformations, so that the local selection rules are inapplicable. They are replaced by the infrared catastrophe: charged objects are accompanied by transverse quanta which are Goldstone excitations in that degenerate vacuum.

The existence of an invariant vacuum was proved in two-dimensional models^[3], and, what is more interesting, in four-dimensional lattice gauge theories in the strong coupling region^[4,5]. Strong coupling implies a large bare coupling constant g_0 and a large bare mass m_0 of the quark (measured in units of the cutoff radius a^{-1}). The state $|0\rangle$ becomes in this limit an eigenstate with the energy

$$V(r) = \sigma r/a.$$

The energy is confined to the lines of the electric field which join the quarks and this is a prototype of the string.

In Lagrangian language in Euclidean space the electric forces manifest themselves as the contribution $\sim \exp\{-\text{area of the quark loop}\}$ ^[2]. More precisely, the contribution of a quark loop (e.g., to two-current Green's function) is proportional to $\exp(-\sigma S/a^2 - \rho P/a)$, where P is the length of the quark loop and S is the area surrounded by it. Summation over all loops and surface areas is understood; the details can be found in

Wilson's paper^[2].

The coefficients σ and ρ depend on the bare parameters g_0 and $m_0 a$. In the local limit $a \rightarrow 0$ these parameters should be varied in such a manner that the zeroes of σ and ρ are determined. Then, most likely, one will arrive at the dual string models^[6].

On the other hand, in the local theory there exists the notorious asymptotic freedom. This means that if we let g_0 tend to zero according to the law $c_1/(c_2 - \ln a)$ with an appropriate constant c_1 we obtain the local limit of the lattice theory. The second bare parameter $m_0 a$ must also be made to tend to zero if γ_5 -invariance, which removes the linear divergences in the self-energy, is respected.

Now there appears a difficulty, since this limit is opposite to the strong-coupling limit where the invariance of the vacuum was proved. A phase transition to the usual vacuum might take place for some g_0 and $m_0 a$, such that $\sigma \equiv 0$. The phase transition problem is related to the existence of fixed points of the renormalization group. If there are no fixed points except the free ultraviolet one then the effective interaction will increase indefinitely in the infrared region, which apparently characterizes the asymptotic prison, i.e., the absence of a phase transition (^[6], and also G. 't Hooft, communication at the Marseille Conference, 1972).

In brief, the situation is as follows: in usual perturbation theory the ultraviolet freedom is obvious and the infrared prison causes problems, whereas in the lattice strong coupling expansion it is the other way around. If, as we hope, both the prison and the freedom coexist in the same theory, a third computational method is needed, which is not related to the strength of the interaction.

We intend to develop numerical renormalization group methods analogous to the recursion equations of statistical mechanics.^[7] The main problem is connected with the requirement of local gauge invariance. In the present paper we propose a first version of a gauge recursion equation which is as yet far from perfect. Nevertheless this equation is sensitive to the existence of phase transitions. We have verified this on the example of the discrete gauge group Z_2 and on the Abelian group $U(1)$, where the existence of a phase transition is known. In the non-Abelian theory the equation yields a phase transition for dimension $D > 4$ and no phase transition for $D \leq 4$.

1. THE EFFECTIVE ACTION OF THE GAUGE FIELD

The classical action of the gauge field proposed by Yang and Mills

$$A_{cl} = - \int d^D x \sum_{\mu} \frac{1}{4g_{cl}^2} \text{Tr}(\partial_\mu B_\nu - \partial_\nu B_\mu + i[B_\mu, B_\nu])^2 \quad (1)$$

needs to be redefined in quantum theory. In addition to the usual ultraviolet divergences related to the infinite number of degrees of freedom per unit volume, the functional integrals contain divergences related to the invariance of the action under local gauge transformations

$$B_\mu \rightarrow S^{-1}(x) B_\mu S(x) - iS^{-1}(x) \partial_\mu S(x). \quad (2)$$

The most adequate method of regularization for our problem is to consider (1) as the limit of a lattice theory. Gauge transformations on a lattice have been considered in [2, 8] and independently by Polyakov in 1974 (private communication). One carries out a Wick rotation, after which the D-dimensional Euclidean space is split up into the cells of a hypercubic lattice. The action of the lattice theory is represented as the sum of the actions of each cell

$$A_{cell} = \sum_i A(x_i). \quad (3)$$

The action $A(x)$ of one cell depends on the loop products

$$v_x = \prod_{\Gamma} \exp(iB_\mu(y) \Delta y_\mu). \quad (4)$$

Here \prod_{Γ} denotes the product of matrices ordered along the loop Γ in the boundary of the cell, Δy_μ are the sides of the loop and $B_\mu(y)$ are the gauge fields at the centers of the sides. Thus, the loop product around the square in Fig. 1 is of the form

$$v_{xx} = \exp\{iB_\mu(x - \frac{1}{2}ae_\mu)\} \exp\{iB_\mu(x + \frac{1}{2}ae_\mu)\} \\ \times \exp\{-iB_\mu(x + \frac{1}{2}ae_\mu)\} \exp\{-iB_\mu(x - \frac{1}{2}ae_\mu)\}. \quad (4')$$

The traces of closed loop products are invariant with respect to generalized gauge transformations

$$\exp\{iB_\mu(y)\} \rightarrow S^{-1}(y - \frac{1}{2}ae_\mu) \exp\{iB_\mu(y)\} S(y + \frac{1}{2}ae_\mu). \quad (5)$$

The traces can be calculated in any representation of the group. The traces in unitary irreducible representations p , i.e., the characters $\chi_p(v)$ of the group element v , will play a distinguished role in the sequel.

A simple example for the cell action has been proposed by Wilson [2]:

$$A(x) = \sum_{\Gamma} \frac{1}{4g_s^2} [\chi_{adj}(v_\Gamma) - \chi_{adj}(I)]. \quad (6)$$

where χ_{adj} is the character in the adjoint representation.

As $a \rightarrow 0$ the loop products reduce to the components of the field strength $B_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu + i[B_\mu, B_\nu]$ so that the classical lattice action (3), (6) reduces to the classical action (1) in the naive local limit ($g_s^2 a^4 \rightarrow 0$ fixed). For this it suffices that the loops Γ be situated in all possible $\mu\nu$ planes leading to the appearance of all terms in the sum

$$\sum_{\mu\nu} \text{Tr } B_{\mu\nu}^2.$$

The existence of the local limit of the classical action does not yet guarantee that the quantum theory will be local. First of all there must exist a sufficient number of connections between the cells, i.e., the same field B_μ must enter into sufficiently many actions of neighboring cells. The number of connections depends on the loops Γ . Thus, in the Wilson model the loops consist of the four edges of the cell (Fig. 2 for $D = 3$). Then each field corresponds to an edge and enters into

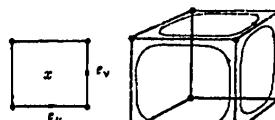


FIG. 1

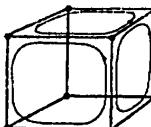


FIG. 2

the actions of $2(D - 1)$ cells with a common edge. This number of connections is sufficient to correlate the quantum fluctuations over the whole lattice. The correlations of fluctuations over distances much larger than the lattice unit must go over into the Green's functions of the local $O(D)$ -invariant theory.

The lattice systems are quantized by means of the usual integration of e^A over the fields. One must only worry about the gauge invariance, and for this one equips the integration with the group invariant measure $d\Omega(e^{iaB})$. The gauge invariance of this measure follows from the multiplicativity

$$d\Omega(v) = d\Omega(vu) = d\Omega(uv). \quad (7)$$

In all practically important cases explicit expressions are known for the group measure. Thus, in the case of $SU(2)$

$$d\Omega(v) = \frac{a}{8\pi^2} \frac{d^3 B}{B^3} \sin^2\left(a \frac{|B|}{2}\right). \quad (8)$$

We have used the spin $\frac{1}{2}$ representation: $B = B \cdot \tau/2$,

For compact groups the integration volume is finite, e.g., $|B| < 4\pi/a$, for $SU(2)$, so that there is no need to add to the action terms which determine the gauge and ensure convergence. In the sequel all integrations over the fields reduce to the orthogonality relation

$$\int d\Omega(v) \chi_p(v) \chi_p(v^\dagger v) = \frac{\chi_p(v) \delta_{p,p}}{d_p}, \quad (9)$$

where $d_p = \chi_p(I)$ is the dimension of the representation p . A more detailed discussion of the formalism of gauge theories on a lattice can be found in [2, 4, 8].

We must now define the effective action. We join 2^D neighboring cells into one cell with twice the edge length and integrate the expression

$$\exp\left\{\sum_{i=1}^D A(x_i)\right\}$$

over all the internal fields, fixing the values of the fields on the boundary. We call this integral the correlation functional Z_{2a} and its logarithms the effective action A_{2a} of the doubled cell. When such an integration is carried out over the whole volume we obtain the doubled lattice with the effective action replacing the bare action. Since the effective action is gauge invariant, it depends on the loop products along the boundaries of the doubled cell. The new loops consist of portions of the old ones and in the general case the number of loops increases. Repeating this operation (this is the recursion) we gradually integrate over all the fields.

The recursion equation which relates cells of sizes $2L$ and L can symbolically be written in the form:

$$Z_{2L} = R(Z_L). \quad (10)$$

It is convenient to separate the averages

$$\langle Z_L \rangle = \int \prod_{\Gamma} d\Omega(v_\Gamma) Z_L, \quad (11)$$

by introducing the normalized correlation functional

$$W_L = Z_L / \langle Z_L \rangle. \quad (12)$$

We are then led to the normalized recursion equation

$$W_L = \hat{R}[W_L]/\langle \hat{R}[W_L] \rangle \quad (13)$$

and to the equation for the average

$$\langle Z_L \rangle = \langle Z_L \rangle^{10} \langle \hat{R}[W_L] \rangle. \quad (14)$$

The latter equation can be solved in general form (we have set $\langle Z_0 \rangle = 1$):

$$\langle Z_L \rangle = \exp \left\{ L^D \sum_{n=1}^{\infty} L_n^{-D} \ln \langle \hat{R}[W_{L-n}] \rangle \right\} \quad (15)$$

$a \ll L, L \gg 2^n a \ll L.$

This quantity is related to the energy spectrum of a cube of size L with periodic boundary conditions^[2]

$$\langle Z_L \rangle = T \exp \{-L \hat{H}(L)\}. \quad (16)$$

For $L \rightarrow \infty$ we obtain the energy density of the vacuum in the infinite system:

$$\epsilon = - \sum_{n=1}^{\infty} L_n^{-D} \ln \langle \hat{R}[W_{L-n}] \rangle. \quad (17)$$

Subtracting L^{D-1} from the Hamiltonian, we obtain the relation

$$\sum_{n=1}^{\infty} L_n^{-D} \ln \langle \hat{R}[W_{L-n}] \rangle = L^{-D} \ln T \exp \{ \epsilon L^D - L \hat{H}(L) \}. \quad (18)$$

The right-hand side contains all possible surface corrections to the vacuum energy density, and the contribution of the excited states is of the order e^{-mLD-D} , where m is the lowest mass. Thus, the asymptotic behavior of the W -functional is related to the mass spectrum.

In principle the lowest mass can be found directly, introducing the sources of the appropriate quantum numbers. We do not intend to discuss this question now, but hope to return to it after the quarks have been included.

The fixed points of the renormalization group are the solutions of the normalized recursion equation which do not depend on L . Asymptotic freedom corresponds to the quadratic action (1) with $g_C^2 \rightarrow 0$, i.e., to a delta-function like fixed point $W \sim \Pi \delta(B_{\mu\nu})$. This fixed point must be realized in nonabelian theories at small distances. The asymptotic prison for $L \rightarrow \infty$ corresponds to vanishing action, i.e., $W = 1$ is the unit fixed point. This fixed point exists on account of the compactness of the gauge group, otherwise the integrals over the fields would diverge in $\hat{R}[W]$ for $W = 1$.

If there are no other fixed points, the W -functional will change from the delta-functional to one as L varies from zero to infinity. The vacuum energy in (17) will diverge for $L \sim a \rightarrow 0$, but the excitation energy will be determined by the region $L^{-1} \sim 1 \text{ GeV}$. Apparently they will correspond to dual models (after quarks are included into the recursion equations).

In order to realize this program one must approximate the functional recursion equations by means of integral equations, reducing the number of degrees of freedom.

2. A TWO-DIMENSIONAL GAUGE THEORY

We start with the trivial example of a two-dimensional theory. Usually the two-dimensional theory is solved in the Coulomb gauge $B_t = 0$, when the commutator $[B_\mu, B_\nu]$ vanishes. This theory exhibits ultra-violet freedom and an infrared prison simply because

the Coulomb potential is proportional to the distance. We reproduce these results with the help of the recursion approach, in order to develop an apparatus which will be useful in the four-dimensional theory.

The elementary cell of the two-dimensional lattice is the square in Fig. 1. There is only one loop product (4') along the perimeter of the square. We consider two neighboring cells 1 and 2 and determine the correlation functional Z_{12} of the joint cell 1 + 2 (Fig. 3). We have to calculate the integral

$$Z_{12} = \int d\Omega(u) Z_{12}(u, u^*) Z_{12}(uu_1) \quad (19)$$

over the internal field $u = \exp[iaB((x_1 + x_2)/2)]$. We have separated from the loop products v_1 and v_2 the matrices u corresponding to the common part of the loops. The matrices u_1 and u_2 correspond to the remaining parts of the contours; their product $v_{12} = u_1 u_2$ corresponds to the perimeter of the joint cell.

The integral is calculated by means of the Fourier expansion on the group

$$Z_{12}(r) = \sum_p Z_{12} d_{p, Y_p}(v). \quad (20)$$

Making use of the orthogonality relation (9) we find

$$Z_{12} = \sum_p Z_{12}^p d_{p, Y_p}(v_{12}). \quad (21)$$

It is clear that the form of the Z -functional reproduces itself when cells are joined together and the Fourier coefficients get multiplied.

It is easy to prove by induction that this rule does not depend on the form and size of the cells. If the boundary between two cells consists of several steps (Fig. 4), the integration with respect to the field of the first edge reduces to a traction, as above, after which the remaining inner fields cancel in the product $v_1 v_2$, since the common part of the loop has opposite orientations in the cells 1 and 2. Now the remaining integrations yield the unit volume of the group.

As a result the Z -functional for a region Γ with area S has the form

$$Z_{\Gamma}(v_{\Gamma}) = \sum_p (Z_{12})^{S/a^2} d_{p, Y_p}(v_{\Gamma}). \quad (22)$$

Here v_{Γ} is the loop product along Γ and S/a^2 is the number of elementary cells. This is the general solution of the 2-dimensional recursion equations.

In the local limit $a \rightarrow 0$ one must take the limit $Z_{a,p} \rightarrow 1 - a^2 \epsilon_p$, so that

$$Z_{\Gamma}(v_{\Gamma}) \rightarrow \sum_p \exp \{-S \epsilon_p\} d_{p, Y_p}(v_{\Gamma}). \quad (23)$$

The loop product v_{Γ} goes over into the T -exponential of the circulation

$$v_{\Gamma} \rightarrow \hat{T} \exp \left\{ i \oint_{\Gamma} B_x dx^x \right\}. \quad (24)$$

The vacuum expectation value corresponds to the zero Fourier coefficient

$$\langle Z_{\Gamma} \rangle = \exp \{ -S z_0 \}, \quad (25)$$

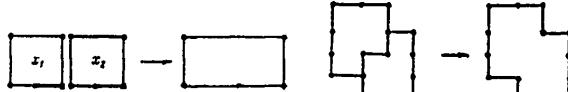


FIG. 3

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so that ϵ_0 is the vacuum energy density.

The normalization corresponds to the subtraction $\epsilon_p \rightarrow \epsilon_p - \epsilon_0$ in (23). These differences must be positive:

$$\epsilon_p - \epsilon_0 = g_s^2 > 0, \quad (26)$$

in order to yield a reasonable W-functional

$$W_s(v_r) = \sum_s \exp(-g_s^2 S) d_s \chi_s(v_r). \quad (27)$$

This functional varies from $W_0 = \delta(v - 1)$ to W_∞ , i.e., no phase transition that would violate the gauge invariance of the vacuum occurs.

We now introduce the fields ψ (colored quarks) belonging to the q-representation of the gauge group. The Green's function of the gauge invariant currents $J_\mu \sim \bar{\psi} \gamma_\mu \psi$ can be represented as sums over closed quark paths Γ of the quantity $\text{Tr } v_\Gamma^\dagger = \chi_q(v_\Gamma^\dagger)$, averaged over the gauge fields with the weight exp[action] (cf.^[2]).

For simplicity we consider only simply connected paths without self-intersections (such paths dominate^[3] for high-rank gauge groups). Integrating $\chi_q(v_\Gamma^\dagger)$ over all the fields we can first integrate over the fields inside Γ , which yields $W_S(v_\Gamma)$ and then outside, which yields $W_{\bar{S}}(v_\Gamma^\dagger)$. The external region S has infinite area, so that $W_{\bar{S}} = 1$. The remaining integrations over the fields on Γ will reduce, on account of the multiplicativity of the measure, to the simple integral over v_Γ :

$$\langle \chi_s \rangle = \int d\Omega(v_r) \chi_s(v_r) W_s(v_r). \quad (28)$$

This integral is easily calculated (only the quark representation contributes), and we find

$$\langle \chi_s \rangle = d_s \exp(-g_s^2 S). \quad (29)$$

This is none other than Wilson's law of areas.^[2]

In the usual solution of the two-dimensional theory this law follows from the one-dimensional Coulomb law $u(x) = g^2(T^2)q|x|$; in place of g^2 in (29) there appears $g^2(T^2)q$, where T^2 is the Casimir operator. The more general law (29) appeared because we have not required that the bare action go over into the Yang-Mills action in the local limit. This requirement is not necessary in the two-dimensional theory, where there is no renormalizability problem.

3. APPROXIMATE RECURSION EQUATIONS

In this section we propose approximate recursion equations for the D-dimensional gauge theory. We first consider the three-dimensional case. The Z-functional of a cube of size $L \gg a$ depends, generally speaking, on all possible loop products along its surface.

We approximate this functional by a function of the average loop products. The average loops are square contours with angles in the middles of the edges of the cube. There are a total of three such loops: γ_{xy} , γ_{yz} and γ_{xz} . They are situated in distinct planes (Fig. 5). We shall consider the average loop products as the independent variables and shall search for the Z-functional in the factorized form:

$$Z_L = F(L, v_{xy}) F(L, v_{yz}) F(L, v_{xz}). \quad (30)$$

When eight L-cubes are joined into one 2L-cube, the average loops are independently joined into larger contours in each plane. Thus, in the xy-plane four loops are joined into a square with transverse coordinate $z = -L/2$ and the other four into a square with

$z = L/2$ (Fig. 6).

The integration over the fields reduces to a contraction as in the two-dimensional case

$$\square = F(L, v) = \sum_s F_s(L) d_s \chi_s(v), \quad (31)$$

$$\square\square = \sum_s F_s(L) d_s \chi_s(v) = \Phi(v). \quad (32)$$

After this the Z-functional of the 2L-cube turns out to be factorized as in (30), but with

$$\Phi(v_{xy}(-L/2)) \Phi(v_{xy}(L/2)) \quad (33)$$

in place of $F(2L, v_{xy}(0))$, and similarly for yz and xz . Here $v_{xy}(z)$ is the loop product over the xy -square with side $2L$ and coordinate z .

As can be seen, our assumption (30) is not reproduced by the recursion equation—the average loop splits into two.

The splitting Δz is smaller than the size of the 2L-loop, so that in a rough approximation we may neglect it. We then obtain a recursion equation for F :

$$F(2L, v) = \left[\sum_s F_s(L) d_s \chi_s(v) \right]^2 \quad (34)$$

or, in the Fourier representation

$$F(2L) = \sum_{p,p_1} F_{p,p_1}(L) F_{p,p_1}(L) C_{p,p_1} \quad (35)$$

where

$$C_{p,p_1} = \frac{d_p d_{p_1}}{d_s} \int d\Omega(v) \chi_{p_1}(v) \chi_{p_1}(v) \chi_{p_1}(v) \chi_{p_1}(v) \quad (36)$$

is the appropriate Wigner coefficient.

We expect this equation to have a quantitative meaning when L is smaller than a typical Compton wavelength of the bound states: in this region there are no dimensional parameters, so that the splitting z should be compared only to $2L$. Then, since the terms linear in z cancel, the error may be small. Below we shall modify this equation somewhat to decrease the error.

First we wish to generalize the equation to the case of arbitrary dimension D of the space. We introduce $D(D-1)/2$ average loops $\gamma_{\mu\nu}$ on the d-dimensional cubic lattice. The angles of the squares $\gamma_{\mu\nu}$ are at the points $(x_\mu, x_\nu, \pm L/2, x_\lambda = 0)$, if the vertices of the cube are at the points $(\pm L/2, \pm L/2, \dots, \pm L/2)$.

In our approximation the Z-functional of the cube will be a product of functions of the average loop products:

$$Z_L = \prod_{\mu<\nu} F(L, v_{\mu\nu}(0)). \quad (37)$$

As above, the integration is carried out independently in each plane, and joining 2^D L-cubes into one 2L-cube, we obtain

$$Z_{2L} = \prod_{\mu<\nu} \prod_{z_\lambda=0} \sum_s F_s(L) d_s \chi_s(v_{\mu\nu}(z_\lambda)), \quad (38)$$

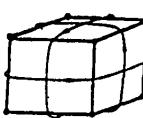


FIG. 5

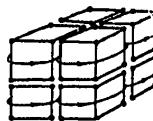


FIG. 6

where $x_{\perp,i} = \pm L/2$ ($i = 1, 2, \dots, D - 2$) are the transverse coordinates of the resulting $2L$ -squares. We now neglect the dependence on x_{\perp} of the $2L$ loop products $v_{\mu\nu}(x_{\perp})$, so that the form (37) is reproduced, and obtain the recursion equation

$$F(2L, v) = \left[\sum_p F_p(L) d_{pX_p}(v) \right]^{2-2}, \quad (39)$$

which generalizes (34).

The second generalization is the transition to an arbitrary change of scale $L \rightarrow \lambda L$ in place of the doubling. If our approach would be exact the results would not depend on λ , but the approximate equation can be improved by varying λ as an independent free parameter.

A scale transformation with nonintegral λ can be defined by means of the following trick. We first consider integral values of λ and find the corresponding recursion equation, joining λ^D cubes into one. Integration with respect to the internal fields yields, in place of (38)

$$Z_{\lambda L} = \prod_{i=1}^D \prod_{x_{\perp,i}} \sum_p F_p(L) d_{pX_p}(v_{\mu\nu}(x_{\perp})), \quad (40)$$

where

$$x_{\perp,i} = \pm \frac{1}{2} L, \pm \frac{1}{2} L, \dots, \pm \frac{1}{2} (\lambda - 1) L; \quad i = 1, 2, \dots, D - 2.$$

Neglecting the splittings $x_{\perp,i}$ we obtain

$$F(\lambda L, v) = \left[\sum_p F_p(L) d_{pX_p}(v) \right]^{2-2} = \hat{R}_\lambda [F(L)]. \quad (41)$$

For noninteger λ we define a recursion operation \hat{R}_λ by means of the same equation (41).

The relations (10)–(19) are also generalized to the case of an arbitrary scale parameter $\lambda \neq 2$. In particular, in place (15) and (16) we have

$$\langle Z_L \rangle = \text{Tr} \exp(-L \hat{R}[f(L)]) = \exp \left\{ L^{\alpha} \frac{D(D-1)}{2} \sum_i L_i^{-\alpha} \ln \langle \hat{R}_i[f(L_{i-1})] \rangle \right\}, \quad (42)$$

where $L_n = \lambda^n a$ and $f(L, v)$ satisfies the normalized equation

$$f(\lambda, L) = \hat{R}_\lambda [f(L)] / \langle \hat{R}_\lambda [f(L)] \rangle. \quad (43)$$

The averaging $\langle \dots \rangle$ denotes here an integration over the normalized group measure; the factor $D(D-1)/2$ in (42) appears on account of factorization.

4. ASYMPTOTIC FREEDOM AND THE INVARIANT VACUUM

The equation (41) is the main result of this paper. In a future paper we shall discuss in detail this equation for different theories. Now we demonstrate the renormalizability and the asymptotic freedom on the example of the gauge group $SU(2)$ and list some results obtained by numerical methods.

A representation of the group $SU(2)$ is characterized by the spin $T = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots$:

$$\chi_r(v) = \frac{\sin(T + \frac{1}{2})\theta}{\sin(\theta/2)}, \quad (44)$$

$$d_r = \chi_r(1) = 2T + 1. \quad (45)$$

In our case the angle θ corresponds to the Yang-Mills field strength.

We introduce the "vertices" $g_n(L)$, such that

$$F(L, v) = \exp \left\{ -g_0(L) - g_1(L) \frac{\theta^0}{2!} - g_2(L) \frac{\theta^0}{4!} - \dots \right\}. \quad (46)$$

The Fourier coefficients

$$F_r(L) = \int \frac{d\Omega}{4\pi} \frac{\sin(\theta/2) \sin(T + \frac{1}{2})\theta}{T + \frac{1}{2}} F(L, v) \quad (47)$$

can be characterized by another set of variables p_i :

$$F_r(L) = \exp \left\{ -p_0 - p_1 \left(T + \frac{1}{2} \right)^0 \frac{1}{2!} - p_2 \left(T + \frac{1}{2} \right)^1 \frac{1}{4!} - \dots \right\}. \quad (48)$$

The inversion formula (47) allows one to express the p_i in terms of the q_j . In terms of the functions $p_i(q_2, q_4, \dots)$ the recursion equation (44) can be rewritten as

$$\lambda^i p_i[q_n(L)] = p_i[\lambda^{1-\alpha} q_n(\lambda L)], \quad i = 2, 4, 6, \dots \quad (49)$$

These equations for $q_i(L)$ can be integrated with respect to the effective coupling constant

$$g^2(L) = 1/q_2(L). \quad (50)$$

As it should be in renormalized perturbation theory, the vertices q_4, q_6, \dots depend on L only through $g^2(L)$:

$$q_n(L) = A_n + B_n g^2(L) + C_n g^4(L) + \dots \quad (51)$$

The coefficients A_n, B_n, C_n, \dots are determined successively from (49) together with the expansion coefficients of $g^2(\lambda L)$ in powers of $g^2(L)$:

$$g^2(\lambda L) = \lambda^{1-\alpha} g^2(L) + \lambda^{1-\alpha} (\lambda^1 - \lambda^{1-\alpha}) g^4(L) + \dots \quad (52)$$

It is convenient to introduce the Gell-Mann–Low function

$$\beta(g^2) = -\frac{\partial g^2}{\partial \ln L} = (D-4)g^2 - \beta_1 g^4 - \beta_2 g^6 + \dots \quad (53)$$

Its coefficients are easily determined by differentiating (52) with respect to $\ln L$ and expressing in the left-hand side $g^2(\lambda L)$ in terms of $g^2(L)$ from (52).

In four-dimensional space we obtain

$$\beta_1 = (\lambda^1 - 1)/12 \ln \lambda, \quad (54)$$

$$\beta_2 = \lambda^3 \beta_1 / 12(\lambda^1 + 1). \quad (55)$$

These coefficients are positive for all λ , so that the effective coupling constant vanishes for $L \rightarrow 0$ according to the law

$$g^2(L) \rightarrow (\beta_1 t + \beta_2 t^2 \ln t)^{-1}, \quad (56)$$

$$t = \ln(L/L_0) \gg 1. \quad (57)$$

Here L_0 is some arbitrary normalization length. When L increases and approaches L_0 perturbation theory becomes inapplicable. In (47) there appear terms of the order

$$g^2(L) \exp \left\{ -\frac{2\pi^4}{g^2(L)} \right\} \sim \exp \left\{ -2\pi^2 \beta_1 \ln \frac{L_0}{L} - \left(3 + \frac{2\pi^2}{\beta_1} \right) \ln \ln \frac{L_0}{L} \right\} \quad (58)$$

determined by the upper integration limit. These terms lead to a rapid growth of the effective coupling constant. It is impossible to follow its behavior further by means of analytic methods and a numerical solution on a computer is required. Such a solution was obtained for $\lambda = \sqrt{2}$, when the equation (41) simplifies in the Fourier representation. The result for $g^2(L)$ is exhibited in Fig. 7.

It can be seen that the solution (56) corresponding to the first corrections of perturbation theory is valid almost up to L_0 . After that $g^2(L)$ increases like

$$g^2(L) \sim \exp \{ \text{const} \cdot (L/L_0)^4 \}. \quad (59)$$

The solution for $f_T(L)$ tends to the unit fixed point $f_T = 8T_0$ according to the law of areas:

$$f_T(L) \sim \exp \{ -\text{const} \cdot T(L/L_0)^4 \}. \quad (60)$$

(We recall that $f_T(L)$ has the meaning of the average

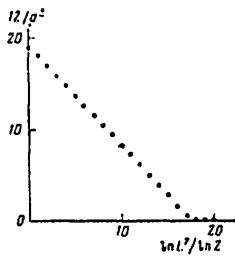


FIG. 7

loop product along the sides of the square of area L^2 , averaged over the fields.) Such a behavior corresponds to the absence of a phase transition.

It is interesting that $D = 4$ is the critical value of the dimension of space. For $D = 4 + \epsilon$ there will be a phase transition for $g_c^2 = \epsilon/\beta_4 + O(\epsilon^2)$, so that $f_T(\omega) = 1$ for $g_0^2 < g_c^2$ and $f_T(\omega) = \delta T_0$ for $g_0^2 > g_c^2$. For $D \leq 4$ there is never a phase transition.

In the general case the absence of a phase transition in a pure gauge theory in four dimensions corresponds to the following behavior of the function $\sigma(g_0^2)$ introduced by Wilson (cf. the Introduction)

$$\sigma(g_0^2) \rightarrow \exp\left(\frac{2\beta_4}{\beta_4^2} \ln \frac{1}{g_0^2}\right) \exp\left(-\frac{2}{\beta_4 g_0^2}\right) (c_1 + c_2 g_0^2 \ln g_0^2 + \dots). \quad (61)$$

The coefficient σ/a^2 in front of the area of the loop (the tension in the string) remains finite in the local limit of the lattice theory. For large g_0 the function $\sigma(g_0^2)$ behaves like $\ln g_0^2 + O(g_0^{-2})^{[2]}$.

The asymptotic behavior of (61) as $g_0^2 \rightarrow 0$, which appears naturally in the recursion approach, seems complicated from the point of view of the strong-coupling expansions. It is possible that such a behavior can be justified on the basis of a modified weak-coupling expansion, taking into account the compactness of the gauge group.

5. DISCUSSION

In our model the vacuum remains invariant in asymptotically free theories. The invariance of the vacuum leads, in particular, to the unobservability of colored objects. To what extent can our model be trusted?

In the weak coupling region it yields the values (54), (55) for the coefficients of the β -function. The exact values of β_4 and β_6 are respectively equal to $11/12\pi^{2/3}$ and $17/48\pi^4$ ^[8]. For $\lambda = 2^{-1/2}$ the error is smaller or approximately equal to 30% in both cases. For $\lambda = 2$

the error is already large, but the signs remain valid for all λ . One can also check that for the group $SU(N)$ the coefficients $\beta_4, \beta_6/\beta_4, \dots$ are proportional to $C_s(G) = N$, as it should be. It is probable that this is true for an arbitrary nonabelian group.

The Abelian group $U(1)$ and the discrete group Z_2 are discussed in a following paper. In both cases the equation yields a correct qualitative picture of the phase transition and correct values for the critical dimensions of the space $D_C = 4$ and $D_C = 2$. The numerical errors in the critical indices and coupling constants are also of the order of 30% for $D = 4$. Thus, our equation is capable of detecting a phase transition and of describing its main properties.

The applicability of the equation for $L > L_0$ is more dubious. For such distances the splitting of the average loop is comparable to L_0 and not to L , so that our approximation can become inapplicable. Nevertheless, we hope that the vacuum energy and the masses of the excitations will be determined by the region $L \lesssim L_0$ and can be estimated by means of recursion equations. For this one must make some more steps, and in the first order of business, include the quarks.

I am grateful to A. Polyakov and K. Wilson for useful discussions and also to E. Bogomol'nyi and V. Lisin for numerically solving the equations.

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Phase transitions in gauge and spin-lattice systems

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A simple recursion equation giving an approximate description of critical phenomena in lattice systems is proposed. The equations for a d -dimensional spin system and a $2d$ -dimensional gauge system coincide. An interesting consequence is the zero transition temperature in the two-dimensional Heisenberg model and four-dimensional Yang-Mills model; this corresponds to asymptotic freedom in field theory.

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INTRODUCTION

Second-order phase transitions possess the remarkable property of universality. In the critical region the micro-structure of the system is unimportant, and only its dimensionality and internal-symmetry group are important. Increasing the internal symmetry makes a phase transition more difficult—the critical dimensionality d_c above which an ordered phase exists is increased. Thus, $d_c = 1$ for the discrete group $SO(1)$ (the Ising Model), while $d_c = 2$ for the continuous groups $SO(n)$ (the Heisenberg model). Recently, gauge systems in which the parameters of the group can depend on the position in the lattice have been introduced^[1]. There is reason to expect that $d_c = 4$ for continuous gauge groups. Such a system corresponds to relativistic field theory with a gauge-invariant spectrum of states. Here the noninvariant objects (quarks) are confined within the invariant ones (hadrons) by long-range forces^[1].

A recursion equation describing critical phenomena in a gauge system was proposed in the author's paper^[2].

Below, using the same methods, we shall obtain a recursion equation for spin systems. As in the gauge equation, the dependence on the dimensionality of space is separated out in explicit form. Here there is a remarkable analogy between a d -dimensional spin system and a $2d$ -dimensional gauge system: the recursion equations for them coincide. From this follow, in particular, the values $d_c = 2$ for the discrete gauge group and $d_c = 4$ for a continuous gauge group. The transition temperature and critical indices, which, in the general case, are determined by solving the recursion equation numerically, can be expanded in powers of $d - d_c$.

The zeroth and first terms of the expansions for the indices are exact. In this respect our equation resembles Wilson's equation^[3], which gives the first terms of the expansion in $4 - d$ for spin systems.

1. THE EXACT EXCURSION EQUATIONS

We shall consider the two-dimensional Heisenberg model and introduce for it a Z-functional—a partition function with pinned spins at the boundary; by definition, the couplings between the spins at the boundary appear with half weight in the energy. As was remarked by Berezinskii^[4], Z-functionals are multiplicative: When neighboring regions are joined into one it is necessary to multiply their Z-functionals and integrate over the spins on the common boundary. It is convenient to consider square regions; then the functional Z_{2L} of a square with side $2L$ is equal to the averaged product of four Z_L -functionals:

$$Z_{2L}(S_r) = \int \Pi(dS_m) \prod_{r=1}^4 Z_L(S_{r_i}), \quad (1)$$

$$(dS) = d^n S \delta(1-S^2) \Gamma(n/2) \pi^{-n/2}. \quad (2)$$

Here $\{S_r\}$ is the set of spins on the boundary of the $2L$ -square, $\{S_{r_i}\}$ are the sets of spins on the boundaries of the L -squares, and $\{S_{int}\}$ are the spins on the internal boundaries of the L -squares (see Fig. 1).

Equation (1) is a functional recursion equation, which must be solved with the following initial condition on the unit cell (Fig. 2):

$$Z_0 = \exp\left(\frac{\beta}{2} \sum_{i=1}^4 S_i S_{i+1} + \frac{h}{2} \sum_{i=1}^4 S_i\right). \quad (3)$$

Analogous equations can be written in d -dimensional space—the number of factors in (1) will then be 2^d . Obviously, we are interested in the free energy in the statistical limit $L \rightarrow \infty$. It can be related, in general form, to the solution of the normalized equation. This is done as follows. From the Z-functionals in (1) we separate out their averages over $\{S\}$, i.e., the usual partition functions:

$$Z_L(S) = \langle Z_L \rangle W_L(S). \quad (4)$$

We then obtain for the correlation functional W a normalized equation of the form

$$W_{2L} = \hat{R}(W_L)/\langle \hat{R}(W_L) \rangle, \quad (5)$$

and we can express the partition function in terms of the correlation functional by the recursion relation

$$\langle Z_{2L} \rangle = \langle Z_L \rangle^4 \langle R(W_L) \rangle. \quad (6)$$

We then find the free energy $-\beta F = \lim L^{-d} \ln \langle Z_L \rangle$:

$$-\beta F(\beta, h) = \sum_{m=1}^{\infty} 2^{-m} \ln \langle \hat{R}(W_{m-1}) \rangle + \ln \langle Z_0 \rangle. \quad (7)$$

As is usual in the recursion approach^[3], the singularities of the free energy are associated with unstable

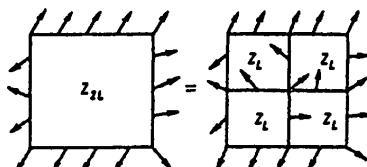


FIG. 1. Exact recursion equations for the correlation functional of the two-dimensional Heisenberg model. The arrows indicate the distribution of spins on the sides of the squares. Averaging is performed over the internal spins.

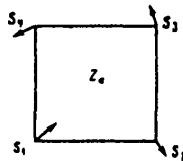


FIG. 2. Correlation functional of a unit cell.

fixed points of the equation for the correlation functional:

$$W_L \rightarrow W_L(S) + (\beta - \beta_c) L^{\nu-\Delta} \Phi_1(S) + h L^{d-\Delta} \Phi_2(S). \quad (8)$$

The critical indices ν and Δ are determined from the equation linearized about W_L : Φ_1 and Φ_2 are its eigenfunctions, with eigenvalues $2^{1/\nu}$ and $2^{d-\Delta}$ respectively. After this, the free energy has the well-known scaling form

$$F(\beta, h) = (\beta - \beta_c)^{\nu/\nu} / (h(\beta - \beta_c)^{1-\nu}) + \text{regular terms} \quad (9)$$

The singular terms are determined by the large distance $2k \sim (\beta - \beta_c)^{-\nu}$ or $2^k \sim h^{-1/(d-\Delta)}$ in the sum (7).

2. LOW-TEMPERATURE APPROXIMATION

Up to now our arguments have been exact and have not differed, in essence, from the general Kadanoff-Wilson scheme^[3].

This scheme acquires practical significance if a successful way of approximating the functional equations by integral equations is found. The well-known approximation of Wilson is valid for $d = 4 - \epsilon$, when the spin fluctuations are close to being Gaussian.

We propose another approximation, which is valid for $d = d_c + \epsilon$, when the transition temperature is low.

In the low-temperature approximation we shall neglect fluctuations of the spins along the side of a square (with $d = 2$, for the present) and shall seek the Z-functional in the form of a product of functions of the average spins of opposite sides:

$$Z_L = F_L(S_1, S_1') F_L(S_2, S_2'). \quad (10)$$

After integrating over the four average internal spins in (1) (Fig. 3), we find

$$F_{LL}(S, S') = (F_L)^2_{SS'}. \quad (11)$$

Here F^2 denotes the contraction

$$(F^2)_{SS'} = \int (dS'') F(S, S'') F(S'', S'). \quad (12)$$

In d -dimensional space we shall associate an average spin with each of the $2d$ faces of a cube and shall seek the Z-functional in the form of a product of d functions $F_L(S_i, S_i')$ of the pairs of spins on opposite faces. Integrating over the spins on the internal faces of the 2^d cubes forming the doubled cube, we find

$$F_{LL}(S, S') = (F_L)^{2^d}_{SS'}. \quad (13)$$

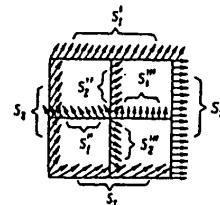
Finally, as in the gauge theory^[2], it will be convenient to generalize the equation to the case of an arbitrary change of scale in place of the doubling. Proceeding analogously, when λ^d cubes are joined together we find the equation

$$F_{LL}(S, S') = (F_L)^{\lambda^d}_{SS'}, \quad (14)$$

where F^λ is the λ -fold contraction.

For noninteger λ this contraction can be defined by means of an eigenfunction expansion on the unit sphere.

FIG. 3. Approximate recursion equation. Spin fluctuations along the sides of the squares are not taken into account.



For the case when there is no magnetic field, so that F depends only on the scalar product (SS') , this expansion has the form

$$F_L = \sum_p f_p(L) \chi_p(SS') N_p. \quad (15)$$

For the Fourier coefficients $f_p(L)$ we obtain from (14) the equation

$$\chi_p(1) f_p(\lambda L) = \int (dS) \left[\sum_q f_q^*(L) \chi_q(SS') N_q \right]^{1/\nu} \chi_p(SS'). \quad (16)$$

This equation goes over into the gauge recursion equation of^[2], if in (16) we replace

$$\lambda \rightarrow \lambda^2, \quad L \rightarrow L^2, \quad d \rightarrow d/2. \quad (17)$$

The spherical functions $\chi_p(z)$ appearing in (15) and (16) coincide for $n = 2$ and 4 with the characters of the groups $U(1)$ and $SU(2)$, respectively. Thus, the XY-model is analogous to photodynamics, i.e., to a lattice Abelian gauge theory, and the four-component Heisenberg model is analogous to the Yang-Mills lattice theory.

These analogies are not accidental. Polyakov has shown by field-theory methods that in four-dimensional photodynamics a phase transition without ordering occurs, as in the two-dimensional XY-model, while in the two-dimensional Heisenberg model there are, at zero temperature, singularities associated with asymptotic freedom, as in the Yang-Mills theory.

In the framework of our approximation the analogy goes further and gives a relation between the critical indices, e.g.,

$$\Delta_{\text{gauge}}(2d)/\Delta_{\text{spin}}(d) = \nu_{\text{spin}}(d)/\nu_{\text{gauge}}(2d) = 2. \quad (18)$$

3. THE ISING MODEL

We shall start from the Ising model, in which the recursion equation (14) can be investigated analytically to completion.

For the coefficients of the normalized correlation functional

$$w_L = 1 + SS' \tanh \beta(L) = e^{\beta(L)SS'}/\cosh \beta(L) \quad (19)$$

the equation reduces to the following:

$$\tanh[\beta(\lambda L)\lambda^{1-\nu}] = \tanh \beta(L), \quad \beta(a) = \beta. \quad (20)$$

Linearizing the equation near the fixed point β_c , we find the index $\Delta' = d - \nu^{-1}$ in (8):

$$\Delta' = (\ln \lambda)^{-1} \ln \left[\frac{\sinh 2\beta_c}{\sinh 2\beta_c \lambda^{1-\nu}} \right]. \quad (21)$$

The second index Δ can be found if we seek the solution in the form

$$w_L = \frac{1}{\cosh \beta_c} \exp(\beta_c SS' + h L^{d-\Delta}(S+S')) \quad (22)$$

and linearize (14) in h . We then obtain

$$\Delta = 1 + 2\beta_c(\lambda^{d-1} - 1)/\ln \lambda. \quad (23)$$

The dependence of the transition point and critical indices on the model parameter λ indicates the inexactness of our approximation.

It is interesting that the indices do not change when λ is replaced by λ^{-1} , whereas the transition temperature acquires a vector λ^{d-1} . From this point of view, the choice $\lambda = 1$ is optimal (the apparent singularities at $\lambda = 1$ cancel in all the quantities). Numerical values of the parameters for $\lambda = 1$ for the two-dimensional model are given in the table.

The critical temperature coincides with the exact answer, the dimension Δ of the order parameter is out by 5% and the dimension $\Delta' = d - \nu^{-1}$ of the energy density is out by 25%. Of course, for the two-dimensional Ising model such a crude approximation is of no value. There exist calculations by Kadanoff, also based on the recursion approach, giving an accuracy of better than 1%. Unfortunately, it has not been possible to generalize these calculations—they use the discreteness of the group in an essential way.

Our equations for the Ising model should become exact for $d \rightarrow 1 + \epsilon$, when the transition temperature tends to zero. In this case we find

$$2\beta_c = \frac{\ln \lambda}{1 - \lambda^{-\epsilon}} + \frac{1 - \lambda^2}{3(1 - \lambda^{-\epsilon})} e^{-\lambda^{-\epsilon}} + O(e^{-\lambda^{-\epsilon}}), \quad (24)$$

$$\Delta' = 1 + \frac{2}{3} \frac{\lambda^2 - 1}{\ln \lambda} e^{-\lambda^{-\epsilon}} + O(e^{-\lambda^{-\epsilon}}), \quad (25)$$

$$\Delta = \frac{1}{3} \frac{\lambda^2 - 1}{\ln \lambda} e^{-\lambda^{-\epsilon}} + O(e^{-\lambda^{-\epsilon}}). \quad (26)$$

The first terms of the ϵ -expansion ($2\beta_c = \epsilon^{-1}$, $\Delta' = 1$, $\Delta = 0$) do not depend on λ , and so it may be hoped that they are exact. We have not succeeded in finding a proof of this hypothesis. It is curious that the first terms of the ϵ -expansion give a fair approximation to the two-dimensional Ising model.

Concerning the gauge-model analog, the following is known^[5].

For $d = 2$ it reduces to the one-dimensional Ising model and is described exactly by our equation. For $d = 3$ the free energy reduces to that of the three-dimensional Ising model with $\beta_c = 0.76$ and $\nu = 0.62$. Finally, the transition temperature is known for $d = 4$: $2\beta_c = \ln(1 + \sqrt{2})$. Our equations (20) with the replacement (17) for $\lambda = 1$ give $\beta_c = 0.9$ and $\nu = 1.05$ for $d = 3$, and $2\beta_c = \ln(1 + \sqrt{2})$ and $\nu = 0.66$ for $d = 4$.

Summarizing, we can say that, by comparison with other recursion methods, our equation describes discrete groups rather crudely. The advantages of our equation will become apparent in the case of continuous groups, where the other methods are inapplicable.

4. CONTINUOUS SYMMETRY GROUPS

In systems with continuous symmetry the critical dimensionality $d_c = 2$. We shall seek a solution of Eq. (19) for $d = 2 + \epsilon$ in Gaussian form:

$$F_L(\cos \theta) \sim \exp(A(L) - \beta(L)\theta^2/2) \quad (27)$$

with a low effective temperature $\beta^{-1}(L)$.

Integrating by the method of steepest descents and retaining terms $\sim \beta$ and ~ 1 , we find a relation for $\beta(L)$:

$$\beta(\lambda L) = \lambda^2 \beta(L) + 1/(n-2) \lambda^2 (1-\lambda) + O(\beta^{-1}). \quad (28)$$

	$\lambda = 1$	Onsager's solution
$2\beta_c$	$\ln(1 + \sqrt{2}) = 0.881$	$\ln(1 + \sqrt{2})$
Δ'	$\sqrt{2} \ln(1 + \sqrt{2}) = 1.246$	1
Δ	$1 - \ln(1 + \sqrt{2}) = 0.119$	$1/8$

From this we find the transition temperature:

$$\beta_c = \frac{n-2}{6} \frac{1-\lambda}{\lambda^{d-1}-1} = \frac{n-2}{6} \frac{1-\lambda}{\ln \lambda} + O(1) \quad (29)$$

and the critical index ν :

$$\nu = \epsilon^{-1} + O(1). \quad (30)$$

The second critical index Δ corresponds to the anisotropic solution

$$F_L \sim \exp(A - \beta_c \theta^2/2 + h L^{d-\epsilon} (S+S') (1+\alpha \theta^2)). \quad (31)$$

Linearizing Eq. (11) in the magnetic field h and integrating by the method of steepest descents, we obtain

$$\alpha = 1/12, \quad (32)$$

$$2^{-\epsilon} = 1 - (n-1)/12\beta_c + O(\beta_c^{-1}). \quad (33)$$

Substituting β_c for $\lambda = 2$ from (29) into this, we find the first term of the ϵ -expansion:

$$\Delta = \frac{n-1}{n-2} \frac{\epsilon}{2} + O(\epsilon^2). \quad (34)$$

The exact values of the linear terms in the ϵ -expansions for the indices have been found by Polyakov by the methods of chiral field theory.

Our results (30) and (34) coincide with the exact results. This is not surprising, inasmuch as the transition temperature vanishes linearly with ϵ , and our model becomes exact in the low-temperature limit. The proportionality coefficient $\epsilon \beta_c$ in (29) depends on λ , and differs from the exact value:

$$\epsilon \beta_c \text{ exact} \sim (n-2)/2\pi. \quad (35)$$

For $\lambda = 1$ the difference will amount to 5%.

But what happens in two-dimensional models? The power temperature singularities as $\epsilon \rightarrow 0$ go over into exponential singularities, e.g.,

$$r \sim \left(1 - \frac{\beta}{\beta_c}\right)^{-1} \sim \exp\left(\frac{\beta \nu}{\beta_c}\right) \sim \exp\left(\frac{2\pi \beta}{n-2}\right). \quad (36)$$

The power dependences on the spatial scale L go over into logarithmic dependences:

$$\beta(L) \sim \beta - \frac{n-2}{2\pi} \ln \frac{L}{a}, \quad (37)$$

$$h L^{d-\epsilon} \sim h L^{\epsilon} \left[\frac{\beta(L)}{\beta} \right]^{(n-1)/4(n-2)}. \quad (38)$$

It is not difficult to verify this by considering the recursion equations for $\epsilon = 0$ in the Gaussian approximation. The zero transition temperature of the two-dimensional Heisenberg model means that ordering is absent at all temperatures, in accordance with Hohenberg's theorem.

The XY-model, in which the corresponding group $SO(2)$ is Abelian, represents a special case. For $\epsilon = 0$, $n = 2$, the transition temperature and critical index Δ in (35) and (34) remain indeterminate. The correlation length (36) is infinite at sufficiently low temperatures, when the Gaussian approximation (27) is applicable. The corrections to the Gaussian approximation are exponen-

tially small, since they are connected with the edges of the range $|\varphi| < \pi$ of integration over the angles of the two-dimensional spin vector.

If we extend the integration to $|\varphi| < \infty$, the Gaussian form with any β will be a fixed point. Linearizing Eq. (11) for $n = 2$ near the degenerate Gaussian point

$$F_1 = \exp \left(A - \frac{\beta}{2} \theta^2 + \frac{h(S+S')}{|S+S'|} L^{1-\alpha} \Psi(\theta) \right), \quad (39)$$

we arrive at the integral equation

$$2^{-\alpha} \Psi(\theta) = \sqrt{\frac{\beta}{\pi}} \int_{-\infty}^{\infty} d\varphi \exp \left(-\beta \left(\varphi - \frac{\theta}{2} \right)^2 \right) \cos \frac{\varphi - \theta}{2} \Psi(\varphi), \quad (40)$$

the solution of which can be found in the form of a double series in θ^2 and $T \equiv \beta^{-1}$:

$$\Psi = 1 - \frac{\theta^2}{24} \left(1 + \frac{77}{90} - \frac{\theta^2}{80} + \dots \right), \quad (41)$$

$$\Delta \ln 2 = \frac{T}{12} - \frac{1}{6} \left(\frac{T}{12} \right)^2 + \dots \quad (42)$$

Solving Eq. (11) numerically for $n = 2$ (without a magnetic field) shows that the initial function $F_0 = \exp(\beta \cos \varphi)$ goes over after several iterations to the Gaussian form $\exp(A - \beta \varphi^2/2)$ with $\beta = \beta + O(1)$. The Gaussian form is held for a very long time for $\beta \gtrsim 1$, and then moves away rapidly to $F = 1$, which corresponds to the disordered phase. For $\beta > \beta_c \approx 1.7$, the Gaussian form remains throughout the entire interval chosen (100 iterations). This means that for $\beta > \beta_c$ the correlation length is effectively infinite, i.e., the region $\beta > \beta_c$ is on a phase-transition line. This corresponds to the curve $T_c(\epsilon)$ (Fig. 4) obtained by solving Eq. (16) numerically for $\lambda = 21/(d-1)$, when this equation simplifies in the Fourier representation.

We recall that, according to the analogy between gauge and spin systems, all that has been said above can be carried over to four-dimensional photodynamics. These results agree with the general conclusions of Berezinskii for the XY-model^[4] and of Polyakov for photodynamics.

CONCLUSION

The results of this paper are summarized in Figs. 5 and 6. Figure 5 enables us to understand intuitively how phase transitions cease at the critical dimensionality of space. Figure 6 shows what happens to the spectrum of dimensions in this case. The behavior of the spectrum for $d = 4 - \epsilon$ is known from Wilson's work^[5]. The upper curves correspond to the dimension $\Delta' = d - \nu^{-1}$ of the energy-density operator. The dimensions of composite operators are not given in this figure. These dimensions, for $d = 2 + \epsilon$, can also be found by linearizing the recursion equations. As regards practical applications of the model, the greatest interest evidently lies in the equation of state in two-dimensional magnets, which can be found by numerical solution of the recursion equations. In this case it is possible to take into account the spin-space anisotropy, which should suppress fluctuations of one or two components of the spin.

In conclusion I wish to thank my colleagues A. M. Polyakov, V. L. Pokrovskii, and S. B. Khokhlachev for numerous discussions and critical comments. I am also extremely grateful to E. B. Bogomol'nyi and V. V.

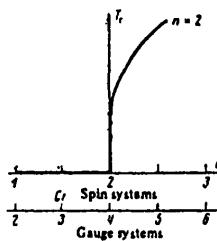


FIG. 4

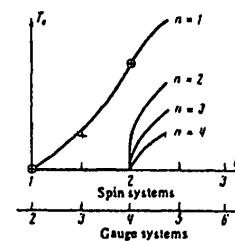


FIG. 5

FIG. 4. Qualitative dependence, found from the recursion equations, of the transition temperature on the dimensionality of space for an $SO(2)$ spin system (XY-model) and a $U(1)$ gauge system (photodynamics).

FIG. 5. Qualitative dependence, found from the recursion equations, of the transition temperature on the dimensionality of space for gauge and spin systems with $SO(n)$ symmetry. The crosses correspond to exact results^[1] for the discrete gauge group $SO(1) = Z_2$; the circles correspond to exact results for the Ising model.

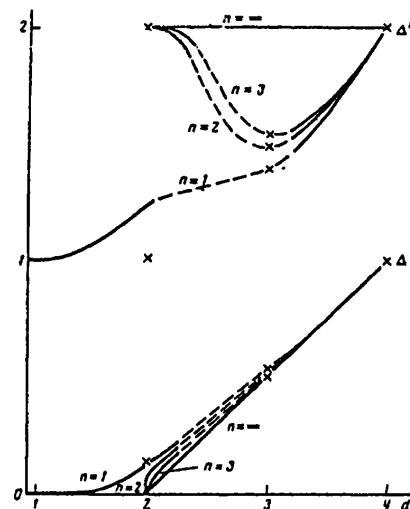


FIG. 6. Qualitative dependence of the dimensions of the spin (Δ) and energy density (Δ') on the dimensionality of space for the generalized $SO(n)$ Heisenberg model. The behavior for $d \rightarrow 1$ and $d \rightarrow 2$ is found from the recursion equations, and for $d \rightarrow 4$ from the ϵ -expansion; the crosses correspond to the known indices of the two- and three-dimensional models.

Vas'kin, who helped me in the numerical solution of the recursion equations.

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Translated by P. J. Shepherd
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Chapter 15

Duality

15.1 Doing Sums

In various parts of this book we have worked with two different kinds of couplings for the Ising model, and for other models as well. In addition to the usual coupling K , we have made use of the dual coupling $\tilde{K} = D(K)$. The word ‘dual’ means that two applications of the dual operation bring a return to the starting point. In symbols,

$$D(D(K)) = K. \quad (15.1)$$

So far, we have employed dual couplings for little tricks, but not for anything very profound. However, duality¹ has a very deep significance. It has important consequences in statistical physics, in field theory, and now in superstring theory. I shall not attempt to do justice to the depth of the concept here. Instead I shall just outline a portion of the idea by suggesting how it applies to two-dimensional statistical problems.²

But before doing two dimensions let us study the much simpler problem of computing sums. Our prototype problem will, in fact, be the calculation of the sum

$$z(K) = K^{1/4} \sum_{n=-\infty}^{\infty} e^{-\pi K n^2}. \quad (15.2)$$

For K very large, the only appreciable term in the sum is the single one in which $n = 0$. This sum is then the analog of calculating the properties of some low temperature system which is stuck in its ground state. For K small, many terms contribute to the sum, and it is like doing quantum statistical mechanics at high temperatures. In fact, for approximate purposes, the sum over n can be replaced by an integral over n and the corresponding Gaussian integral evaluated. However, as we shall see in this section there is a transformation which enables one to determine the result of the large K calculation, knowing the small- K one and vice

¹Originally due to Riemann, the idea was first applied to phase transitions by H. Kramers and G. Wannier, Phys. Rev. 60, 252, 263 (1941).

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versa. Later on, we shall see that it is possible to determine similar relationships between high temperature and low temperature statistical mechanics problems. But for now, let us turn our attention to the sum.

There is a theorem called the *Poisson Sum Formula* which enables us to do summations of slowly varying things in an efficient manner.

To derive this formula let $F(x)$ be a periodic function with period one. It can then be written in a Fourier series in the form

$$F(x) = \sum_{m=-\infty}^{\infty} f(m)e^{2\pi mx} \quad (15.3a)$$

where

$$f(m) = \int_a^{a+1} dy F(y)e^{-2\pi my}. \quad (15.3b)$$

Because of the periodicity, a may be any real number. Combine these two equations to find

$$F(x) = \sum_{m=-\infty}^{\infty} \int_a^{a+1} dy F(y)e^{2\pi im(x-y)}. \quad (15.4)$$

Notice that $F(x)$ is quite arbitrary, except for the requirement that it be periodic. Therefore the only possibility is that the summand in Eq. (15.4)

$$S(x-y) = \sum_{m=-\infty}^{\infty} e^{2\pi im(x-y)}, \quad (15.5)$$

be the periodic equivalent of a delta function. That equivalent is a sum of delta functions of the form:

$$S(x) = \sum_{m=-\infty}^{\infty} e^{2\pi imx} = \sum_{n=-\infty}^{\infty} \delta(x-n). \quad (15.6)$$

Equation (15.6) is an expression of our theorem.

To use this formula imagine that we wanted to calculate a sum, like that in Eq. (15.2), which appears in the form: $\sum_{n=-\infty}^{\infty} G_n$ where G_n is a function known only when n takes on integer values. However, there is a unique analytic function, which we can fit to G_n at the integers and which has no strong non-analyticity at infinity. Let that function have the name $G(x)$. From Eq. (15.6) evaluate the integral

$$\int_{-\infty}^{\infty} dx G(x)S(x),$$

we find that it can be written in two different ways

$$\sum_{n=-\infty}^{\infty} G_n = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} dx G(x)e^{2\pi imx}. \quad (15.7)$$

The result is called the *Poisson Sum Formula*. Notice that the $m = 0$ term expresses the result of replacing the sum by an integral. When $G(x)$ varies smoothly and slowly over a large range of x — a range much bigger than one —, higher m 's give small corrections.

Now consider a specific example in which our function, $G(x)$, is $K^{1/4} \exp(-\pi Kx^2)$ and Eq. (15.7) becomes

$$\begin{aligned} z(K) &= K^{1/4} \sum_{n=-\infty}^{\infty} e^{-\pi K n^2} \\ &= K^{1/4} \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} dx e^{-\pi K x^2} e^{2\pi i m x} \\ &= K^{-1/4} \sum_{m=-\infty}^{\infty} e^{-\pi m^2 / K}. \end{aligned} \quad (15.8)$$

We have, in front of our eyes, an unexpected symmetry property of $z(K)$, namely that

$$z(K) = Z(D(K)) \quad \text{where} \quad D(K) = 1/K. \quad (15.9)$$

As advertised the dual transformation interchanges large K and small, leaving z unchanged.

15.2 Two Dimensions

Before starting out, let us look at some of the properties of vector fields in two-dimensions. (A vector field in two dimensions is a pair of functions of x and y which we interpret as two components of a vector.) Duality has a lot to do with curls and divergences. Let $\mathbf{w}(x, y) = (u(x, y), v(x, y))$ be such a vector field. In the case in which the field is divergence free, so that $u_x + v_y = 0$, one can always write it as a curl, i.e. one can always find a function $\psi(x, y)$, called a *stream function* such that

$$\mathbf{w} = \left(\frac{\partial \psi}{\partial y}, -\frac{\partial \psi}{\partial x} \right), \quad \text{if } \nabla \cdot \mathbf{w} = 0. \quad (15.10a)$$

If, on the other hand, the curl of the field vanishes, i.e.

$$\nabla \times (u, v) = u_y - v_x = 0,$$

then there will always be a *scalar potential* $\phi(x, y)$ which generates the field via a gradient operation

$$\mathbf{w} = \left(\frac{d\phi}{dx}, \frac{d\phi}{dy} \right), \quad \text{if } \nabla \times \mathbf{w} = 0. \quad (15.10b)$$

Notice that Eqs. (15.10a) and (15.10b) have exactly the same structure. To go from one to the other, interchange x and $-y$.

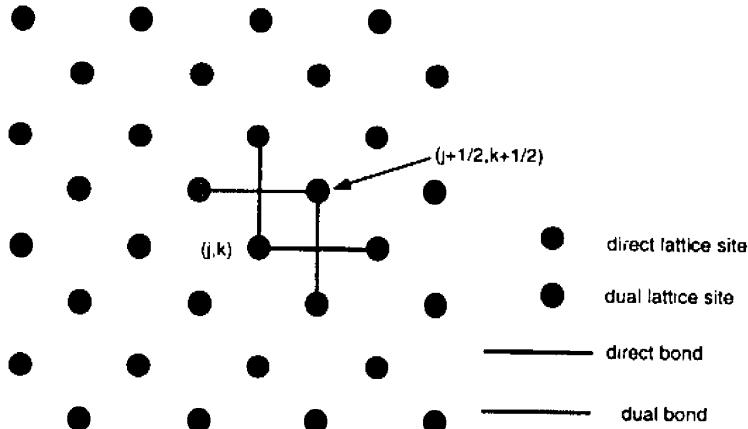


Fig. 15.1. Direct and Dual lattice, shown respectively in black and grey. Take j and k to be integers. The the sites of the dual lattice are labeled by $(j + 1/2, k + 1/2)$. The x -direction bond on the direct lattice is labeled by $(j + 1/2, k)$ as is the y -direction bond on the dual lattice.

All this works equally well on discrete lattices. Figure 15.1 shows a two-dimensional square lattice formed by all the points j, k with integer indices, and also a dual lattice formed by looking at the center of all the squares. Imagine that the lattice has variables defined on the bonds connecting the lattice sites. Thus an x -direction bond would have a variable $\rho(j + 1/2, k)$ while a y -direction bond would have a variable $\eta(j, k + 1/2)$. The vector field is (ρ, η) .

Imagine that the vector field obeys a curl-free condition. That condition implies the vanishing of a path integral like the one shown in Fig. 15.2

$$\oint d\mathbf{r} \cdot (\rho, \eta) = 0$$

to give the condition

$$-\rho\left(j + \frac{1}{2}, k + 1\right) - \eta\left(j, k + \frac{1}{2}\right) + \rho\left(j + \frac{1}{2}, k\right) + \eta\left(j + 1, k + \frac{1}{2}\right) = 0. \quad (15.11)$$

Equation (15.11) is the statement that there is no curl on the site $j + 1/2, k + 1/2$ of the dual lattice. Equation (15.11) will be true if and only if the vector field (ρ, η) is generated as a gradient, i.e. there exists a scalar potential $\phi(j, k)$ such that:

$$\text{gradient : } \rho\left(j + \frac{1}{2}, k\right) = \phi(j + 1, k) - \phi(j, k), \quad (15.12)$$

$$\eta\left(j, k + \frac{1}{2}\right) = \phi(j, k + 1) - \phi(j, k). \quad (15.13)$$

Notice that the ϕ is defined upon the sites j, k of the direct lattice.

There is a direct translation of Eqs. (15.11) and (15.13) into a statement about a divergence-free vector field, which is then generated as a curl. In this formulation, the

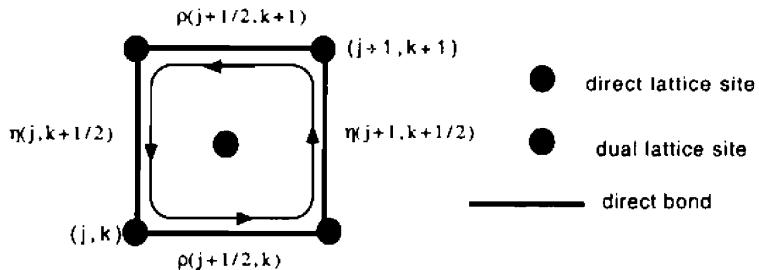


Fig. 15.2. Forming a curl. A closed loop on the direct lattice is shown, along with names of the different bond variables. The bonds with positive direction along the loop make a positive contribution to the curl, the others make a negative one.

dual lattice $(j + 1/2, k + 1/2)$ replaces the direct lattice. Our definition of a divergence-free field on a lattice is that

$$\nabla \cdot (\rho, \eta) = 0$$

when

$$\rho\left(j + \frac{1}{2}, k\right) - \rho\left(j - \frac{1}{2}, k\right) + \eta\left(j, k + \frac{1}{2}\right) - \eta\left(j, k - \frac{1}{2}\right) = 0 \quad (15.14)$$

which will be true if and only if the field is generated as a curl

$$\begin{aligned} \text{curl: } \rho\left(j + \frac{1}{2}, k\right) &= \psi\left(j + \frac{1}{2}, k + \frac{1}{2}\right) - \psi\left(j + \frac{1}{2}, k - \frac{1}{2}\right) \\ \eta\left(j, k + \frac{1}{2}\right) &= -\psi\left(j + \frac{1}{2}, k + \frac{1}{2}\right) + \psi\left(j - \frac{1}{2}, k + \frac{1}{2}\right) \end{aligned} \quad (15.15)$$

for some stream $\psi(j + 1/2, k + 1/2)$ defined on the sites of the dual lattice. A function used to generate a curl in this manner is called a stream function.

In our discussions of duality we shall make heavy use of the relationships given by Eqs. (15.11) and (15.14). However, we shall use them in a slightly more general form. We shall allow the various quantities, ρ, η, ϕ, ψ to take on values of the integers between 1 and p , where p is also an integer. Then we shall weaken Eqs. (15.11) and (15.14) by demanding that they only be true mod p . The two interesting limiting cases, $p = 2$ and $p = \infty$ can be made to correspond respectively to the Ising model and to a kind of Gaussian model.

15.3 Direct Coupling and Dual Coupling

Before doing the two-dimensional case, let us generate analogous but simpler results in one dimension. Imagine a problem with a variable $\phi(j)$ on each site of a one-dimensional lattice $j = 1, 2, \dots, L$. Each ϕ takes on values between 1 and p . We have nearest neighbor couplings with periodic boundary conditions. We assume that the couplings depend upon

the difference $\phi(j+1) - \phi(j)$, where the difference is defined modulus p . Thus the partition function has the form:

$$Z[K] = \text{Tr}_\phi \prod_{j=1}^L \exp \left[K_{j+1/2} \left(\eta \left(j + \frac{1}{2} \right) \right) \right]$$

where

$$\eta \left(j + \frac{1}{2} \right) = \phi(j+1) - \phi(j). \quad (15.16)$$

Here $K_{j+1/2}$ is a coupling which is defined on the bond connecting the lattice sites $j+1$ and j . The coupling term depends upon a bound-coupling variable $\eta(j+1/2)$ which is simply the difference between the two on site variables.

As we know, the partition function in Eq. (15.16) is very simply calculated. We write the coupling as a Fourier series:

$$e^{K(\eta)} = \frac{1}{\sqrt{p}} \sum_{\psi=1}^p e^{\tilde{K}(\psi)} \exp \left(\frac{2\pi i \psi \eta}{p} \right). \quad (15.17)$$

Here we have defined the Fourier coefficient as \tilde{K} . Just as the coupling is a function of a variable, η , with p values, in just the same way the dual coupling is a function of a variable ψ which takes on p different values. The coupling and its dual contain the same information but coded differently. To do the Fourier transforms of all the bonds, we shall need a notation for each Fourier series variable. Naturally, we call the variable on the bond at $j+1/2$, $\psi(j+1/2)$

We have already calculated partition functions almost identical to the one in Eq. (15.16). But for completeness let us calculate this one. We use a slightly different method from the one we have employed before. Equation (15.16) contains L summations and L basic variables $\eta(j+1/2)$. But because of the periodic boundary conditions, $\eta(L+1/2) = \phi(1) - \phi(L)$. For that reason, there is a restriction upon the L difference variables:

$$\sum_{j=1}^L \eta \left(j + \frac{1}{2} \right) = 0, \quad \text{mod } p. \quad (15.18)$$

Thus, we can rewrite the partition function as a sum over the η 's with but one restriction, the one expressed in Eq. (15.18). The restriction is expressed in a factor Δ which is 1 whenever Eq. (15.18) is true and zero otherwise. This factor can be written as

$$\Delta = \frac{1}{p} \sum_{\psi=1}^p \exp \left(-2\pi i \psi \sum_{j=1}^L \frac{\eta(j+1/2)}{p} \right), \quad (15.19)$$

and the partition function is:

$$Z[K] = \text{Tr}_\eta \Delta \exp \left(\sum_{j=1}^L K_{j+1/2} \left(\eta \left(j + \frac{1}{2} \right) \right) \right). \quad (15.20)$$

Substitute the expression (15.19) for Δ in Eq. (15.20). Rearrange the order of the sums, to do the sum over ψ last. The result is

$$Z[K] = \frac{1}{p} \sum_{\psi=1}^p \prod_{j=1}^L \sum_{\eta=1}^p \exp[K_{j+1/2}(\eta)] \exp\left(\frac{2\pi i \psi \eta}{p}\right). \quad (15.21)$$

The rightmost sum defines the Fourier transform of Eq. (15.17). The result is

$$Z[K] = p^{(L-2)/2} \sum_{\psi=1}^p \exp \sum_{j=1}^L \tilde{K}_{j+1/2}(\psi). \quad (15.22)$$

Thus, as before the partition function is reduced to a quite different, dual, expression. When all the couplings are equal, the partition function turns into the simple sum

$$Z[K] = p^{(L-2)/2} \sum_{\psi=1}^p \exp[L \tilde{K}_{k+1/2}(\psi)]. \quad (15.23)$$

For us this calculation contains little that is new. But now turn to two dimensions, which is both more difficult and more interesting.

15.4 Two-Dimensional Calculation

Consider once again a simple square lattice (see Fig. 15.1) defined by variables $\phi(j, k)$ sitting on the lattice sites. Here j and k are integers. We require each of the ϕ 's to be integers in the interval $1 \leq \phi \leq p$. The model is further defined by x -direction couplings $K_x(j+1/2, k)[\phi(j+1, k) - \phi(j, k)]$ and y -direction couplings $K_y(j, k+1/2)[\phi(j, k+1) - \phi(j, k)]$. The coordinate indices $(j + 1/2, k)$ and $(j, k + 1/2)$ indicate that each of these couplings can depend upon lattice position. When this too-heavy notation gets wearisome we write these couplings as $K_x[\rho(j + 1/2, k)]$ and $K_y[\eta(j, k + 1/2)]$ where

$$\begin{aligned} \rho\left(j + \frac{1}{2}, k\right) &= \phi(j + 1, k) - \phi(j, k) \quad \text{and} \\ \eta\left(j, k + \frac{1}{2}\right) &= \phi(j, k + 1) - \phi(j, k). \end{aligned} \quad (15.24)$$

Given these definitions, we write the entire partition function as:

$$Z[K] = \text{Tr}_\phi \prod_{j=1}^L \prod_{k=1}^L \exp \left\{ K_x \left[\rho \left(j + \frac{1}{2}, k \right) \right] + K_y \left[\eta \left(j, k + \frac{1}{2} \right) \right] \right\}. \quad (15.25)$$

We use as usual periodic boundary conditions.

Notice that the trace, Tr_ϕ , is an integral over all L^2 variables $\phi(j, k)$. We have written the action not as a function of these on-site variables, but in terms of the on-bond variables $\rho(j + 1/2, k)$ and $\eta(j, k + 1/2)$. There are a total of $2L^2$ bond variables. Thus, we need to define L^2 constraints in order to get the right variable list. In view of our discussion of vector fields at the head of this chapter, there is one constraint for each site $(j + 1/2, k + 1/2)$ of the dual lattice and the constraint is defined in terms of the variable

$$\begin{aligned} C\left(j + \frac{1}{2}, k + \frac{1}{2}\right) &= \rho\left(j + \frac{1}{2}, k\right) + \eta\left(j + 1, k + \frac{1}{2}\right) \\ &\quad - \rho\left(j + \frac{1}{2}, k + 1\right) - \eta\left(j, k + \frac{1}{2}\right), \end{aligned} \quad (15.26)$$

defined at each site of the dual lattice. The condition is

$$C\left(j + \frac{1}{2}, k + \frac{1}{2}\right) = 0, \quad (\text{mod } p). \quad (15.27)$$

To enforce the constraint, we define a multiplier $\Delta(j + 1/2, k + 1/2)$ which is one whenever the constraint (15.27) is satisfied and zero otherwise. We can write this multiplier as

$$\Delta\left(j + \frac{1}{2}, k + \frac{1}{2}\right) = \frac{1}{p} \sum_{\psi=1}^p \exp\left[-2\pi i \psi C\left(j + \frac{1}{2}, k + \frac{1}{2}\right)/p\right]. \quad (15.28)$$

Since we are going to have one constraint like (15.28) for each dual lattice site, we will have lots of summations over different ψ -variables. From here on we shall call the summation variable in Eq. (15.27) not just plain ψ but $\psi(j + 1/2, k + 1/2)$.

This change is crucial. When we set up our sum, we will have as intermediate summation variables the ψ 's. As we shall set, it will then be easy to sum out the ρ 's leaving us only with the sum over the $\psi(j + 1/2, k + 1/2)$'s. Except for a few tiny changes, like replacing the K 's by dual couplings, the summation problem in the ψ 's will have precisely the same form as the original problem in the ϕ 's. We shall not have solved either problem, but by relating them we shall have learned quite a lot.

So do it. Equation (15.25) can be written as

$$\begin{aligned} Z[K] &= \text{Tr}_\rho \text{Tr}_\eta \prod_{j=1}^L \prod_{k=1}^L \\ &\quad \times \exp\left\{K_x\left[\rho\left(j + \frac{1}{2}, k\right)\right] + K_y\left[\eta\left(j, k + \frac{1}{2}\right)\right]\right\} \Delta\left(j + \frac{1}{2}, k + \frac{1}{2}\right). \end{aligned} \quad (15.29)$$

If we leave the Δ 's in they provide a set of constraints which permit the replacement of the vector fields (ρ, η) by differences of ϕ 's and thus return us to the original problem. But we can, instead, replace the Δ 's by sums of the form (15.28) each with its own summation

variable $\psi(j + 1/2, k + 1/2)$, each one going from 1 to p . The partition function calculation becomes

$$\begin{aligned} Z[K] = \text{Tr}_\rho \text{Tr}_\eta \text{Tr}_\psi \prod_{j=1}^L \prod_{k=1}^L & \exp \left\{ K_x \left[\rho \left(j + \frac{1}{2}, k \right) \right] + K_y \left[\eta \left(j, k + \frac{1}{2} \right) \right] \right\} \frac{1}{p} \\ & \times \exp \left[-2\pi i \psi \left(j + \frac{1}{2}, k + \frac{1}{2} \right) C \left(j + \frac{1}{2}, k + \frac{1}{2} \right) / p \right]. \end{aligned} \quad (15.30)$$

Here the C 's are defined by Eq. (15.26).

It is remarkable to notice that we can do the summations over the bond variables. Each bond variable in Eq. (15.26) appears in precisely three factors. For example $\rho(j + 1/2, k)$ appears in the factors

$$\begin{aligned} F = \sum_{\rho(j+1/2,k)=1}^p & \exp K_x \left[\rho \left(j + \frac{1}{2}, k \right) \right] \exp \left[-2\pi i \psi \left(j + \frac{1}{2}, k + \frac{1}{2} \right) \rho \left(j + \frac{1}{2}, k \right) / p \right] \\ & \times \exp \left[2\pi i \psi \left(j + \frac{1}{2}, k - \frac{1}{2} \right) \rho \left(j + \frac{1}{2}, k \right) / p \right]. \end{aligned} \quad (15.31)$$

Sum expression (15.31) over its ρ and one has precisely the definition of the dual coupling, \tilde{K} . We have

$$F = p^{1/2} \exp \left\{ \tilde{K}_y \left[\psi \left(j + \frac{1}{2}, k + \frac{1}{2} \right) - \psi \left(j + \frac{1}{2}, k - \frac{1}{2} \right) \right] \right\}.$$

Notice that we have defined the Fourier transform of the K_x coupling to be the dual coupling in the y -direction. In the full notation, K_x is $K_x(j + 1/2, k)[\cdot]$ and its dual is $\tilde{K}_y(j + 1/2, k)[\cdot]$. Similarly, the dual of $K_x(j, k + 1/2)[\cdot]$ is $\tilde{K}_y(j, k + 1/2)[\cdot]$. In terms of these dual couplings we write the partition sum as:

$$\begin{aligned} Z[K] = \text{Tr}_\psi \prod_{j=1}^L \prod_{k=1}^L & \exp \tilde{K}_y \left[\psi \left(j + \frac{1}{2}, k + \frac{1}{2} \right) - \psi \left(j + \frac{1}{2}, k - \frac{1}{2} \right) \right] \\ & \times \exp \tilde{K}_x \left[\psi \left(j + \frac{1}{2}, k + \frac{1}{2} \right) - \psi \left(j - \frac{1}{2}, k + \frac{1}{2} \right) \right]. \end{aligned} \quad (15.32)$$

As claimed, this result is precisely the same as our starting point, Eq. (15.25), except that K has been replaced by \tilde{K} and the names of some summation variables have been changed. Notice that the transformation has not changed the value of the partition function. Therefore, our final conclusion is that

$$Z[K] = Z[\tilde{K}]. \quad (15.33)$$

Notice that we have never used any translational invariance condition for the K_x 's and K_y 's. They could all be equal or each one could be different and the calculation would go through in exactly the same way.

15.5 Ising Model

We look to the case $p = 2$. This situation has two possible values of the basic variable ϕ on each state, $\phi = 1$ and $\phi = 2$. Thus it must be in some sense equivalent to the usual Ising model. We do not have to work hard to see the connection. The ϕ -model has a coupling with values $K(1)$ if $\phi = 1$ and $K(2)$ if $\phi = 2$. Since the Ising model has a coupling $K\sigma$, with $K_0 + \sigma = \pm 1$, if we identify $\sigma = 1$ with $\phi = 2$ we have

$$K_0 = \frac{K(1) + K(2)}{2}, \quad (15.34a)$$

$$K = \frac{K(2) - K(1)}{2}. \quad (15.34b)$$

The Fourier series [see Eq. (15.17)] which gives the dual transformation is:

$$\begin{aligned} e^{\tilde{K}(2)} &= \frac{e^{K(2)} + e^{K(1)}}{\sqrt{2}}, \\ e^{\tilde{K}(1)} &= \frac{e^{K(2)} - e^{K(1)}}{\sqrt{2}}. \end{aligned} \quad (15.35)$$

Then from Eq. (15.34), the dual couplings would have the value

$$\tilde{K} = -\frac{1}{2} \ln \tanh K, \quad (15.36a)$$

$$\tilde{K}_0 = K_0 + \frac{1}{2} \ln \frac{\cosh 2K}{2}. \quad (15.36b)$$

We have already said that Eq. (15.36a) can be equivalently written in the symmetrical form:

$$\sinh 2K \sinh 2\tilde{K} = 1. \quad (15.37)$$

To see the consequences of duality, first split off the trivial coupling K_0 from the partition function and write:

$$Z[K] = \exp \left[-F[K] + \sum_{j,k} (K_{x0} + K_{y0}) \right]. \quad (15.38)$$

Here, then, F is a free energy which depends upon the nontrivial coupling of Eq. (15.34b) but not the K_0 's of Eq. (15.34a). Next use a square lattice, so that the interchange of x and y gives no change, and demand that all the couplings be exactly the same, with each and every K_0 having the value zero and all the K 's having the same, nonzero value. Call the value of the free energy, F , in this case $F(K, L)$ where L is the length of the system. Then Eq. (15.33) gives us the relationship between free energies:

$$F(K, L) = F(\tilde{K}, L) + L^2 \ln \frac{\cosh 2K}{\sqrt{2}}. \quad (15.39)$$

We know that the two-dimensional Ising model changes its behavior as a function of K . For small K it is disordered. For large K it has a ferromagnetic order. At some intermediate value of K , K_c , it has a critical point. At this point the free energy has a singularity in which its second derivative with respect to K diverges. From (15.39) it follows that at the critical point, the numerical value of K and of \tilde{K} must be identical so that the singularities on the right and the left hand sides of the equation can arise simultaneously in K . We have two ways of finding this common K value. One is to set both K and \tilde{K} equal to K_c in Eq. (15.37) giving us

$$(\sinh 2K_c)^2 = 1. \quad (15.40a)$$

The other way is to notice that at K_c , the F 's on the right and left hand sides of Eq. (15.39) cancel out, leaving us with the condition

$$\cosh 2K_c = \sqrt{2}. \quad (15.40b)$$

It is pleasing to notice that the two parts of Eq. (15.40) are compatible with one another.

A similar analysis works when the two couplings K_x and K_y are different from one another. Picture the plane with axes K_x and K_y . In this plane, there is a critical line on which the Ising transition occurs. This line is left unchanged by the dual transformation. After the transform, there are new x and y couplings

$$K'_y = D(K_x), \quad (15.41a)$$

$$K'_x = D(K_y). \quad (15.41b)$$

Since we are at a fixed point, the new couplings must equal the old and so $K_y = D(K_x)$. This criticality condition can also be written as

$$\sinh(2K_y) \sinh(2K_x) = 1. \quad (15.41c)$$

which agrees with our previous condition (15.40a) when the two couplings are equal.

There are two remarkable features of the duality transformation. We have just made use of the fact that it connects one problem at the critical point, into another critical problem. The other fact is that, off the critical line, this transformation connects two apparently quite different problems. It takes a problem above the critical temperature and expresses its solution in terms of a problem which is below the critical temperature. These problems are quite different: one problem has long ranged order, the other one does not. Nonetheless, their answers are obtainable from one another.

15.6 XY is Connected to SOS

One can also use duality transforms to connect problems which seem even more different from one another. The transformation we have described works whenever there is a Fourier

transform or a Fourier series. We know for example that a periodic function of θ has a transformation which converts it into a series:

$$\exp(K(\theta)) = \sum_{n=-\infty}^{\infty} \exp(\tilde{K}(n)) \exp(2\pi i n \theta), \quad \text{if } K(\theta + 2\pi) = K(\theta) \quad (15.42a)$$

or inversely,

$$\exp(\tilde{K}(n)) = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} \exp(-2\pi i n \theta) \exp(K(\theta)), \quad \text{if } K(\theta + 2\pi) = K(\theta). \quad (15.42b)$$

An XY model is one in which there is a variable on each site, θ , which takes on values between $-\pi$ and π . This is called an XY model because one visualizes a two-component spin variable, \mathbf{s} , of fixed length and variable direction. This variable can be written as $\mathbf{s} = (\cos \theta, \sin \theta)$ and the couplings between different sites can be considered to depend upon $\mathbf{s} \cdot \mathbf{s}' = \cos(\theta - \theta')$.

In our specific version of the model, the θ -variables are coupled with a bond which produces a weight $\exp[K(\theta - \theta')]$ whenever θ and θ' are nearest neighbor variables, with K being a periodic function of period 2π . Thus, the basic partition function for this model is an integral over all the variables $\theta(j, k)$ over the period 2π with a statistical weight given by the exponential of an action of the form

$$\mathcal{W} = -\beta \mathcal{H} = \sum_{jk} [K_x(\theta(j+1, k) - \theta(j, k)) + K_y(\theta(j, k+1) - \theta(j, k))]. \quad (15.43a)$$

The partition function is given as usual by $Z[K] = \text{Tr}_\theta \exp(\mathcal{W})$. Since θ converts via a Fourier transforms into n , the partition function is equally well given by a sum over a set of dual variables which are integers, n , sitting on sites of the dual lattice and an action

$$\begin{aligned} \mathcal{W} = -\beta \mathcal{H} = & \sum_{jk} \left[\tilde{K}_y \left(n \left(j + \frac{1}{2}, k + \frac{1}{2} \right) - n \left(j + \frac{1}{2}, k - \frac{1}{2} \right) \right) \right. \\ & \left. + \tilde{K}_x \left(n \left(j + \frac{1}{2}, k + \frac{1}{2} \right) - n \left(j - \frac{1}{2}, k + \frac{1}{2} \right) \right) + \ln(2\pi) \right]. \end{aligned} \quad (15.43b)$$

The two actions (15.43a) and (15.43b) generate precisely the same partition function. Thus the problem with a periodic variable at each site (the XY model) has been converted into a very different problem with an integer variable at each site. The latter kind of problem is called a solid on solid model — SOS for short. One thinks of atoms piled up on all the different sites of the dual lattice. One interprets $n(j, k)$ as the height of a stack on its site and says that the statistical weight of neighboring sites is given by a function $\tilde{K}(n - n')$ which depends on the relative height.

Duality relations are very powerful. However, they are also very limited. They need a set of good symmetries in the problem. In the XY case, the required symmetry is one of translating all the θ -variables by the very same angle, and also a symmetry under

independently translating each one of the θ 's through 2π . In the Ising case, you can use duality when you have only a nearest neighbor $K\sigma\sigma'$ coupling, which is invariant under flipping the signs of all the spins, but one cannot get a simple duality relation when there is a symmetry-breaking term like $h\sigma$.

15.7 Gaussian goes into Gaussian

The Fourier transform of a function of a ϕ which goes from minus infinity to infinity is another function $[-\infty, \infty]$. Specifically, the transforms are

$$\exp(w(\phi)) = \int_{-\infty}^{\infty} \frac{d\psi}{\sqrt{2\pi}} \exp(\tilde{w}(\psi)) \exp(i\psi\phi) \quad (15.44a)$$

$$\exp(\tilde{w}(\psi)) = \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi}} \exp(w(\phi)) \exp(-i\psi\phi). \quad (15.44b)$$

The most important example is one in which $w(\phi)$ represents a Gaussian coupling

$$w(\phi) = -\frac{K}{2}\phi^2 + \frac{1}{4}\ln K \quad (15.45a)$$

which has as its dual precisely the same form

$$\tilde{w}(\phi) = -\frac{1}{2K}\phi^2 - \frac{1}{4}\ln K \quad (15.45b)$$

unchanged except that K is replaced by $1/K$. Thus, a Gaussian problem transforms itself into another Gaussian problem, with a revised value of K .

Of course, exactly the same thing happens under a dual transformation in, for example, a two-dimensional system. Imagine a Gaussian problem in which the coupling on each pair of nearest neighboring lattice sites is of the form $w(\phi - \phi')$ with ϕ and ϕ' being the neighboring variables. Notice that this problem is invariant under the displacement of all the ϕ -variables by the same amount. Because of this symmetry, this problem can be transformed directly and exactly into one which has exactly the same form except that K is replaced by $1/K$. If large K represents strong coupling, and small K weak coupling, once again a strong coupling problem has been translated into a weak coupling one, and vice versa.

15.8 Dual Correlations

A dual transformation is a symmetry of a statistical system. For Ising model, one can analyze some of the operators quite directly, and see, for example, that the free energy is even under duality transforms, the energy density minus the critical density is odd, the stress tensor is even, etc. However, it is far less obvious how the spin variables should fit into the transformation scheme.

In this section, I outline a way of seeing how these variables work, and how their dual analogs can be defined. This discussion can be considered to be a kind of prolog to a

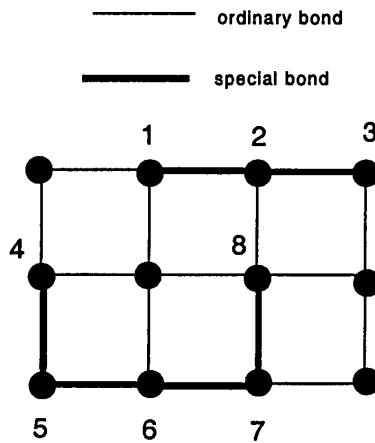


Fig. 15.3. Two paths through the lattice. On the heavy lines the coupling is modified by the addition of $i\pi/2$. The ratio of the modified to the unmodified partition functions for each of the paths determines the correlation function for the four spins at the ends of the path, $\langle \sigma_1 \sigma_3 \sigma_4 \sigma_8 \rangle$.

whole field of activity in which problems in statistical mechanics and quantum field theory give rise to subtle and unexpected excitations and corresponding variables. Start with $Z[K]$, a partition function containing many different couplings. Let us take one of these, a coupling connecting a σ_1 and a σ_2 as $z = \exp(K\sigma_1\sigma_2)$ and change this bond by making the replacement

$$K \rightarrow K' = K + \frac{\pi i}{2}. \quad (15.46a)$$

Correspondingly the statistical weight changes according to

$$z = \exp(K\sigma_1\sigma_2) \rightarrow z' = \exp(K'\sigma_1\sigma_2) = zi\sigma_1\sigma_2. \quad (15.46b)$$

Therefore, if we call the whole set of couplings before the change $[K]$ and the set after the change K' , we find that the partition function has changed according to the rule

$$Z[K] \rightarrow Z[K'] = Z[K]i\langle\sigma_1\sigma_2\rangle \quad (15.46c)$$

where the average on the right is computed with the original set of couplings, K . Similarly if we perform the change of Eq. (15.46a) on two touching bonds (See Fig. 15.3), we obtain

$$Z[K] \rightarrow Z[K'] = Z[K]i^2\langle\sigma_1\sigma_2^2\sigma_3\rangle = Z[K]i^2\langle\sigma_1\sigma_3\rangle. \quad (15.46d)$$

It is easy enough to see how to extend this to many couplings. Imagine that we perform the transformation (15.46a) on n bonds which form a long unbroken path through the lattice. In this way, we get a new partition function. The ratio of the two partition functions is i^n times the average of $2n$ spins. If the bonds form one path through the material then each spin except for the first and the last is counted twice. The net effect of the change is to make a way of calculating the correlation function,

$$\langle\sigma_1\sigma_{n+1}\rangle[K] = i^{-n} \frac{Z[K']}{Z[K]}. \quad (15.47)$$

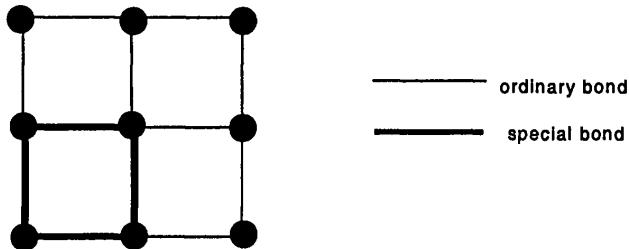


Fig. 15.4. A closed path through the lattice. On each heavy line the coupling is modified by the addition of $i\pi/2$. The modified and unmodified partition functions are exactly equal.

Two such paths are shown in Fig. 15.3. This pair of paths will produce a partition function which will then generate a four-spin correlation function.

Notice that a closed path through the lattice gives each spin raised to an even power. Thus, except for the factor i^{-n} the change (15.46a) produces an invariance on each closed path.

Thus, by varying the coupling constants in the partition function we can calculate all kinds of spin correlation functions. Notice also that if a given spin appears an even number of times inside a average, it disappears from the average. As a consequence we can get the very same correlation function in many different ways. To get a two-spin function, we vary the coupling constants along a path. The beginning and the end of the path determine the spins in the average. Just so long as we have a single-line path, the resulting partition function is independent of the path in question. The test and signal for path independence is that when the couplings are changed on an entire closed path, as in Fig. 15.4, the resulting partition function has as its only change a multiplication by i raised to the number of bonds. Thus, on a closed path, $Z[K'] = \pm Z[K]$.

Thus, varying couplings, in the form (15.46) along a path on the direct lattice determines the spin correlations. The spin variables are said to be order variables because the average of two far-apart spins determines how much long range-order there is in the system. For every single quantity which we might calculate using the direct lattice, there is an analogous quantity for the dual lattice. We might imagine that the dual analog of an order variable, σ , is a disorder variable which we might call μ . The latter has the property that the average of two far-apart disorder variables is zero for T below T_c and gradually rises to unity in the region $T > T_c$. To define such a variable, look back at the relation

$$\sinh(2\tilde{K}) \sinh(2K) = 1.$$

Under the transformation (15.46) $\sinh 2K$ changes sign. Thus the effect of the transformation upon \tilde{K} might be one of two things, either it translates in the same way as K or it changes sign. We have already done the translation. Let us now investigate the consequences of transformations of couplings which change their sign. Imagine that we take a whole region of the lattice enclosing many lattice sites and change the sign of every spin-summation variable in that region. (See Fig. 15.5.) That change is no change at all since the sum is over both signs of all variables. However, that change is equivalent to changing

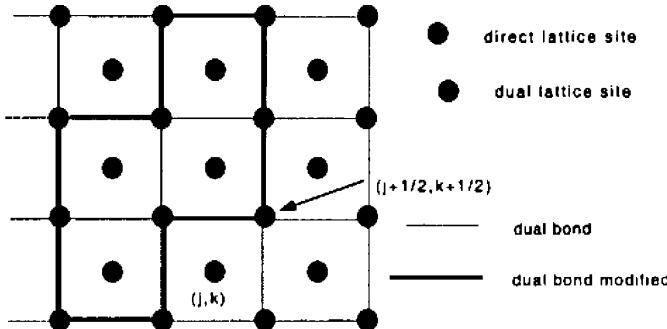


Fig. 15.5. A closed path through the bonds of the dual lattice. On each heavy line the dual coupling is modified by the addition of $i\pi/2$. This is equivalent to changing the signs of all the direct couplings which intersect these dual couplings. Then the transformation can be undone by changing all the signs of all the spins within the path. Thus, modified and unmodified partition functions are exactly equal.

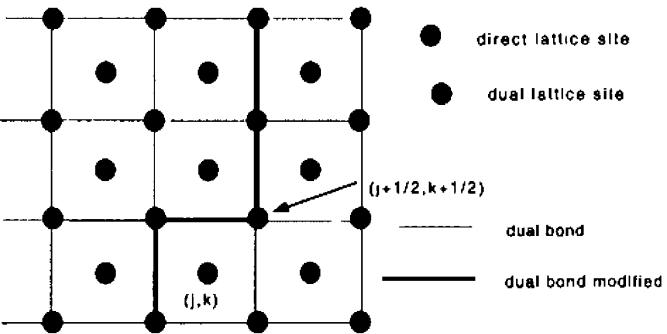


Fig. 15.6. An open path through the bonds of the dual lattice. On each heavy line the dual coupling is modified by the addition of $i\pi/2$. The new partition function is defined to be $\langle \mu_{j-1/2, k-1/2} \mu_{j+1/2, k+5/2} \rangle$ times the old partition function.

the sign of every coupling connecting the region with the remainder of the system. This analysis shows us that a change in sign of all the couplings along a closed path on the dual lattice is an invariance of the partition function.

Accordingly, if we change the sign of all the couplings along an open path (see Fig. 15.6) which produces a new partition function $Z[K']$ which is independent of the path, but only depends upon endpoints. Then we can use the ratio of the old and new partition functions to define a correlation function of disorder variables according to

$$\frac{Z[K']}{Z[K]} = \langle \mu_1 \mu_2 \rangle [K], \quad (15.48)$$

where '1' and '2' label the two endpoints of the path. Thus, we have used to invariance of the system under interchange of the sign of the spin to define an entirely new kind of correlation function.

Duality has paid off for us in three different ways

- (a) in giving relations between high and low temperatures within a given problem.

- (b) in giving unexpected relations among different problems.
- (c) in defining new variables which reflect invariance properties of a given problem.

In recent years, string theorists have gotten even more mileage out of using analogs of duality relations to establish the connections within and among various kinds of string theories.

Homework

Problem 15.1 (Three State Potts Model). This is a problem in which there is a variable on each site, ϕ which can take on three possible values. Let us have a two-dimensional problem with nearest neighbor couplings. Let the statistical weight of a bond be $\exp(K)$ when nearest neighbor variables are the same and 1 when they are different. What is the value of the critical coupling, K_c ?

Problem 15.2 (Poisson Sum Formula). Calculate

$$S[K] = \sum_n e^{-n|K|}$$

both directly and by using the Poisson sum formula.

Chapter 16

Planar Model and Coulomb Systems

16.1 Why Study a Planar Model?

So far we have talked mostly about discrete symmetries. Now we are going to extend our thinking to discuss a two-dimensional rotational symmetry. Imagine that we have a lattice, with lattice sites \mathbf{r} and a variable $\theta_{\mathbf{r}}$ at each lattice site. Here, see Fig. 16.1, θ represents the orientation angle of a two-dimensional vector, $\mathbf{s}(\mathbf{r}) = (s_1(\mathbf{r}), s_2(\mathbf{r})) = (\cos \theta_{\mathbf{r}}, \sin \theta_{\mathbf{r}})$ placed at the lattice site of a regular square lattice.) For simplicity, we will take the magnitude of this vector to be unity, so that it can be completely described by the phase, $\theta_{\mathbf{r}}$.

We study systems composed of many spins arranged on the sites of a regular lattice. (See Fig. 16.2.) The action for this system is based on a set of nearest neighbor bonds, which have the form $K(\theta_{\mathbf{r}} - \theta'_{\mathbf{r}'})$. The action is the sum over all nearest neighbor pairs of bonds of this form:

$$\mathcal{W}[\theta] = \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} K(\theta_{\mathbf{r}} - \theta'_{\mathbf{r}'}) . \quad (16.1)$$

One specific example has the bond being proportional to the dot product of the spins:

$$K(\theta_{\mathbf{r}} - \theta'_{\mathbf{r}'}) = \frac{K}{2\pi} [1 - \mathbf{s}(\mathbf{r}) \cdot \mathbf{s}(\mathbf{r}')] = \frac{K}{2\pi} [1 - \cos(\theta_{\mathbf{r}} - \theta'_{\mathbf{r}'})] . \quad (16.2)$$

Here K is a constant which measures the strength of the bond. The ‘extra’ factor of 2π is inserted here to make some of the later formulas simpler.¹

A model involving a spin variable with two components is called a planar, or XY model. The ‘ XY ’ means that each spin is free to rotate in the plane of some two-dimensional space. This symmetry-space of $\theta_{\mathbf{r}}$ is absolutely not the same as the coordinate space of \mathbf{r} . However,

¹Our work in this and the next chapter is largely based upon the analysis of Jorge V José, Leo P. Kadanoff, Scott Kirkpatrick, David R. Nelson (see Sec. 17.11.3). The ‘extra’ factor of 2π is not in the definition of the K which is used in that work.

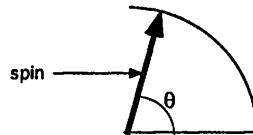


Fig. 16.1. Two-dimensional spins of fixed length are described by an angular variable θ .

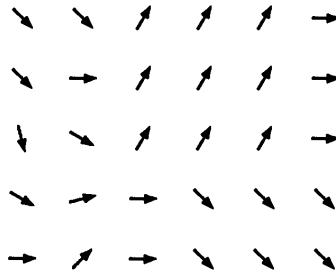


Fig. 16.2. We study a problem in which spins are arranged on a two-dimensional lattice.

some forms of excitation link the two spaces. This linkage is very interesting to both modern physics and also modern mathematics.

The bond (16.2) and the other bonds we use for our planar-model calculations are required to include two important kinds of symmetry. First there is a *global symmetry*. If one rotates every spin in the system by the very same amount, say α ,

$$\theta_{\mathbf{r}} \rightarrow \theta_{\mathbf{r}} + \alpha, \quad (16.3)$$

one leaves the action unchanged. Thus all properties of the model must be invariant under the transformation (16.3). Any invariance produced by the simultaneous and equal change in variables is called a global symmetry.

In addition, we would like to have each and every angular variable behave like a respectable angle. All angles return to themselves after a rotation through 2π . For this reason, we demand that the bond have the periodicity property that

$$K(\theta + 2\pi) = K(\theta). \quad (16.4a)$$

Once we make that condition hold then the problem is periodic in each one of the θ -variables. That is to say that $\mathcal{W}[\theta]$ is invariant under

$$\theta_{\mathbf{r}} \rightarrow \theta_{\mathbf{r}} + 2\pi \quad \text{for any } \mathbf{r}. \quad (16.4b)$$

These two invariance properties will play a large role in determining the behavior of our XY -system.

In view of the symmetry (16.4) all statistical sums are done as integrals over an interval of size 2π . Thus

$$\text{tr}_{\theta} = \int_{-\pi}^{\pi} d\theta. \quad (16.5)$$

An invariance like the one in Eq. (16.3) which is developed as an equal transformation upon all of the variables which make up the system is called a *global* invariance. One like (16.4) which applies to each variable separately is called a *gauge* invariance.² Modern statistical and particle physics is very interested in establishing the effect of both kinds of symmetries upon the long-range correlations in statistical system. The planar problem studied here is the simplest problem having a gauge symmetry reflecting the invariance of an angle under a 2π rotation. Problems in particle physics often have this symmetry and in addition other, more complex symmetries. So we study the simplest case here.

16.2 One-Dimensional Case

The partition function for this case is given in the familiar form:

$$\begin{aligned} Z &= \text{Tr}_\theta \prod_{j=1}^N \exp[K(\theta_{j+1} - \theta_j)], \\ \text{Tr}_\theta &= \prod_{j=1}^N \int_{-\pi}^{\pi} d\theta_j, \end{aligned} \quad (16.6)$$

with the boundary condition that $\theta_{N+1} = \theta_1$.

As we have done before, we solve this problem using a Fourier transform procedure. We write

$$\exp[K(\theta)] = \sum_{n=-\infty}^{\infty} \exp \tilde{K}(n) \exp(-in\theta). \quad (16.7)$$

The partition function in Eq. (16.6) is then calculated quite directly as

$$Z = (2\pi)^N \sum_{n=-\infty}^{\infty} \exp(N\tilde{K}(n)). \quad (16.8)$$

If N is large, the sum on the right is dominated by its one largest term. If the bond coupling $K(\theta)$ is real, then the real part of $\tilde{K}(n)$ is largest for $n = 0$. Thus for large N we find

$$\ln Z = N \ln 2\pi + N\tilde{K}(0). \quad (16.9)$$

A similarly easy calculation gives the correlation between spins at two different sites. The basic spin variable is a two component vector, (s_1, s_2) . It is convenient to store this vector, which has unit length, as a complex number by using the pair of variables:

$$s_1 \pm is_2 = e^{\pm i\theta}. \quad (16.10)$$

²The prototype and simplest gauge invariance is the gauge transformation of the scalar and vector potentials in electrodynamics. In quantum mechanics, this same transformation is accompanied by a transformation of the phase of wave functions. The phase variable has properties very similar to our θ_r .



Fig. 16.3. Two-dimensional spins of fixed length are described by an angular variable θ . Here, these spins are arranged on a one-dimensional lattice.

One can calculate the correlation function

$$\rho(k - j) = \langle [s_1(j) + is_2(j)][s_1(k) - is_2(k)] \rangle \quad (16.11)$$

as a function of the distance between the two spins, $|k - j|$. After a brief calculation [see Problem (16.1)], we find that, for $N \gg |k - j| \gg 1$, the correlation function has the value

$$\rho(k - j) = \exp[-|k - j|(\tilde{K}(0) - \tilde{K}(1))]. \quad (16.12)$$

Since $\tilde{K}(0)$ is larger than $\tilde{K}(1)$, this correlation function always drops off as an exponential function of separation. This exponential fall-off of the correlation function is indicative of a disordered phase. We conclude that any near neighbor interaction model with a planar symmetry is disordered in one dimension.³ The basic reason for the disorder is shown in Fig. 16.3. No matter how strong is the interaction between nearest neighbor spins, they may each be rotated by a small amount relative to one another. There is nothing then to prevent many small changes from adding up to a big change. (In fact the changes will — by a random walk process — certainly become large whenever the region considered is sufficiently large.) The big change will, in turn, imply that in one dimension the system will always be in a disordered phase, except perhaps at zero temperature.

16.3 Phases of the Planar Model

Thus, for one dimension, the planar model will certainly be in a disordered phase. For dimensions greater than 2, the behavior of this model is well-understood and is basically similar to the models we have discussed heretofore. If the nearest neighbor couplings are ferromagnetic, i.e. if the bond $K(\theta - \theta')$, takes on its largest values for $\theta = \theta'$, then the system can fall into the usual three phases, described by a complex order parameter

$$\text{order parameter} = \langle \exp(i\theta_r) \rangle. \quad (16.13)$$

- (1) For weak couplings the system is in a disordered phase, with the order parameter, $m = \langle \exp(i\theta_r) \rangle$ equal to zero. This system then has a correlation function,

$$\rho(r, r') = \langle \exp(i\theta_r) \exp(-i\theta_{r'}) \rangle,$$

which falls off exponentially with separation, $|r - r'|$.

³As argued by Lev Landau, one-dimensional systems must be disordered at nonzero temperatures. Consider first a situation in which the local ordering variable takes on discrete values, e.g. $\sigma = \pm 1$. For the system to be ordered, information must travel from one end of the system to the other. A Bloch wall cuts this flow of information, since each such wall will separate this system into uncorrelated regions. With continuous symmetry, the ordering variable can change gradually, thus producing an increased potential for disorder. As a result, one-dimensional systems cannot be ordered except in extreme limits, like zero temperature.

- (2) At some critical coupling the system falls into a critical phase in which the average of $\exp[i(\theta_{\mathbf{r}} - \theta_{\mathbf{r}'})]$ decays algebraically as $|\mathbf{r} - \mathbf{r}'|$ is increased

$$\rho(\mathbf{r}, \mathbf{r}') \sim |\mathbf{r} - \mathbf{r}'|^{-2x}.$$

This critical behavior, too, is quite standard. Here x is a critical index which is universal, i.e. it depends on dimensionality but not upon the details of the coupling scheme.

- (3) For strong couplings the system falls into an ordered phase in which the order parameter, $s(\mathbf{r}) = \exp(i\theta_{\mathbf{r}})$, has a nonzero average. Fluctuations in the order parameter called spin waves produce a spin correlation function

$$\rho(\mathbf{r}, \mathbf{r}') = \langle \exp(i(\theta_{\mathbf{r}} - \theta_{\mathbf{r}'})) \rangle - \langle \exp(i\theta_{\mathbf{r}}) \rangle^2 \sim |\mathbf{r} - \mathbf{r}'|^{-2z}, \quad (16.14)$$

which decays algebraically as $|\mathbf{r} - \mathbf{r}'|$ is increased. For a given dimension, the spin correlation index, z , is universal.

This algebraic behavior⁴ in an ordered phase is entirely different from any behavior we have encountered so far in this course. Its explanation is both deep and interesting. Consider how information about ordering passes along the lattice. Whenever there is a discrete symmetry, one can only pass a discrete number of bits of information at every step. Thus, at each step, some information about the ordering might be lost. The net result of many small losses is an exponential decay of correlations. In this case, any fluctuation which arises in the system dies away after a short distance and the resulting correlation length is finite. However, when there is an ordered phase in which a continuous symmetry is broken, then there is a possibility for continuously varying excitation in which the order parameter varies quite gradually. Since the slow variation is a small change from an unvarying order parameter, in the quantum interpretation of the problem, the increase in the system's energy is quite small. The small increase goes to zero as the wavelength becomes infinite. If the energy change vanishes as the wave length goes to infinity, the excitation has an infinite correlation length, and thus represents a particle with mass equal to zero. Thus an ordered state with a broken continuous symmetry has a massless excitation and a critical behavior. This argument was originally given by Y. Nambu and J. Goldstone. The excitation is called a Goldstone or Nambu–Goldstone boson. These excitations form a most interesting part of condensed matter physics and of particle physics.

In the X - Y case considered here, the basic variable is a two-dimensional spin with components s_1 and s_2 . The ordering picks a direction for that vector. When the direction varies slowly in space, we can get a zero-mass excitation and critical correlation like that shown in Eq. (16.14).

At $d = 2$, something different occurs. The first two phases are familiar to us. At weak couplings this system falls into a disordered phase with exponential decay of fluctuations.

⁴The basic theory of spin waves in the XY model is due to V. L. Berezinskii (JETP **34**, 610 (1971) and REPRINT: Sec. 16.7.1).

As usual, there is a critical value of the coupling that produces a critically ordered phase with algebraic correlation. The new features arise at stronger couplings. Instead of the phase described by number 3 above we have:

- (3') In two dimensions, the average order parameter is zero for all finite values of the coupling.⁵ Hence there is no ordered phase in the low temperature system. However, there is excellent evidence, e.g. from high temperature series,⁶ that the system does have a phase transition. As we shall see below, the system falls into a situation in which the order parameter is zero, but there are continuously varying critical indices. Thus, we have a phase which remains critically ordered over a whole range of coupling strengths.

16.4 The Gaussian Approximation

One way to see what is going on is to assume that we are at very strong coupling.⁷ Then the system comes very close to falling into a locally ordered state, in that nearby vectors point in almost the same direction, so that for all d we can expand about that state. Assume that the variables, $\phi = \theta_{\mathbf{r}} - \theta'_{\mathbf{r}}$, are all small and then expand the cosine in the bond (16.2), in the form $\cos \phi \approx 1 - \phi^2/2$ to obtain the action

$$\mathcal{W}[\theta] = -\frac{K}{4\pi} \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} (\theta_{\mathbf{r}} - \theta_{\mathbf{r}'})^2. \quad (16.15)$$

There are two steps in our method of deriving a Gaussian approximation. The first is the replacement of the basic interaction by using the approximation of Eq. (16.15). The second is to extend all $\theta_{\mathbf{r}}$ integrals to go from minus infinity to infinity. Both steps are accurate when K is sufficiently large. In this way, we obtain a completely Gaussian problem. This approximate restatement is called the *spin wave* approximation to the planar model. It is reliable for all dimensions if K is large enough.

This is, however, a special Gaussian model. Because of the global symmetry,

$$\theta_{\mathbf{r}} \rightarrow \theta_{\mathbf{r}} + \alpha, \quad (16.16)$$

this Gaussian model is always precisely at the critical point, as can be seen by a comparison back to Eq. (3.20).

At this point, we begin to calculate averages like

$$\langle \exp(i\theta_{\mathbf{r}}) \exp(-i\theta_{\mathbf{r}'}) \rangle = \langle [s_1(\mathbf{r}) + is_2(\mathbf{r})][s_1(\mathbf{r}') - is_2(\mathbf{r}')] \rangle. \quad (16.17)$$

⁵See M. D. Mermin and H. Wagner, Phys. Rev. Letts. **17**, 133 (1966) and also P. Hohenberg, Phys. Rev. **158**, 383 (1967).

⁶DGL: Volume 3, D. D. Betts, page 569 (1974).

⁷See V. L. Berezinskii's work reprinted in Sec. 16.7.1.

To attack averages of this kind, let us recall the general result for Gaussians and work from there. We wish to find the average of $\exp(iX)$ and X is a sum of the form

$$X = \sum_{j=1}^M q_j \theta_{\mathbf{r}_j}. \quad (16.18)$$

To describe this average, we shall call q_j the ‘charge’ at the point \mathbf{r}_j . As we shall see, for $d = 2$, there is a strong analogy between this system and a two-dimensional Coulomb gas. We shall limit ourselves to integer values of q_j . When this charge is plus one $\exp(iX)$ contains a factor of the the complex order parameters, $e^{i\theta_{\mathbf{r}_j}}$. When the charge is minus one, the corresponding factor $e^{-i\theta_{\mathbf{r}_j}}$. From Eq. (3.7), we see that the average of $\exp(iX)$ has the form

$$\langle \exp(iX) \rangle = \exp \left[- \sum_{jk} q_j q_k G(\mathbf{r}_j - \mathbf{r}_k) \frac{2\pi}{K} \right] \quad (16.19)$$

where $G(\mathbf{r})$ is the lattice Green function, and has the form given in Eq. (3.19):

$$G(\mathbf{r}) = \int_{-\pi}^{\pi} \frac{d\mathbf{k}}{(2\pi)^d} \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sum_{a=1}^d 4(1 - \cos k_a)}. \quad (16.20)$$

Consider the very simplest example of a correlation of the form (16.19). We consider one charge, with $\theta = \pm 1$, at \mathbf{r} . Then we discover that in the Gaussian approximation

$$\langle e^{iq\theta_{\mathbf{r}}} \rangle = \exp \left[-G(0)q^2 \frac{2\pi}{K} \right]. \quad (16.21)$$

There is difference between the two cases $d > 2$ and $d \leq 2$. Look at the integral (16.20). For all values of \mathbf{r} , not just $\mathbf{r} = 0$, the small- k form of the integration has a potential infinity in it. The result is

$$G(0) = \int \frac{d\mathbf{k}}{(2\pi)^d} \frac{1}{2k^2} + \text{higher } k\text{-contributions} \sim \int k^{d-1} dk \frac{1}{k^2} + \dots. \quad (16.22)$$

For $d > 2$ the low- k contributions are finite and cause no problem. In that case, $G(0)$ is finite and the order parameter (16.21) is nonzero. Thus, we get a conventional ordered state.

The situation is different for $d \leq 2$. In that case, according to Eq. (16.22), $G(\mathbf{r})$ diverges to plus infinity because of the small- q zero in the denominator in Eq. (16.20). If $G(0)$ is infinite, the order parameter defined by Eq. (16.21) is zero. Thus for dimensions less than or equal to two, the order parameter vanishes. Now there are, once more, two different situations. Either $d < 2$ or $d = 2$. The only physical case with $d < 2$ is dimension one, where there is no ordering.

Dimension two is truly interesting. According to the Gaussian approximation the order parameter is zero.⁸ However the correlation functions need not vanish so long as the total charge

$$Q = \sum_{j=1}^M q_j \quad (16.23)$$

does indeed vanish. Whenever such a vanishing takes place, there is a nonzero correlation function. The simplest case is the two-point function

$$\langle \exp(i\theta_r) \exp(-i\theta_{r'}) \rangle = \exp\left(\frac{g(r - r')}{K}\right). \quad (16.24)$$

Here $g(|r - r'|)$ is obtained from Eq. (16.19) by combining the four terms in the exponent of that equation.⁹ Then $g(r) = 4\pi[G(\mathbf{0}) - 2G(r)]$, and thus

$$g(r) = 2\pi \int_{-\pi}^{\pi} \frac{dk}{(2\pi)^d} \frac{1 - \cos \mathbf{k} \cdot \mathbf{r}}{\sum_{a=1}^d 2(1 - \cos k_a)}. \quad (16.25)$$

If one specializes that result to the long-wavelength limit, by expanding the denominator in Eq. (16.20) one finds

$$g(r) = 2\pi \int_{-\pi}^{\pi} \frac{dk}{(2\pi)^d} \frac{1 - \cos \mathbf{k} \cdot \mathbf{r}}{k^2}. \quad (16.26)$$

Notice that the small- k divergence has canceled out in g . If \mathbf{r} has a length which extends over many lattice sites, then the small k contribution to the integral in Eq. (16.26) is, for $d = 2$,

$$g(r) \approx \int_{1/r}^{\pi} \frac{dk}{k} \approx \ln \frac{r}{ac}, \quad (16.27)$$

where a is the nearest neighbor separation distance and c is a constant which can be determined by numerical integration of Eq. (16.25). We thus obtain the algebraically decaying correlation function

$$\langle \exp(i\theta_r) \exp(-i\theta_{r'}) \rangle \approx \left[\frac{|r - r'|}{ac} \right]^{-1/K}. \quad (16.28)$$

⁸According to a careful analysis carried out by H. Wagner, M. D. Mermin and P. Hohenberg the average of $\cos \theta(\mathbf{r})$ will always vanish for any two-dimensional situation with the XY symmetries. In fact, the Gaussian analysis qualitatively gives the ‘right answers’ for the existence of ordering in this model. See M. D. Mermin and H. Wagner, Phys. Rev. Letts. **17**, 133 (1966).

⁹The careful reader will wonder whether one can get valid and correct results by adding and subtracting infinite quantities. The answer is sometimes one can. For example one can do the entire analysis in a box of finite size. Then the integral over wave vectors is replaced by a sum. The zero-charge condition eliminates the zero wave-vector term. The remaining terms are finite and may be manipulated. Then, in the final answer, take the limit as the volume goes to infinity. The final answer is the same as given in the text.

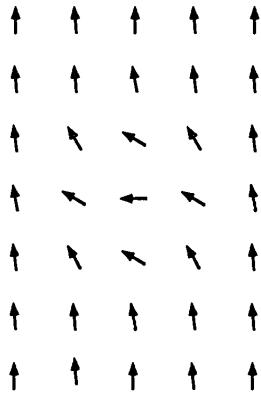


Fig. 16.4. Two-dimensional spins of fixed length can rotate slowly in space in response to a single spin which is held in place. Here, the central spin is held to point toward the left while the spins at infinity point to the top of the page.

Thus the correlation function dies off algebraically, with a power which depends upon the coupling K .

In some respects this is a typical critical point result. At criticality, the order-parameter correlation function usually has a power-law dependence upon distance. However, this situation is different from the usual critical one in two respects: First, the system is not in at a critical point but is instead in its low-temperature region. Equation (16.28) applies when the coupling, K , is large. Second, instead of having a universal value of the critical index, the index in Eq. (16.28) has a value, $1/K$, which is a continuously varying function of the coupling constant. Such continuous variation is not characteristic of the usual critical problems.

We should certainly ask why the two-dimension planar model shows these logarithmic correlations. The answer is connected with the kinds of excitations which can appear in the system. Start from a situation in which we fix some of the spins. In particular, we hold the spins at infinity to point upward. (See Fig. 16.4). One additional spin is held fixed and points, say, to the left. Every other spin then rotates a bit to find its position to minimize the total bond energy. Notice how the angular deviations between neighboring spins decrease as one moves away from the center of the disturbance. A precise calculation, using lattice Green functions shows that the angular deviation dies away as $1/r$. As a result each bond energy, proportional to $1 - \cos(\theta - \theta')$, increases by $1/r^2$. The total energetic cost out to distance R is obtained by integrating

$$\int_1^R d^2\mathbf{r} \frac{1}{r^2} \sim \ln R. \quad (16.29)$$

Therefore each excitation costs an energetic factor of the form $\exp(bK \ln R)$, where b depends on the detailed form of the excitation. The exponential of a logarithm is a power, and here the power varies with K . This power is the cause of the ‘pseudo-critical’ behavior of the low temperature two-dimensional planar model. The sort of excitation just discussed is called a ‘spin-wave’.

According to our argument, since the Gaussian approximation is accurate for strong coupling, the strong coupling model shows critical behavior with continuously varying critical indices. In fact, the Gaussian approximation for the two-dimensional planar model is essentially correct for all couplings strengths above a characteristic critical coupling, K_c . The only error made by the Gaussian approach is that the value of the critical index x_1 is not $1/(2K)$ but $1/(2K_{\text{eff}})$ where the effective coupling must be determined by a renormalization procedure. (See the next chapter.)

It is important to notice that $\exp(-i\theta_r)$ and $\exp(i\theta_r)$ appear naturally in the theory outlined above because they represent the basic spin operators. This information about the spin operators is not really included in the Gaussian theory. It is added from outside to make the Gaussian theory fit with the planar model. The Gaussian theory itself would permit the consideration of operators like $\exp(-i\theta_r\sqrt{2})$ or $\exp(\pi\theta_r)$ but these are ruled out by our insistence upon a physical interpretation.

16.5 Two-Dimensional Coulomb Systems

So far we have considered spin wave excitations, and their logarithmic correlations. Lines of charge also¹⁰ have logarithmic interactions. Consequently charges q_1 and q_2 at positions r_1 and r_2 have an interaction potential which is

$$-q_1 q_2 \frac{\ln|r_1 - r_2|}{\epsilon},$$

where ϵ is the dielectric constant of the medium.

Our spin wave approximation to the planar model has very much the same behavior. The basic operators are described by their charge q , which must be ± 1 . Thus we write the operator as

$$O_q(r) = \exp(iq\theta_r). \quad (16.30)$$

We form the most general operator that we can by constructing the product

$$\mathcal{P} = \prod_{j=1}^M O_{q_j}(r_j) = \exp \left(i \sum_{j=1}^M q_j \theta_{r_j} \right). \quad (16.31)$$

In a situation in which the total charge is zero, one can rewrite Eq. (16.19) in terms of g as

$$\langle \mathcal{P} \rangle = \exp \left[\sum_{j < k=1}^M \frac{q_j q_k}{K} g(r_j - r_k) \right]. \quad (16.32)$$

¹⁰For an exposition of the role of coulomb systems in two-dimensional phase transitions, see B. Nienhuis in DGL: Volume 11, page 1 (1987).

Consider the situation in which all separations are large compared to a lattice constant, and then replace the g by logarithms of distances [see Eq. (16.27)] to find

$$\langle \mathcal{P} \rangle = \exp \left[\sum_{j < k=1}^M \frac{q_j q_k}{K} \ln \left(\frac{|\mathbf{r}_j - \mathbf{r}_k|}{ac} \right) \right], \quad (16.33)$$

as a form for the correlation function of many charges placed in two-dimensional space. For Eq. (16.33) to be correct, the total charge contained in \mathcal{P} must be zero. Equation (16.33) has exactly the form we might expect. The charges interact via logarithmic potentials. The constant multiplier, c , in Eq. (16.33), arose from the corresponding multiplier in Eq. (16.27). Notice how the coupling constant, K , serves the role of the dielectric constant in this formula for charge-charge interactions. This role of the coupling will have an important consequence for the renormalization of the planar system.

We are going to use Eq. (16.33) to illustrate some of the concepts about local critical operators which we outlined in Chapter 12. We saw there that the product of two nearby operators must have an expansion in terms of the other operators in the system.

16.6 Multipole Expansion

Let us bring two equal but opposite charges close together to form a product

$$\mathcal{Q} = O_q \left(\mathbf{R} + \frac{\mathbf{r}}{2} \right) O_{-q} \left(\mathbf{R} - \frac{\mathbf{r}}{2} \right), \quad (16.34)$$

by adding two more equal charges to the list already present. The distance r will be taken to be very small. From Eq. (16.33) the correlation among these $M + 2$ charges obeys

$$\langle \mathcal{Q} \mathcal{P} \rangle = \langle \mathcal{P} \rangle \langle \mathcal{Q} \rangle e^\Gamma \quad (16.35)$$

$$\Gamma = \frac{q}{K} \sum_{j=1}^M q_j \left\{ \ln \left| \mathbf{r}_j - \mathbf{R} - \frac{\mathbf{r}}{2} \right| - \ln \left| \mathbf{r}_j - \mathbf{R} + \frac{\mathbf{r}}{2} \right| \right\}. \quad (16.36)$$

In working in two dimensions, it is helpful to use a complex notation for vectors. So instead of $\mathbf{r} = (x, y)$, use $z = x + iy$. Notice that the magnitude of a vector is the same as that of a complex number, $|\mathbf{r}|^2 = zz^*$, where z^* is the complex conjugate of z . Use the notation in which z_j is the complex version of $\mathbf{r}_j - \mathbf{R}$. We evaluate expression (16.36) by using the fact that $|z|$ is much smaller than $|z_j|$. Then Γ simplifies as

$$\begin{aligned} \ln \left| \mathbf{r}_j - \mathbf{R} - \frac{\mathbf{r}}{2} \right| - \ln \left| \mathbf{r}_j - \mathbf{R} + \frac{\mathbf{r}}{2} \right| &= \frac{1}{2} \ln \frac{z_j - z}{z_j + z} + \text{complex conjugate} \\ &= \left(\frac{-z}{z_j} \right) + \left(\frac{-z^*}{z_j^*} \right) + \text{order} \left(\frac{z}{z_j} \right)^3, \end{aligned}$$

so that e^Γ becomes

$$\begin{aligned} e^\Gamma = 1 - \sum_{j=1}^M \frac{q_j q}{K} & \left\{ \left(\frac{z}{z_j} \right) + \left(\frac{z^*}{z_j^*} \right) \right\} \\ & + \sum_{j=1}^M \sum_{k=1}^M \frac{q^2 q_j q_k}{2K^2} \left\{ \left(\frac{z}{z_j} \right) + \left(\frac{z^*}{z_j^*} \right) \right\} \left\{ \left(\frac{z}{z_k} \right) + \left(\frac{z^*}{z_k^*} \right) \right\}. \end{aligned} \quad (16.37)$$

To interpret Eq. (16.37), notice that the content of the operator product expansion, Eq. (12.60),

$$O_\alpha \left(\mathbf{R} + \frac{\mathbf{r}}{2} \right) O_\beta \left(\mathbf{R} - \frac{\mathbf{r}}{2} \right) = \sum_\gamma C_{\alpha\beta\gamma}(\mathbf{r}) O_\gamma(\mathbf{R}), \quad (16.38)$$

is that an operator product can be expanded as a sum of the basic operators in the theory (O) with coefficients (C) which depend upon distance. Use Eq. (16.37) to replace the Γ in Eq. (16.36) and find:

$$\begin{aligned} O_q \left(\mathbf{R} + \frac{\mathbf{r}}{2} \right) O_{-q} \left(\mathbf{R} + \frac{\mathbf{r}}{2} \right) \approx & \left[\frac{r}{ac} \right]^{-q^2/K} \left[1 + \frac{qz}{K} \mathcal{D}(\mathbf{R}) + \frac{qz^*}{K} \mathcal{D}^*(\mathbf{R}) + \frac{q^2 z^2}{2K^2} \mathcal{Q}(\mathbf{R}) \right. \\ & \left. + \frac{q^2 z^{*2}}{2K^2} \mathcal{Q}^*(\mathbf{R}) + \frac{q^2 z z^*}{2K^2} \mathcal{M}(\mathbf{R}) \right]. \end{aligned} \quad (16.39)$$

This result consists of a sum of six different terms, each representing a different operator, O_γ . We list them here:

The first term, unity, on the right hand side of Eq. (16.39) gives a result which is independent of the position, \mathbf{R} . This term comes from the simplest of all fluctuation operators, the constant. The correlator of anything with this operator, 1, is given by

$$\langle \mathcal{P} | 1 \rangle = \langle \mathcal{P} \rangle \quad (16.40)$$

just as one might expect for a unit operator.

In the next two terms \mathcal{D} and \mathcal{D}^* are dipole operators, expressed in a complex notation in which the respective operators have the same rotational properties as $(x - iy)$ and $(x + iy)$. The operators are complex conjugates of one another. The correlator of a dipole operator with a bunch of charges is given by Eq. (16.37) as

$$\langle \mathcal{D}(\mathbf{R}) | \mathcal{P} \rangle = \langle \mathcal{P} \rangle \sum_{j=1}^M \frac{q_j}{Z - z_j}. \quad (16.41)$$

Here, Z is the complex version of the coordinate \mathbf{R} while z_j is the complex representation of \mathbf{r}_j . The operator \mathcal{P} , is an abbreviation for the product of M charged operators as given in Eq. (16.31).

Next, come the quadrupole operators \mathcal{Q} and \mathcal{Q}^* . These operators are the two components of a second rank tensor which has the correlation property

$$\langle \mathcal{Q}(\mathbf{R}) \mathcal{P} \rangle = \langle \mathcal{P} \rangle \sum_{j,k=1}^M \frac{q_j q_k}{(Z - z_j)(Z - z_k)}. \quad (16.42)$$

The dipole and quadrupole operators show in Eqs. (16.41) and (16.42) exactly the interaction properties which one would have expected from looking at the charge multipole interaction potentials in two-dimensional electrostatics. The quadrupole operators also serve as the stress tensors which can produce distortions in the coordinates in the problem.

Last turn to \mathcal{M} which has correlations

$$\langle \mathcal{M}(\mathbf{R}) \mathcal{P} \rangle = \langle \mathcal{P} \rangle \sum_{j,k=1}^M \left[\frac{q_j q_k}{(Z - z_j)(Z - z_k)^*} + \text{complex conjugate} \right]. \quad (16.43)$$

Notice that \mathcal{M} has the same scaling properties as $1/R^2$. Thus it is a marginal operator. In fact, it is precisely the local version of the operator which is required to produce changes in the dielectric constant K .

We can rearrange Eq. (16.43) into a form which will prove useful in the next chapter. This rearrangement comes from grouping the diagonal and off-diagonal terms as:

$$\begin{aligned} \langle \mathcal{M}(\mathbf{R}) \mathcal{P} \rangle &= \langle \mathcal{P} \rangle \sum_{j < k} 2q_j q_k \left[\frac{1}{(Z - z_j)(Z - z_k)^*} \right. \\ &\quad \left. + \frac{1}{(Z - z_j)^*(Z - z_k)} - |Z - z_j|^{-2} - |Z - z_k|^{-2} \right] \end{aligned} \quad (16.44)$$

We shall make a detailed use of this expression in calculating the renormalization properties of the planar model.

Homework

Problem 16.1 (Correlations in One-Dimensional Planar Model).

- (a) Show that Eq. (16.12) is correct. Require $|k - j|$ to be much smaller than N .
- (b) What is the value of $\langle \exp(i\theta(j)) \exp(-i\theta(k)) \rangle$?

(c) Calculate the average of

$$\exp(i\theta(j_1)) \exp(-i\theta(j_2)) \exp(i\theta(j_3)) \exp(-i\theta(j_4)).$$

Problem 16.2 (Operator Product in $d = 2$ Coulomb Model).

- (a) What do you expect to be the result of bringing together the position of two operators $\exp(iq_1\theta_{\mathbf{r}_1})$ and $\exp(iq_2\theta_{\mathbf{r}_2})$.
- (b) Calculate the leading order of the operator product expansion for two operators with charges q_1 and q_2 .

Problem 16.3 (A Numerical Integration). Do the appropriate integrals and find the numerical value of the constant c which appears in Eq. (16.27).

Problem 16.4 (A Localized Excitation). We wish to construct the situation shown in Fig. 16.4. Allow the spins at infinity to point to the right and the one at $(0, 0)$ to point perpendicular to these. Use the spin wave approximation to calculate the average spin as a function of position. Draw a better version of Fig. 16.4.

Problem 16.5 (Criticality and Invariance of Gaussian Model). Consider a Gaussian model in which the action depends upon variables $\phi_{\mathbf{r}}$ and is a quadratic function of these variables. Show that this model is critical whenever an invariance like (16.16) holds. That is, the model is critical whenever

$$\phi_{\mathbf{r}} \rightarrow \phi_{\mathbf{r}} + \alpha$$

leaves the action unchanged. Is the converse true?

16.7 Reprint on Spin Waves

16.7.1 V. L. Berezinskii JETP 34 610 (1971). An Overview of Problems with Continuous Symmetry

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DESTRUCTION OF LONG-RANGE ORDER IN ONE-DIMENSIONAL AND TWO-DIMENSIONAL SYSTEMS POSSESSING A CONTINUOUS SYMMETRY GROUP. II. QUANTUM SYSTEMS

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The asymptotic behavior of the correlations in the low-temperature phase are found for the following two-dimensional quantum systems: a two-dimensional lattice of plane rotators, two-dimensional magnetic substances having an easy plane of magnetization, a two-dimensional Bose liquid (Sec. 1), and a two-dimensional isotropic Heisenberg ferromagnet (Sec. 2). The nature of the change of the asymptotic behavior with increasing temperature is investigated for the systems considered in Sec. 1. The nature of the change of the asymptotic behavior with increasing temperature is investigated for the systems considered in Sec. 1. The nature of the low-temperature phase consists in the superfluidity of a two-dimensional Bose liquid; the corresponding property can also be formulated in terms of magnetic substances.

In the previous article^[1] by the author, the correlation functions were determined at low temperatures in two-dimensional systems of classical spins and in other two-dimensional systems possessing a continuous symmetry group. In the present article similar results are derived for two-dimensional quantum systems: in Sec. 1 the correlations are investigated in a two-dimensional lattice of planar rotators, in a two-dimensional Bose liquid, and in planar magnetic substances (these three problems are equivalent), and in Sec. 2 the correlations in a two-dimensional Heisenberg ferromagnet are investigated. To within quantities of the order of the cut-off parameter r_0 , these correlations coincide with the correlations in classical systems, which were found in^[1]. The nature of the temperature-dependent corrections to the found expressions is briefly described in Sec. 1, and the question of the nature of the low-temperature phase, which was treated incorrectly in article^[1], is touched upon: The characteristic of the low-temperature phase is not an infinite susceptibility, as was erroneously asserted in^[1], but rather the superfluidity of a two-dimensional Bose liquid and the corresponding property of two-dimensional magnetic substances. The author hopes to return to this question, too. One-dimensional systems are not considered in this article.

1. TWO-DIMENSIONAL LATTICE OF PLANAR ROTATORS AND SYSTEMS EQUIVALENT TO IT (TWO-DIMENSIONAL BOSE LIQUID AND PLANAR MAGNETIC SUBSTANCES)

Lattice of Planar Rotators

This system corresponds to a two-dimensional lattice with lattice constant a (the notation for the lattice sites is the same as in^[1]), where a planar rotator described by the dynamical variables φ_r (angle) and $\hat{v}_r = i\partial/\partial\varphi_r$ (angular momentum) is associated with each site r . The wave function of the system must be periodic with respect to each of the variables φ_r with period 2π , and the eigenvalues \hat{v}_r are integers. We take the Hamiltonian of the system in the form

$$H = \sum_r \frac{1}{2m} \hat{v}_r^2 + \frac{1}{2} \sum_{|r-r'|=a} \sum_{m=-\infty}^{+\infty} H_{mr}, \quad (1)$$

where only nearest neighbors interact ($|r - r'| = a$; $|a| = a$) and the interaction energy is an even periodic function of the difference $v_{r,r'} = \varphi_{r'} - \varphi_r$, having a single minimum at $v_{r,r'} = 0$ in the interval $|v_{r,r'}| < \pi$, that is, the interaction is ferromagnetic:

$$H_{rr'} = J(v_{r,r'}) = \sum_{m=-\infty}^{+\infty} J_m e^{im(v_{r,r'})}, \quad (2)$$

$$J(0) = \sum_{m=-\infty}^{+\infty} J_m = 0, \quad J = J''(0) = \sum_{m=-\infty}^{+\infty} m^2 J_m > 0. \quad (3)$$

For the time being we shall forget about the periodicity conditions on the wave function, regarding it as a function of the variables φ_r , which vary over the entire axis $-\infty < \varphi_r < +\infty$. The potential energy then has minima for configurations satisfying the conditions

$$\varphi_r - \varphi_{r'} = 2\pi n_{rr'} \quad (|r - r'| = a), \quad (4)$$

where $n_{rr'}$ is an arbitrary integer function, defined on neighboring pairs of sites r and r' such that $n_{r'r} = -n_{rr'}$. Each such configuration corresponds to the minimum configuration (4). We assume that near this minimum one can replace the Hamiltonian by its quadratic expansion with respect to small deviations from (4), which gives

$$H \approx H_{(4)} = \sum_r \frac{1}{2m} \hat{v}_r^2 + \frac{1}{2} \sum_{|r-r'|=a} \sum_{m=-\infty}^{+\infty} \frac{1}{2} (v_{r'} - \varphi_r - 2\pi n_{rr'})^2. \quad (5)$$

We have a situation which is similar to the one which is encountered in the well-known method of Heitler and London, viz., in different regions of configuration space the Hamiltonian separates differently into the major part and the perturbation ("asymmetrical perturbation theory," see^[2]). In the first approximation the eigenfunctions of the initial Hamiltonian will be linear combinations of the eigenfunctions of the Hamiltonians (5). In order to find these linear combinations it is, in general, necessary to solve the secular equation, but allowance for the symmetry requirements simplifies this problem. In the present case the total wave function

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must be periodic in all the variables φ_r , that is, invariant with respect to the substitution $\varphi_r \rightarrow \varphi_r + 2\pi n_r$, where n_r is an arbitrary integer lattice function. Upon making such a substitution, $n_{rr'}$ in the Hamiltonian (5) goes over into another function $\bar{n}_{rr'}$, which is related to the previous $n_{rr'}$ by the equation

$$n_{rr'} = \bar{n}_{rr'} + n_r - n_{r'}. \quad (6)$$

We shall call the two functions $n_{rr'}$ and $\bar{n}_{rr'}$ \sim -equivalent if they are related by equation (6) for a certain integer lattice function n_r . One can easily verify that (6) is an equivalence relation and hence it divides the set of functions $n_{rr'}$ into nonintersecting classes of \sim -equivalent functions. If $\bar{n}_{rr'}$ is a certain (arbitrary) representation of a given class \mathcal{D} , then all the others are obtained from it by formula (6), when n_r takes all possible values of the integer lattice functions. The summation over a given class \mathcal{D} therefore reduces to a summation over n_r . Let $\psi_n^{(E)}(\dots, \varphi_r, \dots)$ denote the eigenfunction of (5) with energy E . The summation of all such functions for $n_{rr'}$, corresponding to a given class \mathcal{D} , has the form

$$\Psi_{\mathcal{D}}^{(E)}(\dots, \varphi_r, \dots) \sim \sum_{\dots} \sum_{n_r} \psi_n^{(E)}(\dots, \varphi_r + 2\pi n_r, \dots). \quad (7)$$

where $\bar{n}_{rr'}$ is a certain (arbitrary) representation of the class \mathcal{D} . Since (7) is an eigenfunction with the same energy E , the approximate eigenfunctions of the initial Hamiltonian must be linear combinations of the functions (7) in order to satisfy the periodicity condition.

Let us consider the physical meaning of the states described by the functions (7). Let r_0, r_1, \dots, r_l be a certain closed path (contour) along the bonds of the lattice ($r_0 = r_l$, r_i and r_{i+1} are neighbors). Let us call

$$K = \sum_{i=0}^{l-1} n_{r_i r_{i+1}}$$

the quantity K , the circulation of $n_{rr'}$ along the contour. It is easy to see that if $n_{rr'}$ and $\bar{n}_{rr'}$ are equivalent in the sense of (6), then their circulations along any arbitrary contour coincide, so that the set of circulations over all contours is an invariant of the class \mathcal{D} and uniquely describes this class. It is sufficient to specify the circulation along the minimum contour—that is, along the boundaries of the elementary squares (faces) of the lattice. One can associate each face having a nonvanishing circulation with a defect, which we shall call a “vortex,” since for the case of a Bose liquid (see below) these defects correspond to the well-known quantized vortices (see [3]).

Thus, each class \mathcal{D} corresponds to a definite distribution of the vortices over the faces of the lattice. The states without vortices correspond to the class \mathcal{D}_0 , having as one of its representations the function $\bar{n}_{rr'} = 0$ (that is, consisting of functions $n_{rr'}$ of the form $n_r - n_{r'}$). For the class \mathcal{D}_0 the Hamiltonian (5) goes over into the Hamiltonian for a system of harmonic oscillators, having an energy spectrum for the low-lying excited states of the form¹⁾ (here and in what follows, k

¹⁾The condition for the applicability of “asymmetric perturbation theory” is a small overlap of the eigenfunctions of the Hamiltonian (5) for a different $n_{rr'}$. For functions of the class \mathcal{D} , this reduces to $(\langle \hat{\phi}_r - \phi_r \rangle)^2 \ll 1$. By calculating the standard deviation of the difference $\hat{\phi}_{r'} - \phi_{r'}$ from the wave function for the ground state of the system of oscillators, we obtain the condition for the validity of the method in the form $(J\eta)^{-1} \gg 1$.

denotes the quasi-momentum)

$$\omega_k = \hbar\omega_0 - hc|k| + o(|k|), \quad c = (\alpha/\hbar)\sqrt{J}/\eta. \quad (8)$$

For classes \mathcal{D} different from \mathcal{D}_0 , (5) is the Hamiltonian of a system of “displaced” harmonic oscillators and its energy spectrum is shifted with respect to (8) by an amount $\Delta E_{\mathcal{D}}$, equal to the minimum of the inhomogeneous quadratic form in (5).²⁾ By virtue of this, taking the classes $\mathcal{D} \neq \mathcal{D}_0$ into consideration should give corrections of the order of $\exp(-\Delta E_{\mathcal{D}}/T)$ and at low temperatures one can confine attention to only the contributions from the class \mathcal{D}_0 . Thereby the calculation of the averages reduces to the similar problem for a system of harmonic oscillators having the spectrum (8).

In fact, let the averaging (with a Gibbs weight function) be carried out with respect to the approximate eigenfunctions (7) of the class \mathcal{D}_0 and the averaged quantity is a periodic function $F_{\text{per}}(\varphi_{r_1}, \dots, \varphi_{r_n})$ of the angles φ_{r_s} . Then each term of the summation (7) gives the same contribution to the average, and it coincides with the average of $F_{\text{per}}(\hat{\varphi}_{r_1}, \dots, \hat{\varphi}_{r_n})$ over the system of oscillators. In particular, for integer values of m_s one can write

$$\left\langle \exp\left\{ i \sum_{s=1}^n m_s \varphi_{r_s}(t_s) \right\} \right\rangle = \exp\left\{ -\frac{1}{2} \sum_{s_1, s_2=1}^n m_s m_{s'} \langle \hat{\varphi}_{r_s}(t_s) \hat{\varphi}_{r_{s'}}(t_{s'}) \rangle_0 \right\} \quad (9)$$

where $\langle \hat{\varphi}_{r_s}(t) \hat{\varphi}_{r_{s'}}(t') \rangle_0$ is the correlation function for the coordinates of the harmonic oscillators. One can easily deduce Eq. (9) for a system of harmonic oscillators for arbitrary values of m_s , but, according to what was said above, in that case when m_s is an integer and hence the averaged function is periodic, its average with respect to the system of oscillators coincides (for $T/J \ll 1$) with the Gibbs average over the initial system.

For $t_s \neq t_{s'}$ the correlation function $\langle \varphi_{r_s}(t_s) \varphi_{r_{s'}}(t_{s'}) \rangle_0$ depends on the method of ordering the noncommuting operators $\varphi_r(t)$, but at large distances these differences are of the order of $1/u_{ss'}$, where $u_{ss'}$ is defined as

$$u_{ss'} = \begin{cases} |r_s - r_{s'}| & \text{if } |r_s - r_{s'}| > c|t_s - t_{s'}| \\ c|t_s - t_{s'}| + \gamma c^2 (t_s - t_{s'})^2 - (r_s - r_{s'})^2 & \text{if } |r_s - r_{s'}| < c|t_s - t_{s'}| \end{cases} \quad (10)$$

that is, the operators $\varphi_r(t)$ at remote points asymptotically commute.

For $u_{ss'} \gg 1$ the asymptotic form of the correlators in (9) has the form

$$\langle \hat{\varphi}_{r_s}(t_s) \hat{\varphi}_{r_{s'}}(t_{s'}) \rangle \approx O\left(\ln \frac{R}{a}\right) - (1 - \delta_{ss'}) a \ln \frac{u_{ss'}}{r_0}, \quad (11)$$

where the following notation is used ($\gamma = 0.5772 \dots$ is Euler's constant)

$$a = T/2\pi J, \quad r_0 = 2e^{-\gamma} hc/T \approx 1.28 hc/T \quad (12)$$

and $\delta_{ss'} = 1$ for $s = s'$ and $\delta_{ss'} = 0$ for $s \neq s'$ for integer values of s, s' . The

²⁾Configurations of vortices with non-vanishing total circulation have an energy of the order of $\ln(R/a)$, where R is the size of the system, and these configurations drop out of the partition function. The minimum $\Delta E_{\mathcal{D}} = \pi^2 J$ corresponds to a pair of vortices with $K = +1$ and $K = -1$, situated in neighboring faces.

first term in (11) is a logarithmically divergent constant (for $R \rightarrow \infty$, where R is the size of the system).

Substituting (11) into (9) and taking into consideration that the first term from (11) gives a factor $\exp\{-O(l \ln(R/a)(m_1 + \dots + m_n)^2\}$ to the right-hand side of Eq. (9), which is equal to $\delta_{m_1 + \dots + m_n, 0}$ in the limit $R \rightarrow \infty$, we obtain the following result for $u_s, s' \gg a$:

$$\begin{aligned} & \left\langle \exp\left\{\sum_{s=1}^n m_s \hat{q}_{r_s}(t_s)\right\} \right\rangle \\ & \cong \delta_{m_1 + \dots + m_n, 0} \prod_{s=1}^n \prod_{r_s=r_0}^R \left(\frac{u_{r_s}}{r_s}\right)^{m_s} \quad (m_s - \text{integers}). \end{aligned} \quad (13)$$

Correlations involving the participation of $\nu_r(t) = \eta d\varphi_r/dt$ are of the same order, $O(1/u_{ss'})$, as the terms connected with the noncommutativity of the $\varphi_r(t)$ which were thrown away earlier, so that at large distances one can neglect them and assume

$$\langle e^{im_r \nu_r(t_s)} \rangle \approx 0, \quad \langle \nu_r(t_s) \nu_{r'}(t_s') \rangle \approx 0 \quad (u_s \gg a). \quad (14)$$

Formulas (13) and (14) enable us to calculate the asymptotic behavior for any arbitrary correlation function. For $t_s = t_s'$ expression (13) is equivalent to formula (21) from [1], but with a different value of the cutoff parameter r_0 .³⁾

Two-dimensional Bose Liquid

Now let us show that the long-range correlations in a two-dimensional neutral Bose liquid can be calculated on the basis of an equivalent Hamiltonian isomorphic to (1). Let us assume that the Bose condensate only exists in the ground state (for $T = 0$), and for $T \neq 0$ it is destroyed by the fluctuations of the phase, a description of which we also wish to derive. We introduce the following notation: m denotes the mass of the atoms, $\bar{\rho} = 1/l^2$ is the number of particles per unit area (l is the average distance between the particles), c_s is the speed of sound, $\kappa = \partial N/\partial \mu = 1/m c_s^2$ is the compressibility in the ground state. There are two correlation lengths in the problem: the average de Broglie wavelength $\xi = \hbar/m c_s$ and r_c —the radius of correlation for fluctuations of the phase; at $T = 0$ (in the ground state) $r_c = \infty$, but at low temperatures $r_c \gg \xi$ and has a macroscopic value.⁴⁾ Therefore, one can separate the entire system into cells, having macroscopic dimensions a such that $\xi \ll a \ll r_c$; for simplicity we shall assume that these cells are the cells of a square lattice, and their centers coincide with the lattice sites r .

Let us represent the Hamiltonian of the system in the form of a sum of Hamiltonians of the individual cells and of terms describing the transitions between the cells. If at first we neglect the latter, then the Hamiltonian separates into the sum of independent Hamiltonians for the individual cells. In this connection one can construct the low-lying eigenstates as products of the

³⁾ In the classical case the cutoff is due to the short-wavelength behavior of ω_k and $r_0 \approx a$. In the quantum case the cutoff is due to the Planck distribution for $\hbar\omega_k \approx T$, $r_0 \approx \hbar\omega_k/T \gg a$.

⁴⁾ Fulfillment of the condition of quantum degeneracy, $\xi \gg l$, is necessary for the very existence of the Bose liquid.

⁵⁾ As we shall see below (see Eq. (20)), $r_c/\xi \approx (\kappa T)^{-1} \exp[-O(\xi^2/l^2 \kappa T)]$.

eigenstates of the individual cells with quantum numbers differing slightly from the equilibrium number $N_a = \bar{\rho}a^2$. Namely, let us denote the ground state of the r -th cell by $|\nu_r\rangle_r$ when the number of particles in it is given by $N_r = N_a + \nu_r$; then one can associate a state $|\nu\rangle = \prod_r |\nu_r\rangle_r$ (the product over all cells) to each distribution $\{\dots, \nu_r, \dots\} = \{\nu\}$ of the particles over the cells, in which $N_a + \nu_r$ particles fall into the r -th cell (and where $\sum \nu_r = 0$).

The energy of this state is composed of the energies of the individual cells and is equal to $E(\nu) = E_0 + \sum (2\kappa N_a)^{-1} \nu_r^2 + O(\nu_r^2)$ (the linear terms in ν_r drop out due to the fact that $\sum \nu_r = 0$). Since the quadratic terms in ν_r are small (they are of the same order as the terms associated with transitions between the cells, which have been discarded), so the states $|\nu\rangle$ form an almost degenerate system of states. According to perturbation theory for this case, in the first-order approximation the energies are determined as the eigenvalues of an effective Hamiltonian which is equal to $H_{\text{eff}} = \hat{P}H\hat{P}$, where \hat{P} is a projection operator on a subspace spanned by the states $|\nu\rangle$. More precisely

$$H_{\text{eff}} = E_0 + \sum_r \frac{1}{2\kappa N_a} \hat{\nu}_r^2 + \sum_{|r-r'|=1} \sum_{\nu} \hat{P} H_{rr'} \hat{P}, \quad (15)$$

where $\hat{\nu}_r$ is the operator multiplying the state $|\nu\rangle$ by the number ν_r , and $\hat{P}H_{rr'}\hat{P}$ is the term in the Hamiltonian corresponding to transitions from cell r to cell r' , from which only the matrix elements $\langle \nu' | H_{rr'} | \nu \rangle$ are left. It is obvious that these matrix elements will differ from zero only for transitions $\{\nu\} \rightarrow \{\nu'\}$ such that ν particles go from cell r to the neighboring cell r' but the number of particles in the remaining cells does not change. Let us denote the value of such a matrix element by J_ν ; then one can write the operators $\hat{P}H_{rr'}\hat{P}$ in the form

$$\hat{P}H_{rr'}\hat{P} = \sum_{\nu=-\infty}^{+\infty} J_\nu (\hat{R}_r)^\nu (\hat{R}_{r'})^{-\nu}, \quad (16)$$

where $(\hat{R}_r)^\nu$ denotes the operator which changes the number of particles in the r -th cell by ν , leaving the number of particles in the other cells unchanged.

In order to see the equivalence of the Hamiltonians (1) and (15), let us pass to a representation where the operators \hat{R}_r are diagonal. Let $|\varphi\rangle_r = \sum \nu e^{i\varphi\nu} |\nu\rangle_r$ (the summation is over the integers ν) denote the state of the r -th cell containing an indeterminate number of particles, but the phase φ of the condensate is fixed. If a state $|\varphi\rangle = \prod_r |\varphi_r\rangle_r$ is associated with each set of phases $\{\dots, \varphi_r, \dots\} = \{\varphi\}$, then the two sets of basis functions $|\varphi\rangle$ and $|\nu\rangle$ are unitarily equivalent, and since

$$\hat{\nu}_r |\varphi\rangle = -i \frac{\partial}{\partial \varphi_r} |\varphi\rangle, \quad (\hat{R}_r)^\nu |\varphi\rangle = e^{i\varphi\nu} |\varphi\rangle, \quad (17)$$

then (15) actually coincides with (1) for $\eta = \kappa N_a$. The quantity corresponding to \bar{J} (see Eq. (3)) can be expressed in terms of the parameters of a Bose liquid by using the f-sum rule

$$\langle N | [\{\hat{\rho}_k, H\} \hat{\rho}_{-k}] | N \rangle = \frac{N}{m} \hbar^2 k^2$$

(see [4, 5]), where $\hat{\rho}_k \approx \sum_r (N_a + \hat{\nu}_r) e^{ik \cdot r}$ are the Fourier components of the density, $|N\rangle \approx (\text{const}) \sum |\nu\rangle$ is the

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ground state (the summation extends over all r such that $-(\Delta N_a) \leq r \leq (\Delta N_a)$, where $\Delta N_a = O(\sqrt{N_a})$ denotes the fluctuations of the number of particles in a cell). This gives $\bar{J} = \bar{\rho} \hbar^2/m$, so that the parameters appearing in (13) are given by

$$\alpha = \frac{Tm}{2\pi\hbar^2}, \quad c = \sqrt{\frac{1}{m\lambda}} = c_{ss}, \quad r_s \approx 1.28 \frac{\hbar c_s}{T}. \quad (18)$$

For these values of the parameters, formulas (13) and (14) permit us to determine the asymptotic form of the average of any function of $\hat{\varphi}_r$ and $\hat{\nu}_r$. It is necessary to associate the operators $\hat{P}\hat{A}$ with the quantities A of the initial system; if \hat{A}_s is a local operator pertaining to the neighborhood of the point r_s , then $\hat{P}\hat{A}_s\hat{P}$ is expressed in terms of $\hat{\varphi}_{r_s}$ and $\hat{\nu}_{r_s}$, and since by virtue of (14) one can set $\nu_r \approx 0$ in evaluating the correlations at widely separated points, then the averages of the products $\Pi \hat{A}_s$ in the initial system coincide (for widely separated points r_s) with the averages of products of the operators $\mathcal{A}_s(\hat{\varphi}_{r_s})$, where $\mathcal{A}_s(\varphi)$ is the Bogolyubov quasi-average of the operator \hat{A}_s (see [6]), expressed as a function of the phase φ of the Bose condensate, that is, $\hat{A}_s \rightarrow \mathcal{A}_s(\hat{\varphi}_{r_s})$, where $\mathcal{A}_s(\varphi)$ is defined as

$$\mathcal{A}_s(\varphi) = \lim_{N \rightarrow \infty} \sum_{n=-\infty}^{+\infty} e^{in\varphi} \langle N | \hat{A}_s | N + n \rangle = \langle \psi | A_s | \psi \rangle. \quad (19)$$

In particular, according to this rule the operator $\psi(r, t)$ corresponds to the expression $\sqrt{\rho_0} \exp(i\varphi_r(t))$, where ρ_0 denotes the density of the Bose condensate; for the asymptotic form of the average $\langle \psi(r, t)\psi(r', t') \rangle$ (for $t = t'$, when $u_{r,t}(r, t'; r', t') = |r - r'|$) we have

$$\langle \psi(r)\psi(r') \rangle \approx \rho_0 |(r - r')/r_s|^{-\alpha} \quad (|r - r'| \gg a). \quad (20)$$

This formula was previously derived in [7] and [8].

Anisotropic Planar Magnetic Substances

These systems are considered in [9] where, in particular, their equivalence with Bose systems is mentioned. In the notation of [9] the rules giving the correspondences between the parameters, similar to (18), have the form: $\alpha = T/2\pi\rho_s$ and $c = (\rho_s/\chi_s)^{1/2}$ (the values of ρ_s and χ_s are taken for $T = 0$).

The Nature of the Corrections to (13) and the Nature of the Low-temperature Phase

The following approximations were made in the derivation of the asymptotic expressions (13) for the correlation functions: In the first place, the contributions from classes $\mathcal{D} \neq \mathcal{D}_0$ were neglected, i.e., quantized vortices were not considered; in the second place, in calculating the contributions from the class \mathcal{D}_0 the quadratic expansion of the Hamiltonian near the minimum was used. It is not difficult to take the corrections associated with the breakdown of the latter approximation into account by using perturbation theory; here the usual diagram technique is applicable, in which the lines correspond to the correlation functions $\langle \varphi_r(t)\varphi_{r'}(t') \rangle_0$ for a system of harmonic oscillators, and the vertices correspond to terms of the fourth-order and higher orders in the expansion of the Hamiltonian in powers of $v_{r,\delta}$. Since the factors $v_{r,\delta} = i(k \cdot \delta)\varphi_k + o(k)$ (the

Fourier transforms of $v_{r,\delta}$) appear in the vertices, then as $k \rightarrow 0$ the "polarization operator" $\Pi(k) \sim k^2$; if ρ_s^0 is introduced according to the equation

$$\lim_{k \rightarrow 0} \Pi(k)/k^2 = (J - \rho_s^0)/T,$$

then as $k \rightarrow 0$ the Fourier transform of the total correlation function $\langle \varphi_k \varphi_{-k} \rangle = (T/\rho_s^0)k^{-2}$; from here follow (11) and (13) with $\alpha = T/2\pi\rho_s^0$. For example, for the two-point correlation function one will have

$$\langle \exp\{i(\varphi_r - \varphi_{r'})\} \rangle \approx C(T) |r - r'|^{-\alpha} \quad (|r - r'| \gg a). \quad (21)$$

Let us consider one more quantity $\Delta\mathcal{F}(A)$ —the change of the free energy due to the influence of an external vector potential $A_{r,\delta}$ (the corresponding Hamiltonian is obtained from (1) by making the substitution $v_{r,\delta} \rightarrow v_{r,\delta} + A_{r,\delta}$). Let $A_{r,\delta} = (A(r) \cdot \delta)$, where $A(r) = \{A_i(r)\}$ is a slowly varying vector function of the coordinates. The diagram technique described above gives

$$\Delta\mathcal{F}(A) = \frac{1}{2} \rho_s \sum_i \sum_{n=1,2} \int (A_n)_i (A_{-n})_i \left(\delta_{nn} - \frac{k_n k_n}{k^2} \right) (dk) + o(A^4), \quad (22)$$

where $\rho_s = \rho_s^0$ and $(A_k)_i$ is the Fourier transform of the function $A_i(r)$.

One can clarify the role of the corrections associated with the classes $\mathcal{D} \neq \mathcal{D}_0$ (i.e., with the vortices) in the example of a classical system (with the same Hamiltonian (1)). For this system one is able to construct a systematic low-temperature expansion, which the author proposes to describe in a separate article. We shall, however, discuss some of the conclusions here. (It is clear that the behavior of the correlation functions at large distances is identical in the quantum and in the classical systems; we prove this below in Sec. 2 (see Eq. (34)). It turns out that the vortices are equivalent to the particles of a certain lattice gas (on the dual lattice, whose sites r_* lie at the centers of the "faces" of the initial lattice). The states of the gas are specified by distributions of the "charges" K_{r*} (the vortex circulations), where each K_{r*} independently takes integer values $0, \pm 1, \pm 2, \dots$, and the energies of the states are given by

$$E(\dots, K_{r*}, \dots) = 4\pi^2 \rho_s^0 \sum \sum K_{r*} K_{r'} G_{r,r'}$$

(the sum goes over all pairs r_*, r'_* , where $G_{r,r'} \approx 2\pi^{-1} \ln(R/|r_* - r'_*|)$ for $|r_* - r'_*| \gg a$ (R denotes the size of the lattice)). One can prove that in such a gas at low temperatures all of the particles are bound into neutral "quasi-molecules" (i.e., groups of vortices having a total circulation equal to zero), and the decay of the latter is related to a certain phase transition (the situation does not resemble a gas with a Coulomb interaction $\sim |r_* - r'_*|^{-1}$, where there is a non-vanishing concentration of ions at any arbitrary temperature!). Upon taking the vortices into account we again have (21) and (22), where

$$\alpha = \frac{1}{2\pi} \left(\frac{T}{\rho_s^0} + 4\pi^2 \bar{d}^2 \right) \quad \rho_s = \rho_s^0 \left(1 - \frac{4\pi^2 \bar{d}^2}{T} \rho_s^0 \right) \quad (23)$$

(the mean-square "dipole moment of the molecules" is denoted by \bar{d}^2). The phase transition occurs at a temperature T_c such that

$$\rho_s(T_c) = 0. \quad (24)$$

In addition, it is evident in Eq. (21) that $C(T) \rightarrow 0$ as $T \rightarrow T_c$.

The author of [1] justified the necessity of a phase transition by the fact that at low temperatures the susceptibility $\chi = (\partial \langle m \rangle / \partial h)_{h=0}$ is infinite (the average moment $\langle m \rangle$ in the field h is given by formula (40), see below). The transition to the usual dependence $\langle m \rangle \sim h$ occurs when $\alpha = 2$. Although the value of $\alpha(T_c)$ is unknown, by taking the interaction with the external field in the form $h \cos m\varphi_r$, we obtain a similar transition when $\alpha = 2/m^2$ (where m is an arbitrary integer). These transitions pertain to the system with $h \neq 0$, but not to the initial system with $h = 0$, and an infinite susceptibility cannot be regarded as an indication of a separate phase (see footnote⁶⁾ below).

The true nature of the low-temperature phase (as the author now understands it) consists in the fact that a two-dimensional Bose liquid is superfluid; the corresponding property can also be formulated in terms of magnetic substances. In this connection the quantity ρ_s from (22) corresponds to the density of the superfluid component in the two-fluid hydrodynamics of the Bose liquid or the "coefficient of rigidity" for magnetic substances, which was introduced in [6].

Formula (22) and the correlation function of the currents corresponding to it,

$$\langle j_k, j_{-k, \delta} \rangle = T(\rho - \rho_s)(\delta\delta') + T\rho_s(k\delta')(k\delta')/k^4 \quad (25)$$

($j_{k, \delta}$ denotes the Fourier transform of the current $j_{x, \delta} = -\partial H / \partial v_{r, \delta}$; $\rho = \langle \delta^2 H / (\delta v_{r, \delta})^2 \rangle$), express the fact that, as has been noted by many authors (see [6, 10, 11]), a "rigidity" with respect to transverse influences is the characteristic property of the superfluid state. Another characteristic property consists in the presence of spatially-inhomogeneous metastable states, described by an additional variable $v_g(r)$ ("states associated with the superfluid current")⁶⁾. Within the framework of the approximation which only takes the class \mathcal{D}_0 into consideration, these states are obtained from the states (7) by making the transformation $\varphi_r \rightarrow \varphi_r + \varphi_r$ (a displacement of the coordinates of the oscillators), where $\varphi_{r'} - \varphi_r = (v_g(r) \cdot \delta)$. The energy density ϵ and the entropy density s for the states with $v_g \neq 0$ are given by

$$\epsilon = \epsilon_0 + 1/2 \rho_s v_g^2, \quad s(\epsilon) = s_0(\epsilon - 1/2 \rho_s v_g^2) \approx s_0 - 1/2 \rho_s v_g^2 / T. \quad (26)$$

From (26) one can infer two-fluid hydrodynamics and the corresponding theory for magnetic substances (see [11, 9]), also including Eq. (25), in exactly the same way as for three-dimensional systems. Thus, as illustrated by the two-dimensional systems under consideration, it is clear that, contrary to common opinion, a spontaneous violation of the phase symmetry is not

⁶⁾According to Landau and Lifshitz (see [12], Sec. 81) a system has many phases if it has spatially-inhomogeneous equilibrium states. The critical point is best defined as the point at which a system of many phases becomes a single-phase system. This definition can be made completely rigorous by using the concept of "Gibbs states of infinite systems" which has been recently introduced (see [13]).

necessary for the existence of superfluidity.⁷⁾

2. ISOTROPIC SYSTEMS OF QUANTUM SPINS. HEISENBERG FERROMAGNETS

Let us show that the problem of calculating the long-range correlations for isotropic systems of quantum spins reduces to the corresponding problem for classical spins, which was solved in [1] (for low temperatures).

First let us consider a single spin. As is well known, the components $\hat{s}^{(\alpha)}$ ($\alpha = x, y, z$) are the generators of the representations $\hat{\mathcal{D}}(u)$ of the group SU_2 ($\hat{\mathcal{D}}(u)$ is the matrix which corresponds in a given representation to the element u of the rotation group). One can parameterize the elements of the group SU_2 , which is the universal covering group of the rotations, in the same way as the elements of the rotation group,—that is, by the Euler angles ϑ, φ, ψ , only the period with respect to the angle ψ will not be 2π , but 4π . If the irreducible representation corresponding to total spin S is considered, then the well-known orthogonality relations (see [14]) hold for the elements of the $2S+1$ -dimensional matrices of the representation $D(u)$; these relations will be used below in the following form (which is equivalent to the usual formulation): For any operator $\hat{F} = F_{MM'}$ acting on the $2S+1$ -dimensional space of the representation, and for any normalized vector $| \cdot \rangle$ of this space, the following identity is satisfied:

$$\text{Sp } \hat{F} = \sum_{M=-S}^S F_{MM} = (2S+1) \int \langle \cdot | \hat{\mathcal{D}}^*(u) \hat{F} \hat{\mathcal{D}}(u) | \cdot \rangle (du), \quad (27)$$

where the integral is taken over the group SU_2 , and $(du) = \sin \vartheta d\vartheta d\psi / 16\pi^2$ is the volume element on the group.

Now let us consider a lattice in which a spin \hat{s}_r is associated with each lattice site r (all of the spins have the same magnitude, $(\hat{s}_r)^2 = S(S+1)$). We associate its own independent SU_2 -transformation u_r with each site r , and the corresponding operator $\hat{\mathcal{D}}_r(u_r)$, which operates only on the variables pertaining to the spin \hat{s}_r . Then each lattice function $u = \{\vartheta, \varphi, \psi\}$ (i.e., the triplet of functions $\vartheta_r, \varphi_r, \psi_r$) can be assigned an operator $\mathcal{D}[U] = \prod \mathcal{D}_r(u_r)$ (the product runs over all sites r) which transforms the states of the entire system. This transformation can be regarded as the same as a transformation of operators whereby each operator $\hat{F} = F(\dots, \hat{s}_r, \dots)$, which acts on the space of states of the system, corresponds to a transformed operator given by

$$\hat{F}(u) = \hat{\mathcal{D}}^*(u_r) \hat{F} \hat{\mathcal{D}}(u_r) = F(\dots, \hat{s}_r(u_r), \dots). \quad (28)$$

If the operator \hat{F} is expressed in terms of \hat{s}_r , then the transformed operator (28) is obtained from this expression by replacing each of the $\hat{s}_r^{(\alpha)}$ by

$$\hat{s}_r^{(\alpha)}(u_r) = \hat{\mathcal{D}}_r^*(u_r) \hat{s}_r^{(\alpha)} \hat{\mathcal{D}}_r(u_r) = R_{\alpha\beta}(u_r) \hat{s}_r^{(\beta)}, \quad (29)$$

⁷⁾One can describe the properties of the "two-dimensional crystals" considered in [1] in a similar fashion. The components of the deformation tensor are the additional thermodynamical variables which serve to describe the metastable states. Transverse waves exist in the system, so that this model describes a solid, notwithstanding the absence of long-range crystalline order.

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where $R_{\alpha\beta}(u) = R_{\alpha\beta}(\vartheta, \varphi, \psi)$ is the matrix for a finite rotation characterized by the Euler angles ϑ, φ , and ψ (here and in what follows, summation over repeated Greek subscripts $\alpha, \beta, \dots = x, y, z$ is to be understood).

We obtain the following result for the trace of an arbitrary operator \hat{F} , acting on the states of the entire system (by taking successively the traces with respect to the variables pertaining to each site, and each time applying Eq. (27)):

$$\text{Sp } \hat{F} = (2S+1)^N \int \dots \int \langle 0 | \hat{F}(u) | 0 \rangle \prod (du_r). \quad (30)$$

Here N denotes the total number of lattice sites, $\hat{F}(u)$ is the operator given by Eq. (28), and $|0\rangle$ is any arbitrary normalized vector from the space of states of the lattice. Our discussion will be based on the utilization of the identity (30).

Let us consider a two-dimensional Heisenberg ferromagnet. Let

$$H = \frac{1}{2} J \sum_{|r-r'|=1} \sum s_r \cdot s_{r'} \quad (31)$$

denote the Hamiltonian of the system; we shall utilize the identity (30), having taken as $|0\rangle$ the ground state of (31) such that $\hat{z}_r^{(2)}|0\rangle = +S|0\rangle$ for all r . For the average of an arbitrary operator \hat{A} we then obtain

$$\langle \hat{A} \rangle = (2S+1)^N \int \dots \int \langle 0 | \hat{A}(u) \exp \left(-\frac{\mathcal{F} - H(u)}{T} \right) | 0 \rangle \prod (du_r), \quad (32)$$

where \mathcal{F} denotes the free energy, determined from the requirement $\langle 1 \rangle = 1$. The integrand in Eq. (32) actually does not depend on the angles ψ_r . In fact, from the identity

$$\mathcal{D}(\vartheta, \varphi, \psi) = \mathcal{D}(\vartheta, \varphi, 0) \exp(i\psi_r S_r)$$

it is clear that the states $\mathcal{D}\{u\}|0\rangle$ depend on ψ_r only through the factors $\exp(i\psi_r S_r)$, which are cancelled in (32) by the conjugate factors coming from $\langle 0 | \mathcal{D}^\dagger \{u\} | 0 \rangle$. Therefore, in Eq. (32) one can omit the integrations over $d\psi_r$ and by u_r understand $\{\vartheta_r, \psi_r, 0\}$, which simplifies the calculations.

Now let us introduce the functional $\Delta\mathcal{F}\{u\}$ defined by the equation

$$\langle 0 | \exp \left(-\frac{1}{T} H(u) \right) | 0 \rangle = \exp \left(-\frac{E_0}{T} \right) \exp \left(-\frac{1}{T} \Delta\mathcal{F}(u) \right) \quad (33)$$

(E_0 is the energy of the ground state). Furthermore, if we calculate the average of a product of local operators A_s pertaining to widely separated points r_s (such that $|r_s - r'_s| \gg a$) is calculated, then according to the principle of the decay of correlations (the ergodic property) we have in the present case (for the state $|0\rangle$)

$$\begin{aligned} & \langle 0 | \left(\prod_i \hat{A}_i(u_i) \right) \exp \left(-\frac{1}{T} \hat{H}(u) \right) | 0 \rangle \\ & \approx \left(\prod_i \langle 0 | \hat{A}_i(u_i) | 0 \rangle \right) \exp(-E_0/T) \exp \left(-\frac{1}{T} \Delta\mathcal{F}(u) \right). \end{aligned} \quad (34)$$

Substituting this expression into (32), we see that the quantum-mechanical average of the product of local operators A_s , pertaining to widely separated points r_s , coincides with the average over the equivalent classical system, in which the configurations are described by

functions $u_r = \{\vartheta_r, \psi_r, 0\}$, the energy of the configurations is given by the functional $\Delta\mathcal{F}\{u\}$, and the correspondence between physical quantities is realized according to the following rule: The quantum-mechanical quantity \hat{A}_s is associated with the classical quantity

$$\mathcal{A}_s(\vartheta_r, \psi_r) = \langle 0 | \hat{A}_s(u_r) | 0 \rangle.$$

In particular, here the components $s_r^{(\alpha)}$ of the spin are related to the classical quantities $S_n^{(\alpha)}$, where n_r is a unit vector having the direction $\vartheta_r, \psi_r - (\pi/2)$ in the spherical coordinate system:

$$s_r - S_n = S \{ \sin \vartheta_r \sin \psi_r, -\sin \vartheta_r \cos \psi_r, \cos \vartheta_r \}. \quad (35)$$

In order to use the results of the investigation of the classical system carried out in Sec. 2 of article^[1], it is only necessary to determine the expression for the equivalent energy $\Delta\mathcal{F}\{u\}$. In this connection it is very important that the entire investigation in^[1] was only based on the expression for the energy of slowly varying configurations, that is, configurations in which the differences $d_\delta u_r = u_{r+\delta} - u_r$ are sufficiently small for $|\delta| = a$.

One can find the expression for the equivalent energy of slowly varying configurations correct to within terms of second order in $d_\delta u_r$ by using the corresponding expansion of the transformed Hamiltonian:

$$H(u) = H + \hat{H}_1(u, d_\delta u_r) + \hat{H}_2(u, d_\delta u_r) + o((d_\delta u_r)^2), \quad (36)$$

where \hat{H} is the initial Hamiltonian (31), $\hat{H}_1\{\dots\}$ and $\hat{H}_2\{\dots\}$ are the terms of first and second order in $d_\delta u_r$ and $o(\dots)$ are the terms of higher orders. Actually $\hat{H}\{u\}$ is obtained from (31) by making the substitution $s_r \cdot s_{r'} \rightarrow s_r(u_r) \cdot s_{r'}(u_{r'})$ for each pair of neighboring sites $r, r' = r + \delta$. The term of zero order in the expansion of $s_r(u_r)s_{r+\delta}(u_{r+\delta})$ in powers of $d_\delta u_r$ is then equal to $s_r s_{r+\delta}$, because the scalar product does not change upon an identical rotation of both spins. Thus, the term of zero order in (36) coincides with the initial Hamiltonian (31) (which is simply a consequence of the invariance of H with respect to the simultaneous rotation of all the spins through identical angles). One can obtain explicit expressions for the terms of first and second order with respect to $d_\delta u_r$ in Eq. (36) by using formula (29) and by calculating the expansion of $R_{\alpha\gamma}(u)R_{\beta\gamma}(u + du)$ in powers of du based on the well-known expressions for $R_{\alpha\beta}(u)$ in terms of the Euler angles (see^[14]). We shall not present these calculations here, and we shall not even write down the final expressions for $H_1\{\dots\}$ and $H_2\{\dots\}$, limiting our attention to only a description of the method used to obtain these results.

In virtue of (36) one can use perturbation theory to calculate the values of the functional $\Delta\mathcal{F}\{u\}$ for slowly varying configurations, regarding the first term on the right hand side of (36) as the major term and treating the terms H_1 and H_2 as perturbations. Thus, we arrive at an expansion of $\Delta\mathcal{F}\{u\}$ in powers of the differences $d_\delta u_r$, where the first-order term vanishes and the second-order term is given by

$$\Delta\mathcal{F}\{u\} = \langle 0 | H_1 | 0 \rangle - \frac{T}{2} \int d\tau \int d\tau' \langle 0 | H_1 e^{-iH_1 T} H_2 | 0 \rangle. \quad (37)$$

The second term on the right-hand side of Eq. (37) can

be represented in the form of a summation over intermediate states, where only states corresponding to single spin waves with quasimomenta k give any contribution. The first term can also be represented in the form of a sum over k . Comparing these sums and taking into consideration that, as follows from^[1], only wavelengths in the region $\ln(|k|a) \leq -O(1/T)$ are important, one can see that the second term from (37) is negligible in this region in comparison with the first term, so that $\Delta_2 \mathcal{F}\{u\}$ is given simply by the average value $\langle 0 | H_2 \{u, d_\delta u\} | 0 \rangle$. Evaluating this average value with the aid of the explicit expression for $H_2 \{u, d_\delta u\}$ (which is not written down above), and replacing $d_\delta \mathbf{J}_r$ and $d_\delta \varphi_r$ by $(\delta \cdot \nabla) \mathbf{J}_r$ and $(\delta \cdot \nabla) \varphi_r$, and also replacing the sum over r by an integral, we obtain the following result for the energy of the slowly changing configurations

$$\Delta_2 \mathcal{F}\{u\} \simeq \frac{1}{4} JS^2 \int (dr) ((\nabla \theta_r)^2 + (\nabla \varphi_r)^2 \sin^2 \theta_r). \quad (38)$$

This expression coincides with the corresponding expression for the energy of the slowly varying classical configurations (see^[1], formula (38)), on which the conclusions reached in^[1] were based. Therefore, one can immediately apply these conclusions to the present case. In particular, for the asymptotic form of the pair correlation function we obtain (taking (35) into consideration):

$$\langle s_s s_{r'} \rangle \simeq S^2 |(r - r')/r_0|^{-\alpha} \quad (|r - r'| \gg a), \quad (39)$$

and for the specific magnetic moment in a weak external field, $h \ll J$, we obtain

$$\langle m \rangle = \langle S^{(0)} \rangle = S (ChS/J)^{\alpha/(1-\alpha)} + \dots, \quad (40)$$

where $C \sim a^2/r_0^2$ is a certain constant, and in the present case $\alpha = T/\pi J$. The magnitude of the cutoff parameter r_0 and the constant C of Eq. (40) can be found from the correspondence with the expressions given by the theory of spin waves (the regions of applicability of Eqs. (39) and (40) and the theory of spin waves overlap for distances $a \ln(|r - r'|/r_0) \ll 1$ and for fields $h \gtrsim T$). In this connection, for the cutoff parameter r_0 we obtain $r_0/a = (1/2) \sqrt{JS/T}$.

Other isotropic spin systems can be treated in analogous fashion, but since in the general case the exact ground state and the low-lying excited states are unknown, the constant appearing in front of (38) cannot be explicitly expressed in terms of the parameters of the initial Hamiltonian, and must be treated as a phenomenological parameter.

In conclusion I wish to thank A. I. Larkin, V. L. Pokrovskii, and Yu. N. Ovchinnikov for a discussion of the questions considered in Sec. 1. V. N. Popov has courteously informed me that he has arrived at similar

results (in regard to the superfluidity of a two-dimensional Bose liquid and the power-law nature of the asymptotic behavior), by starting from the formalism^[15] developed by him.

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Chapter 17

XY Model, Renormalization, and Duality

17.1 Plan of Action

In the last chapter we discussed the low temperature form of spin correlations for the planar model. We saw how a spin wave approximation led to an algebraic decay of correlation functions for large separations. The main result was that, for large values of K ,

$$\langle \exp(i\theta_{\mathbf{r}}) \exp(-i\theta_{\mathbf{r}'}) \rangle = \left[\frac{|\mathbf{r} - \mathbf{r}'|}{ca} \right]^{-1/K}. \quad (17.1)$$

Large K implies low temperatures. In this limit, the spin wave approximation is correct and the correlation function decays as a power of the separation, $|\mathbf{r} - \mathbf{r}'|$, for large separations.

However, we were left with a mystery. Equation (17.1) cannot possibly be true for high temperatures, i.e. small values of K . In that limit, the system falls into a typical high temperature phase in which all correlations drop off exponentially with distance. Nonetheless Eq. (17.1) seems to be essentially right in the large K -limit. Our next job is to study the low temperature phase more precisely and describe how the high temperature, disordered, phase arises. In doing this we are following the paths of previous workers who derived the basic properties of this model, and its phase transition.¹

We would like to stick as close as possible to the Gaussian model, because it gives attractive low-temperature results. We might be dissatisfied with this spin wave approximation, however, because it fails to include the gauge symmetry of Eq. (16.4b). The first step in our calculation is to choose a potential form, the ‘Villain potential’,² which looks Gaussian,

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but which includes the gauge symmetry. In the next step, we construct the dual form of the problem. This dual form enables one to see immediately the form of the high temperature phase. Then, a use of the Poisson sum formula Eq. (15.6) converts the problem into one which is simple at low temperatures, and which, strangely enough, looks like a set of interacting charges in two dimensions. The latter is analyzed via renormalization group arguments, originally due to Kosterlitz and Thouless.³

17.2 Villain Representation of the Basic Bonds

We need an accurate discussion of the planar model, which includes all symmetries, but is erected upon a Gaussian structure. We shall obtain this starting point by changing the functional form of the coupling term while maintaining all the symmetry properties of the system.

But, you might ask, is it fair to change the problem about? After all, when we started discussing the planar model, we began by thinking about a problem in which the basic coupling was proportional to $\cos(\theta - \theta')$. To go further, we invoke the concept of universality. We hope and expect that the most important properties of the planar model, particularly the algebraic correlations at low temperatures, are universal. That is we suggest that they depend mostly upon the global and gauge symmetries and very little upon the specific interactions used. Thus we can allow ourselves to change the potential by constructing a bond which looks Gaussian in character.

In a Gaussian theory, the variables, ϕ go from minus infinity to infinity. If the basic bond is of the form $-\pi K(\phi - \phi')^2$ so that its exponential can be written in a Fourier transform representation as

$$K^{1/4} \exp\left[-\frac{K}{4\pi}(\phi - \phi')^2\right] = K^{-1/4} \int dx \exp\left[i(\phi - \phi')x - \frac{\pi x^2}{K}\right]. \quad (17.2)$$

Of course, this structure is not translationally invariant so that ϕ cannot have the meaning of an angle. There are two different ways of constructing a pseudo-Gaussian function of angles. The first is to periodically repeat the structure (17.2) giving:

$$B(\theta - \theta') = K^{1/4} \sum_{m=-\infty}^{\infty} \exp\left[-\frac{K}{4\pi}(\theta - \theta' - 2\pi m)^2\right]. \quad (17.3)$$

Another, different way of writing a pseudo-Gaussian but periodic bond is to replace (17.2) by a Fourier sum as

$$B(\theta - \theta') = K^{-1/4} \sum_{l=-\infty}^{\infty} \exp\left[i(\theta - \theta')l - \frac{\pi l^2}{K}\right]. \quad (17.4)$$

The two expressions (17.3) and (17.4) are different ways of making the expression (17.2) periodic. They look entirely different from one another. However, as one can see by applying

³See footnote 1.

the Poisson sum formula (see homework 17.1) they are really precisely and identically the same expression. This form for the bond was first proposed by J. Villain (see footnote 3) and later used for this problem by José *et al.*⁴ As we shall see it provides a convenient, even elegant, starting point for dealing with the planar model.⁵

We now set up a planar model calculation in two dimensions, using this basic bond. The partition function is written as a nearest neighbor coupling on a two-dimensional lattice as:

$$Z = \text{Tr}_\theta \prod_{jk} B(\theta_{j,k+1} - \theta_{j,k})B(\theta_{j+1,k} - \theta_{j,k}). \quad (17.5)$$

17.3 Duality Transformation

The duality transformation involves replacing the basic bond by its Fourier transform. Here the variables for the system are angle variables with a periodicity of 2π , and consequently the Fourier transform is the Fourier sum of Eq. (17.4). Thus the dual bond is

$$\tilde{B}(l) = K^{-1/4} \exp \left[-\frac{\pi l^2}{K} \right], \quad (17.6)$$

where l is an integer. Recall the general discussion of duality in Chapter 15. There are two bond variables, $l_x(j + 1/2, k)$ and $l_y(j, k + 1/2)$, are respectively attached to each x - and y -direction bond on the direct lattice. The partition function is a sum over these l -variables and an integral over each of the θ -variables. The integral produces a restriction on the l 's which is the requirement that these vector variables have zero divergence. In symbols

$$l_x \left(j + \frac{1}{2}, k \right) - l_x \left(j - \frac{1}{2}, k \right) + l_y \left(j, k + \frac{1}{2} \right) - l_y \left(j, k - \frac{1}{2} \right) = 0. \quad (17.7)$$

This divergence-free condition requires that the l 's are curls defined by integer variables, $n(j + 1/2, k + 1/2)$, defined on the dual lattice. The definition is (see Eq. (15.15))

$$\begin{aligned} l_x \left(j + \frac{1}{2}, k \right) &= n \left(j + \frac{1}{2}, k + \frac{1}{2} \right) - n \left(j + \frac{1}{2}, k - \frac{1}{2} \right), \\ l_y \left(j, k + \frac{1}{2} \right) &= -n \left(j + \frac{1}{2}, k + \frac{1}{2} \right) + n \left(j - \frac{1}{2}, k + \frac{1}{2} \right). \end{aligned} \quad (17.8)$$

To find the dual partition function, one sums over each of these dual variables:

$$\text{Tr}_n = \prod_{jk} \sum_{n(j+1/2,k+1/2)=-\infty}^{\infty}, \quad (17.9)$$

⁴REPRINT: Sec. 17.11.3.

⁵One might think that (17.2) and (17.3) will be little different if K is large. This view might arise because, in that case, only one term in the summation of (17.3) would ever give a large result. Can't that term be the one listed in (17.2)? Are not then the two expressions equivalent? The answer is no. Imagine that $\theta = \pi - \epsilon$, where ϵ is a small positive number, while θ' is $-\pi + \epsilon$. Then the angles are really close together because $\theta - \theta' = 2\pi - 2\epsilon$. But the term which dominates the sum is not the $m = 0$ term, but the $m = 1$ term. So (17.2) and (17.3) are not equal even for large K and angles in the interval $[-\pi, \pi]$.

with a weight which is an exponential of an action depending on nearest neighbor n -variables:

$$\begin{aligned}\mathcal{W}[n] &= \sum'_{j,k} \{\ln \tilde{B}(n(j,k) - n(j-1,k)) + \ln \tilde{B}(n(j,k) - n(j,k-1))\} \\ &= \sum'_{j,k} \left\{ -\frac{1}{2} \ln K - \frac{\pi}{K} [n(j,k) - n(j-1,k)]^2 - \frac{\pi}{K} [n(j,k) - n(j,k-1)]^2 \right\}. \quad (17.10)\end{aligned}$$

In writing Eq. (17.10) we have used a notation in which the prime on the sum over j and k means that the sum is to cover all values on the dual lattice. Thus all the values of j and k in a primed sum are half integers. The partition function is

$$Z = \text{Tr}_n \exp(\mathcal{W}[n]). \quad (17.11)$$

17.4 Two Limits

We look at this result in two different limiting cases. In the low temperature case, K is very large. Then, the sums over n are slowly varying and contain many terms which are of the same size. In that situation, we can approximately replace the sum over the n 's by integrals over the n 's which go from $-\infty$ to ∞ . These Gaussians generate algebraic decay of correlations.⁶ Thus, we see once more that the low temperature phase has algebraic order.

In the opposite limit in which K goes to zero, the direct problem has weak couplings among the different sites. Then the dual problem (see Eq. (17.10)) has a very strong coupling, among the n -variables. As a result, the dual model falls into a phase which has an entirely different character from that of the Gaussian problem. The strong couplings tend to produce long ranged correlations among the n 's. Each ordered phase is labeled by its average value of n , which we call n^* . The interactions tend to keep each n the same as its neighbors'. So, as K goes to zero, most of the n 's have the value n^* , with a few sites fluctuating away from this value. The most likely excitations are localized to one dual site. It is likely that all the surrounding dual sites will have $n = n^*$.

Imagine that, at the particular dual site, n is not equal to n^* . Instead, it has the value, $n = n^* \pm 1$. As one can see from Eq. (17.10), this changes costs a probability factor $\exp(-4\pi/K)$. All other changes have a smaller probability factor. Thus the high temperature phase is one of frozen n . Each different value of n^* represents a different phase of the dual system. However, the θ description is invariant under a uniform shift of all the n 's

$$n \left(j + \frac{1}{2}, k + \frac{1}{2} \right) \rightarrow n \left(j + \frac{1}{2}, k + \frac{1}{2} \right) + 1.$$

Consequently, in the θ -description there is only one high temperature phase.

⁶Our work in Chapter 3 shows that Gaussian problems are always critical if they have an invariance under shifting each variable by the same amount. In this case, the mass of the excitation is zero. See also Problem 16.5.

When one translates the frozen n back into the situation described by the angular variables, θ , one finds that the $\exp(\pm i\theta)$ -variables show exponentially decaying order. Thus, we see that at high temperatures we get ordered n and disordered $\exp(\pm i\theta)$. Conversely, at low temperatures, both kinds of variables have algebraic correlations.

17.5 Vortex Representation

To understand the phase transition, we need a more exact theory which includes both the high temperature limit and the low temperature one, and gives a representation of the basic states of the system, along with the excitation properties.

We do understand the predominant natural excitations in the system at high temperatures. They are local variation in n away from n^* . Next we would like to understand excitations at low temperatures. This understanding requires that we set up a formal mechanism for treating corrections to the low-temperature Gaussian theory. We have set up all the machinery for doing this through the use of the Poisson sum formula which says that a slowly varying sum over n can effectively be replaced by a rapidly decreasing sum over m in the form:

$$\sum_{n=-\infty}^{\infty} F(n) = \sum_{m=-\infty}^{\infty} \int d\phi F(\phi) \exp(2\pi im\phi). \quad (17.12)$$

Make the replacement (17.12) at each and every lattice site. After this replacement, the trace operation becomes:

$$\text{Tr}_\phi \text{Tr}_m = \prod_{j,k} \left[\int_{-\infty}^{\infty} d\phi \left(j + \frac{1}{2}, k + \frac{1}{2} \right) \sum_{m(j+1/2,k+1/2)=-\infty}^{\infty} \right]. \quad (17.13)$$

The new action is derived from Eq. (17.10) with an added term of the form $2\pi im\phi$, so that the new action is

$$\begin{aligned} \mathcal{W}'[\phi, m] &= \mathcal{W}[n] + \sum_{j,k} 2\pi im(j, k)\phi(j, k) = \sum_{j,k} \left\{ -\frac{1}{2} \ln K + 2\pi im(j, k)\phi(j, k) \right. \\ &\quad \left. - \frac{\pi}{K} [\phi(j, k) - \phi(j-1, k)]^2 - \frac{\pi}{K} [\phi(j, k) - \phi(j, k-1)]^2 \right\}. \end{aligned} \quad (17.14)$$

In this writing, and below, we have used the symbols j and k to define locations on the *dual* lattice.

In the usual way, to calculate an average of anything we write

$$\langle X \rangle = \text{Tr}_\phi \text{Tr}_m X \frac{\exp(\mathcal{W}'[\phi, m])}{Z}, \quad (17.15)$$

where the partition function is

$$Z = \text{Tr}_\phi \text{Tr}_m \exp(\mathcal{W}'[\phi, m]). \quad (17.16)$$

Equation (17.14) is an completely exact representation of the original problem: calculating the properties of the planar model with a coupling of the Villain form. Notice that the problem has a Gaussian form in the x -variables so that all the integrals over ϕ in Eqs. (17.15) and (17.16) can be performed exactly. Then, the problem gets a new formulation in which the only remaining sums are sums over the m -variables. The formulation is that whenever X depends upon the m 's but not upon the ϕ -variables:

$$\langle X \rangle = \text{Tr}_m X \frac{\exp(C[m])}{Z}. \quad (17.17)$$

Here, the ‘coulomb’ action is the result one gets by doing the Gaussian integrals in Eq. (17.14), namely,

$$C[m] = - \sum_{\mathbf{r}, \mathbf{r}'} m(\mathbf{r})m(\mathbf{r}')G(\mathbf{r} - \mathbf{r}')K + \text{constant}. \quad (17.18)$$

This quadratic structure is exactly the same as the one in Eqs. (3.18) and (16.19) and the Green's function, G is exactly the one in Eqs. (3.20) and also in (16.20). Thus, we have come right back to the structure of our original coulomb problem, as discussed in the previous chapter. In that chapter, we had a set of variables, q 's, which we called electrical charges. Now we have a dual problem with a different set of integer variables. We need a name for them. Long ago P. A. M. Dirac argued that one could reformulate electrodynamics to include quantized magnetic monopoles, which were the duals of the electric charges. In fact the duality relation discussed here is remarkably similar to the one discussed by Dirac in this entirely different context.⁷ We therefore call the m 's monopole charges or magnetic charges.

This problem may be further simplified by noticing that the probability of any configuration will be vanishing small unless the total magnetic charge

$$M_T = \sum_{\mathbf{r}} m(\mathbf{r}) \quad (17.19)$$

is zero. We previously [see Eq. (16.23)] argued that the analogous total electric charge must vanish also. [See discussion around Eq. (16.22).] Using $M_T = 0$, we can simplify the expression for the action to read⁸

$$C[m] = \sum_{\text{pairs}} m(\mathbf{r})m(\mathbf{r}')g(\mathbf{r} - \mathbf{r}')K. \quad (17.20)$$

The Green function in Eq. (17.20), $g(\mathbf{r})$ was previously discussed. (See Eqs. (3.20) and (16.26).) Equation (16.27) gives $g(\mathbf{r})$ as

$$g(\mathbf{r}) \approx \ln \left(\frac{|\mathbf{r}|}{ac} \right), \quad (17.21)$$

for large values of the ratio of the distance, r to the lattice constant a .

⁷See also the discussion by G. 't Hooft in Nucl. Phys. B79, 276 (1974).

⁸In writing Eq. (17.20) we have dropped an additive constant which is independent of $\{m\}$, the set of monopole strengths, but does depend upon the k 's.

The ‘magnetic’ problem described by Eq. (17.20) looks very much like the ‘electrical’ problem discussed in the previous chapter. But there are two big changes. Because of the dual transformation the K in Eq. (16.19) has been replaced by a $1/K$ in Eq. (17.18). Thus this formulation involves a very strong coupling among the m ’s at low temperatures and a weak correlation at high temperatures.

The second change is that the formulation of the problem automatically brings in statistical sums over all the m -variables, one on each of the sites of the dual lattice. (Recall that the ‘electrical’ charges entered the problem as a set of operators, $\exp(iq(r)\theta_r)$, with fixed position and charge. So the electrical charges are all specified while the magnetic ones are summation variables.) In the summation in the magnetic problem, each m takes on all possible integer values, according to

$$\text{Tr}_m = \prod'_{j,k} \sum_{m(j,k)=-\infty}^{\infty} . \quad (17.22)$$

After all this, the monopole summation problem can be described by the partition function is:

$$Z = \text{Tr}_m \exp \mathcal{C}\{m\}, \quad (17.23)$$

where the action is given by Eq. (17.20).

17.6 The Magnetically Charged System

In Fig. 16.4 we plotted out the kind of changes in the direction of the spin $(\cos \theta, \sin \theta)$ which can be produced by an excitation of the charged type, $\exp(\pm i\theta_r)$. Notice that the spin directions are fully aligned far away from the center.

However, the spin waves — like those shown in Fig. 16.4 — do not take full advantage of all the symmetries of the system. The spins waves produce a relatively low energy by making use of the global symmetry in which all arrows may rotate together. However, they take no advantage of the particularly angular nature of the variable θ_r . They would equally well exist in a system which did not have the gauge symmetry $\theta_r \rightarrow \theta_r + 2\pi n(r)$.

One can produce a configuration which does take advantage of this symmetry. Look at Fig. 17.1. This is the pattern of $(\cos \theta, \sin \theta)$ produced in a low temperature planar system when there is a magnetic ‘charge’ at the center of the picture. The algebra which gets us this pattern is a little long-winded. We do not include it here.

Instead, look at the pattern. It has several interesting properties. First, note that there is a singularity at the center of the pattern. Next, imagine summing up the angular changes as we walk along a path in the lattice, like the two paths shown in the figure, thereby forming

$$S = \sum \delta \mathbf{s} \cdot \text{Trunc}(\theta_r - \theta_{r'}) . \quad (17.24)$$

Here \mathbf{s} is a unit vector directed along the path while $\text{Trunc}(\theta)$ stands for a function which has values $\theta - 2\pi n$ with n being an integer. This integer is always picked so as to keep the

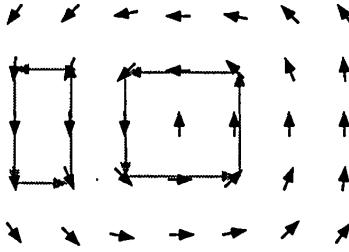


Fig. 17.1. Two-dimensional spins arrayed in a vortex. The dark arrows are spin directions; the light ones describe paths through the lattice. Notice the singularity at the center. The central vector can point in any direction without changing the action. The angles between nearest neighbor spins fall off as one over the distance from the center, so that the total change in the action diverges as the logarithm of the size of the system. Note the two paths in the picture. The sums up all the angular changes around the central path is 2π . A similar sum around the path on the left is zero.

value of Trunc in the interval between $-\pi$ and π . Many paths in the system will give a sum, S , which is zero. For example in Fig. 17.1 any path which does not enclose the ‘singularity’ at the center of the figure will give a sum zero. Conversely any path which winds around the singularity precisely once in the clockwise sense will give a result 2π . The monopole moment of a given point is defined to be $1/(2\pi)$ times the sum around that point. This monopole is an example of a topological quantum number, i.e. one which exists because of changes in space defined by a symmetry group.

Together spin waves and magnetic excitations like the one shown provide the complete low temperature excitation spectrum of the planar system. The excitation shown in Fig. 17.1 is very unlikely to appear alone in any significant fashion in statistical sums since its probabilistic cost is $\exp[-KG(0)]$ and $G(0)$ diverges logarithmically with the size of the system. However, it is perfectly possible to have two such vortices with equal and opposite magnetic charge. Hence we focus our attention upon those configurations in which the logarithmic infinity does not appear, i.e. those with total magnetic charge, M_T , equal to zero. Then the sum in Eq. (17.23) may be written as

$$Z = \text{Tr}_m \delta(M_T, 0) \exp \left[\sum_{\text{pairs}} K g(\mathbf{r} - \mathbf{r}') m(\mathbf{r}) m(\mathbf{r}') \right]. \quad (17.25)$$

Equation (17.25) and the earlier Eq. (17.21) show that the correlation between two unlike magnetic charges drops off algebraically. Thus, the magnetically charged system forms a kind of Coulomb gas in which the coupling K serves as a charge squared

$$K \text{ replaces } \frac{e^2}{\epsilon}. \quad (17.26)$$

For large K , the system has a strong tendency for charges to be paired up into overall neutral structures (like atoms!) while as we shall see, for smaller K the atoms tend to fall apart and the system forms a kind of plasma. Separating these two phases, there is a phase transition: the *Kosterlitz–Thouless transition*, named the two physicists who predicted and explained it.

To explain why and how there is a qualitative difference between strong couplings and weak, we must explain a little about the properties of this ‘coulomb’ gas. To start, imagine that there are but two sites in the system. The charge neutrality condition requires that the magnetic charge at the two sites be equal and opposite. These charges must be integers. In the end, we find that the probability of a charge m at \mathbf{r} and a charge $-m$ at \mathbf{r}' is

$$\rho_m = z^{-1} \exp[-m^2 g(\mathbf{r} - \mathbf{r}')K] \quad (17.27)$$

where z is a partition function for this small system. Note that g is necessarily positive. In the limit as K becomes quite large, the probability drops off quite rapidly as m^2 is increased. For this reason, we only hold on to terms in which m equals 0 or ± 1 . If we do this,

$$z = 1 + 2 \exp[-g(\mathbf{r} - \mathbf{r}')K].$$

We can evaluate $g(\mathbf{r} - \mathbf{r}')$ when $\mathbf{r} - \mathbf{r}'$ is a lattice vector, using Eq. (16.25). Thus, in this case, the probability of having $m = 1$ is

$$\rho_1 = \frac{Y^2}{1 + 2Y^2} \quad \text{with} \quad Y = \exp\left[-\frac{K\pi}{4}\right].$$

For large K , we see that the probability of this pairwise excitation is quite small. Equation (17.21) holds for a system with but two monopoles. If these sites happen to be separated by a large distance, the probability of finding monopoles of charge 1 at \mathbf{r} and -1 at \mathbf{r}' is

$$\rho(\mathbf{r} - \mathbf{r}') = \frac{y^2}{|\mathbf{r} - \mathbf{r}'|^K}, \quad \text{where} \quad y^2 = (ac)^K, \quad (17.28)$$

when $|\mathbf{r} - \mathbf{r}'|$ is large compared with a lattice constant.

On the full lattice which has many different lattice sites, Eq. (17.28) still works. Once again it describes the probability that we will find two elementary excitations, one with $m = +1$ and the other with $m = -1$ separated by a vector $\mathbf{r} - \mathbf{r}'$. This result is correct in a dilute gas approximation in which we may neglect the effect of all the other magnetic charges in the system. Then K serves as a descriptor of the long ranged behavior of the correlations, while y describes the probability that they might be found.

When y is small, the formula (17.28) is the lowest order term in an expansion in y . Fluctuations produced by the remaining charges within the system modify this formula. Imagine that $\mathbf{r} - \mathbf{r}'$ is a huge separation compared to the nearest neighbor distance. Then some of the remaining charges would be found in the region between these two, and serve to screen the charges. This screening would, as in any dielectric material (or here diamagnetic material) serve to reduce the strength of the long ranged interaction. We would then have

$$\rho(\mathbf{r} - \mathbf{r}') = \frac{y_\infty^2}{|\mathbf{r} - \mathbf{r}'|^{K_\infty}}, \quad \text{for large } |\mathbf{r} - \mathbf{r}'|, \quad (17.29)$$

where here K_∞ is an effective renormalized value of the coupling constant and y_∞ is a renormalized value of the probability of finding a nearby pair. In an electrical description K_∞ is simply e^2/ϵ where ϵ is the dielectric constant. Thus the main effect of the renormalization is to weaken the bare ‘magnetic charge’ and replace it by an effective charge.

17.7 Correlation Calculation

Before we start the renormalization calculation we have to describe the calculation of correlation functions in somewhat more detail. We deal with an action in which we calculate the average of an operator \mathcal{Q} in which we demand that the system contains precisely N charges at positions \mathbf{r}_j . The charge at the j th site is m_j , which takes on the values ± 1 . The total magnetic charge must be zero. Thus, our basic operator is

$$\mathcal{Q}[m] = \prod_{j=1}^N \delta(m(\mathbf{r}_j), m_j). \quad (17.30)$$

In our notation, $[m]$ is the set of all nonzero m 's defined by the operator $\mathcal{Q}[m]$.

To calculate the $\langle \mathcal{Q} \rangle$ employ the action

$$\mathcal{C}_0[m] = K \sum_{j < k}^N m(\mathbf{r}_j)m(\mathbf{r}_k) \ln(|\mathbf{r}_j - \mathbf{r}_k|) + \sum_{j=1}^N m(\mathbf{r}_j)^2 \ln y. \quad (17.31)$$

The main simplification that we have made so far is to replace the Green function, g , by the logarithmic form appropriate for large separations.

As usual, in statistical physics, we start out by calculating a partition function, which is a sum over all fluctuations of the exponential of the action. In this case, the fluctuations consist of magnetic charges $[m']$ which are different from zero. Thus the partition function is

$$Z = \text{Tr}_{[m']} e^{\mathcal{C}_0[m']}. \quad (17.32)$$

If the fugacity, y , is small, the partition function can be found as an expansion in y^2 , with the first two terms being

$$Z = 1 + y^2 \sum_{\mathbf{r} \neq \mathbf{r}'} |\mathbf{r} - \mathbf{r}'|^{-K}. \quad (17.33)$$

Here the sums cover the entire lattice.

A similar calculation applies to $\langle \mathcal{Q}[m] \rangle$. This average is

$$\langle \mathcal{Q}[m] \rangle = Z^{-1} \text{Tr}_{[m']} e^{\mathcal{C}_0[m+m']}. \quad (17.34)$$

Here, $[m']$ is the set of all magnetic charges produced by fluctuations while $[m]$ is the set of specified charges. Naturally, $m'(\mathbf{r})$ is zero on all the sites, \mathbf{r}_j , for which the $[m]$ is specified.

Like the partition function, the correlation function has an expansion in y^2 . The result is, to second order,

$$\begin{aligned} \langle \mathcal{Q}[m] \rangle &= Z^{-1} e^{\mathcal{C}_0[m]} \left[1 + y^2 \sum_{\mathbf{r} \neq \mathbf{r}'} |\mathbf{r} - \mathbf{r}'|^{-K} e^{V[m]} + \dots \right], \\ V[m] &= K \sum_j m(\mathbf{r}_j) \ln \frac{|\mathbf{r}_j - \mathbf{r}|}{|\mathbf{r}_j - \mathbf{r}'|}. \end{aligned} \quad (17.35)$$

If we put this together with the similar result for the partition function (Eq. 17.33)), we find a perturbation theory result for the correlation function

$$\langle Q[m] \rangle = e^{C_0[m]} \left[1 + y^2 \sum_{\mathbf{r}, \mathbf{r}'} |\mathbf{r} - \mathbf{r}'|^{-K} (e^{V[m]} - 1) \right]. \quad (17.36)$$

We can think of the structure of this result as having $\langle Q[m] \rangle$ be a sum of two terms, one involving no fluctuation pairs, and having the value e^{C_0} and the other involving Q together with an extra two charges. This perturbation term has the structure SQ , with S being the dipole operator

$$S(\mathbf{R}, \mathbf{r}) = \delta \left(m \left(\mathbf{R} + \frac{\mathbf{r}}{2} \right), 1 \right) \delta \left(m \left(\mathbf{R} - \frac{\mathbf{r}}{2} \right), -1 \right). \quad (17.37)$$

Equation (17.36) can therefore be written in symbolic form as

$$\langle Q[m] \rangle = \langle Q[m] \rangle_0 + \sum_{\mathbf{R}, \mathbf{r}} [\langle S(\mathbf{R}, \mathbf{r}) Q \rangle_0 - \langle S(\mathbf{R}, \mathbf{r}) \rangle_0 \langle Q \rangle_0], \quad (17.38)$$

where the average $\langle \rangle_0$ entirely leaves out the effect of fluctuating magnetic charges.

17.8 The Renormalization Calculation

The main effect of the $e^{V[m]} - 1$ term in Eq. (17.36) is the screening of the particles with magnetic charge m . To calculate the effect of the screening we explicitly calculate the correlations induced by fluctuations-produced pairs with all separations which obey

$$|\mathbf{r}| < ae^\lambda. \quad (17.39)$$

Thus, λ describes the cutoff scale. Our renormalization will change that cutoff distance. We go ahead by dividing the fluctuations $[m']$ into two classes, $[m''](\lambda)$ and $[m']_\lambda$. The first class describes pairs with a separation distance which obeys Eq. (17.39); the latter describes far-separated magnetic charges. Our renormalization calculation will involve summing over the set $[m''](\lambda)$ for successively larger and larger values of λ . Let us do this for the partition function:

$$Z = \text{Tr}_{[m']_\lambda} \{ \text{Tr}_{[m'']} e^{C_0[m'' + m'']} \}. \quad (17.40)$$

We describe the close-together pairs by second order perturbation theory in y and obtain a result with the same structure as Eq. (17.36). The result is

$$Z = \text{Tr}_{[m']_\lambda} e^{C_0[m']_\lambda} \left(1 + y^2 \sum_{\mathbf{r}, \mathbf{r}'} |\mathbf{r} - \mathbf{r}'|^{-K} e^{V[m']_\lambda} \right), \quad (17.41)$$

$$\langle Q[m] \rangle = \text{Tr}_{[m']_\lambda} e^{C_0[m + m']_\lambda} \left[1 + y^2 \sum_{\mathbf{r}, \mathbf{r}'} |\mathbf{r} - \mathbf{r}'|^{-K} (e^{V[m + m']_\lambda} - 1) \right]. \quad (17.42)$$

We now define a renormalized action by

$$e^{\mathcal{C}_\lambda[m]} = e^{\mathcal{C}_0[m]} \left[1 + y^2 \sum_{\mathbf{r}\mathbf{r}'} \frac{e^{V[m]} - 1}{|\mathbf{r} - \mathbf{r}'|K} \right]. \quad (17.43)$$

We are about to calculate the averages on the right hand side of Eq. (17.43) and thereby find the form of the renormalized action, $\mathcal{C}_\lambda[m]$. We assume a form involving purely coulombic interactions

$$\mathcal{C}_\lambda[m] = K(\lambda) \sum_{j < k}^N m(\mathbf{r}_j)m(\mathbf{r}_k) \ln(|\mathbf{r}_j - \mathbf{r}_k|) + \sum_{j=1}^N m(\mathbf{r}_j)^2 \ln y(\lambda). \quad (17.44)$$

Here, $K(\lambda)$ is an effective coupling and $y(\lambda)$ a fugacity, depending upon the cutoff. This action differs in details from the action defined by the lattice system above. In particular, it has holes of linear dimension $a e^\lambda$ in its lattice. Nonetheless it is close enough to sit within the same universality class as the usual planar model. Analysis of this model will tell us how the planar model behaves.

In writing Eq. (17.44) in terms of the two couplings $K(\lambda)$ and $y(\lambda)$, we are making a brave assumption. We have guessed that the entire effect of the fluctuations in the system is to leave us with interactions of precisely the same form as in Eq. (17.31), except that the coupling constants K and y are changed by the interaction. This assumption would be quite foolhardy, except for the fact that we have ‘read ahead’ by studying the work in the literature and we know that this assumption will work.

The actual renormalization calculation starts with Eq. (17.43) and evaluates the average on the right hand side. The clue for how to do this step in the calculation is Eq. (16.39). When one fixes the charges, the electrical and the magnetic case are precisely the same except that whenever one sees a K in one situation one replaces it by K^{-1} to get the other situation. Just as before, we consider the limiting case in which the pair separation distance, r , is quite small in comparison with any of the other distances in the problem. In that case one can evaluate $\mathcal{S}(\mathbf{R}, \mathbf{r})$ in terms of an operator product or short distance expansion. We already know something about the operators which might appear, because they were analyzed in the discussion following Eq. (16.39). In this case, the expansion is⁹

$$\begin{aligned} \mathcal{S}(\mathbf{R}, \mathbf{r}) \longrightarrow & \frac{y^2}{r^K} \left[1 - Kz\mathcal{D}(\mathbf{R}) - Kz^*\mathcal{D}^*(\mathbf{R}) - \frac{K^2 z^2}{2} \mathcal{Q}(\mathbf{R}) \right. \\ & \left. - \frac{K^2 z^{*2}}{2} \mathcal{Q}^*(\mathbf{R}) - \frac{K^2 z z^*}{2} \mathcal{M}(\mathbf{R}) + \dots \right]. \end{aligned} \quad (17.45)$$

The calculation continues by substituting Eq. (17.45) into Eq. (17.38) and then evaluating the relevant averages.

⁹We use the same names for the operators in Eq. (17.45) as were previously used in Eq. (16.39). A more careful analysis, involving correlations between magnetic and electrical charge, shows that they are indeed the same set of operators modulo multiplication by -1 and powers of K .

In the subsequent analysis, the operator $\mathcal{M}(\mathbf{R})$ will be our main concern. We have already identified this operator as a marginal operator which has the effect of changing the value of the coupling, K . By the same argument as in the previous chapter (see Eq. (16.44)), it has a correlation

$$\langle \mathcal{M}(\mathbf{R})\mathcal{Q} \rangle = -\langle \mathcal{Q} \rangle \sum_{j < k} 2m_j m_k \left[2 \frac{(\mathbf{R} - \mathbf{r}_j) \cdot (\mathbf{R} - \mathbf{r}_k)}{(|\mathbf{R} - \mathbf{r}_j|^2)(|\mathbf{R} - \mathbf{r}_k|^2)} - |\mathbf{R} - \mathbf{r}_j|^{-2} - |\mathbf{R} - \mathbf{r}_k|^{-2} \right]. \quad (17.46)$$

As we discussed above [see the discussion below Eq. (16.39)] the various terms in Eq. (17.45) have simple physical interpretations. To calculate the change in the action, we take these terms and average them over position and angular orientation. The dipole and quadrupole terms disappear when they are averaged over angle, and hence, to linear order, produce no important change in the action. The unit operator just adds a constant to the action. That addition also has no effect. The net result is that instead of Eq. (17.45), we can use the simpler replacement

$$\mathcal{S} \longrightarrow -\frac{y^2}{r^K} \frac{K^2 r^2}{2} \mathcal{M}(\mathbf{R}), \quad (17.47)$$

and therefore rewrite Eq. (17.42) in the form

$$\langle \mathcal{Q}[m] \rangle = \text{Tr}_{[m']} \langle \mathcal{Q}[m + m'] \rangle_\lambda. \quad (17.48)$$

Here $\langle \mathcal{Q} \rangle_\lambda$ is an average which includes (to lowest order) all fluctuations with separations up to the cutoff set by λ . From Eq. (17.42), we compute the correction to the action produced by the small-separation terms. To order y^2 , we find

$$\langle \mathcal{Q}[m] \rangle_\lambda = e^{\mathcal{C}_\lambda[m]} = \left[e^{\mathcal{C}_0[m]} - \int_{r < ae^\lambda} dr \int d\mathbf{R} \frac{K^2 r^2}{2} \frac{y^2}{r^K} \langle \mathcal{Q}[m] \mathcal{M}(\mathbf{R}) \rangle_\lambda \right]. \quad (17.49)$$

Thus, we can conclude this section with an explicit formula which will be used for the calculation of $\mathcal{C}_\lambda[m]$, namely

$$\mathcal{C}_\lambda[m] = \mathcal{C}_0[m] - \int_{r < ae^\lambda} \frac{K^2 r^2}{2} dr \int d\mathbf{R} \frac{y^2}{r^K} \frac{\langle \mathcal{Q}[m] \mathcal{M}(\mathbf{R}) \rangle_\lambda}{\langle \mathcal{Q}[m] \rangle_\lambda}. \quad (17.50)$$

The appearance of the subscript, λ , on the right hand side of Eq. (17.50) is an indication that we are actually considering effects beyond linear order in y^2 . The derivation given here is only accurate to order y^2 . But, the structure looks plausible enough so that we keep the higher order corrections.

17.9 Spatial Averages

We have seen that the pairs can be replaced by the marginal operator, $\mathcal{M}(\mathbf{R})$. There are now two spatial averages to be performed. One is over the average position of the pair, \mathbf{R} .

The second is over the distance between pairs, r . We will do position-averages first. Go back to Eq. (17.46), which implies that

$$\int d\mathbf{R} \langle \mathcal{M}(\mathbf{R}) \mathcal{Q} \rangle = \langle \mathcal{Q} \rangle \sum_{j < k} m_j m_k J(\mathbf{r}_j, \mathbf{r}_k)$$

with

$$J(\mathbf{r}_j, \mathbf{r}_k) = 2 \int d\mathbf{R} \left[-2 \frac{(\mathbf{R} - \mathbf{r}_j) \cdot (\mathbf{R} - \mathbf{r}_k)}{(|\mathbf{R} - \mathbf{r}_j|^2)(|\mathbf{R} - \mathbf{r}_k|^2)} + |\mathbf{R} - \mathbf{r}_j|^{-2} + |\mathbf{R} - \mathbf{r}_k|^{-2} \right]. \quad (17.51)$$

Equation (17.51) involves an integrals over \mathbf{R} , which gains a logarithmically divergent contribution whenever \mathbf{R} approaches \mathbf{r}_j or \mathbf{r}_k .¹⁰ We say that the smallest possible distance is one lattice constant and find that the contribution of these divergent terms gives an a -dependent result

$$J(\mathbf{r}_j, \mathbf{r}_k) = 8\pi \ln \frac{1}{a} + \dots$$

The term left out is independent of the cutoff a . The natural spatial range of the integral is up to where all three distances $|\mathbf{R} - \mathbf{r}_j|$, $|\mathbf{R} - \mathbf{r}_k|$, and $|\mathbf{r}_j - \mathbf{r}_k|$ are of the same order of magnitude. When \mathbf{R} is much farther away than the distance between charges, the integral converges quite rapidly. Thus the contribution from logarithmically divergent terms gives

$$J(\mathbf{r}_j, \mathbf{r}_k) = 8\pi \ln \frac{|\mathbf{r}_j - \mathbf{r}_k|}{a} + \dots \quad (17.52)$$

Here the correction term is of order unity and does not count in comparison to the logarithm.

This part of the calculation may be finished by substituting the result of Eq. (17.52) back into Eq. (17.51) to find

$$\int d\mathbf{R} \langle \mathcal{M}(\mathbf{R}) \mathcal{Q}[m] \rangle = \langle \mathcal{Q}[m] \rangle \sum_{j < k} m_j m_k 8\pi \ln \frac{|\mathbf{r}_j - \mathbf{r}_k|}{a}. \quad (17.53)$$

A comparison back to Eq. (17.31) shows that the effect of the marginal operator is to change the K -value in $\langle \mathcal{Q}[m] \rangle$, since

$$\int d\mathbf{R} \langle \mathcal{M}(\mathbf{R}) \mathcal{Q}[m] \rangle = 8\pi \frac{\partial}{\partial K} \langle \mathcal{Q}[m] \rangle. \quad (17.54)$$

Here the derivative is to be taken at constant values of y .

¹⁰In two dimensions an integral $\int d\mathbf{R}/R^2$ diverges logarithmically. If the upper and lower cutoff on the R -integral are a and L , the integral has the value $2\pi \ln L/a$.

17.10 The Actual Renormalization

Now we can begin. From Eqs. (17.50) and (17.54), we find

$$C_\lambda[m] - C_0[m] = - \int_{r < ae^\lambda} dr \frac{y^2}{r^K} K^2 r^2 4\pi \frac{\partial}{\partial K} C_\lambda[m]. \quad (17.55)$$

We asserted in Eq. (17.44) that the entire effect of a renormalization would be to change the values of K and y in an effective action. Now Eq. (17.55) gives us a justification for this statement. If y is small so that the change on the left is small, we can evaluate it in terms of derivatives, and find:

$$[K(\lambda) - K(0)] \frac{\partial}{\partial K} C_0[m] = - \int_a^{ae^\lambda} dr \frac{y^2}{r} \frac{K^2 r^4 8\pi^2}{r^K} \frac{\partial}{\partial K} C_0[m]. \quad (17.56)$$

The factors of involving $C_0[m]$ can be canceled out. If the resulting equation is differentiated with respect to λ , one finds the renormalization equation

$$\frac{dK}{d\lambda} = -K^2 \frac{y^2}{r^{K-4}} 8\pi^2, \quad (17.57)$$

with r being the cutoff distance defined as ae^λ . The r -dependent combination of factors which enters here is

$$y(\lambda) = yr^{(2-K/2)} = y[ae^\lambda]^{(2-K/2)}. \quad (17.58)$$

Then coupling, K , and the effective fugacity, y , obey the renormalization equations

$$\frac{d}{d\lambda} K(\lambda)^{-1} = [y(\lambda)]^2 8\pi^2, \quad (17.59)$$

$$\frac{d[y(\lambda)]^2}{d\lambda} = [y(\lambda)]^2 (4 - K(\lambda)). \quad (17.60)$$

This last equation is obtained by differentiating Eq. (17.58) with respect to λ , while neglecting the λ -dependence of K . Equations (17.59) and (17.60) are only correct to second order in y . Nonetheless, we shall use these equations to calculate higher order effects of the magnetic charges.

The main doubt about these equations is whether the system can be described as having coulomb interactions, even in the presence of fluctuations. The derivation of the renormalization equations supports the notion that the system will retain its coulomb-like behavior, even after renormalization. Thus the use of the renormalization Eqs. (17.59) and (17.60), is very, very plausible — but it is not fully proven.

The effect of the renormalization is to increase the value of the cutoff, ae^λ , from some small value to some very large one. As the cutoff is increased, the effect of more and more of the fluctuating charges are taken into account — until at λ equals infinity, they are all included. As this takes place, according to Eq. (17.59), K decreases. Let us trace out

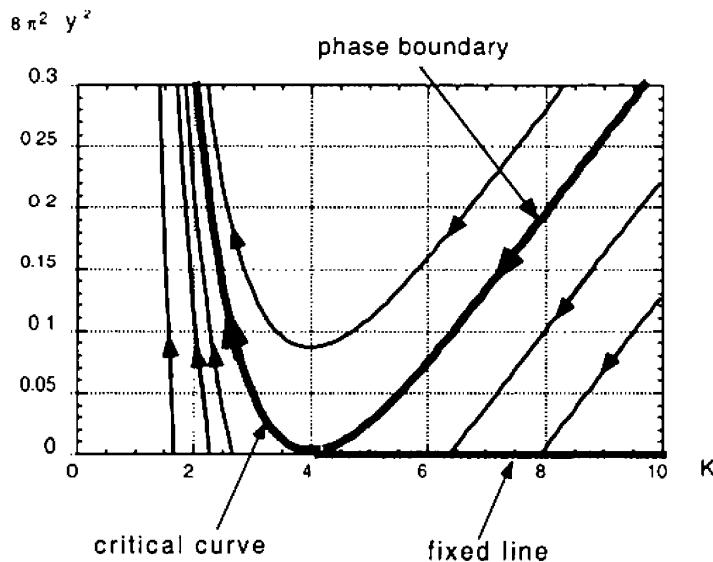


Fig. 17.2. Flow diagram for the planar model. The arrows describe the direction of the renormalization group flow. As the trajectory hits the x -axis all motion stops. Thus, the x -axis is a fixed line of the flow. The heavy curve is a critical trajectory, separating the different phases.

the phase diagram produced by the pair of flow Eqs. (17.59) and (17.60). These flows are plotted out in Fig. 17.2. To get the plots, one divides (17.59) by (17.60) and notes that $(dx/d\lambda)/(dw/d\lambda) = dx/dw$ so that

$$\frac{d}{dy^2} \frac{1}{K} = \frac{8\pi^2}{4 - K}, \quad (17.61)$$

so that the trajectory of y versus K is determined by:

$$8\pi^2(y^2 - c) = 4K^{-1} + \ln K, \quad (17.62)$$

where c is a constant of integration, which differentiates among the different trajectories. The direction of the arrows shows the flow. Notice that y increases with λ for $K < 4$, but decreases for $K > 4$.

If $y(\lambda)$ is always small, the decrease is moderate. If $y(\lambda)$ becomes large, the decrease is substantial. According to Eq. (17.60) while λ increases, $y(\lambda)$ will decrease whenever $K(\lambda)$ is greater than four. This decrease then permits the effect of the normalization to be just the production of a finite change in K . However, as soon as the renormalized K decreases to a value below four, then y starts to rise. With further increase in λ , y grows without bound and correspondingly K goes to zero. We call the value of K at λ equal to infinity, the renormalized K or K_∞ . The phases of the system are described by the corresponding destinations of K after a full renormalization. The low temperature phases are the magnetically charged atoms in which a coupling K_∞ bigger than four holds together opposite magnetic charges and restrains the screening. Then any magnetic charges in the system have algebraic correlations with one another. When the initial value of y is too large, the system renormalizes itself to the weak coupling phase with K_∞ equal to zero.

The atoms come apart, the screening is strong, and the correlation die off exponentially. If $K_\infty = 4$, one has a special critical phase.

One good way of describing this situation is by talking about the fixed points and fixed lines of the pair of Eqs. (17.59) and (17.60). There is a fixed line at $y = 0$ and any value of K . This line is unstable if K is less than four and stable if K is greater than 4. In the unstable region the system flows to a $y = \infty, K = 0$ fixed point.

This mathematical structure can be traced out by looking at the flow diagram which shows the changes in couplings as a is changed. These flows are plotted out in Fig. 17.2.

Thus, in the end, this remarkable renormalization analysis originally due to Kosterlitz and Thouless explains the main qualitative properties of the two-dimensional planar model, the coulomb gas, the solid upon solid system. Two-dimensional melting, the superfluid transition of bose systems, and many other systems besides.¹¹

Homework

Problem 17.1 (Two Kinds of Periodic Bonds). Prove that the expressions on the right hand sides of Eqs. (17.3) and (17.4) are identical to one another.

Problem 17.2 (High Temperature Planar Model). In the limit of high temperatures, most of the n -variables are frozen to a single integer value, n^* . In this limit, what is the probability that

- (a) A given site will have n equal to $n^* + \delta$.
- (b) Two nearest-neighbor sites will have n equal to $n^* \pm 1$.
- (c) Two neighbor sites will have n equal to $n^* \pm 1$.

Problem 17.3 (Vortex Energy). The caption of Fig. 17.1 states: ‘Notice the singularity at the center. The central vector can point in any direction without changing the action. The angles between nearest neighbor spins fall off as $1/r$ so that the total change in the action diverges as the logarithm of the size of the system’. Justify these statements.

17.11 Reprints on Planar Model

¹¹For a review see David Nelson in DGL: Volume 7 page 1 (1983).

17.11.1 The Kosterlitz–Thouless Theory

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Ordering, metastability and phase transitions in two-dimensional systems

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Abstract. A new definition of order called topological order is proposed for two-dimensional systems in which no long-range order of the conventional type exists. The possibility of a phase transition characterized by a change in the response of the system to an external perturbation is discussed in the context of a mean field type of approximation. The critical behaviour found in this model displays very weak singularities. The application of these ideas to the xy model of magnetism, the solid–liquid transition, and the neutral superfluid are discussed. This type of phase transition cannot occur in a superconductor nor in a Heisenberg ferromagnet, for reasons that are given.

1. Introduction

Peierls (1935) has argued that thermal motion of long-wavelength phonons will destroy the long-range order of a two-dimensional solid in the sense that the mean square deviation of an atom from its equilibrium position increases logarithmically with the size of the system, and the Bragg peaks of the diffraction pattern formed by the system are broad instead of sharp. The absence of long-range order of this simple form has been shown by Mermin (1968) using rigorous inequalities. Similar arguments can be used to show that there is no spontaneous magnetization in a two-dimensional magnet with spins with more than one degree of freedom (Mermin and Wagner 1966) and that the expectation value of the superfluid order parameter in a two-dimensional Bose fluid is zero (Hohenberg 1967).

On the other hand there is inconclusive evidence from the numerical work on a two-dimensional system of hard discs by Alder and Wainwright (1962) of a phase transition between a gaseous and solid state. Stanley and Kaplan (1966) found that high-temperature series expansions for two-dimensional spin models indicated a phase transition in which the susceptibility becomes infinite. The evidence for such a transition is much stronger for the xy model (spins confined to a plane) than for the Heisenberg model, as can be seen from the papers of Stanley (1968) and Moore (1969). Low-temperature expansions obtained by Wegner (1967) and Berezinskii (1970) give a magnetization proportional to some power of the field between zero and unity, and indicate the possibility of a sharp transition between such behaviour and the high-temperature régime where the magnetization is proportional to the applied field.

In this paper we present arguments in favour of a quite different definition of long-range order which is based on the overall properties of the system rather than on the

behaviour of a two-point correlation function. In the cases we consider, the usual correlation function, such as the spin-spin correlation function, vanishes at any finite temperature in contrast to the corresponding cases in three dimensions. This type of long-range order, which we refer to as topological long-range order, may exist for the two-dimensional solid, neutral superfluid, and for the *xy* model, but not for a superconductor or isotropic Heisenberg model. In the case of a solid, the disappearance of topological long-range order is associated with a transition from an elastic to a fluid response to a small external shear stress, while for a neutral superfluid it is associated with the instability of persistent currents. Recently, Berezinskii (1971) has put forward similar arguments, but there are some important differences in our results. A brief account of this theory has already been given (Kosterlitz and Thouless 1972).

The definition of long-range order which we adopt arises naturally in the case of a solid from the dislocation theory of melting (Nabarro 1967). In this theory, it is supposed that a liquid close to its freezing point has a local structure similar to that of a solid, but that in its equilibrium configurations there is some concentration of dislocations which can move to the surface under the influence of an arbitrarily small shear stress, and so produce viscous flow. In the solid state there are no free dislocations in equilibrium, and so the system is rigid. This theory is much easier to apply in two dimensions than in three since a dislocation is associated with a point rather than a line.

Although isolated dislocations cannot occur at low temperatures in a large system (except near the boundary) since their energy increases logarithmically with the size of the system, pairs of dislocations with equal and opposite Burgers vector have finite energy and must occur because of thermal excitation. Such pairs can respond to an applied stress and so reduce the rigidity modulus. At sufficiently high temperatures, the largest pairs become unstable under an applied shear stress and produce a viscous response to the shear.

The presence or absence of free dislocations can be determined in the following manner. We suppose that the system has a fair degree of short-range order so that a local crystal structure can be identified. To be definite we take the crystal structure to be a simple square lattice with spacing a . Using the local order, we attempt to trace a path from atom to atom which, in the perfect crystal, would be closed. Mermin (1968) has commented that the thermal motion does not necessarily destroy the correlation in orientation of the crystal axes at large distances, but even if this is destroyed, the direction taken in one region can be defined in terms of that taken in a previous region in the same neighbourhood. Local defects can be avoided by small deformations of the path. This procedure is possible provided there are no grain boundaries. If there are free dislocations present, the number of dislocations contained within the region surrounded by the contour will be proportional to the area of the region. Since the Burgers vectors of the individual dislocations can point in two possible directions, the average total Burgers vector will be proportional to the square root of the area. The path will fail to close by an amount proportional to L , the length of the path. If there are only pairs of dislocations present, only those pairs which are cut by the contour will contribute to the total Burgers vector. The number of pairs cut by the path is proportional to Lr where r is the mean separation of the pairs. Averaging over the possible orientations of the individual Burgers vectors, we see that the path will fail to close by an amount proportional to $(Lr)^{1/2}$. This allows us to determine the presence or absence of topological long-range order in the system.

We can obtain estimates of the transition temperature for the systems discussed by arguments similar to those used by Thouless (1969) for a one-dimensional Ising model

with an interaction falling off at large distances as r^{-2} . At large distances from a dislocation (or vortex in the case of the xy model and neutral superfluid) the strain produced is inversely proportional to the distance and so the energy of a single dislocation depends logarithmically on the size of the system. In fact, the energy of an isolated dislocation with Burgers vector of magnitude b in a system of area A is (Friedel 1964)

$$E = \frac{vb^2(1 + \tau)}{4\pi} \ln \frac{A}{A_0} \quad (1)$$

where v and τ are the two-dimensional rigidity modulus and Poisson's ratio respectively, and A_0 is an area of the order of b^2 . The entropy associated with a dislocation also depends logarithmically on the area, and, since there are approximately A/A_0 possible positions for the dislocation, the entropy is

$$S = k_B \ln \frac{A}{A_0} + O(1) \quad (2)$$

where k_B is the Boltzmann constant.

Since both energy and entropy depend on the size of the system in the same way, the energy term will dominate the free energy at low temperatures, and the probability of a single dislocation appearing in a large system will be vanishingly small. At high temperatures, dislocations will appear spontaneously when the entropy term takes over. The critical temperature at which a single dislocation is likely to occur is the temperature at which the free energy changes sign, namely (Kosterlitz and Thouless 1972)

$$k_B T_c = \frac{vb^2(1 + \tau)}{4\pi} . \quad (3)$$

Identical considerations for the xy model give

$$k_B T_c = \pi J \quad (4)$$

where J is the spin-spin coupling constant and

$$k_B T_c = \frac{\pi \hbar^2 \rho}{2m} \quad (5)$$

for the neutral superfluid where ρ is the density of particles per unit area and m is the effective atomic mass which is not necessarily the same as the atomic mass for a particle moving on a substrate.

That these estimates are upper bounds can be seen by the following argument. Although the formation of isolated dislocations will not occur at low temperatures, there can always be production of a pair of dislocations with equal and opposite Burgers vector, since the strain produced by such a pair falls off sufficiently rapidly at large distances so that the energy is finite. The critical temperatures as calculated above are the temperatures at which a pair of dislocations (or vortices) will dissociate, ignoring the effect of other pairs in the system. These other pairs will relax in the field of the first pair thereby renormalizing the rigidity modulus etc. downwards and consequently reducing the critical temperature. Most of the rest of the paper is devoted to a detailed study of this phenomenon in the systems discussed.

2. A model system

The statistical problem we are faced with is essentially that of a two-dimensional gas of particles with charges $\pm q$ interacting via the usual logarithmic potential, the number of particles being constrained only by the requirement that the system has overall electrical neutrality. The only essential modification necessary to treat the dislocation problem is to allow for the two different possible orientations of the Burgers vector. The hamiltonian for such a system is

$$H(r_1 \dots r_N) = \frac{1}{2} \sum_{i \neq j} U(|r_i - r_j|) \quad (6)$$

where

$$\begin{aligned} U(|r_i - r_j|) &= -2q_i q_j \ln \left| \frac{r_i - r_j}{r_0} \right| + 2\mu & r > r_0 \\ &= 0 & r < r_0. \end{aligned}$$

Here q_i and r_i are the charge and position of the i th particle, 2μ is the energy required to create a pair of particles of equal and opposite charge a distance r_0 apart, and r_0 is some suitable cutoff to avoid spurious divergences at small separations. We expect that the cutoff r_0 is of the order of the particle diameter or, for a lattice, the lattice spacing. In such a lattice near the critical point, we will be able to replace sums over the lattice sites by an integral over the whole system since the important contributions to the sum will come from the long-range part of the interaction, that is $|r_i - r_j| \gg r_0$.

To obtain a tractable theory, we further assume that the chemical potential μ is sufficiently large that there are very few particles present in the system. Since we have such a dilute gas, the configurations of least energy are those where equal and opposite charges are closely bound in dipole pairs, well separated from one another. At low temperatures, therefore, the fluctuations of charge within a given region are restricted, while at high temperatures charges may occur in isolation so much larger fluctuations may occur. For such configurations, we see that the mean square separation of the particles making up a dipole pair (ignoring for the present interactions between the pairs) is

$$\langle r^2 \rangle = \frac{\int_{r_0}^{\infty} dr r^3 \exp\{-2\beta q^2 \ln(r/r_0)\}}{\int_{r_0}^{\infty} dr r \exp\{-2\beta q^2 \ln(r/r_0)\}} = r_0^2 \frac{\beta q^2 - 1}{\beta q^2 - 2} \quad (7)$$

where $\beta = 1/k_B T$. The probability of finding a pair within a given area is found by summing $\exp\{-2\beta\mu - 2\beta q^2 \ln(|r_i - r_j|/r_0)\}$ over all values of r_i and r_j in the area. The double sum can be replaced by a double integral if we normalize by a factor of order r_0^{-4} , so that the mean separation d between such pairs is given in the same approximation by

$$\begin{aligned} \frac{1}{d^2} &\approx \frac{e^{-2\beta\mu}}{r_0^4} \int d^2r \exp\{-2\beta q^2 \ln(r/r_0)\} + O(e^{-4\beta\mu}) \\ &= \frac{\pi}{r_0^2} e^{-2\beta\mu} \frac{1}{\beta q^2 - 1}. \end{aligned} \quad (8)$$

Here we can see the necessity for a large chemical potential μ , since already in calculating d^{-2} , any terms beyond first order in $\exp(-2\beta\mu)$ become intractable. Thus

$$\langle (r/d)^2 \rangle \approx \frac{\pi e^{-2\beta\mu}}{\beta q^2 - 2} \ll 1 \quad \text{for} \quad \beta q^2 < 2. \quad (9)$$

We can already see that a phase transition to a conducting state will take place at a temperature T_c given by

$$k_B T_c \approx \frac{1}{2}q^2 \quad (10)$$

since, in this simple approximation the polarizability, which is proportional to $\langle r^2 \rangle$, diverges. The closely bound dipole pairs will separate to give a uniform two-dimensional plasma of oppositely charged particles. The free energy of an isolated charge is

$$F = E - TS \approx \frac{1}{2}q^2 \ln(R^2/r_0^2) - k_B T \ln(R^2/r_0^2) \quad (11)$$

where R is the radius of the system. Thus we see that isolated charges can appear spontaneously when the temperature reaches T_c as given by equation (10). We are therefore particularly interested in values of βq^2 near 2.

Hauge and Hemmer (1971) have investigated the two-dimensional Coulomb gas under very different conditions. In the limit of vanishing particle size, they find a transition at $kT = q^2$ (in our units), the temperature at which pairs begin to form as $kT \rightarrow q^2$ from above. We look at a different temperature range and find a transition near $kT = \frac{1}{2}q^2$, when the largest pairs dissociate as the transition is approached from below. The main difference between the two models is the presence of a finite cutoff in this paper, which makes the potential well behaved at small distances, while Hauge and Hemmer allow the potential to be singular at the point of closest approach.

The divergence of the polarizability as the transition temperature is approached from below suggests that the most important effect of the interactions between different pairs may be described by the introduction of a dielectric constant. The field of a pair separated by a small distance of the order of r_0 does not extend much beyond the distance of separation of the two charges and from equation (8) it is very unlikely that there will be another pair in their immediate vicinity. Thus the dielectric constant appropriate for the expression of the energy of such a pair is unaffected by the polarizability of the other pairs. It is only for charges separated by an amount greater than the mean separation d of pairs that the energy is modified by the presence of other smaller pairs lying within the range of the field. The effective dielectric constant, therefore, becomes larger as we consider larger and larger pairs, so that the problem becomes a sort of iterated mean field approximation. We are therefore faced with problems similar to those which led to rescaling in the paper of Anderson *et al* (1970).

Within the range of a pair with large separation $r \gg r_0$ it is expected that there will be other pairs with separation up to $r \exp(-\beta\mu)$. The effect of these will be to reduce the interaction energy of the large pair by introducing an effective dielectric constant $\epsilon(r)$. To calculate this dielectric constant we consider pairs with separations lying in a small interval between r and $r + dr$ with $dr \ll r$, and consider terms to first order only in dr . Using the standard methods of linear response theory, we apply a weak electric field E at an angle θ to the line joining the two charges. The polarizability per pair is given by

$$p(r) = q \frac{\partial}{\partial E} \langle r \cos \theta \rangle \Big|_{E=0} \quad (12)$$

where the average is taken over the annulus $r < r' < r + dr$ with Boltzmann factor

$$\exp\{-\beta U(r)\} = \left(\frac{r}{r_0}\right)^{-2\beta q^2/\epsilon(r)} \exp(\beta Erq \cos \theta). \quad (13)$$

Although formally the factor $\exp(\beta Erq \cos \theta)$ will cause a divergence in the integrals of equation (12), we can argue that we can carry out the differentiation with respect to E

and take the limit $E \rightarrow 0$ before integrating as follows. Inside the medium the effective field is set up by the two charges, and falls off rapidly at distances greater than the separation between the charges and so has a finite range. Moreover, since the dipole pairs within this field have a separation very much less than the separation of the two charges of interest, the field experienced by the dipole pairs is effectively constant over them. Thus, our method of calculating the polarizability of a given pair from equation (12) is justified. We easily obtain

$$p(r) = \frac{1}{2}\beta q^2 r^2. \quad (14)$$

The density of such pairs is, by the same argument that leads to equation (8),

$$dn(r) = \frac{1}{r_0^4} \int_0^{2\pi} d\theta \int_r^{r+dr} dr' r' \exp\{-\beta U_{\text{eff}}(r')\} + O(e^{-4\beta\mu}) \quad (15)$$

where $U_{\text{eff}}(r)$ is the energy of two charges separated by r in such a dielectric medium. The terms $O(e^{-4\beta\mu})$ correspond to the fact that in the normalization of the probability for seeing such pairs there are terms corresponding to seeing no pairs, one pair etc, all of which we ignore except for the no-pair term. Another complication arises at this point because the energy $U_{\text{eff}}(r)$ is given by

$$U_{\text{eff}}(r) = 2\mu + 2q^2 \int_{r_0}^r \frac{dr'}{r'\epsilon(r')}.$$

As it stands, we cannot evaluate equation (16) because of the unknown function $\epsilon(r)$. However, assuming that $d\epsilon^{-1}(r)/dr$ is sufficiently small, we can write

$$U_{\text{eff}}(r) = \frac{2q^2 \ln(r/r_0)}{\epsilon(r)} \quad (17)$$

and check the consistency of this assumption *a posteriori*. We finally obtain the susceptibility due to these pairs

$$d\chi(r) = \pi\beta q^2 e^{-2\beta\mu} \left(\frac{r}{r_0}\right)^{-2\beta q^2/\epsilon(r)+4} d\left(\ln\frac{r}{r_0}\right). \quad (18)$$

Lastly, we change variables to

$$x = \ln\frac{r}{r_0} \quad \text{and} \quad y(x) = \frac{2\beta q^2}{\epsilon(x)} - 4$$

to obtain the differential equation

$$\frac{dy}{dy} = -\pi^2 e^{-2\beta\mu} (y+4)^2 e^{-x} \quad (19)$$

which is subject to the boundary conditions

$$y(0) = 2\beta q^2 - 4 \quad \text{and} \quad y(\infty) = \frac{2\beta q^2}{\epsilon} - 4 \quad (20)$$

where ϵ is the macroscopic dielectric constant. Since, as discussed previously, when $x = 0, r = r_0$ so that the interaction of a pair separated by r_0 is unaffected by any other pairs, so that $\epsilon(x=0) = 1$. Similarly, as $x \rightarrow \infty$, the effective interaction is reduced by a factor $\epsilon(x=\infty)$, which must be the same as the dielectric constant as measured by application of an external field to a macroscopic region of the medium. We can simplify

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equation (19) further by noticing that, since the derivative dy/dx is proportional to $e^{-2\beta\mu}$, the difference $y(0) - y(\infty)$ for $y(0) > y_c(0)$ must also be very small (in fact $y(0) - y(\infty) < O(e^{-\beta\mu})$) so that we can replace the factor $(y + 4)^2$ in equation (19) by $(y(0) + 4)^2$.

The problem is now reduced to solving the equation

$$\frac{d\tilde{y}}{d\tilde{x}} = - \exp(-\tilde{x}\tilde{y}) \quad (21)$$

where we have rescaled $x = (\pi e^{-\beta\mu}(y(0) + 4))^{-1} \tilde{x}$ and $y = (\pi e^{-\beta\mu}(y(0) + 4)) \tilde{y}$ to eliminate the constant multiplying the exponential. This equation does not possess an analytic solution but the solutions fall into two classes (see Appendix)

$$\begin{aligned} \text{(i)} \quad & \frac{q^2}{k_B T \epsilon(T)} - 2 > 0 && \text{for } T < T_c \\ \text{(ii)} \quad & \frac{q^2}{k_B T \epsilon(T)} - 2 \rightarrow -\infty && \text{for } T > T_c. \end{aligned} \quad (22)$$

We interpret this sudden change in the behaviour of $\epsilon(T)$ as T passes through T_c as a phase transition to the conducting state where the pairs become unbound. The critical temperature T_c is given by

$$\frac{q^2}{k_B T_c} = 2 \left[1 + \left\{ \tilde{y}_c(0) \pi \exp\left(\frac{-\mu}{k_B T_c}\right) \right\} \right] \quad (23)$$

and the critical value of the dielectric constant at the transition temperature is given by

$$\frac{q^2}{k_B T_c} - 2\epsilon(T_c) = 0. \quad (24)$$

To determine the values of T_c and ϵ_c and to investigate the nature of the phase transition, it is necessary to find an approximate solution of equation (21). This can be done in two limiting cases, $T \ll T_c$ and $T \gtrsim T_c$. In the first case, $y(0) \approx y(\infty) > 0$ so we can immediately integrate equation (21) by replacing $y(x)$ by $y(0)$ in the exponential to obtain

$$\epsilon \approx 1 + \frac{\pi^2 \beta q^2 e^{-2\beta\mu}}{\beta q^2 - 2}. \quad (25)$$

In the second case $T \gtrsim T_c$, equation (21) may be solved approximately by the methods described in the Appendix to obtain $\tilde{y}_c(0) = 1.3$ so that

$$\frac{q^2}{k_B T_c} \approx 2 \left\{ 1 + 1.3 \pi \exp(-\mu/k_B T_c) \right\} \quad (26)$$

and

$$\left(\frac{q^2}{k_B T \epsilon(T)} - 2 \right)_{T \rightarrow T_c} \sim \exp \left\{ - \left(\ln \frac{T_c}{T_c - T} \right)^{1/2} \right\}. \quad (27)$$

This singularity in $\epsilon(T)$ is of a most unusual type but, since we have used a mean field theory, this form of the singularity is unlikely to be the correct one. Note in particular that $\epsilon(T_c)$ is finite so that the susceptibility does not diverge at the critical temperature as one would expect from the simple arguments presented earlier.

We are now in a position to check our assumption that $d\epsilon^{-1}(r)/dr$ is sufficiently small to do the integration in equation (16). Clearly, for $T \ll T_c$, the replacement of $\epsilon^{-1}(r)$ by a constant is valid. The most unfavourable case is for the critical trajectory when $y(\infty) = 0$ and $d\epsilon^{-1}(r)/dr$ is largest. The condition for the replacement to be valid is

$$\frac{d\epsilon^{-1}(r)}{dr} \underset{r \rightarrow \infty}{\ll} \frac{1}{r \ln r}. \quad (28)$$

The critical solution of equation (21) is, as can be verified by direct substitution

$$\tilde{y}(x) \underset{x \rightarrow \infty}{\sim} \frac{2 \ln \tilde{x}}{\tilde{x}} - \frac{\ln \ln \tilde{x}}{\tilde{x}} + \dots \quad (29)$$

Remembering that $\tilde{x} \propto \ln r/r_0$, this gives

$$\frac{d\epsilon^{-1}(r)}{dr} \underset{r \rightarrow \infty}{\sim} \frac{1}{r \ln r} \frac{\ln \ln r}{\ln r} \ll \frac{1}{r \ln r}. \quad (30)$$

The free energy has a singularity at the critical temperature but it is so weak that any observable except the dielectric constant is finite and all derivatives are finite and bounded for $T < T_c$. Not surprisingly, this is in agreement with the results obtained by Anderson and Yuval (1971) for the one-dimensional Ising model with inverse square interaction, which can be treated with our methods to obtain most of their results. The energy of a pair of charges is

$$U = \frac{q^2 \int_0^\infty dx x \epsilon^{-1}(x) \exp\{-2(\beta q^2 \epsilon^{-1}(x) - 1)x\}}{\int_0^\infty dx \exp\{-2(\beta q^2 \epsilon^{-1}(x) - 1)x\}} \quad (31)$$

where we have substituted $x = \ln(r/r_0)$. Since the specific heat C is proportional to $dU/d\beta$, any singularities in C will show up in integrals of the form

$$\int_0^\infty dx x^n \frac{\partial \epsilon^{-1}(x)}{\partial \beta} \exp\{-2(\beta q^2 \epsilon^{-1}(x) - 1)x\} \approx \int_0^\infty dx x^n e^{-\alpha x} \frac{\partial y(x)}{\partial y(0)} \quad (32)$$

where we have used the fact that $\beta q^2 \epsilon^{-1}(x) - 1 \approx \text{const} > 0$ for $T < T_c$. This integral will certainly be finite except possibly at $T = T_c$, in which case we want the asymptotic form of $y(x)$ as given by equation (29), since it is clear that $\partial y(x)/\partial y(0)$ is singular only at infinity.

Differentiating equation (21) with respect to $\tilde{y}(0)$ and using equation (29) we obtain

$$\frac{\partial}{\partial \tilde{x}} \left(\frac{\partial \tilde{y}(\tilde{x})}{\partial \tilde{y}(0)} \right) \underset{x \rightarrow \infty}{\sim} \frac{\partial \tilde{y}(\tilde{x})}{\partial \tilde{y}(0)} \frac{\ln \tilde{x}}{\tilde{x}} \quad (33)$$

which has the solution

$$\frac{\partial \tilde{y}(\tilde{x})}{\partial \tilde{y}(0)} \underset{x \rightarrow \infty}{\sim} \exp\{\frac{1}{2}(\ln \tilde{x})^2\}. \quad (34)$$

The integrals of the form (32) in the expression for C are thus all finite since the $e^{-\alpha x}$ factor ensures convergence. We can similarly show that all derivatives of C of finite order are finite and bounded at the critical temperature, which strongly indicates that C is analytic there.

It must be borne in mind that mean field approximations are notoriously bad in predicting the form of the singularities in specific heats etc, since such a theory ignores fluctuations in the internal field. We therefore expect that our value of T_c is an overestimate and that in an exact treatment there may be a weak singularity in C .

Just above the critical temperature, the largest pairs will dissociate and be able to carry charge so that the medium will conduct. Assuming that the mobility of a free charge behaves smoothly at T_c , the behaviour of the DC conductivity as $T \rightarrow T_c$ from above will be determined by that of the density of dissociated pairs $\delta n(T)$. This number may be estimated by calculating the number of pairs whose separation is less than R , where R is defined by $y(R) = 0$. When the separation r increases so that $y(r) < 0$, the trajectory $y(x)$ ($x = \ln(r/r_0)$) falls off rapidly to minus infinity (see figure A1). We interpret this failure of the theory as the complete dissociation of such a pair. We find that R is given by (see Appendix)

$$\ln \frac{R}{r_0} \underset{T \rightarrow T_c^+}{\sim} \exp \left\{ \left(\ln \frac{1}{T - T_c} \right)^{1/2} \right\}. \quad (35)$$

The density of pairs with separation less than R is

$$\begin{aligned} n(R) &\approx \frac{2\pi}{r_0^2} \int_{r_0}^R \frac{dr}{r_0} \left(\frac{r}{r_0} \right)^{-(2\beta q^2/\epsilon(r)-1)} \\ &\approx \frac{\pi}{r_0^2} \frac{1 - (R/r_0)^{-2(\beta q^2-1)}}{\beta q^2 - 1} \end{aligned} \quad (36)$$

where we have taken $\epsilon(r) \approx 1$ throughout the region of integration. This is justified here because $\{\beta q^2/\epsilon(r)\} - 1 \approx 1$ near T_c for all r . Thus, the density of dissociated pairs $\delta n(T)$ is given by

$$\ln \frac{\delta n(T)}{n} \underset{T \rightarrow T_c^+}{\sim} - \exp \left\{ \left(\ln \frac{1}{T - T_c} \right)^{1/2} \right\} \quad (37)$$

where $2n$ is the total density of charges. Also

$$\frac{d}{dT} \ln \frac{\delta n(T)}{n} \underset{T \rightarrow T_c^+}{\sim} \frac{\exp([\ln\{1/(T - T_c)\}]^{1/2})}{T - T_c} \quad (38)$$

so that

$$\frac{\delta n(T)}{n} \underset{T \rightarrow T_c^+}{\rightarrow} 0 \quad (39)$$

and

$$\frac{dr}{dT} \frac{\delta n(T)}{n} \underset{T \rightarrow T_c^+}{\rightarrow} 0. \quad (40)$$

Thus, the DC conductivity tends to zero with all derivatives zero as the critical temperature is approached from above.

To conclude this section on the model system, we would like to point out that the assumption of a very dilute system ($e^{-2\beta\mu} \ll 1$) is not necessarily valid in a real system. However, we expect that the qualitative arguments will go through even in such a case and the general form of the results will be unchanged. We can imagine increasing the cutoff r_0 to some value R_0 such that the energy of two charges a distance R_0 apart is $2\mu(R_0)$ where $\exp\{-2\mu(R_0)\beta\} \ll 1$. For charges further apart than R_0 , we can use the theory as outlined previously. The boundary conditions given by equation (20) will be changed to

$$y(0) = \frac{2q^2}{k_B T \epsilon(R_0)} - 4 \quad (41)$$

with $\epsilon(R_0)$ an unknown function. The critical temperature and the dielectric constant will now be determined in terms of $\epsilon(R_0)$ and $\mu(R_0)$. To determine these two quantities, a more sophisticated treatment is required, but we expect that the behaviour of the dielectric constant and specific heat at the critical temperature will be unchanged.

3. The two-dimensional *xy* model

The two-dimensional *xy* model is a system of spins constrained to rotate in the plane of the lattice which, for simplicity, we take to be a simple square lattice with spacing a . The hamiltonian of the system is

$$H = -J \sum_{\langle ij \rangle} S_i \cdot S_j = -J \sum_{\langle ij \rangle} \cos(\phi_i - \phi_j) \quad (42)$$

where $J > 0$ and the sum $\langle ij \rangle$ over lattice sites is over nearest neighbours only. We have taken $|S_i| = 1$ and ϕ_i is the angle the i th spin makes with some arbitrary axis. Only slowly varying configurations, that is, those with adjacent angles nearly equal, will give any significant contribution to the partition function so that may expand the hamiltonian up to terms quadratic in the angles.

It has been shown by many authors (Mermin and Wagner 1966, Wegner 1967, Berezinskii 1970) that this system does not have any long-range order as the ground state is unstable against low-energy spin-wave excitations. However, there is some evidence (Stanley 1968, Moore 1969) that this system has a phase transition, but it cannot be of the usual type with finite mean magnetization below T_c . As we shall show, there exist metastable states corresponding to vortices which are closely bound in pairs below some critical temperature, while above this they become free. The transition is characterized by a sudden change in the response to an applied magnetic field.

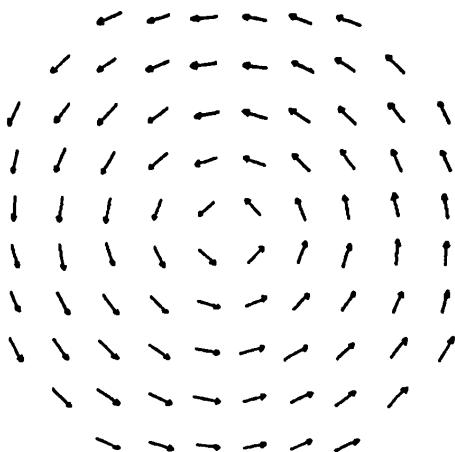
Expanding about a local minimum of H

$$H - E_0 \approx \frac{1}{2} J \sum_{\langle ij \rangle} (\phi_i - \phi_j)^2 = J \sum_r (\Delta\phi(r))^2 \quad (43)$$

where Δ denotes the first difference operator, $\phi(r)$ is a function defined over the lattice sites, and the sum is taken over all the sites. If we consider the system in the configuration of figure 1, its energy is, from equation (43)

$$H - E_0 \approx \pi J \ln \frac{R}{a} \quad (44)$$

where R is the radius of the system. Thus we have a slowly varying configuration, which we shall call a vortex, whose energy increases logarithmically with the size of the system.

Figure 1. An isolated vortex in the xy model.

From the arguments of the Introduction, this suggests that a suitable description of the system is to approximate the hamiltonian by terms quadratic in $\Delta\phi(r)$ and split this up into a term corresponding to the vortices and another to the low-energy excitations (spin waves).

We extend the domain of $\phi(r)$ to $-\infty < \phi(r) < \infty$ to allow for the fact that, in the absence of vortices, $\langle(\phi(r) - \phi(r'))^2\rangle$ increases like $\ln(|r - r'|)$ (Berenzinskii 1971). Thus, at large separations, the spins will have gone through several revolutions relative to one another. If we now consider a vortex configuration of the type of figure 1, as we go round some closed path containing the centre of the vortex, $\phi(r)$ will change by 2π for each revolution. Thus, for a configuration with no vortices, the function $\phi(r)$ will be single-valued, while for one with vortices it will be many-valued. This may be summarized by

$$\sum \Delta\phi(r) = 2\pi q \quad q = 0, \pm 1, \pm 2 \dots \quad (45)$$

where the sum is over some closed contour on the lattice and the number q defines the total strength of the vortex distribution contained in the contour. If a single vortex of the type shown in figure 1 is contained in the contour, then $q = 1$.

Let now $\phi(r) = \psi(r) + \bar{\phi}(r)$, where $\bar{\phi}(r)$ defines the angular distribution of the spins in the configuration of the local minimum, and $\psi(r)$ the deviation from this. The energy of the system is now

$$H - E_0 \approx J \sum_r (\Delta\psi(r))^2 + J \sum_r (\Delta\bar{\phi}(r))^2 \quad (46)$$

where

$$\sum \Delta\psi(r) = 0 \quad \text{and} \quad \sum \Delta\bar{\phi}(r) = 2\pi q. \quad (47)$$

The cross term vanishes because of the condition (47) obeyed by $\psi(r)$. Clearly the configuration of absolute minimum energy corresponds to $q = 0$ for every possible contour when $\bar{\phi}(r)$ is the same for all lattice sites. We see from equation (45) that, if we shrink the contour so that it passes through only four sites as in figure 2, we will obtain the strength

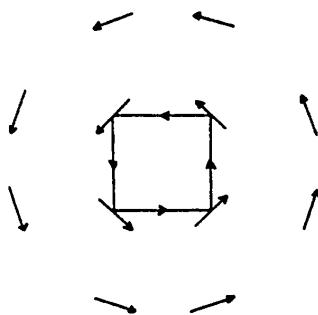


Figure 2. Contour around centre of vortex.

of the vortex whose centre we can take to be located on a dual lattice whose sites r^* lie at the centres of the squares of the original lattice (Berezinskii 1971). This procedure enables us to define the vortex distribution function $\rho(r^*)$ given by

$$\rho(r^*) = \sum_e q_e \delta_{r^*, r_e}. \quad (48)$$

Going now to a continuum notation for convenience, using equation (47), we can easily find the equation obeyed by $\bar{\phi}(r)$

$$\nabla^2 \bar{\phi}(r) = 2\pi\rho(r). \quad (49)$$

In terms of ρ , the energy of the system in a given configuration is

$$H - E_0 = J \int d^2r (\nabla \psi)^2 - 4\pi^2 J \int \int d^2r d^2r' \rho(r) g(r - r') \rho(r') + 2\pi J \int \int d^2r d^2r' \rho(r) \rho(r') \ln \frac{R}{r_0} \quad (50)$$

where R is the radius of the system, r_0 is a cutoff of the order of the lattice spacing a and $g(r)$ is the Green function of the square lattice defined so that $g(0) = 0$ (Spitzer 1964). The last term of equation (50) requires that $\sum q_e = 0$ which is the condition that the total vorticity of the system vanishes, and corresponds to the requirement of electrical neutrality in the model system. The first term produces the spin-wave excitations and is responsible for destroying long-range order, and the second term is the interaction energy of the vortices which cause the phase transition.

If we ignore all vortex configurations, we obtain for the spin-spin correlation function

$$\langle S_i \cdot S_j \rangle = \langle \exp\{i(\phi_i - \phi_j)\} \rangle = \exp\left(-\frac{k_B T}{2J} g(r_i - r_j)\right) \quad (51)$$

where (Spitzer 1964)

$$g(r) \approx \frac{1}{2\pi} \ln \left| \frac{r}{r_0} \right| \quad (52)$$

and

$$\frac{r_0}{a} = \frac{e^{-\gamma}}{2\sqrt{2}} \quad (\gamma = \text{Euler's constant}).$$

Thus

$$\langle S_i S_j \rangle \underset{|r_i - r_j| \gg a}{\approx} \left| \frac{r_i - r_j}{r_0} \right|^{-k_B T / 4\pi J} \quad (53)$$

and we can see that the spin-wave excitations are responsible for destroying any long-range order in the system, but have nothing to do with any phase transition which may occur.

The energy E_v of the vortex configuration is now simply

$$E_v \underset{|r_i - r_j| \gg a}{\approx} -2\pi J \sum_{i \neq j} q_i q_j \ln \left| \frac{r_i - r_j}{r_0} \right| \quad (54)$$

where q_i is the strength of the i th vortex whose centre is located at r_i . We no longer distinguish between the original and dual lattices. This asymptotic expression for the energy is in fact a very good estimate even down to $|r| = a$ (Spitzer 1964) so we can use it for all $|r| > a$. Since in our approximation, the spin-waves and vortices do not interact with one another, the problem is now reduced to that of the model system with the vortices playing the rôle of the charged particles and

$$\begin{aligned} E_v &= -2\pi J \sum_{i \neq j} q_i q_j \ln \left| \frac{r_i - r_j}{a} \right| - 2\pi J \sum_i q_i^2 \ln \frac{r_0}{a} && \text{for } |r_i - r_j| > a \\ &= 0 && \text{otherwise.} \end{aligned} \quad (55)$$

The chemical potential μ of a single vortex of unit strength is

$$\mu = -2\pi J \ln \frac{r_0}{a} = 2\pi J(\gamma + \frac{3}{2} \ln 2) \quad (56)$$

which is to be compared with the exact expression for the energy of two vortices separated by a single lattice spacing

$$\mu = \pi^2 J \quad (57)$$

which is obtained from equation (50) using the exact value of $g(a) = \frac{1}{4}$. The critical temperature T_c at which the transition takes place is given by the solution of the equation

$$\begin{aligned} \frac{\pi J}{k_B T_c} - 1 &\approx \pi \tilde{y}_c(0) \exp\left(\frac{-\pi^2 J}{k_B T_c}\right) \\ &\approx 0.12. \end{aligned} \quad (58)$$

Below T_c , the vortices will be bound in pairs of zero total vorticity, while above T_c they are free to move to the surface under the influence of an arbitrarily weak applied magnetic field, thereby causing a sudden change in the form of the response to the applied field.

One way of seeing the effect of the transition is to consider the spin-spin correlation function $\langle S_i \cdot S_j \rangle$. Taking the vortices into account, this is modified to

$$\langle S_i \cdot S_j \rangle = \langle \exp\{i(\psi_i - \psi_j)\} \rangle \langle \exp\{i(\bar{\phi}_i - \bar{\phi}_j)\} \rangle. \quad (59)$$

Since the vortices and spin waves do not interact in our approximation, the two averages are taken independently. The average $\langle \exp\{i(\psi_i - \psi_j)\} \rangle$ is taken over all possible values of ψ_i , and is given by equation (53) and $\langle \exp\{i(\bar{\phi}_i - \bar{\phi}_j)\} \rangle$ is taken over all possible vortex distributions. In our mean field approximation, we can estimate the latter term as follows

$$\langle \exp\{i(\bar{\phi}_i - \bar{\phi}_j)\} \rangle = \langle \bar{S}_i \cdot \bar{S}_j \rangle \underset{|r_i - r_j| \rightarrow \infty}{\equiv} K(T) \quad (60)$$

where \bar{S}_i is the spin on the i th site in the absence of spin-wave excitations. Thus,

$$K(T) = \bar{\sigma}^2 \quad (61)$$

where $\bar{\sigma}$ is the mean magnetization of the metastable configurations without the spin-wave excitations. Thus, $\bar{\sigma}$ corresponds exactly to ϵ^{-1} of the model system so that $K(T) = O(1)$ for $T < T_c$ and vanishes discontinuously at $T = T_c$ according to equation (27).

Since the spin waves and vortices do not interact, the system of vortices alone is equivalent to a system of freely moving, straight parallel current-carrying wires whose number is not conserved, located at the centres of the vortices. The sign of the forces between the wires is reversed, and $I_i = q_i/\sqrt{2\pi J}$, I_i being the current in the i th wire in suitable units. The chemical potential $\mu = \pi^2 J$ is the energy required to 'create' a wire with no current. The sum of the currents in the wires is contained to be zero, corresponding to the condition $\sum q_i = 0$. This analogy tells us that, on applying a magnetic field in the plane of the system, the vortices will tend to move at right angles to the field, the direction determined by the sign of q_i .

4. Two-dimensional crystal

For simplicity, we consider a crystal with a square lattice of spacing a , and when possible as a continuum with a short distance cutoff r_0 of the order of the lattice spacing a . As far as any critical phenomena are concerned, this will make no essential difference. The short-distance behaviour will affect quantities like the effective chemical potential, but for our purposes we require only that this is sufficiently large. We can therefore use standard linear elasticity theory to describe our crystal (Landau and Lifshitz 1959).

The stress σ_{ij} is related to the strain u_{ij} for an isotropic medium by

$$\sigma_{ij} = 2v u_{ij} + \lambda \delta_{ij} u_{kk} \quad (62)$$

and the internal energy by

$$U = \frac{1}{2} \int d^2r u_{ij} \sigma_{ij}. \quad (63)$$

As mentioned in the Introduction, there is no long-range order of the usual type in this system, exactly as for the xy model of the previous section. Writing the energy in terms of the displacement field $u(r)$, which describes the displacement of the lattice sites from their equilibrium positions, and expanding to terms quadratic in $u(r)$, we can show that the mean square deviation of a site from its equilibrium position increases logarithmically with the size of the system (Peierls 1935, Berezinskii 1970). This destruction of long-range order is caused by the low-energy phonon modes, and the phase transition from the solid to the liquid state by the dislocation configurations. Since in our approximation, the phonons and dislocations do not interact, we may treat them separately. As in the magnetic case, we may decompose the displacement field as

$$u(r) = v(r) + \bar{u}(r) \quad (64)$$

where

$$\oint v(r) dl = 0 \quad \text{and} \quad \oint \bar{u}(r) dl = b \quad (65)$$

where the integral is taken round some closed contour and \mathbf{b} is the total Burger's vector of the dislocation distribution contained within the contour. $\mathbf{v}(\mathbf{r})$ is the displacement field of the phonons and $\bar{\mathbf{u}}(\mathbf{r})$ that of the dislocations. If the contour in equation (65) is taken round only one dislocation it gives the Burger's vector \mathbf{b} of that dislocation. For simplicity we shall assume that $|\mathbf{b}|$ is the same for all dislocations and the most likely value of $|\mathbf{b}|$ will be the smallest possible, that is $|\mathbf{b}| \approx a$.

The most convenient way of treating a medium with dislocations is to introduce a stress function $\chi(\mathbf{r})$ which is related to the stress $\sigma_{ij}(\mathbf{r})$ by (Friedel 1964, Landau and Lifshitz 1959)

$$\sigma_{ij}(\mathbf{r}) = \epsilon_{ik}\epsilon_{jl} \frac{\partial^2 \chi(\mathbf{r})}{\partial x_k \partial x_l} \quad (66)$$

where

$$\epsilon_{12} = +1, \quad \epsilon_{21} = -1, \quad \epsilon_{ij} = 0 \text{ otherwise.}$$

We can then define a source function $\eta(\mathbf{r})$ describing the distribution of dislocations so that $\chi(\mathbf{r})$ obeys the equation

$$\nabla^4 \chi(\mathbf{r}) = K\eta(\mathbf{r}) \quad (67)$$

where

$$K = \frac{4v(v + \lambda)}{2v + \lambda} = 2v(1 + \tau). \quad (68)$$

$\eta(\mathbf{r})$ is given by (Friedel 1964)

$$\eta(\mathbf{r}) = \sum_a \epsilon_{ij} b_j^{(a)} \frac{\partial}{\partial x_i^{(a)}} \delta^{(2)}(\mathbf{r} - \mathbf{r}^{(a)}) \quad (69)$$

where $\mathbf{r}^{(a)}$ and $\mathbf{b}^{(a)}$ are the position and Burger's vector respectively of the a th dislocation.

Having set up such a formalism, we can investigate the response of a medium containing dislocations to an applied stress in exact analogy to the electrostatic case. In our case, σ_{ij} and u_{ij} correspond respectively to the electric field \mathbf{E} and displacement field \mathbf{D} . The strain energy of the medium due to the dislocations is

$$\begin{aligned} U &= \frac{1}{2} \int d^2 r \chi(\mathbf{r}) \eta(\mathbf{r}) \\ &= \frac{1}{2} K \int d^2 r d^2 r' \eta(\mathbf{r}) g(\mathbf{r} - \mathbf{r}') \eta(\mathbf{r}') + O\left(\sum_{\alpha\beta} \mathbf{b}^{(\alpha)} \cdot \mathbf{b}^{(\beta)} \ln \frac{R}{a}\right) \end{aligned} \quad (70)$$

where $g(\mathbf{r})$ is the Green function of equation (67)

$$g(\mathbf{r}) \underset{|\mathbf{r}| \gg a}{\approx} \frac{1}{8\pi} r^2 \ln \left| \frac{\mathbf{r}}{r_0} \right| \quad (71)$$

and

$$g(0) = 0.$$

Using those equations, we can immediately see that the energy of an isolated dislocation increases logarithmically with the area of the system. The strain energy of a pair of dislocations with equal but oppositely directed Burger's vectors is easily found to be (Friedel 1964)

$$U_{\text{pair}}(\mathbf{r}) \underset{|\mathbf{r}| \gg a}{\approx} \frac{Kb^2}{4\pi} \left(\ln \left| \frac{\mathbf{r}}{a} \right| - \frac{1}{2} \cos 2\theta \right) + 2\mu \quad (72)$$

where $|r|$ is the separation of the two dislocations, θ the angle between b and r , and 2μ the energy required to create two dislocations one lattice spacing apart. This result implies that, at low temperatures, the dislocations tend to form closely bound dipole pairs. Clearly, the condition $\sum b^{(\alpha)} = 0$ must be satisfied so that at low temperatures the energy of the system is finite, corresponding to the condition of electrical neutrality in the model system.

The next step is to identify a quantity analogous to the dielectric constant. Consider the stress function $\chi^{(\alpha)}(r)$ due to the α th dipole with source function $\eta^{(\alpha)}(r)$, (cf Jackson 1962)

$$\chi^{(\alpha)}(r) = K \int d^2 r' \eta^{(\alpha)}(r') g(r - r^{(\alpha)} - r') \quad (73)$$

where $r^{(\alpha)}$ denotes the centre of the α th dipole. Assuming the dipoles are very small, we expand in powers of r' for $|r'| \ll |r - r^{(\alpha)}|$

$$\chi^{(\alpha)}(r) = K \int d^2 r' \eta^{(\alpha)}(r') g(r - r^{(\alpha)}) + \frac{1}{2} K \int d^2 r' \eta^{(\alpha)}(r') x'_i x'_j \frac{\partial^2 g(r - r^{(\alpha)})}{\partial x_i^{(\alpha)} \partial x_j^{(\alpha)}} + \dots \quad (74)$$

since the linear term vanishes for a dipole. We can now define the macroscopic stress function by averaging over a region ΔA such that $\langle r^2 \rangle \ll \Delta A \ll A$, where $\langle r^2 \rangle$ is the mean square separation of the dipole and A is the area of the system.

$$\chi(r) \approx K \int d^2 r' \eta(r') g(r - r') + K \int d^2 r' C_{ij}(r') \frac{\partial^2 g(r - r')}{\partial x'_i \partial x'_j} \quad (75)$$

where

$$\eta(r) = \left\langle \sum_{\alpha} \int d^2 r' \eta^{(\alpha)}(r') \delta(r - r^{(\alpha)}) \right\rangle_{\Delta A} n(r) \quad (76)$$

and

$$C_{ij}(r) = \frac{1}{2} \left\langle \sum_{\alpha} \int d^2 r' \eta^{(\alpha)}(r') x'_i x'_j \delta(r - r^{(\alpha)}) \right\rangle_{\Delta A} n(r)$$

where $n(r)$ is the density of dipoles.

Simple tensor analysis shows that, for an isotropic medium, C_{ij} is given in terms of the applied stress σ_{ij} by

$$C_{ij} = \epsilon_{ik} \epsilon_{kl} (C_1 \sigma_{kl} + C_2 \delta_{kl} \sigma_{mm}) + O(\sigma^2) \quad (77)$$

where C_1 and C_2 are to be determined by a model calculation. From equation (75), we find after an integration by parts

$$\chi(r) = \frac{K}{1 - K(C_1 + C_2)} \int d^2 r' \eta(r') g(r - r'). \quad (78)$$

Thus, the effect of the dislocation pairs is to renormalize $K^{-1} \rightarrow K^{-1} - (C_1 + C_2)$, and we immediately see that the quantity corresponding to the dielectric constant $\epsilon(r)$ is $\epsilon(r) = 1 - K\{C_1(r) + C_2(r)\}$. Using simple linear response theory as in the model system, we obtain

$$\begin{aligned} C_1(r) &= -\frac{1}{4} \beta b^2 n \langle r^2 \rangle \\ C_2(r) &= \frac{1}{8} \beta b^2 n \langle r^2 \cos 2\theta \rangle \end{aligned} \quad (79)$$

where the averages are to be taken with Boltzmann factor $\exp\{-\beta U_{\text{eff}}(r)\}$ and

$$U_{\text{eff}}(r) = \frac{b^2 K}{4\pi\epsilon(r)} \left(\ln \left| \frac{r}{r_0} \right| - \frac{1}{2} \cos 2\theta \right) + 2\mu. \quad (80)$$

Provided we choose the cutoff r_0 sufficiently large so that our continuum approximation holds, and that μ is large enough, we only have to show that the average over θ does not change the analogy with the model system of § 2. We can easily show that equation (19) is modified to

$$\frac{dy}{dx} = -\pi^2 e^{-2\beta\mu} (y+4)^2 \left(1 - \frac{I_1(2+\frac{1}{2}y)}{2I_0(2+\frac{1}{2}y)} \right) e^{-xy}, \quad (81)$$

with

$$y(x) = \frac{\beta b^2}{4\pi K\epsilon(x)} - 4$$

and $I_v(z)$ is the v th-order modified Bessel function (Ambramowitz and Stegun 1965). Provided μ is sufficiently large, $y(x)$ is very small for all x , so that the Bessel functions occurring in equation (81) are essentially constant. Thus we can immediately apply all the results of § 2 to this case.

5. Neutral superfluid

The same type of argument can be applied to a neutral superfluid in two dimensions. All that is required is that Bose condensation should occur in small regions of the system, so that locally a condensate wavefunction can be defined. The argument of Hohenberg (1967) shows that the phase of the condensate wavefunction fluctuates over large distances so that the type of order defined by Penrose and Onsager (1956) cannot occur. If a condensate wavefunction can be defined in a local region, it should be possible to explore the variation of its phase from one region to a neighbouring region. The total vorticity within a region is found by the change of phase along the boundary, divided by 2π . Just as the energy of a vortex in the magnetic system or dislocation in the crystal, so the energy of a superfluid vortex increases logarithmically with the size of the system. At low temperatures, there will be no free vortices, only clusters of zero total vorticity. Neglecting the interaction between clusters, the critical temperature is given by equation (5). The analogy with the model system is close as there is only one type of vortex which may have either sign. As in this model, we expect the interaction between vortex clusters to lower the critical temperature from the estimate of equation (5). The lattice Bose gas has been discussed in detail by Berezinskii (1971) who finds the parameters of the Bose gas to be related to those of the magnetic system by

$$J = \frac{\rho\hbar^2}{m} \quad \text{and} \quad r_0 \approx 1.28 \frac{\hbar c}{T}$$

where c is the speed of sound. Using these parameters, we can estimate the value of T_c from equation (58) and the superfluid density $\rho_s(T_c)$ which is nonzero in contrast to the result of Berezinskii.

Below the critical temperature, for a lattice Bose system with periodic boundary conditions, superfluid flow is stable in the thermodynamic limit, since a state with flow is one in which the phase of the order parameter changes by a multiple of 2π round the

system. The system can change from one such state to another by the creation and separation of a pair of vortices, one of which passes right round the system before recombining with the other, but there is a high energy barrier which prevents this process. The different states of superfluid flow are topologically distinct states which do not make transitions between one another at low temperatures. The phase transition is characterized by these states becoming mutually accessible above the transition temperature, so that the flow states are no longer metastable.

Experiments on the onset of superfluid flow for thin films—see, for example, Symonds *et al* (1966), Chester *et al* (1972) and Herb and Dash (1972)—show a strong depression of the temperature as the film becomes thinner. According to the considerations of this paper the critical temperature should be given by

$$k_B T_c = \frac{\pi \hbar^2 \rho_s}{2m^*} \quad (82)$$

where ρ_s is the density of superfluid particles per unit area and m^* is the effective mass of the helium atoms in the film. If ρ_s is taken to be the bulk value multiplied by the film thickness and m^* is taken to be unaffected by the substrate, and so equal to the atomic mass, this formula gives too high a value for T_c , so the effect of the boundaries in reducing ρ_s must be important. The value of ρ_s at the onset temperature must be nonzero: for a film thickness 1.5 nm at 1.5 K the superfluid density given by equation (81) is about 0.22 times the particle density, if m^* is taken equal to the atomic mass. It is not surprising that the specific heat maximum occurs at a higher temperature than the onset of superfluidity, since a considerable degree of short-range order is necessary before the considerations of this paper have any relevance. De Gennes has made a relevant comment on this matter (see Symonds *et al* 1966).

For a charged superfluid (superconductor) the argument cannot be carried through because, as a result of the finite penetration depth λ , the energy of a single flux line is finite. The circulating current density inside a thin superconducting film of thickness $d \ll \lambda$ is (Pearl 1964)

$$\begin{aligned} J(r) &\approx \frac{\hbar c^2}{4e} \frac{d}{\lambda^2} \frac{1}{r} & r \ll \frac{\lambda^2}{d} \\ &\approx \frac{\hbar c^2}{4\pi e} \frac{1}{r^2} & r \gg \frac{\lambda^2}{d} \end{aligned} \quad (83)$$

where r is the distance from the flux line. The repulsion energy between two vortices with opposite circulation falls off like r^{-1} instead of increasing as $\ln r$ for large separations. The self energy of a single flux line is thus determined by the current near the flux line and is approximately (De Gennes 1966)

$$U \approx \left(\frac{\hbar c}{4e}\right)^2 \frac{d}{\lambda^2} \ln \frac{\lambda^2}{d\xi} \quad (84)$$

where ξ is the ‘hard core’ radius of the flux line.

6. Isotropic Heisenberg model in two dimensions

The isotropic Heisenberg model for a two-dimensional system of spins is quite different from the xy model. To show the nature of this difference, we consider a large system

with periodic boundary conditions, but similar considerations apply to other boundary conditions. In the xy model at low temperatures, the direction of magnetization in a region is defined by a single angle ϕ which varies slowly in space. Although the angle ϕ fluctuates by a large amount in a large system, the number of multiples of 2π it changes by on a path that goes completely round the system is a topological invariant, so that

$$n_x = \frac{1}{2\pi} \int_0^{L_x} \frac{\partial \phi}{\partial x} dx \quad n_y = \frac{1}{2\pi} \int_0^{L_y} \frac{\partial \phi}{\partial y} dy \quad (85)$$

are numbers defining a particular metastable state. Transitions can only take place from one metastable state to another if a vortex pair is formed, the two vortices separate and recombine after one has gone right round the system. Such a process will cause a change of one in either n_x or n_y , but there is a logarithmically large energy barrier to prevent such a transition.

In the case of the isotropic Heisenberg model, the direction of magnetization is defined by two polar angles θ and ϕ . A quantity such as

$$\frac{1}{2\pi} \int_0^{L_x} \frac{\partial \phi}{\partial x} dx$$

is not a topological invariant. A twist of the angle ϕ by 2π across the system can be changed continuously into no twist by changing the other polar angle θ (which we take to be the same everywhere) from $\frac{1}{2}\pi$ to zero. There is in fact a single topological invariant for the Heisenberg model in two dimensions, which is

$$N = \frac{1}{4\pi} \iint \sin \theta \left(\frac{\partial \theta}{\partial x} \frac{\partial \phi}{\partial y} - \frac{\partial \theta}{\partial y} \frac{\partial \phi}{\partial x} \right) dx dy. \quad (86)$$

If we regard the direction of magnetization in space as giving a mapping of the space on to the surface of a unit sphere, this invariant measures the number of times the map of the space encloses the sphere. This invariant is of no significance in statistical mechanics, because the energy barrier separating configurations with different values of N is of order unity. To show this, we consider how a configuration with N equal to unity can be transformed continuously into one with N equal to zero.

A simple example of a configuration with $N = 1$ is one in which θ is a continuous function of $r = (x^2 + y^2)^{1/2}$, equal to π for r greater than some value a , and equal to zero at the origin. The angle ϕ is assumed to be equal to $\tan^{-1}(y/x)$. The energy of a slowly varying configuration is proportional to

$$\frac{1}{2} \iint ((\nabla \theta)^2 + \sin^2 \theta (\nabla \phi)^2) dx dy$$

which, for the configuration described above

$$= \pi \int_0^a \left\{ \left(\frac{d\theta}{dr} \right)^2 + \frac{1}{r^2} \sin^2 \theta \right\} r dr. \quad (87)$$

Even if θ varies linearly between the origin and $r = a$, this integral is finite and independent of a . The configuration can be changed continuously into a configuration with $N = 0$ by letting a tend to zero. Of course, for small values of a , this expression for the energy is invalid, but the number of spins in a disc of radius a is then small so that any energy barrier is small.

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We must conclude that there is no topological long-range order in the Heisenberg model in two dimensions. Supposing that the occurrence of a phase transition is really connected with the existence of long-range order we would conjecture that the *xy* model has a phase transition but the Heisenberg model does not. Such a conjecture does not seem to be in conflict with the evidence provided by the analysis of power series for the models by Stanley (1968) and Moore (1969).

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Appendix. Solution of $dy/dx = -e^{-xy}$

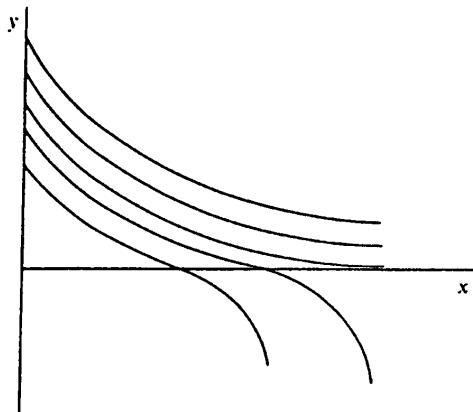


Figure A1. Trajectories of $dy/dx = e^{-xy}$.

From the method of isoclines, we see that the trajectories $y(x)$ behave as plotted in figure A1 with the singular point at infinity. It is easy to see that the solutions fall into two classes

- | | | | |
|------|---------------------------------|--------------------|-------|
| (i) | $y(\infty) \geq 0$ | $y(0) \geq y_c(0)$ | |
| (ii) | $y(\infty) \rightarrow -\infty$ | $y(0) < y_c(0)$ | (A.1) |

corresponding to equation (22). For convenience, we make a transformation of variables to bring the singular point to the origin by defining

$$z = \frac{1}{xy} \quad w = xy - \ln \frac{x}{y} \quad (A.2)$$

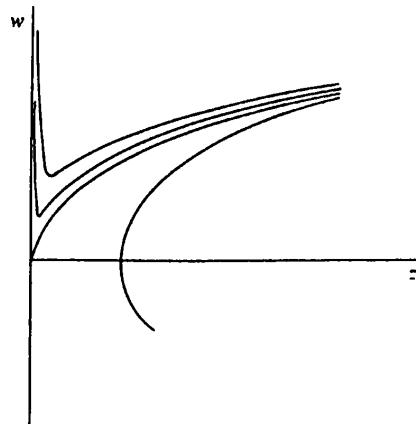


Figure A2. Trajectories in transformed variables.

so that

$$\frac{dw}{dz} = -\frac{1}{z^2} + \frac{1}{z} \coth \frac{1}{2}w. \quad (\text{A.3})$$

The trajectories $w(z)$ have the form displayed in figure A2, where the trajectories corresponding to $y(0) \geq y_c(0)$ are those with $w(z) \geq 0$. We can find approximate solutions in the three regions

- (i) $w \sim 0, \quad z \sim 0$
- (ii) $w \rightarrow \infty, \quad z \sim 0$
- (iii) $w \rightarrow \infty, \quad z \rightarrow \infty$

and match the solutions at $w = 2$. In region (i)

$$\frac{dw}{dz} \approx -\frac{1}{z^2} + \frac{2}{wz}. \quad (\text{A.4})$$

Changing variables to $2t = (1/z) - w$ we obtain

$$z(t) \approx e^{t^2} \int_t^{t_1} e^{-s^2} ds \quad (\text{A.5})$$

where $t_1 \rightarrow \infty$ as $y(0) \rightarrow y_c(0)$ from above. In regions (ii) and (iii)

$$w(z) \approx \frac{1}{z} + \ln z + 2 \ln y \quad (\text{A.6})$$

where $y = y(\infty)$ in (ii) and $y = y(0)$ in (iii).

We can make the best match at $w(z) = 2$, where the gradients in the three regions are equal. However, the numbers are not too good because $\coth 1 \approx \frac{2}{3}$, while we have taken $\coth \frac{1}{2}w = 1$ in regions (ii) and (iii). The points at which we match are defined by the intersections of the curves

$$z(t) = \frac{1}{2(t+1)} \quad \text{and} \quad z(t) = e^{t^2} \int_t^{t_1} e^{-s^2} ds. \quad (\text{A.7})$$

The match between regions (i) and (ii) corresponds to the intersection at $t \rightarrow \infty$, that is

$$t \approx t_1 - \frac{\ln t_1}{2t_1}. \quad (\text{A.8})$$

At the other intersection, we put $t = t_c + \delta$, where t_c is defined by

$$z_c(t_c) = \frac{1}{2(t_c + 1)} = e^{t_c^2} \int_{t_c}^{\infty} e^{-s^2} ds. \quad (\text{A.9})$$

Numerical calculations give $t_c \approx -0.84$. Expanding $z(t)$ to first order in δ we obtain

$$t \approx t_c + \frac{(t_c + 1)e^{t_c^2}}{(-2t_c - 1)} \frac{e^{-t_c^2}}{t_1}. \quad (\text{A.10})$$

Using equations (A.6) to (A.10), we obtain

$$y(\infty) \approx \sqrt{2t_1} e^{-t_1}$$

$$y(0) - y_c(0) \approx \frac{(1 + t_c)^2 \exp(t_c^2 - 2t_c)}{2y_c(0)} \frac{e^{-t_c^2}}{t_1} \quad (\text{A.11})$$

where

$$y_c^2(0) = 2(t_c + 1)e^{-2t_c} \approx 1.7. \quad (\text{A.12})$$

Taking logarithms of equation (A.11) eliminating t_1 , we obtain the leading singularity in $y(\infty)$ for $y(0) \gtrsim y_c(0)$

$$\ln y(\infty) \sim - \left(\ln \frac{1}{y(0) - y_c(0)} \right)^{1/2}. \quad (\text{A.13})$$

Substituting the expressions for $y(\infty)$ and $y(0)$ given by equation (20), and ignoring all but the most singular terms, we immediately obtain equation (27).

Just above the critical temperature where $y(0) \leq y_c(0)$, the appropriate solution of equation (A.4) is

$$z(t) = e^{t^2} \int_t^{\infty} e^{-s^2} ds + Ke^{t^2} \quad (\text{A.14})$$

where $K \geq 0$. In the region $w \rightarrow -\infty$, $z \rightarrow +\infty$

$$w(z) \approx \frac{1}{z} - \ln z - 2 \ln X \quad (\text{A.15})$$

where X is defined by $y(X) = 0$. We can now carry out exactly the same procedure as above to estimate the behaviour of X for $y(0) \rightarrow y_c(0)$ when $K \rightarrow 0^+$ by matching the solutions (A.6), (A.14) and (A.15) at $w = \pm 2$. We find

$$\ln X \underset{y(0) \rightarrow y_c(0)}{\sim} \{-\ln(y_c(0) - y(0))\}^{1/2}. \quad (\text{A.16})$$

Using the expressions for $y(0)$ and $y_c(0)$ of equation (20), we immediately obtain equation (35).

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17.11.2 Kosterlitz: On Renormalization of the Planar Model

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The critical properties of the two-dimensional *xy* model

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Abstract. The critical properties of the *xy* model with nearest-neighbour interactions on a two-dimensional square lattice are studied by a renormalization group technique. The mean magnetization is zero for all temperatures, and the transition is from a state of finite to one of infinite susceptibility. The correlation length is found to diverge faster than any power of the deviation from the critical temperature. Analogues of the strong scaling laws are derived and the critical exponents, η and δ , are the same as for the two-dimensional Ising model.

1. Introduction

In a previous paper (Kosterlitz and Thouless 1973, to be referred to as I), we investigated the possibility of a phase transition in a number of two-dimensional systems with short-range interactions. In such systems the absence of conventional long-range order has been demonstrated rigorously by Mermin (1968), Mermin and Wagner (1966) and Hohenberg (1967). By studying the low-temperature behaviour on the basis of an iterated mean-field theory we showed that it is possible to define long-range order, called topological order, and that there is a phase transition characterized by a sudden change in the response of the system to an external perturbation.

In this paper we study in more detail the *xy* model of ferromagnetism with nearest-neighbour interactions, both above and below the critical temperature, and evaluate the critical exponents for the system. From work done on spin systems with lattices of higher dimension (Wilson 1971, Wilson and Fisher 1972, Wilson and Kogut 1972), we expect that the critical exponents will be independent of the details of the lattice structure and the range of the interaction, provided it is sufficiently short-ranged. The mechanism of the transition was explained in I. Besides the usual spin-wave excitations which are responsible for ensuring that the mean magnetization is zero at all temperatures, there are other equilibrium configurations which are not taken into account in the usual treatments. These are analogous to dislocations in a crystal or vortices in a superfluid and are characterized by the phase of the spins going through a multiple of 2π as we go round a contour enclosing the vortex. As discussed in I, the energy of an isolated vortex configuration of unit strength in such a spin system described by the hamiltonian

$$H_0 = -J \sum_{\langle ij \rangle} \mathbf{s}_i \cdot \mathbf{s}_j \quad (1.1)$$

is

$$E \approx 2\pi J \log R/\tau \quad (1.2)$$

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where R is the radius of the system and τ the lattice spacing. For definiteness, we take the lattice to be square. Since there are $(R/\tau)^2$ possible positions for the vortex, its entropy is

$$S \approx 2k_B \log R/\tau + O(1) \quad (1.3)$$

where k_B is Boltzmann's constant. The free energy is

$$F \approx 2(\pi J - k_B T) \log R/\tau. \quad (1.4)$$

At sufficiently low temperatures, the energy dominates so that it is unfavourable for isolated vortices to occur, while at high temperatures the entropy term takes over and isolated vortices occur. The critical temperature is approximately

$$k_B T_c \approx \pi J. \quad (1.5)$$

In this crude approximation interactions between the vortices have been ignored and most of the rest of this paper is devoted to a detailed study of their effects on the critical behaviour.

Within the limitations of our approximations we confirm the hypothesis of Stanley (1968) that the susceptibility is infinite for all temperatures below the critical temperature and is finite above. We find that at $T \rightarrow T_c$, the correlation length ξ and the susceptibility χ diverge according to the asymptotic laws

$$\begin{aligned} \xi &\sim \exp(bt^{-1/2}) & t > 0 \\ &= \infty & t < 0 \end{aligned} \quad (1.6)$$

where $t = (T - T_c)/T_c$ and $b \approx 1.5$, and

$$\begin{aligned} \chi &\sim \xi^{2-\eta} & t > 0 \\ &= \infty & t < 0 \end{aligned} \quad (1.7)$$

where the exponent $\eta = \frac{1}{4}$ has the same value as in the two-dimensional Ising model (Kaufman and Onsager 1949). This means that we cannot define the conventional exponents ν and γ since ξ diverges faster than any power of t . This is not inconsistent with some tentative results of Moore (private communication) who found that, on the basis of series expansions, γ did not settle to a constant value but continued to increase, indicating that the susceptibility diverges faster than a power of t . We further find that the singular part of the free energy behaves above T_c as

$$F \sim \xi^{-2} \quad t > 0 \quad (1.8)$$

and that, in a weak external magnetic field h the magnetization m is asymptotically

$$m \sim h^{1/\delta} \quad t = 0 \quad (1.9)$$

with $\delta = 15$. We thus see that the usual strong scaling laws are obeyed, provided they are expressed in terms of the correlation length, ie

$$\begin{aligned} \tilde{\gamma} &= 2 - \eta \\ \tilde{\alpha} &= -d \\ \delta &= (d + 2 - \eta)/(d - 2 + \eta) \end{aligned} \quad (1.10)$$

where $\tilde{\gamma}$ and $\tilde{\alpha}$ are defined by $\tilde{\gamma} = \gamma/\nu$, $\tilde{\alpha} = \alpha/\nu$ so that

$$\chi \sim \xi^{\tilde{\gamma}}$$

$$C_h \sim \xi^{\tilde{\alpha}}.$$

2. The model

The two-dimensional xy model is a system of spins confined to rotate in the plane of the lattice, which we take to be a simple square lattice with spacing τ . The hamiltonian of the system is

$$H_0 = -J \sum_{\langle ij \rangle} \mathbf{s}_i \cdot \mathbf{s}_j = -J \sum_{\langle ij \rangle} \cos(\phi_i - \phi_j) \quad (2.1)$$

where $J > 0$ and the sum $\langle ij \rangle$ over the lattice sites is over nearest neighbours only. We have taken $|\mathbf{s}_i| = 1$, and ϕ_i is the angle the i th spin makes with some arbitrary axis. Only slowly varying contributions, that is those with adjacent angles nearly equal, will contribute significantly to the partition function. We may thus expand the hamiltonian about a local minimum up to terms quadratic in $\phi_i - \phi_j$.

$$H = H_0 - E_0 = \frac{1}{2}J \sum_{\langle ij \rangle} (\phi_i - \phi_j)^2 = J \int d^2r (\nabla \phi(r))^2 \quad (2.2)$$

where we use a continuum notation for convenience. We expect that the critical properties of the system will be dominated by long-range effects where a continuum approximation will be sufficiently accurate.

As discussed in the Introduction, we must take into account the vortex configurations as well as the spin-wave excitations which are responsible for destroying the conventional long-range order. The vorticity q of a given region may be defined by

$$\oint d\phi(r) = 2\pi q \quad (2.3)$$

where the integral is taken round the boundary of the region. This suggests that we define

$$\phi(r) = \psi(r) + \bar{\phi}(r) \quad (2.4)$$

where $\bar{\phi}(r)$ defines the angular distribution in the configuration of the local minimum of H and $\psi(r)$ defines the deviations from this. Clearly the absolute minimum of H is given by $\bar{\phi}(r) = \text{const}$.

Since $\bar{\phi}(r)$ obeys Laplace's equation except at isolated points (the centres of the vortices), we can introduce the conjugate function $\bar{\phi}'(r)$ defined by

$$f(z) = \bar{\phi}(r) + i\bar{\phi}'(r) \quad (2.5)$$

where $z = x + iy$, $r = (x, y)$. These obey the Cauchy–Riemann relations so that, using equation (2.3), we find

$$\nabla^2 \bar{\phi}'(r) = -2\pi\rho(r) \quad (2.6)$$

where $\rho(r) = \sum_i q_i \delta(r - r_i)$ is the distribution function of the vortices, and q_i is the strength of the i th vortex centred at r_i .

The solution of equation (2.6) on a square lattice is

$$\bar{\phi}'(r) = -2\pi \int d^2r' \rho(r') g(r - r') + O\left(\log(R/r_0) \int \rho(r) d^2r\right) \quad (2.7)$$

where $g(r)$ is the Green function on a two-dimensional square lattice defined so that $g(0) = 0$. An excellent approximation for $g(r)$ for all $r \geq \tau$ is (Spitzer 1964)

$$g(r) = \frac{1}{2}\pi \log \frac{r}{r_0} \quad (2.8)$$

where $\tau/r_0 = 2\sqrt{2}e^\gamma$. The second term in equation (2.7) demands that

$$\int \rho(r) d^2r = 0 \quad \text{or} \quad \sum q_i = 0. \quad (2.9)$$

Thus, using equation (2.5), we see that $\bar{\phi}(r)$ is given by the imaginary part of

$$f(z) = -2\pi \sum_i q_i g(z - z_i) = -\sum_i q_i \log\left(\frac{z - z_i}{r_0}\right) \quad (2.10)$$

where the branch of $\log z$ is chosen so that

$$\log z = \log |z| + i \arg z. \quad (2.11)$$

Using the Cauchy–Riemann relations we find that

$$\int d^2r (\nabla \phi(r))^2 = \int d^2r (\nabla \phi'(r))^2 \quad (2.12)$$

so that for a configuration of $2n$ vortices in zero external field, from equations (2.6) to (2.8),

$$H_{2n}(r_1 \dots r_{2n}) = J \int d^2r (\nabla \psi(r))^2 - 2\pi J \sum_{i \neq j}^{2n} q_i q_j \log \left| \frac{r_i - r_j}{\tau} \right| + \mu \sum_i q_i^2 \quad (2.13)$$

where $2\mu q^2 = 4\pi J q^2 \log(\tau/r_0) \approx 2\pi^2 J q^2$ is the energy of a pair of vortices of opposite vorticity q separated by a single lattice spacing τ . The exact value of μ is unimportant as it affects only the numerical value of the critical temperature and has no effect on the form of the critical singularities. The only restriction on μ is that $\mu/k_B T_c$ is sufficiently large so that there is a low concentration of vortices near T_c in order to obtain a tractable theory. For the xy model, μ is determined by J , which in turn determines T_c so that $\mu/k_B T_c \approx \pi$ which is just large enough to obtain a selfconsistent theory. For simplicity we make the further assumption that only vortices of unit strength are present since these will be much more favourable than vortices with $|q| > 1$.

The partition function Z may now be written as

$$Z = \text{Tr} \exp(-\beta H_{2n}) \quad (2.14)$$

where

$$\text{Tr} \equiv \int \delta\psi(r) \sum_{n=0}^{\infty} \frac{1}{(n!)^2} \int_{D_{2n}} d^2r_{2n} \dots \int_{D_1} d^2r_1 \quad (2.15)$$

and $\beta = 1/k_B T$. The functional integral over the angle $\psi(r)$ is carried out for $-\infty < \psi(r) < +\infty$, although, strictly speaking $|\psi(r)| < \pi$. Since the hamiltonian is quadratic in $\psi(r)$, such a change should have a negligible effect. We must then further integrate over all possible positions of the vortices which are allowed to go over the whole plane subject only to the restriction $|r_i - r_j| \geq \tau$. Finally we sum over all possible numbers of vortices and include a statistical factor $(n!)^{-2}$ to allow for the fact that there are two sets of n vortices of equal but opposite vorticity.

3. The scaling equations

In this section we concentrate our attention on the contribution of the vortex configura-

tions to the partition function. In the Appendix we show that, on scaling the lattice spacing τ to $\tau + d\tau$, we recover the partition function with unchanged functional form but with scaled interaction parameters given by equations (A.14) to (A.17). There is a fixed point solution to these equations at $K\tau^2 = 0$ and $\beta p^2 - 2 = 0$ which, in accordance with the hypothesis of Wilson (1971), we interpret as signalling the presence of a phase transition. Writing these equations in differential form and linearizing about the fixed point,

$$dx = -y^2 \frac{d\tau}{\tau} \quad (3.1)$$

$$dy^2 = -2xy^2 \frac{d\tau}{\tau} \quad (3.2)$$

$$dF = \frac{1}{8\pi} y^2 \frac{d\tau}{\tau^3} \quad (3.3)$$

where $x = \beta p^2 - 2 = 2(\pi\beta J - 1)$, $y = 4\pi K\tau^2$ and dF is the free energy due to the configurations where pairs of vortices are separated by $\tau < r < \tau + d\tau$, which have been averaged out.

These equations have an almost identical structure to those discussed by Anderson *et al* (1970, 1971), and are easily solved to obtain

$$x^2 - y^2 = x_0^2. \quad (3.4)$$

It can be shown that $x_0^2 = -Ct$ and a crude numerical calculation gives $C \approx 2.1$ for the xy model. The trajectories of equation (3.4) are plotted in figure 1 for various values of t .

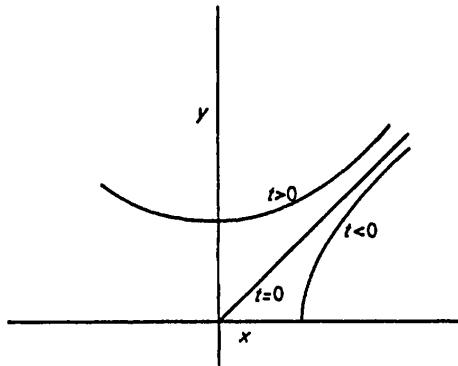


Figure 1. The trajectories of equation (3.4) for various values of t .

The critical temperature T_c is found by putting $x_0^2 = 0$ in equation (3.4), so that it is given by the solution of

$$\pi J/k_B T_c - 1 = 2\pi \exp(-\pi^2 J/k_B T_c). \quad (3.5)$$

This value of T_c is obtained by approximating $\epsilon(r) = \epsilon$ in the mean-field theory of I so that the effective energy of a pair of vortices is scaled by the same factor ϵ . We are unable to say which theory is more realistic, but the numerical differences are very small.

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The solutions of the scaling equations for x and y as functions of τ have been obtained by Anderson *et al* (1970, 1971). In the region below T_c , x and y are positive for all τ , so that, using equations (3.1), (3.2) and (3.4) we find, for large τ

$$x(\tau) \approx x_0(1 + (\tau/\tau_i)^{-2x_0})(1 - (\tau/\tau_i)^{-2x_0})^{-1}. \quad (3.6)$$

At $T = T_c$, when $x_0 = 0$, this becomes

$$x(\tau) \approx (\log \tau/\tau_i)^{-1}. \quad (3.7)$$

We see that for sufficiently large τ , $x(\tau)$ has lost all knowledge of its initial value $x_i = x(\tau_i)$ provided only that $x_0 \ll x_i$. As $\tau \rightarrow \infty$, $x(\tau) \rightarrow x_0$. The same is true for $y(\tau)$ which tends to zero as $\tau \rightarrow \infty$. The behaviour of $x(\tau)$ and $y(\tau)$ is shown in figure 2. We interpret this as

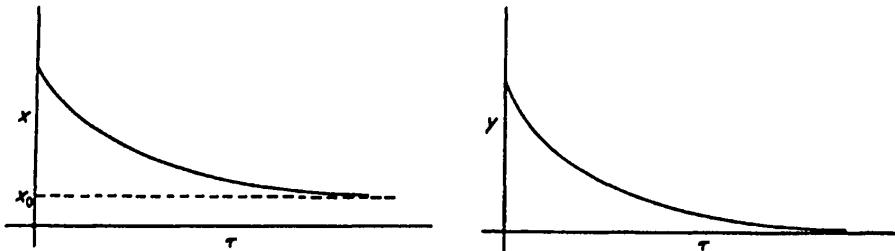


Figure 2. The scaling parameters x and y as functions of τ for $t < 0$.

meaning that, when the lattice spacing is scaled to infinity, all the vortices are scaled out of the problem since the chemical potential of a vortex becomes infinite. If we now identify the maximum value of τ before deviations from the fixed point become significant as the correlation length ξ , we have

$$\xi = \infty \quad t < 0. \quad (3.8)$$

This is a rather surprising result but it has a simple physical explanation. The correlation between two spins is determined by two factors, the spin waves and the vortices. Below the critical temperature, the most favourable configuration of the vortices is for them to be bound together in close pairs of zero vorticity. The effect of a close pair on a spin far distant from the pair is very small since they almost cancel each other out. Even as $T \rightarrow T_c^-$ the mean separation of such pairs is finite (see I) so that as far as the average correlation of two widely separated spins is concerned, the vortices are still in small pairs. They have only a small effect and the correlation is determined by the spin waves which in turn implies an infinite correlation length.

Above the critical temperature, $t > 0$, the situation is not so clear cut. We make an analytic continuation $x_0 = iy_0$, y_0 real, so that $y_0^2 = Ct$, and now the solution of the scaling equations is

$$\frac{\tau}{\tau_i} = \exp \left\{ \frac{1}{y_0} \left(\tan^{-1} \frac{y_0}{x} - \tan^{-1} \frac{y_0}{x_i} \right) \right\}. \quad (3.9)$$

We must choose the branch of \tan^{-1} to be $0 < \tan^{-1} < \pi$ so that τ is an increasing function of x as x decreases from $x_i > 0$ through zero to negative values (see figure 3). For large values of τ equation (3.8) becomes

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$$\frac{\tau}{\tau_i} \approx \exp\left(\frac{\pi}{y_0}\right) \exp\left\{-\left(\frac{1}{|x_{\max}|} + \frac{1}{x_i}\right)\right\} \quad (3.10)$$

where $-|x_{\max}| \ll -y_0$ is the value of x where deviations from the fixed point behaviour

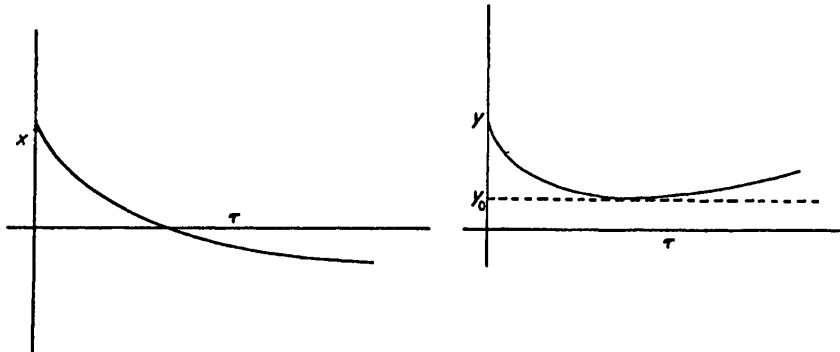


Figure 3. The scaling parameters x and y as functions of τ for $t > 0$.

become significant and the renormalization is stopped. Identifying the correlation length with the corresponding value of τ we obtain

$$\xi_{t \rightarrow 0^+} \sim \exp\left(\frac{\pi}{y_0}\right) \sim \exp(bt^{-1/2}) \quad (3.11)$$

where $b \approx 1.5$. We thus have our first critical quantity ξ , which diverges as $t \rightarrow 0^+$ faster than any power of t and remains infinite for all $t \leq 0$. In this model, the exponent v defined by $\xi \sim t^{-v}$ does not exist.

4. The two-point correlation function

In this section we study the two-point correlation function

$$\Gamma(r - r') = \langle s(r) \cdot s(r') \rangle \quad \text{for } |r - r'| \gg \tau \quad \text{as } t \rightarrow 0^+.$$

The method used is very similar to that of the Appendix, so we only sketch the calculation. In terms of the angles $\phi(r)$, the two-spin correlation function is

$$\begin{aligned} \Gamma(r - r') &= \langle \cos(\phi(r) - \phi(r')) \rangle \\ &= \langle \cos(\bar{\phi}(r) - \bar{\phi}(r')) \cos(\psi(r) - \psi(r')) \rangle \\ &\equiv \Gamma_v(r - r') \Gamma_s(r - r') \end{aligned} \quad (4.1)$$

since the average $\langle \sin \psi \rangle$ vanishes. Fortunately, the two averages can now be carried out separately since H is a sum of two terms containing $\bar{\phi}(r)$ and $\psi(r)$ only.

Since H is quadratic in ψ , the average over ψ gives (Berezinskii 1970)

$$\Gamma_s(r) \underset{|r| > \tau}{\approx} \left| \frac{r}{\tau} \right|^{-\frac{1}{4\pi\beta J}}. \quad (4.2)$$

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To evaluate $\Gamma_v(r)$ we write, explicitly displaying the cut-off,

$$\Gamma_v(r - r'; \tau) = \langle \exp \{2\pi i \operatorname{Im} \sum_k q_k [g(z - z_k) - g(z' - z_k)]\} \rangle \quad (4.3)$$

where $q_k = \pm 1$, $\sum_k q_k = 0$ and we have used equation (2.10). This can be scaled by a slight generalization of the method described in the Appendix to obtain

$$\Gamma_v(r - r'; \tau) = \Gamma_v(r - r'; \tau + dt) \exp \left\{ -\frac{1}{8} y^2 \frac{dt}{\tau} \log \left| \frac{r - r'}{\tau} \right| \right\} \quad (4.4)$$

where

$$\Gamma_v(r - r'; \tau + dt) = \langle \exp i(\bar{\phi}(r) - \bar{\phi}(r')) \rangle. \quad (4.5)$$

The average in equation (4.5) is taken with the hamiltonian appropriate to the scaled cut-off $\tau + dt$. Equations (4.4) and (4.5) are sufficient to find the behaviour of $\Gamma_v(r)$.

Let us first consider the correlation function below the critical temperature. In this region, the correlation length is infinite and so we can continue the scaling procedure up to $\tau = r$, since at this stage the two spins under consideration are one lattice spacing apart. We then expect that

$$\Gamma_v(r - r'; \tau = |r - r'|) = O(1) \quad (4.6)$$

so that the correlation function is given by

$$\Gamma_v(r) = \exp \left\{ -\frac{1}{8} \int_{x_i}^r \frac{d\tau}{\tau} y^2 \log \frac{r}{\tau} \right\} \quad (4.7)$$

where $r = |r - r'|$.

To evaluate the critical exponent η defined by $\Gamma(r) \sim_{r \rightarrow \infty} r^{-\eta}$ in two dimensions, we consider equation (4.7) for $t = 0$. Using the scaling equations (3.1), (3.2), (3.4) and (3.7) we have

$$\begin{aligned} \Gamma_v(r) &= \exp \left\{ \frac{1}{8} \int_{x_i}^{x(r)} dx \log r - \frac{1}{8} \int_{x_i}^{x(r)} dx \log \tau \right\} \\ &\approx \exp \left\{ \frac{1}{8} (x(r) - x_i) \log r - \frac{1}{8} \log x(r) \right\} \\ &\approx r^{-\frac{1}{8}x_i} (\log r)^{\frac{1}{8}} r^{-1/8 \log r}. \end{aligned} \quad (4.8)$$

The last factor in equation (4.8) is $O(1)$, so that, ignoring the logarithmic term

$$\Gamma_v(r) \sim r^{-\frac{1}{8}x_i} \quad t = 0. \quad (4.9)$$

Combining equations (4.2) and (4.9) and working to first order in x_i as we have been doing throughout, the total correlation function at $t = 0$ is

$$\Gamma(r) \sim r^{-\frac{1}{4}} \quad (4.10)$$

whence $\eta = \frac{1}{4}$. The value $\frac{1}{4}$ of the exponent η comes from a conspiracy between the spin-wave and vortex contributions. The spin-waves alone give $\eta = \frac{1}{4}k_B T_c / \pi J$. If we use the simple free energy arguments of the Introduction we would find $\eta = \frac{1}{4}$ since, in this case, the noninteracting vortices do not contribute to η but serve only to determine $k_B T_c / \pi J = 1$. When we consider the interactions between the vortices, the critical temperature is reduced, but now the vortices contribute to η the exact amount required to

bring η back to $\frac{1}{4}$. For $t < 0$, $\Gamma(r)$ falls off somewhat more slowly than $r^{-1/4}$, but its precise behaviour is not of interest. However, we have, from the fluctuation-dissipation theorem,

$$\chi \sim \int d^2r \Gamma(r) = \infty \quad t < 0. \quad (4.11)$$

These are two of the main results of this paper. In particular, the results $\eta = \frac{1}{4}$ is encouraging because the exact solution of the two-dimensional Ising model also gives $\eta = \frac{1}{4}$. This is not in complete agreement with our expectations as experience with the expansions of Wilson and Fisher (1972) indicate that the exponents depend on the number of degrees of freedom of the order parameter, so that one might expect that η for the xy model should differ slightly from $\frac{1}{4}$. However, we are working in a region where the methods of Wilson are inapplicable so when we are unable to say more about this question at this stage.

The situation for $t > 0$ is similar to that of the previous section in our discussion of the correlation length. We can explicitly follow the renormalization for $x_i > x(r) > -x > -1$, but when $x = O(1)$ our equations are no longer valid. However, in this region, as discussed by Anderson *et al.*, we are in a very simple regime where $K\tau^2$ is large so that we have a very large number of vortices present and we are at very high temperatures. In effect, when we reach this stage we must calculate $\Gamma_v(r)$ for high temperatures.

By integrating equation (4.4) up to $\tau = \xi$ so that $-1 < x(\tau) < -y_0$, we find, for $r > \xi$,

$$\Gamma_v(r/\tau_i) = \Gamma'_v(r/\xi) (r/\xi)^{-\frac{1}{4}|x|} (r/\tau_i)^{-\frac{1}{4}x_i} \quad (4.12)$$

where Γ'_v is to be calculated with the hamiltonian appropriate for $\tau = \xi$. As argued above, this corresponds to calculating the correlation function in the high temperature régime where we expect it to fall off very rapidly with increasing values of r/ξ . We may thus write for $t > 0$

$$\Gamma(r) \sim r^{-\frac{1}{4}} f(r/\xi) \quad (4.13)$$

where $f(r/\xi)$ falls off rapidly for $r/\xi > 1$.

The susceptibility becomes

$$\chi \sim \int_{\xi}^{\infty} d^2r r^{-\frac{1}{4}} f(r/\xi) \sim \xi^{2-\frac{1}{4}}. \quad (4.14)$$

We have heuristic arguments which suggest that the contribution to χ from the region $r < \xi$ behaves like $\xi^{2-1/4-\alpha}$ where $\alpha \geq 0$ so that the susceptibility scales as equation (4.14).

5. The exponent δ

In a finite magnetic field h , the partition function becomes

$$Z = \text{Tr} \exp \left\{ -\beta H + \beta h \int d^2r \cos \phi(r) \right\}. \quad (5.1)$$

The change in the free energy due to the magnetic field is

$$\beta\Delta F(h) \approx \left\langle \exp \left\{ \beta h \int d^2r \cos \phi(r) \right\} \right\rangle. \quad (5.2)$$

Expanding equation (5.2), we obtain terms of the form

$$\int d^2r_1 \dots \int d^2r_m (\beta h)^n \langle (\cos \phi(r_1))^{p_1} \dots (\cos \phi(r_m))^{p_m} \rangle \quad (5.3)$$

where p_i are positive integers and $\sum_i p_i = n$. Writing $\cos \phi = \frac{1}{2}(\exp(i\phi) + \exp(-i\phi))$, we are led to consider averages of the form

$$\langle \exp \{ i \sum_k m_k \phi(r_k) \} \rangle = \langle \exp \{ i \sum_k m_k \bar{\phi}(r_k) \} \rangle \langle \exp \{ i \sum_k m_k \psi(r_k) \} \rangle. \quad (5.4)$$

Berezinskii (1970) has shown how to evaluate the average over the spin-wave excitations which can be done in the same way as for the two-point correlation function

$$\langle \exp \{ i \sum_k m_k \psi(r_k) \} \rangle = \prod_{k \neq k'} \left| \frac{r_k - r_{k'}}{\tau_0} \right|^{-m_k m_{k'}/8\pi\beta J} \delta_{0, \sum m_k}. \quad (5.5)$$

By a simple generalization of the method used to scale the two-point correlation function we find

$$\langle \exp \{ i \sum_k m_k \bar{\phi}(r_k) \} \rangle_{(t)} = \langle \exp \{ i \sum_k m_k \bar{\phi}(r_k) \}_{(t+d_t)} \exp \left\{ \frac{1}{16} y^2 \frac{d\tau}{\tau} \sum_{k \neq k'} m_k m_{k'} \log \left| \frac{r_k - r_{k'}}{\tau} \right| \right\} \rangle \quad (5.6)$$

where we explicitly display the cut-off by which the averages are taken. Integrating equation (5.6) at $t = 0$, and ignoring any logarithmic factors

$$\langle \exp \{ i \sum_k m_k \bar{\phi}(r_k) \} \rangle_{(t=0)} \sim \prod_{k \neq k'} \left| \frac{r_k - r_{k'}}{\tau_0} \right|^{+m_k m_{k'}/x_i} \quad (5.7)$$

so that, to first order in x_i

$$\langle \exp \{ i \sum_k m_k \phi(r_k) \} \rangle \sim \prod_{k \neq k'} \left| \frac{r_k - r_{k'}}{\tau_0} \right|^{+m_k m_{k'}}. \quad (5.8)$$

Consider now a term of the form (5.3) with all $p_i = 1$ and scale $r_k = Rr'_k$, with R the radius of the system. Then the contribution to $\Delta F(h)$ from terms with all $p_i = 1$ is

$$\begin{aligned} & \sum_{n=0}^{\infty} C_n (\beta h)^n \int d^2r_1 \dots \int d^2r_n \prod_{k \neq k'} \left| \frac{r_k - r_{k'}}{\tau_0} \right|^{+m_k m_{k'}} \\ &= \sum_{n=0}^{\infty} C_n (\beta h)^n R^{n(2-\frac{1}{4})} \int_{|r_1| < 1} d^2r_1 \dots \int_{|r_n| < 1} d^2r_n \left| \frac{r_k - r_{k'}}{\tau_0} \right|^{+m_k m_{k'}}. \end{aligned} \quad (5.9)$$

We now demand that, as $R \rightarrow \infty$, the free energy per unit area has a finite limit

$$\frac{\Delta F(h)}{R^2} = \Delta f(h) \quad (5.10)$$

and look for solutions of the form

$$\Delta F(h) = a_0 u^{b_0} \quad (5.11)$$

where $u = \beta h R^{(2-\frac{1}{4})}$. Using equations (5.10) and (5.11), we find that

$$\Delta f(h) \sim h^{16/15}. \quad (5.12)$$

By similar arguments it can be shown that the terms (5.3) with any $p_i > 1$ give contributions to $\Delta f(h)$ which vanish with a higher power of h as $h \rightarrow 0$. Provided the series converges

$$\Delta f(h) \underset{h \rightarrow 0}{\sim} h^{16/15}. \quad (5.13)$$

Thus, the mean magnetization $m \sim h^{1/\delta}$ with $\delta = 15$.

6. Free energy and thermal properties

For $t < 0$, the free energy is calculated in exactly the same way as in Anderson *et al* (1970, 1971) by integrating equation (3.3).

$$F_{t < 0} \sim \exp \left\{ \frac{-\text{const}}{t^{1/2}} \right\} + \text{analytic part.}$$

Similarly, for $t > 0$, remembering that we must cut the integrals off at $x \sim -1$

$$F_{t > 0} \sim \exp(-2\pi/y_0) + \text{analytical part.}$$

Thus, the specific heat is regular at $t = 0$ since all derivatives of the singular part of F vanish at $t = 0$. As expected, as $t \rightarrow 0^+$

$$F_{\text{sing}} \sim \xi^{-2}.$$

Appendix

We derive the scaling equations for the system in zero magnetic field and discuss the relation to the two-dimensional classical plasma consisting of n positively and n negatively charged particles interacting with the usual logarithmic Coulomb potential. The contribution of a vortex configuration to the hamiltonian is

$$H_{2n}(r_1 \dots r_{2n}) = - \sum_{i \neq j} p_i p_j \log \left| \frac{r_i - r_j}{\tau} \right| + 2n\mu \quad (\text{A.1})$$

where $p_i = \pm(2\pi J)^{1/2}$ and $\sum p_i = 0$. This has an identical structure to the hamiltonian for the classical plasma with charges $p_i = \pm p$ except for the chemical potential μ . However, if we form the grand partition function for such a system

$$Z = \sum_n \frac{1}{(n!)^2} K^{2n} \int d^2 r_{2n} \dots \int d^2 r_1 \exp \{-\beta H_{2n}\} \quad (\text{A.2})$$

where $K\tau^2 = \exp(-\beta\mu)$ and with the restriction that the system is dilute, so that $\mu/k_B T$ is large, we have precisely the same problem as before. In this case τ is the diameter of the particles. One may worry about the fact that the integrations over the r_i restrict the range to $|r_i - r_j|/\tau > 1$, but one can always redefine the size of the particles by suitably redefining μ so that this restriction still holds. Provided the system is sufficiently dilute, the condition that $\mu/k_B T$ is large will still hold. Thus, if we can solve the problem of the two-dimensional classical plasma we solve the xy model at the same time.

For generality, we include an electric field E , which has no easily realizable physical

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analogue in the *xy* model, so that the partition function becomes

$$Z = \sum_n \frac{1}{(n!)^2} K^{2n} \int_{D_{2n}} d^2 r_{2n} \dots \int_{D_1} d^2 r_1 \exp \left\{ \beta \sum_{i \neq j} p_i p_j \log \left| \frac{r_i - r_j}{\tau} \right| + \beta \sum_i p_i E \cdot r_i \right\} \quad (\text{A.3})$$

where we keep the order of the integrations fixed and D_k is the whole plane except for the circles $|r_k - r_j| < \tau$, $j = k + 1, k + 2, \dots, 2n$. In I we investigated this by an iterated mean-field approximation which yielded a solution to the problem for $T < T_c$, but did not give much information for $T > T_c$.

Anderson *et al* (1970, 1971) have studied a similar partition function for the one-dimensional case corresponding to the Kondo problem and the Ising model with interactions falling off at long distances as r^{-2} . Their methods are directly applicable to our problem. The idea is to scale the lattice spacing or minimum particle separation from τ to $\tau + d\tau$ with $d\tau \ll \tau$ and find the partition function for this new problem which should be of the same functional form as the initial one. To $O(d\tau)$ we can rearrange the integrals of equation (A.3) as

$$\begin{aligned} \int_{D_{2n}} d^2 r_{2n} \dots \int_{D_1} d^2 r_1 &= \int_{D'_{2n}} d^2 r_{2n} \dots \int_{D'_1} d^2 r_1 + \frac{1}{2} \sum_{i \neq j} \int_{D'_{2n}} d^2 r_{2n} \dots \int_{D'_{j+1}} d^2 r_{j+1} \\ &\times \int_{D'_{j-1}} d^2 r_{j-1} \dots \int_{D'_{i+1}} d^2 r_{i+1} \int_{D'_{i-1}} d^2 r_{i-1} \dots \int_{D'_1} d^2 r_1 \int_{\bar{D}_j} d^2 r_j \int_{\delta_i(j)} d^2 r_i \end{aligned} \quad (\text{A.4})$$

where D'_k is defined as for D_k except that τ is replaced by $\tau + d\tau$, $\delta_i(j)$ is the annulus $\tau < |r_i - r_j| < \tau + d\tau$, and \bar{D}_j is the whole plane except for the circles of radius τ about the other $2n - 2$ points, r_k , $k \neq i, j$. The integral over the domain $\delta_i(j)$ selects particle i and pairs it with particle j . The integral over \bar{D}_j then takes this pair over the whole allowed region of the plane. The sum $\frac{1}{2} \Sigma_{i \neq j}$ selects each possible pair once. The main contribution to Z will come from pairing particles with opposite charge so that may restrict the sum over i and j in equation (A.4) to be over particles with $p_i = -p_j$. These three operations have the effect of averaging out the contribution to Z of all close pairs or particles, thereby producing a new problem where the minimum spacing is $\tau + d\tau$.

To proceed, we must carry out the integrations over $\delta_i(j)$ and \bar{D}_j . We select all the terms in $H(r_1 \dots r_{2n})$ containing r_i and r_j and consider

$$\begin{aligned} \int_{\delta_i(j)} d^2 r_i \exp \left\{ 2\beta \left(\sum_k p_i p_k \log \left| \frac{r_i - r_k}{\tau} \right| + \sum_k p_j p_k \log \left| \frac{r_j - r_k}{\tau} \right| \right) \right. \\ \left. + \beta E \cdot (p_i r_i + p_j r_j) \right\}. \end{aligned} \quad (\text{A.5})$$

Since $p_i = -p_j$ and $r_i - r_j = \tau$ we obtain

$$\tau d\tau \int_0^{2\pi} d\theta \prod_k \left(1 + \frac{2\tau \cdot (r_j - r_k)}{|r_j - r_k|^2} + \frac{\tau^2}{|r_j - r_k|^2} \right)^{\beta p_i p_k} \exp \{ \beta p_i E \cdot \tau \} \quad (\text{A.6})$$

where θ is the angle τ makes with some axis. Using the fact that, provided $K\tau^2$ is sufficiently small, we can expand out the product in equation (A.6) to $O(\tau^2/|r_j - r_k|^2)$ since the probability of having three particles (remember that there is a neutral pair at r_j) close together (ie $|r_i - r_k| = O(\tau)$) is very low, so that the main contribution to Z will come

from the regions where $|r_j - r_k| \gg \tau$. Carrying out the expansion to this order and to terms linear in E and doing the integrals over θ we obtain

$$2\pi\tau d\tau \left\{ 1 + \beta^2 p^4 \sum_k \frac{\tau^2}{|r_j - r_k|^2} + \beta^2 p^2 \sum_{k \neq l} p_k p_l \frac{\tau^2 (r_l - r_k) \cdot (r_j - r_l)}{|r_j - r_k|^2 |r_j - r_l|^2} + \beta^2 p^2 \sum_k p_k \frac{\tau^2 E \cdot (r_j - r_k)}{|r_j - r_k|^2} \right\} \quad (\text{A.7})$$

The integration of equation (A.7) over \bar{D}_j is tedious but elementary and our final result is

$$2\pi\tau d\tau \left[A - 2\pi\tau^2 \beta^2 p^2 \sum_{k \neq l} p_k p_l \log \left| \frac{r_k - r_l}{\tau} \right| \right] \quad (\text{A.8})$$

where A is the area of the system.

Using equations (A.4) and (A.8) and rearranging the summation over n we may write the partition function as

$$Z = \sum_n \frac{1}{(n!)^2} K^{2n} \int_{D'_{2n}} d^2 r_{2n} \dots \int_{D'_1} d^2 r_1 \left[1 + \frac{K^2}{(n+1)^2} \sum_{i=1}^{n+1} \sum_{j=1}^{n+1} 2\pi\tau d\tau \times \left(A - 2\pi\tau^2 \beta^2 p^2 \sum_{k \neq l} p_k p_l \log \left| \frac{r_k - r_l}{\tau} \right| \right) \right] \exp \left\{ \beta \sum_{k \neq l} p_k p_l \log \left| \frac{r_k - r_l}{\tau} \right| + \beta \sum_k p_k E \cdot r_k \right\}. \quad (\text{A.9})$$

We notice that on integrating equation (A.5) over the domains $\delta_i(j)$ and \bar{D}_j all dependence on the labels i and j has dropped out so that the summation over i and j in equation (A.9) simply gives a factor $(n+1)^2$. Since we are working to $O(d\tau)$ we may take the exponential of the factor in square brackets in equation (A.9) so that the partition function becomes

$$Z = \exp \{ 2\pi K^2 \tau d\tau A \} \sum_n \frac{1}{(n!)^2} K^{2n} \int_{D'_{2n}} d^2 r_{2n} \dots \int_{D'_1} d^2 r_1 \exp \left\{ \beta \left(1 - (2\pi)^2 \beta p^2 \times (K\tau^2)^2 \frac{d\tau}{\tau} \right) \sum_{i \neq j} p_i p_j \log \left| \frac{r_i - r_j}{\tau} \right| + \beta \sum_i p_i E \cdot r_i \right\}. \quad (\text{A.10})$$

The last step is to change $\tau \rightarrow \tau + d\tau$ in the integrand of equation (A.10) since this will bring the partition function into exactly the same functional form as the initial one except that the cut-off, or minimum particle separation, has been increased to $\tau + d\tau$. This can easily be seen to change the activity $K\tau^2$ since the relevant part of equation (A.10) transforms as

$$K^{2n} \exp \left\{ -\beta \sum_{i \neq j} p_i p_j \log \tau \right\} = \left[K \left(1 - \beta p^2 \frac{d\tau}{\tau} \right) \right]^{2n} \exp \left\{ -\beta \sum_{i \neq j} p_i p_j \log (\tau + d\tau) \right\}. \quad (\text{A.11})$$

We now have

$$Z(\beta p^2, K\tau^2) = Z_0 Z(\tilde{\beta} p_2, \tilde{K}\tau^2) \quad (\text{A.12})$$

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where $Z(\tilde{\beta}p^2, \tilde{K}\tau^2)$ is the partition function for the new problem with cut-off $\tau + d\tau$ and

$$Z_0 = \exp \{2\pi K^2 \tau d\tau A\} \quad (\text{A.13})$$

is the partition function of the pairs with separations between τ and $\tau + d\tau$ which have been averaged out. From equations (A.10) and (A.11), we see that the interaction parameters βp^2 , $K\tau^2$ and Ep have been scaled according to

$$\beta p^2 \rightarrow \tilde{\beta}p^2 = \beta p^2 \left(1 - (2\pi)^2 (\beta p^2) (K\tau^2)^2 \frac{d\tau}{\tau} \right) \quad (\text{A.14})$$

$$K\tau^2 \rightarrow \tilde{K}\tau^2 = K\tau^2 \left(1 - (\beta p^2 - 2) \frac{d\tau}{\tau} \right) \quad (\text{A.15})$$

$$Ep \rightarrow \tilde{Ep} = Ep. \quad (\text{A.16})$$

The free energy per unit area of the particles which have been averaged out is

$$dF = 2\pi K^2 \tau d\tau. \quad (\text{A.17})$$

Equations (A.14), (A.15) and (A.17) are those used in § 3, while equation (A.16) is relevant only to the plasma. Exactly as for the *xy* model, as we scale $\tau \rightarrow \infty$ for $T < T_c$, the total free energy is given by integrating equation (A.17) so that the specific heat is regular as $T \rightarrow T_c^-$. Similar arguments above T_c show that the specific heat is also regular as $T \rightarrow T_c^+$. The critical temperature T_c is given by the solution of the equation

$$\frac{p^2}{k_B T_c} - 2 = 2\pi \exp \left(-\frac{\mu}{k_B T_c} \right) \quad (\text{A.18})$$

obtained by integrating equations (A.14) and (A.15). The behaviour of the dielectric constant ϵ is found from equation (A.16), which on integrating gives

$$E(\tau) = E(\tau_i) \exp \left\{ \frac{1}{4} (x_i - x(\tau)) \right\} \quad (\text{A.19})$$

where $x = \beta p^2 - 2$. When $\tau \rightarrow \infty$, all the particles are scaled out of the problem, so that the dielectric constant $\epsilon(\infty) = 1$ and the actual dielectric constant $\epsilon = \epsilon(\tau_i)$ is given by

$$E(\infty) = \epsilon(\tau_i) E(\tau_i) \quad (\text{A.20})$$

so that

$$\epsilon = \exp \frac{1}{4} (x_i - x_0) \approx 1 + \frac{1}{4} (x_i - x_0) \quad (\text{A.21})$$

for $x \ll 1$. Remembering that $x_0 \propto (T_c - T)^{1/2}$, the dielectric constant approaches its critical value as

$$\epsilon(T_c) - \epsilon(T) \sim (T_c - T)^{1/2} \quad (\text{A.22})$$

which is to be compared with the singularity obtained in I by the mean-field approximation. Within the context of a mean-field theory, equation (A.21) is obtained by assuming that the effective energy of a pair of oppositely charged particles is

$$E_{\text{eff}} = \frac{2p^2}{\epsilon} \log r/\tau$$

while in I we assumed that ϵ was dependent upon r , the distance between the particles. We cannot say at this stage which theory is more accurate.

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*J M Kosterlitz***Acknowledgments**

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Renormalization, vortices, and symmetry-breaking perturbations in the two-dimensional planar model

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The classical planar Heisenberg model is studied at low temperatures by means of renormalization theory and a series of exact transformations. A numerical study of the Migdal recursion relation suggests that models with short-range isotropic interactions rapidly become equivalent to a simplified model system proposed by Villain. A series of exact transformations then allows us to treat the Villain model analytically at low temperatures. To lowest order in a parameter which becomes exponentially small with decreasing temperature, we reproduce results obtained previously by Kosterlitz. We also examine the effect of symmetry-breaking crystalline fields on the isotropic planar model. A numerical study of the Migdal recursion scheme suggests that these fields (which must occur in real quasi-two-dimensional crystals) are strongly relevant variables, leading to critical behavior distinct from that found for the planar model. However, a more exact low-temperature treatment of the Villain model shows that hexagonal crystalline fields eventually become irrelevant at temperatures below the T_c of the isotropic model. Isotropic planar critical behavior should be experimentally accessible in this case. Nonuniversal behavior may result if cubic crystalline fields dominate the symmetry breaking. Interesting duality transformations, which aid in the analysis of symmetry-breaking fields are also discussed.

I. INTRODUCTION

A. Planar model

We wish to examine the low-temperature properties of the classical planar Heisenberg model of ferromagnetism in two dimensions. Thus, we consider a reduced Hamiltonian or "action" of the form

$$A[\theta] = \frac{-H}{k_B T} = - \sum_{\langle \vec{r}, \vec{r}' \rangle} K \{ 1 - \cos[\theta(\vec{r}) - \theta(\vec{r}')]\} + \sum_{\vec{r}} \sum_p h_p \cos[p\theta(\vec{r})], \quad (1.1)$$

where the sums over \vec{r} index the sites of a two-dimensional lattice, the symbol $\langle \vec{r}, \vec{r}' \rangle$ indicates a sum over nearest-neighbor lattice sites only, and

$$K = J/k_B T. \quad (1.2)$$

The quantity J is an exchange coupling entering a nearest-neighbor interaction between fixed length spins on the lattice of the form $J\vec{S}(\vec{r}) \cdot \vec{S}(\vec{r}')$, and $\theta(\vec{r})$ is the angle the spin $\vec{S}(\vec{r})$ makes with some arbitrary axis. The second term in (1.1) involves a sum over possible symmetry-breaking fields h_p ,

indexed by a positive integer p .

With all symmetry-breaking fields h_p set to zero, the Hamiltonian (1.1) has been studied quite extensively. Although evidence from high-temperature series expansions¹⁻³ suggests that the susceptibility of the planar model diverges at some finite T_c , the lack of long-range order at any temperature has been proven rigorously.⁴⁻⁶

Wegner⁷ and Berezinskii⁸ and later Zittartz⁹ have produced "spin wave" theories for the planar model which should be accurate at sufficiently low temperatures. This class of theories leads to a power-law decay of correlation functions at all temperatures, suggesting that the model has a line of critical points with continuously variable critical exponents. Taken literally, the spin-wave results suggest that this line extends out to infinite temperature.

Kosterlitz and Thouless¹⁰ and Berezinskii¹¹ suggested that the spin-wave theories should be modified in an important way by the presence of vortex excitations in the model. Below a certain critical temperature, bound vortex-antivortex pairs should populate an "ordered phase," coexisting with the spin-wave excitations. Above T_c , these pairs are expected to dissociate. Kosterlitz¹² subsequently produced a quantitative analysis

which makes this picture concrete. He constructed a simple renormalization-group transformation which contains a line of fixed points, corresponding physically to a line of critical points terminating in a finite $T_c < \infty$.¹³

In this paper, we focus especially upon the region $T < T_c$. Two methods of attack are developed here. First, the planar model is examined directly via a lattice recursion scheme introduced by Migdal.¹⁴ When applied to fixed-length spins in $2 + \epsilon$ dimensions, this scheme is known to yield results equivalent to those obtained in a more sophisticated theory^{15,16} to first order in ϵ . Second, we argue that there is another model—a generalized Villain^{17,18} model—which has exactly the same symmetry properties as the planar model but is easier to analyze. The original Villain model makes the Kosterlitz-Thouless decomposition into spin waves and vortices particularly simple because the spin waves are described by a purely Gaussian (and hence soluble) interaction. Our generalized Villain model includes (in addition to the coupling strength K) a parameter y which determines the strength of the coupling of vortices into the spin-wave system. In the low-temperature region, one can gain very useful results by expanding in the additional parameter y .

Our plan of attack will be to use the Migdal approximation to understand in a semiquantitative fashion the planar model's behavior. We will argue that this approximation gives recursion relations which become more and more quantitatively correct as the temperature goes to zero. Unfortunately, some of the apparent qualitative features of the exact problem—in particular the existence of a fixed line—are not correctly given by the Migdal scheme. But, the fixed line is almost¹⁹ present so that one can gain useful insight from this approach.

Then, armed with this insight, we pass from the Migdal approximation to the generalized Villain model. This interaction will very naturally lead to a perturbation scheme. This scheme will be very similar to the Kosterlitz-Thouless decomposition into spin waves and vortices, followed by an expansion in the vortex variables. We shall argue that this expansion converges for all temperatures lower than the Kosterlitz-Thouless transition temperature T_c at which the vortices can become unbound.

From the theoretical point of view, our major result will be that the Gaussian spin-wave theory is quantitatively exact for predicting the large-distance correlation functions of the planar model at any temperature below T_c . In particular the correlation function for $\cos p\theta(r)$ is given by the spin-wave result

$$\langle \cos p\theta(r) \cos p\theta(r') \rangle \sim (|r - r'|^{2/p^2 K_{\text{eff}}})^{-1} \quad (1.3)$$

for all values of p equal to integers. This result, we argue, is true for large $|\vec{r} - \vec{r}'|$ for all the models in question whenever the symmetry-breaking terms [defined by h_p in Eq. (1.1)] are zero. The models differ in that K_{eff} depends differently upon K for the various cases. But in all cases $K_{\text{eff}} \rightarrow K$, as $K \rightarrow \infty$ ($T = 0$). As the temperature increases, K decreases and so does K_{eff} —albeit in a model-dependent fashion. This decrement in K_{eff} continues until

$$2\pi K_{\text{eff}} = 4, \quad (1.4)$$

whereupon we observe an unbinding of the vortices and a transition to an entirely different mode of behavior.

B. Symmetry-breaking fields

From the experimental point of view, our most important results relate to the effect of symmetry-breaking fields like h_p . In recent years, it has become possible to study experimentally critical phenomena in crystals which are effectively two-dimensional. Indeed, Birgeneau *et al.*²⁰ have measured critical exponents for the Ising-like quasi-two-dimensional antiferromagnetic K_2NiF_4 , which are strikingly similar to those expected for the two-dimensional Ising model.

One might hope that similar substances with the XY symmetry of the planar model could also be studied experimentally.²¹ However real magnetic crystals are subject to symmetry-breaking crystalline fields in addition to an isotropic exchange coupling. Thus, one must consider the more general Hamiltonian (1.1) with at least one of the h_p 's nonzero. In practice, we expect to encounter crystalline anisotropies with $p = 2-4$ and 6. The effect of an applied external magnetic field is given by $p=1$.

Although Eq. (1.1) is difficult to analyze directly, we may form conclusions about the h_p perturbations both from the Migdal scheme and also from the generalized Villain model. The Migdal scheme implies that as $T \rightarrow 0$ all h_p perturbations are strongly relevant variables. Recursion by recursion, an h_p perturbation will grow and grow finally forcing the system into a state of broken symmetry in which one of the directions $\theta = 2\pi n/p$, $n = 0, 1, \dots, p-1$, is especially preferred. Thence any h_p perturbation will force the system away from a planar model behavior if T is sufficiently small.

The generalized Villain model then gives a precise meaning to "sufficiently small" T . If this model lies in the same universality class as the planar model, then a small perturbation with in-

dex p will be relevant if

$$8\pi K_{\text{eff}} > p^2. \quad (1.5)$$

If this inequality is satisfied, the planar model system will be unstable against ordering via h_p -type perturbations. Equations (1.4) and (1.5) then imply together that the Gaussian spin-wave behavior of the planar model (and its universality "cousins") is stable against symmetry-breaking perturbations and destruction via vortices provided

$$4 < 2\pi K_{\text{eff}} < \frac{1}{4}p^2. \quad (1.6)$$

There is no such stability region for uniaxial perturbations ($p=2$) or triangular perturbations ($p=3$). The square perturbations have a vanishing stability region. But a real planar system with hexagonal perturbation may be expected to show typical critical planar model behavior for

$$4 < 2\pi K_{\text{eff}} < 9.$$

We hope that experimentalists will attempt to find and study such a system.

Phase diagrams for $p=6$ and $p=4$ are shown in Fig. 1. The lines of asterisks at $h_p=0$ indicate the Kosterlitz-Thouless line of critical points with continuously variable exponents. On lowering the temperature of fixed $h_p \neq 0$, one first crosses an upper critical temperature $T_1(h_p)$ into a planar model "phase" of critical points with continuously variable exponents. There is a second transition at temperature $T_2(h_p)$ into a discrete planar ordered phase, where the system orders into one of the six preferred directions selected by the symmetry-breaking perturbation. The susceptibility diverges exponentially fast [i.e., as in Eq. (5.7)] on approaching $T_1(h_p)$ from above or $T_2(h_p)$ from below, and remains infinite between these temperatures. For the Villain models considered here, we find $\eta = \frac{1}{4}$ as T goes to $T_1(h_p)$ from below and $\eta = \frac{1}{9}$ as T tends to $T_2(h_p)$ from above.

The predictions for $p=4$ are also rather striking. The three lines of critical points shown in Fig. 1(b) correspond to three distinct lines of fixed points! Thus, they are denoted by asterisks to show that all three display continuously variable exponents. The second-order phase transition into an ordered four-state phase for $h_4 \neq 0$ should display conventional power law singularities, but with *nonuniversal* critical exponents. Although we find $\eta = \frac{1}{4}$ at the confluence of these critical lines, we have not completely reconciled this result with the predictions of Luther and Scalapino¹³ (see Sec. V).

The stability of various h_p perturbations was analyzed previously within spin wave theory by Prokrovsky and Uimin,²² while Kosterlitz and

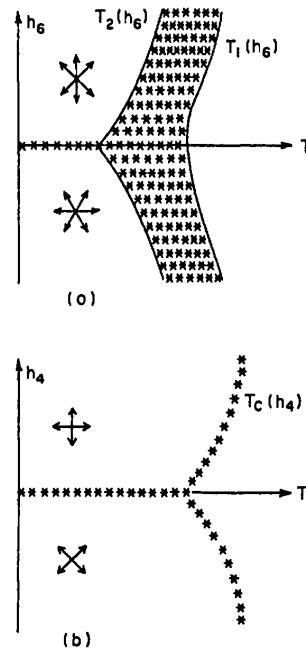


FIG. 1. Phase diagrams in the h_p - T plane for $p=6$ and $p=4$. The asterisks denote critical points with continuously variable critical exponents.

Thouless have shown how this analysis is modified by vortices in a recent review article.²³ Both sets of authors suggested that there would be two phase transitions for $p>4$. In Sec. V C, we present a nonlinear recursion analysis which refines and considerably sharpens this picture. The results lead directly to the phase diagrams shown in Fig. 1, and allow detailed predictions to be made about the associated critical behavior for small h_p . We have been unable to ascertain the small h_p structure of the phase diagrams for $p=2$ and $p=3$.²⁴

As pointed out by Kosterlitz and Thouless,²³ isotropic planar behavior should be very difficult to see experimentally in quasi-two-dimensional magnetic systems, because of an unusually strong crossover to three-dimensional behavior. Hopefully, experimental analogues of the models studied here can be found elsewhere in nature, perhaps in systems exhibiting nonmagnetic phase transitions.

C. Outline

In Sec. II we discuss various transformations on the action (1.1) which are useful both in the context of the Migdal approximation and in the analytic treatment. Section III describes the results which can be obtained from the Migdal recursion

relation, both with and without symmetry-breaking perturbations. In Sec. IV we demonstrate explicitly that the generalized Villain model collapses readily into the Coulomb gas system treated by Kosterlitz and determine the first correction to the Berezinskii results in a cumulant expansion. Finally, in Sec. V we rederive results obtained by Kosterlitz, and present a more detailed analysis of symmetry-breaking perturbations. We also summarize our conclusions and speculations about the isotropic planar model at this point. Appendix A shows how symmetry-breaking fields can be treated within the spin-wave approximation, and Appendix B discusses a generalization of the Migdal approach which allows for symmetry-breaking interactions. Appendix C explains certain features of the cumulant expansion of Sec. IV, whereas Appendix D proves a duality transformation result given in Sec. V.B.

II. TRANSFORMATIONS OF THE ACTION

A. Fourier analysis and the Villain model

The planar model has a coupling between nearest-neighbor "spins" of the form

$$V(\theta - \theta') = -K[1 - \cos(\theta - \theta')]. \quad (2.1)$$

Of course a periodic function like this can always be written in a Fourier series

$$e^{V(\theta)} = \sum_{s=-\infty}^{\infty} e^{is\theta + \tilde{V}(s)}, \quad (2.2)$$

where the Fourier coefficient is given by

$$e^{\tilde{V}(s)} = \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-is\theta + V(\theta)}. \quad (2.3)$$

The coupling (2.1) has $\tilde{V}(s)$ given in terms of a Bessel function of imaginary argument

$$e^{\tilde{V}(s)} = e^{-K} I_s(K). \quad (2.4)$$

In the limit of large and small couplings this reduces to

$$e^{\tilde{V}(s)} = \begin{cases} (1/s!)(\frac{1}{2}K)^s, & K \rightarrow 0, \\ e^{-s^2/2K}/(2\pi K)^{1/2}, & K \rightarrow \infty. \end{cases} \quad (2.5)$$

For small K the sum in Eq. (2.2) converges quite rapidly with only the $s=0$ and ± 1 terms contributing. However, for large K the summation converges very slowly. To get a more rapidly converging result, we use the Poisson summation formula, which in its simplest form states that the sum over s of any function $g(s)$ can be written

$$\sum_{s=-\infty}^{\infty} g(s) = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{+\infty} d\phi g(\phi) e^{-2\pi im\phi}. \quad (2.6)$$

Hence, Eq. (2.2) can be rewritten in terms of a

sum over m as

$$e^{V(\theta)} = \sum_m e^{V_0(\theta+2\pi m)}, \quad (2.7)$$

where V_0 is given as a Fourier integral

$$e^{V_0(\theta)} = \int d\phi e^{\tilde{V}(\phi)+i\phi\theta}. \quad (2.8)$$

At low temperatures the sum over m in Eq. (2.7) will converge quite rapidly. In fact, the integers m in this formula will describe the quantum numbers of vortices in the system, while the integration variable ϕ in Eq. (2.8) will represent the spin waves.

Notice that the summation over m in Eq. (2.7) automatically enforces the periodicity of $V(\theta)$. Hence, V_0 may itself be a nonperiodic function. The simplest choice of V_0 was made by Villain¹⁷ who took

$$V_0(\theta) = -\frac{1}{2}K_V\theta^2, \quad (2.9a)$$

which implies the simple Gaussian form for $\tilde{V}(\phi)$

$$\tilde{V}(\phi) = -\phi^2/2K_V. \quad (2.9b)$$

In Sec. III we arrive at the Villain coupling in a different way. The Migdal procedure starts from any interaction function between nearest-neighbor spins—say the interaction (2.1)—and replaces it with a new interaction function $V'(\theta - \theta')$ generated from an approximate decimation renormalization-group transformation. After a few iterations of this procedure, we find that any interaction function at reasonably low temperatures appears to generate a new interaction of the form

$$e^{V_V(\theta-\theta')} = \sum_{m=-\infty}^{\infty} e^{-K_V(\theta-\theta+2\pi m)^2/2}, \quad (2.10)$$

with $K_V \approx K$. This correspondence is important because (2.10) is the model proposed by Villain,¹⁷ which does have some properties which are much simpler than those of the original planar model. The Migdal-style analysis suggests that the two interaction models can indeed have very similar critical properties.

In particular, we suggest that the critical properties of the two models will be identical if we choose K_V to be some function of K :

$$K_V = f(K).$$

A comparison of the interaction form for weak and strong couplings show them to be identical if

$$f(K) = \begin{cases} K & \text{for } K \rightarrow \infty, \\ [2 \ln(2/K)]^{-1} & \text{for } K \rightarrow 0. \end{cases} \quad (2.11)$$

B. Duality transformations

We can make use of the tricks described in Sec. II A to perform a duality transformation on a pla-

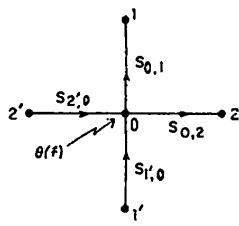


FIG. 2. Five vertices of a square lattice populated with "angle" variables $\theta(\vec{r})$. Four integer variables s populate the bonds connecting to the central vertex. The arrows suggest our convention for ordering adjacent θ variables in the Fourier transform of the nearest-neighbor potential.

nar model with arbitrary nearest-neighbor interaction. That is, we consider an action of the form

$$A[\theta] = \sum_{\langle \vec{r}, \vec{r}' \rangle} V(\theta(\vec{r}) - \theta(\vec{r}')) \quad (2.12)$$

entering a partition sum

$$Z = \int d[\theta] e^{A[\theta]} = \left(\prod_{\vec{r}} \int_0^{2\pi} \frac{d\theta(\vec{r})}{2\pi} \right) e^{A[\theta]}. \quad (2.13)$$

For definiteness, imagine that the sums run over the sites of a square lattice, although the transformations described below are easily generalized.

The first step is to write every term in $A[\theta]$ as an expansion of the form (2.1). In writing (2.1) for a particular lattice bond, we shall always choose θ to be either to the left of or below θ' . These substitutions yield a partition function which depends both on the angle $\theta(\vec{r})$ at a lattice site and on integers $S(\vec{r}, \vec{r}')$ which populate the lattice bonds:

$$Z = \int d[\theta] \prod_{\langle \vec{r}, \vec{r}' \rangle} \sum_{S(\vec{r}, \vec{r}')=-\infty}^{\infty} \exp[\tilde{V}(S(\vec{r}, \vec{r}')) + iS(\vec{r}, \vec{r}') \times [\theta(\vec{r}) - \theta(\vec{r}')]]. \quad (2.14)$$

The θ integrals can be performed immediately. A typical integral is represented by Fig. 2. The $e^{is\theta}$ terms just give Kronecker δ functions restricting the sums over s . For example, the case shown in Fig. 2 gives

$$\Delta(\vec{r}) = \delta_{S_{0,1}+S_{0,2}+S_{1',0}+S_{2',0}}. \quad (2.15)$$

Thus, Z reduces to a sum over bond variables $S(\vec{r}, \vec{r}')$ with a set of δ function symbols at every site:

$$Z = \sum_{\{S(\vec{r}, \vec{r}')\}} \left(\prod_{\vec{r}} \Delta(\vec{r}) \right) \exp \sum_{\langle \vec{r}, \vec{r}' \rangle} \tilde{V}(S(\vec{r}, \vec{r}')). \quad (2.16)$$

For a lattice of N sites, there are clearly $2N$ summation variables and N restrictions represented by the $\Delta(\vec{r})$'s. The restrictions can be thought of as requirements that the net $S(\vec{r}, \vec{r}')$ "flowing" into any site vanish. This "zero divergence" condition can, in fact, be met by choosing the $S(\vec{r}, \vec{r}')$ field to be the "curl" of a new field

$S(\vec{R})$. With this in mind, we choose a new set of integer variables $\tilde{S}(\vec{R})$ defined at the centers of the cells of the old lattice. A set of four cells is shown in Fig. 3.

Now make the ansatz that each $S(\vec{r}, \vec{r}')$ can be written in terms of differences of the $S(\vec{R})$:

$$\begin{aligned} S_{0,1} &= S_A - S_B, & S_{0,2} &= S_B - S_C, \\ S_{1',0} &= S_D - S_C, & S_{2',0} &= S_A - S_D. \end{aligned} \quad (2.17)$$

With this new set of variables, the $N\Delta(\vec{r})$ constraints are satisfied automatically, and the $2N$ sums become N unconstrained sums over the variables $S(\vec{R})$ populating the dual lattice. The function $\tilde{V}(S(\vec{r}, \vec{r}'))$ now becomes a nearest neighbor coupling $V(S(\vec{R}) - S(\vec{R}'))$ between these new variables. We are left with the problem of evaluating

$$Z[S] = \sum_{\{S(\vec{R})\}} \exp \left(\sum_{\langle \vec{R}, \vec{R}' \rangle} \tilde{V}(S(\vec{R}) - S(\vec{R}')) \right), \quad (2.18)$$

where each $S(\vec{R})$ is summed over the set of integers.¹⁸

Equation (2.18) is an exact rewriting of the partition function. Unfortunately, we do not have much experience in statistical mechanics in evaluating sums of this kind. Furthermore, we do not expect the sums in (2.18) to converge very rapidly at low temperatures. Both difficulties can be eliminated by performing the transformation (2.6) on each $S(\vec{R})$ sum to obtain

$$\begin{aligned} Z = \sum_{\{m(\vec{R})\}} & \left(\prod_{\vec{R}} \int_{-\infty}^{\infty} d\phi(\vec{R}) \right) \exp \left(\sum_{\langle \vec{R}, \vec{R}' \rangle} \tilde{V}(\phi(\vec{R}) - \phi(\vec{R}')) \right. \\ & \left. + \sum_{\vec{R}} 2\pi i m(\vec{R}) \phi(\vec{R}) \right). \end{aligned} \quad (2.19)$$

Equation (2.19) is our final result for the partition function. As we shall see, $\phi(\vec{R})$ describes the spin-wave degrees of freedom, while $m(\vec{R})$ is a quantum number for a vortex excitation. In the limit of low temperatures, the sums over $m(\vec{R})$ should converge quite rapidly.

C. Dual transformations on correlation functions

Similar tricks can be used to transform correlation functions, e.g.,

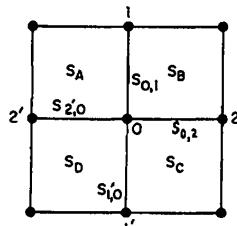


FIG. 3. Representation of the bond integers variable by integer variables on the dual lattice whose "curl" automatically satisfies the divergence condition.

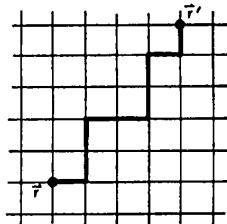


FIG. 4. Bonds entering the representation of the correlation function $g_p(\vec{r} - \vec{r}')$.

$$g_p(\vec{r} - \vec{r}') \equiv \langle e^{ip[\theta(\vec{r}) - \theta(\vec{r}')]}\rangle, \quad (2.20)$$

where p is an integer. The expectation is to be taken in the ensemble specified by the action (2.12). With $p=1$, the real part of (2.20) is just the average of the vector product of two spins located at sites \vec{r} and \vec{r}' . The other values of p are related to various symmetry-breaking perturbations, as we shall see.

First, imagine we wish to determine $Z g_p(\vec{r} - \vec{r}')$, where \vec{r} and \vec{r}' are nearest-neighbor sites. Dual transformations on this object carry through exactly as before, except that the bond connecting r and r' has a new statistical weight, namely

$$\begin{aligned} e^{V'[\theta(\vec{r}) - \theta(\vec{r}')]}) &= e^{V[\theta(\vec{r}) - \theta(\vec{r}')]}) e^{ip[\theta(\vec{r}) - \theta(\vec{r}')]}) \\ &= \sum_s \exp\{is[\theta(\vec{r}) - \theta(\vec{r}')] + \tilde{V}(s-p)\}. \end{aligned} \quad (2.21)$$

Thus, the effect of the factor $e^{ip[\theta(\vec{r}) - \theta(\vec{r}')]})$ is to shift the argument in one of the \tilde{V} by an amount p . The conclusion is that in the nearest-neighbor case

$$g_p(\vec{r} - \vec{r}') = Z'/Z, \quad (2.22)$$

where Z is given by (2.18), and Z' has a similar form,

$$Z' = \sum_{\{S(\vec{R})\}} \exp\left(\sum_{(\vec{R}, \vec{R}')} \tilde{V}(S(\vec{R}) - S(\vec{R}') - \eta_{\vec{R}\vec{R}'} p)\right). \quad (2.23)$$

Here $\eta_{\vec{R}\vec{R}'}$ is a "projection operator" which is unity on the dual image of the special nearest-neighbor bond and zero everywhere else.

Now consider correlations over longer distances. An expression such as (2.20) can be written as the average of a product of nearest-neighbor terms $e^{ip[\theta(\vec{r}_j) - \theta(\vec{r}_{j+1})]})$. For example, the correlation shown in Fig. 4 can be represented as a product

$$Z' \equiv \langle e^{ip[\theta(\vec{r}_0) - \theta(\vec{r}_N)]}\rangle = Z \left\langle \prod_{j=0}^N e^{ip[\theta(\vec{r}_j) - \theta(\vec{r}_{j+1})]}\right\rangle. \quad (2.24)$$

Consequently, a path can be chosen running from \vec{r}_0 to \vec{r}_N as shown in Fig. 4, and the Z' of Eq. (2.24) can be calculated as in the nearest-neighbor case. The result is that Z' has the form (2.23) but with the projection operator $\eta_{\vec{R}, \vec{R}'}$, given by

$$\eta_{\vec{R}, \vec{R}'} = \begin{cases} 0 & \text{if the path does not cut the bond } \vec{R}\vec{R}', \\ +1 & \text{if } \vec{R} \text{ lies just to the left of the path and } \vec{R}' \text{ just to the right,} \\ -1 & \text{if } \vec{R}' \text{ lies just to the left of the path and } \vec{R} \text{ just to the right.} \end{cases} \quad (2.25)$$

Or employing the Poisson sum formula once again, we obtain our final result

$$g_p(\vec{r} - \vec{r}') = Z^{-1} \left(\prod_{\vec{R}} \int_{-\pi}^{\pi} d\phi(\vec{R}) \right) \sum_{\{m(\vec{R})\}} \exp\left(\sum_{(\vec{R}, \vec{R}')} \tilde{V}(\phi(\vec{R}) - \phi(\vec{R}') - \eta_{\vec{R}\vec{R}'} p) + 2\pi i \sum_{\vec{R}} m(\vec{R}) \phi(\vec{R})\right). \quad (2.26)$$

III. MIGDAL APPROXIMATION

A. Isotropic planar model recursion relation

The Migdal recursion scheme¹⁵ has recently been reviewed and rederived by a potential-moving technique.²⁵ It is this potential-moving point of view we will take here.

We first review the decimation recursion relations for the isotropic planar model (1.1) (with all h_p 's set to zero) in one dimension; that is, we explicitly integrate out the angle variables at every other site in a linear chain. It is easily shown^{15,25} that the Fourier components of an arbitrary nearest-neighbor potential obey an exact recursion formula

$$\tilde{V}'(s) = 2\tilde{V}(s), \quad (3.1)$$

where $\tilde{V}'(s)$ represents the new Fourier component obtained after decimation. If $b-1$ out of b sites are summed over the resulting interaction is

$$\tilde{V}'(s) = b\tilde{V}(s). \quad (3.2)$$

The Migdal approach can be viewed as a procedure for bootstrapping equations like (3.2) into higher dimensions.²⁵ The basic ideas are summarized in Fig. 5. First one moves the vertical bonds in every row of a square lattice, as shown in Fig. 5(b). The spins indicated by an x in Fig. 5(b) are then removed by a one-dimensional decimation to give Fig. 5(c). Finally, the lattice is rotated by 90° and the entire operation is repeated. We refer the reader to the literature for a detailed discussion of the validity of this procedure.

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RENORMALIZATION, VORTICES, AND SYMMETRY-BREAKING...

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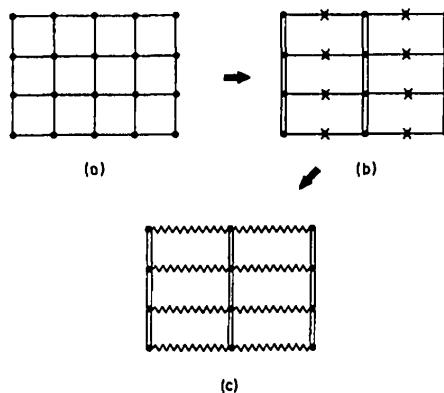


FIG. 5. One half of the Migdal transformation on a two-dimensional lattice. New vertical bonds are obtained by moving every other vertical bond on top of a remaining bond. New horizontal bonds are then obtained by decimating out the isolated vertices.

For any $b > 1$, this interpretation of the Migdal scheme introduces anisotropic horizontal and vertical couplings, even if these are initially identical.²⁵ Thus, it is necessary to consider recursion relations for both x - and y -direction nearest-neighbor Fourier components $\tilde{V}_x(s)$ and $\tilde{V}_y(s)$. These recursion relations are

$$e^{\tilde{V}_x(s)} = \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-is\theta} \left(\sum_{s_1} e^{is_1\theta} e^{b\tilde{V}_x(s_1)} \right)^b, \quad (3.3a)$$

$$e^{\tilde{V}_y(s)} = \left[\frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-is\theta} \left(\sum_{s_1} e^{is_1\theta} e^{\tilde{V}_y(s_1)} \right)^b \right]^b. \quad (3.3b)$$

The new interactions in real space can be recovered by summing a Fourier series

$$e^{V_x(\theta)} = \sum_s e^{is\theta} e^{\tilde{V}_x(s)}, \quad (3.4a)$$

$$e^{V_y(\theta)} = \sum_s e^{is\theta} e^{\tilde{V}_y(s)}. \quad (3.4b)$$

Note the symmetry between the recursion formulas for the x and y bonds: To obtain the x recursion (with, say, $b = 2$) we first double the interaction in Fourier space, and then double the interaction in real space. To obtain the y recursion, we perform these same operations in the reverse order.

The Migdal recursion relation becomes isotropic as $b \rightarrow 1$, so it is of interest to consider (3.3) in this limit. On expanding in $b - 1 \approx \ln b$, we obtain recursion relations for a single isotropic set of Fourier coefficients

$$\begin{aligned} \frac{d e^{V(s)}}{d l} = V(s) + \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-is\theta} & \left(\sum_{s_1} e^{is_1\theta} e^{V(s_1)} \right) \\ & \times \ln \left(\sum_{s_2} e^{is_2\theta} e^{V(s_2)} \right), \end{aligned} \quad (3.5)$$

where

$$l = \ln b \quad (3.6)$$

is the logarithm of the change in length scale. Although it is isotropic, this set of equations is rather difficult to work with. Equations (3.3) (with integer b) are easier to treat with high precision on a computer. The bulk of our numerical calculations were done on Eq. (3.3b), with $b = 2$, which can be rewritten as a single summation

$$e^{\tilde{V}_y(s)} = \left(\sum_{s_1} e^{\tilde{V}_y(s_1)} e^{\tilde{V}_y(s-s_1)} \right)^2. \quad (3.7)$$

B. Numerical analysis and fixed points

Given functional recursion relations such as (3.3) or (3.7), we want to follow the progress under repeated iterations of various initial interaction functions. Of course, fixed points are of particular interest. An infinite temperature fixed point would correspond to an interaction independent of θ , $V(\theta) = \text{const}$. A zero-temperature fixed-point function would be infinite everywhere except at $\theta = 0$ or 2π , on a scale chosen such that $V(\theta = 0) = 0$.

Figure 6 illustrates what happens to an initial interaction

$$V_y(\theta) = K(1 - \cos\theta). \quad (3.8)$$

After three or four iterations of the transformation (3.7), a limiting function is apparently reached which depends on the initial coupling K in (3.8). Limiting fixed-point functions are shown for $K^{-1} = 0.5$ and 0.8 . These functions are periodic in θ , although certainly not cosines, and are approached for all $K \geq 1$. For $K \leq 1$, any initial function tends toward a high-temperature fixed point. Very similar behavior was found for (3.3a) with $b = 2$. These qualitative properties of the transformation (3.3) were first discovered by Migdal.¹⁵

If the planar model had a conventional critical point in two dimensions, we would expect a single isolated unstable fixed point, in addition to the zero- and infinite-temperature fixed points. However, the behavior described in the preceding paragraph suggests that the planar model has a line of fixed points at low temperatures. This indicates the existence of a line of critical points, with continuously variable critical exponents. Clearly, it is important to investigate this point further.

To help visualize what is at issue, we have sum-

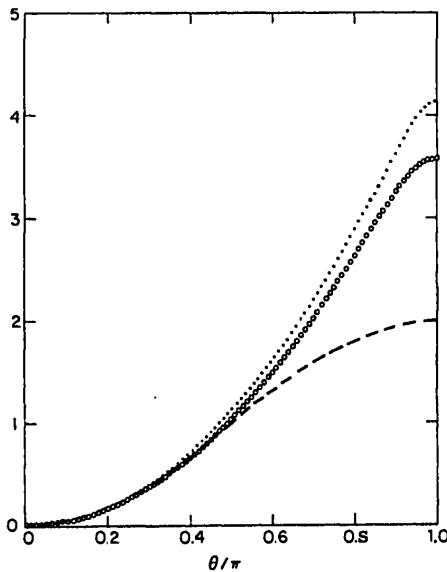


FIG. 6. Invariant interaction functions $V_x(\theta)$ approached by the Migdal transformation for initial interaction strengths $K^{-1} = 0.5$ (dots) and $K^{-1} = 0.8$ (circles). The initial interaction functions are proportional to $1 - \cos\theta$ (dashed line).

marized the properties of the interaction functions at each iteration by just two parameters, an effective "temperature" T_{eff} and a barrier height B given by

$$T_{eff}^{-1} = \frac{-d^2V(\theta)}{d\theta^2} \Big|_{\theta=0} = \sum_s s^2 e^{V(s)} / \sum_s e^{V(s)} \quad (3.9)$$

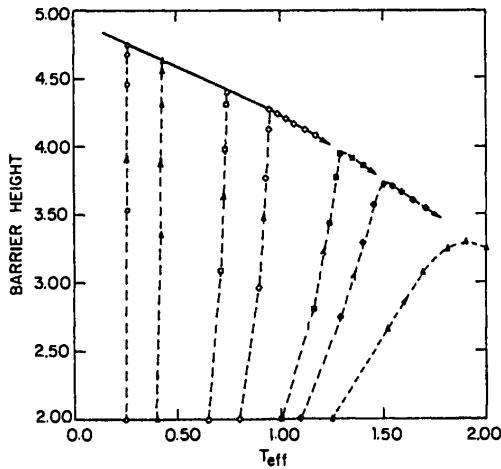


FIG. 7. The Migdal transformation parametrized by an effective temperature and barrier height. The circles, triangles, etc., indicate iterations of the $b = 2$ transformation from the line of barrier height = 2.0.

$$B = T_{eff}[V(\theta=0) - V(\theta=\pi)]. \quad (3.10)$$

For the interaction (3.8), $T_{eff} = K^{-1} = k_B T/J$, and $B = 2.0$ initially. The renormalization flows in (T_{eff}, B) space are shown in Fig. 7. Initial interactions with $B = 2.0$ and $T_{eff} \leq 0.8$ iterate rapidly to an apparent fixed line. For $T_{eff} \geq 0.8$, the iterations eventually bend toward high temperatures and low barriers along a universal trajectory.

Let us try to guess the approximate fixed-point function which is approached for $T_{eff} \leq 0.8$. It turns out that the Villain model is an extremely good guess. On substituting the ansatz

$$e^{\tilde{V}(s)} = e^{-s^2/2K_V} \quad (3.11)$$

into Eqs. (3.3a) or (3.3b) and approximating the sums by integrals, we obtain

$$e^{\tilde{V}(s)} = \text{const} \times e^{-s^2/2K_V}. \quad (3.12)$$

Absorbing the constant into a redefinition of the free energy, we see that the s dependence of the new interaction is identical to the old. In Fig. 8, we compare various apparent fixed-point functions found by iterating (3.7) with the Villain model for an appropriately chosen K_V . The Villain model is a rather accurate representation for all $T_{eff} \leq 0.8$, corresponding to the apparent fixed line in Fig. 6.

Unfortunately, the Villain model does not actually

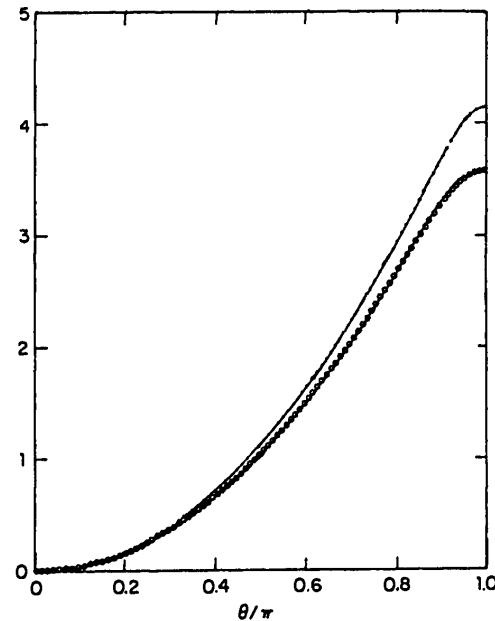


FIG. 8. Comparison of apparent fixed-point functions found with the Migdal transformation, and an appropriately chosen Villain model for $K^{-1} = 0.5$ (dots) and $K^{-1} = 0.8$ (circles).

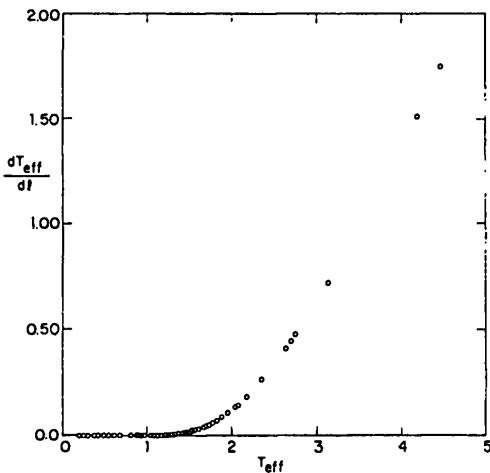


FIG. 9. Change in effective temperature with iteration dT_{eff}/dl for the Migdal transformation. This quantity is almost identically zero until $T_{\text{eff}} \approx 1.0$.

represent a family of exact fixed-point functions of the Migdal transformation. We can see this, for example, by calculating the error introduced at low temperatures in Eq. (3.7) by approximating the sum by an integral

$$\begin{aligned} e^{\bar{V}_z'(s)} &= \sum_{s_1=-\infty}^{\infty} e^{-s_1^2/K_V} e^{-(s-s_1)^2/K_V} \\ &= \sum_{m=-\infty}^{\infty} \int_{-\infty}^{+\infty} d\phi e^{-\phi^2/K_V} e^{-(s-m)^2/K_V} e^{2\pi i m \phi} \\ &= (\frac{1}{2}\pi K_V)^{1/2} e^{-s^2/2K_V} [1 + 2 \cos(\pi s) e^{-r^2 K_V/2}]. \end{aligned} \quad (3.13)$$

The Villain model fails exponentially to be a fixed point.

To see if there really is a one-parameter family of fixed-point functions (which is presumably "close" to a family of Villain models), we investigate very precisely changes in the effective temperature with iteration. Consider the quantity

$$\frac{dT_{\text{eff}}}{dl} = \frac{T'_{\text{eff}} - T_{\text{eff}}}{\ln 2} \quad (3.14)$$

for the transformation (3.7); this should be identically zero along a fixed line. In Fig. 9 we have plotted dT_{eff}/dl along the apparent fixed line versus T_{eff} . The change in T_{eff} appears to be identically zero until $T_{\text{eff}} \approx 1.0$, which would be consistent with a fixed line. However, appearances can be deceiving. In Fig. 10, $\log_{10}(dT_{\text{eff}}/dl)$ is plotted against $1/T_{\text{eff}}$. The "differential" change dT_{eff}/dl decreases exponentially in $1/T_{\text{eff}}$ over at least 20 decades! To a good approximation,

$$\frac{dT_{\text{eff}}}{dl} = 79.4 e^{-13.2/T_{\text{eff}}} \quad (3.15)$$

at low temperatures, suggesting that dT_{eff}/dl is positive for all nonzero temperatures and that there is no phase transition.

This conclusion, that there is almost, but not quite a fixed line within the Migdal approximation, was reached previously by Wilson,¹⁹ who showed analytically that

$$\frac{dT_{\text{eff}}}{dl} \sim \exp(-4\pi^2/3 T_{\text{eff}}), \quad (3.16)$$

at low temperatures. The number $\frac{4}{3}\pi^2$ is very close to 13.2.

It is interesting to contrast the Migdal approximation to the planar model, summarized in Fig. 10 with the corresponding quantity for the two-dimensional Ising model, shown in Fig. 11. Within the Migdal scheme, it is known analytically that^{15,25}

$$\frac{dT_{\text{eff}}}{dl} = -T_{\text{eff}} - \frac{T_{\text{eff}}^2 \tanh(1/T_{\text{eff}}) \ln[\tanh(1/T_{\text{eff}})]}{1 - \tanh^2(1/T_{\text{eff}})}, \quad (3.17)$$

where $T_{\text{eff}} = k_B T/J$ in this case. The Migdal transformation does predict rather bizarre behavior for the planar model at $T=0$. Given the form (3.15) it is possible to show that the susceptibility diverges as the exponential of an exponential as $T \rightarrow 0$,

$$\chi \sim \exp(AT^2 e^{B/T}), \quad (3.18)$$

where A and B are constants. Similar behavior has

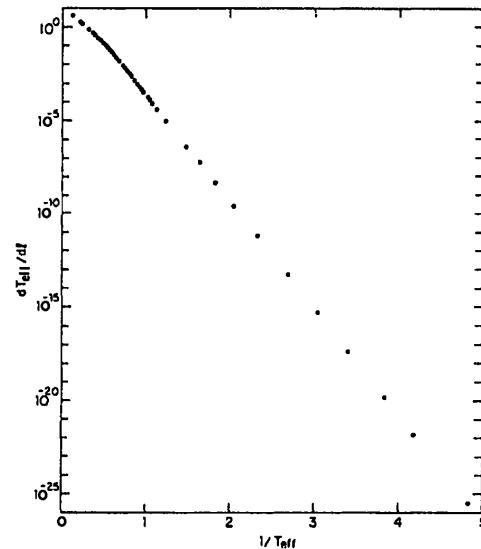


FIG. 10. Plot of dT_{eff}/dl vs $1/T_{\text{eff}}$. The graph is linear over about 20 decades in dT_{eff}/dl .

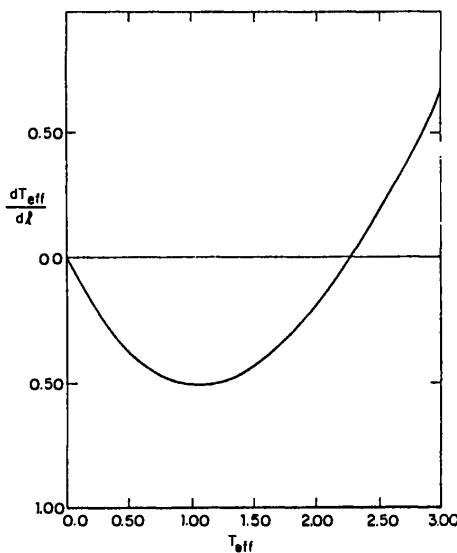


FIG. 11. Differential recursion relation dT_{eff}/dl obtained from Migdal's recursion formula for the two-dimensional Ising model.

been found in the correlation length of a "truncated tetrahedron" Ising model.²⁶

We do not yet know if we should believe the detailed predictions of the Migdal theory. Although the rapid approach of an initial interaction to something resembling a Villain model is probably qualitatively correct, we shall suggest in Sec. IV that the approximation does not treat vortices properly along the apparent fixed line. In any event, it is clear from Fig. 9 that the Migdal approach simulates a fixed line remarkably well, as first observed by Migdal himself.¹⁴

C. Symmetry-breaking interactions

We now investigate the symmetry-breaking perturbations displayed in Eq. (1.1). In Appendix A we deduce the renormalization-group eigenvalues of these fields along the fixed line in the spin-wave approximation. A small field h_p should obey the recursion law

$$h'_p \approx b^{\lambda_p(T)} h_p, \quad (3.19)$$

with

$$\lambda_p(T) = 2 - (k_B T / 4\pi J) p^2. \quad (3.20)$$

Apparently, the h_p variables should be strongly relevant at low temperatures ($\lambda_p > 0$). An initially small crystalline field will grow rapidly, leading to behavior quite different from that found for $h_p = 0$. However, (3.20) also suggests that some of

these fields may become *irrelevant* ($\lambda_p < 0$) at sufficiently high temperatures. The h_p 's would then become smaller with iteration, and would not affect the isotropic planar model behavior. The borderline between relevancy and irrelevancy of a particular field h_p occurs at a temperature

$$k_B T_m = 8\pi J/p^2. \quad (3.21)$$

At $T = T_m$, the eigenvalue is *marginal* ($\lambda_p = 0$).

We first want to calculate the $\lambda_p(T)$ in the framework of the Migdal theory. The spin-wave approximation is certainly suspect at higher temperatures, although it does suggest that $\lambda_0(T)$ is more likely to become irrelevant than $\lambda_2(T)$. The second aim of this section will be to investigate the critical behavior which occurs if the $\lambda_p(T)$ are relevant. We have done this numerically, and have relegated the necessary generalization of the Migdal scheme to Appendix B.

The characteristic behavior of $\lambda_p(T)$ in the Migdal approximation can be seen by carrying out a one-dimensional decimation with $h_p \neq 0$ for some p , approximating $V(\theta)$ by a Gaussian $-\theta^2/2T_{\text{eff}}$ and expanding to first order in h_p . The result

$$h' = h(1 + e^{-b^2 T_{\text{eff}}/4}) \quad \text{for } b = 2 \quad (3.22)$$

gives $\lambda_p > 0$ for all p and T_{eff} . Combining (3.22) with a bond-shifting transformation, as described in Appendix B, we obtain the eigenvalues $\lambda_p(T)$ for $p = 1-4$ and 6 shown in Fig. 12.

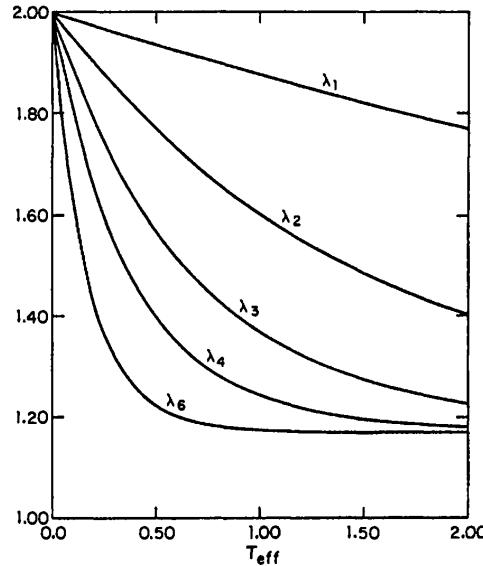


FIG. 12. Eigenvalues $\lambda_p(T)$ of various symmetry-breaking perturbation along the apparent fixed line in the Migdal recursion relation.

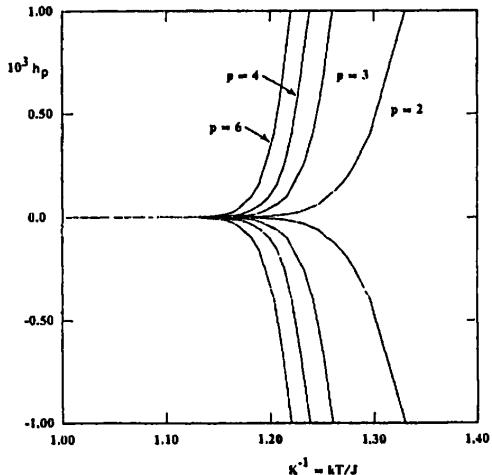


FIG. 13. Phase diagrams in the $h_p - K^{-1}$ plane for $p = 2, 3, 4$, and 6 as given by Migdal transformation. The lines are lines of second-order phase transitions with exponents characteristic of a p -state planar model.

At low temperatures $\lambda_p(T)$ decreases from 2.0 in proportion to $p^2 T$ for all p , and all eigenvalues saturate at the same value at high temperatures. This high-temperature limit depends upon the scale factor b and the free parameter α whose choice is discussed in Appendix B. For all physically sensible values of b and α , the Migdal scheme gives $\lambda_p(T) \geq 0$ as $T \rightarrow \infty$. We shall see in Sec. IV that $\lambda_p(T)$ actually does go negative at rather low temperature for $p > 4$, although the Migdal approximation may be qualitatively correct for $p = 1-3$.

We have also tracked the effective interactions which result as the h_p 's iterate toward larger values (in Secs. IV and V, we will only be able to treat the small- h_p limit). It appears that the on-site potentials h_p become unboundedly large with many iterations of the Migdal recursion relation. Consequently, the Hamiltonian (1.1) (with a single nonzero h_p) rapidly becomes equivalent to a planar model with p discrete allowed states.

As discussed in Sec. III D, we expect these p -state models to have at least one phase transition as the temperature is varied²⁷ for $p \geq 2$ ($p = 2$ is an Ising model). Thus an $h_p - K^{-1}$ plane of initial Hamiltonians divides into two regions, one which maps under the Migdal transformation into a p -state model above its critical point, and one which goes into a p -state model below T_c . The phase boundaries obtained in this way for $p = 2-4$ and 6 are shown in Fig. 13. Each curve is a line of second-(or possibly first) order phase transitions with exponents appropriate to the corresponding p -state planar model. For small h_p and $K^{-1} = k_B T$ these

lines are given by

$$h_p \sim e^{-AT^2 e^{B/T}}, \quad (3.22)$$

where A and B are constants. This prediction is consistent with the zero critical temperature found earlier for the isotropic planar model in this approximation.

We emphasize that there are strong reasons to suspect the phase boundaries shown in Fig. 13 for $p \geq 4$ (see the Introduction and Sec. V). The plots for $p = 2$ and $p = 3$ may be qualitatively correct, however.

D. Discrete planar models

Motivated by the numerical results of Sec. III C, we consider the limiting case of the discrete models which are approached by (1.1) after many iterations. For simplicity imagine taking one of the h_p 's infinite and setting the rest to zero in (1.1). This class of models should describe the properties of the critical lines shown in Fig. 13. The spins at each site can now assume only p -discrete angles $\theta_n = 2\pi n/p$, $n = 1, \dots, p$. The interaction energy between two nearest-neighbor angles $\theta(\vec{r})$ and $\theta(\vec{r}')$ in states n and n' is then

$$V(\theta_n(\vec{r}) - \theta_{n'}(\vec{r}')) = K[1 - \cos[\theta_n(\vec{r}) - \theta_{n'}(\vec{r}')]]. \quad (3.23)$$

Although the h_p do appear to iterate to infinity when they perturb an isotropic planar model, the isotropic part of the interaction $V(\theta)$ is also changing with iteration. Consequently, (3.23) should be replaced by

$$V_n(\theta_n(\vec{r}) - \theta_{n'}(\vec{r}')), \quad (3.24)$$

this being the limiting function $V(\theta)$ approached as h_p iterates to infinity. The precise limiting function is rather difficult to ascertain numerically, and will in fact depend on the initial temperature variable K . Thus we feel it is reasonable to apply the Migdal transformation to $V(\theta)$ in the form

$$e^{V^*(\theta_n)} = \sum_{n'=1}^p \exp[2V(\theta_n) + 2V(\theta_n - \theta_{n'})] \quad (3.25)$$

in the expectation that the result $V^*(\theta_n)$ of many iterations of (3.25) will not differ essentially from $V_n(\theta_n)$. The coupling K appearing in (3.23) must now be interpreted as an effective coupling approached as h_p goes to infinity, and should not be identified with the "bare" or initial temperature variable.

With these caveats and simplifications, it is straightforward to analyze the p -state planar models within the Migdal approximation. The manipulations are very similar to those required for the s -state Potts models described in Ref. 25. We have plotted dT_{eff}/dt for these models in Fig. 14.

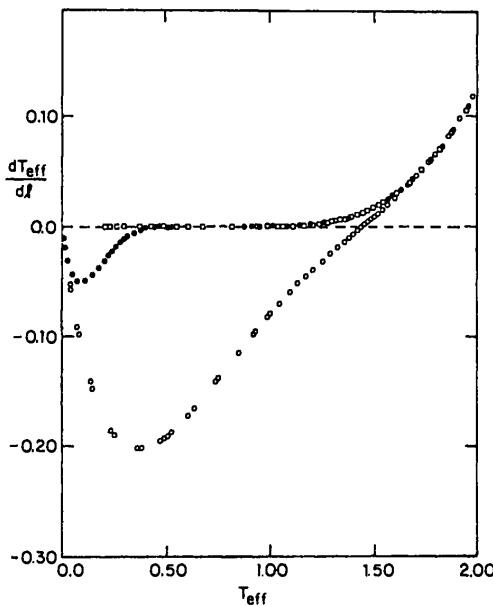


FIG. 14. Differential recursion relations for discrete planar models with $p = 6$ (circles) and $p = 12$ (dots) states.

T_{eff} for the discrete models is defined by $V(0) - V(2\pi/p) = 2\pi^2 J/p^2 T_{\text{eff}}$, which becomes equivalent to the previous definition (3.9) in the limit $p \rightarrow \infty$. All models with $p \geq 2$ appear to have a conventional second-order phase transition at a finite T_c . For $p \geq 8$, dT_{eff}/dl was found to agree closely with the result for the continuous model (Fig. 8) at all temperatures above T_c . Effects of the discreteness of the models were only apparent below T_c . This result is suspect at large p , because it is known that the Migdal transformation fails to predict the first-order character of the transition of s -state Potts models with large s . The critical exponent $\nu(p)$ for these models (which is just the reciprocal of the slope of dT_{eff}/dl through its nontrivial zero) are shown in Fig. 15. As $p \rightarrow \infty$, ν diverges, which is not surprising since we should recover an isotropic planar model in this limit.²⁸ From Fig. 15 we find that $\nu \propto e^{1.5p}$ for $p \geq 10$.

$$Z = \sum_{\{\phi(\vec{R})\}} \left(\prod_{\vec{R}} \int_{-\infty}^{\infty} \frac{d\phi(\vec{R})}{2\pi K} \right) \exp \left(-\frac{1}{2K} \sum_{\langle \vec{R}, \vec{R}' \rangle} [\phi(\vec{R}) - \phi(\vec{R}')]^2 + \sum_{\vec{R}} 2\pi i m(\vec{R}) \phi(\vec{R}) \right). \quad (4.2)$$

This exact representation of the partition sum is the result of a dual transformation on the zero-field (all $h_\mu = 0$) Villain model. Notice that the quadratic coupling term in (4.2) is multiplied by K^{-1} , in contrast to the original problem in which

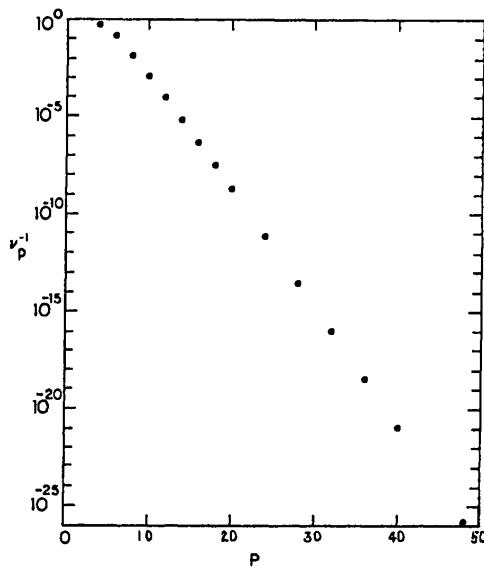


FIG. 15. The critical exponent ν_p^{-1} for a p -state discrete model obtained from the Migdal approximation.

IV. LATTICE COULOMB GAS AND LOW-TEMPERATURE ANALYSIS

A. Generalized Villain model

We now turn to a more direct and systematic analysis of the low-temperature properties of the planar model. For simplicity we will deal with the Villain model, taking the Fourier-transformed interaction to be

$$\tilde{V}(s) = -s^2/2K_V - \frac{1}{s} \ln(2\pi K_V). \quad (4.1)$$

The normalizing constant part of (4.1) is chosen for convenience; we will henceforth drop the subscript on K_V . Recall that the interaction appearing in (1.1) became very similar to the Villain model after a few iterations of the Migdal transformation.

With the choice (4.1), the expression (2.19) for the planar model partition function becomes²⁹

the coupling was proportional to K at low temperatures. This mapping of a strong-coupling problem into a weak-coupling one (and vice versa) is typical of a dual transformation.

For large K , each $\phi(\vec{R})$ in (4.2) undergoes small

fluctuations, and the terms with various $m(\vec{R})$'s different from zero are suppressed. If all the $m(\vec{R})$'s were zero, the mathematics of evaluating (4.2) would be identical to that described in the simple spin-wave analysis of Appendix A. In a limit where finite m excitations can be ignored, we would expect the line of low-temperature fixed

$$Z(y_0) = \sum_{m(\vec{R})} \left(\prod_{\vec{R}} \int_{-\infty}^{\infty} \frac{d\phi(\vec{R})}{2\pi} \right) \exp \left(-\frac{1}{2} K \sum_{(\vec{R}, \vec{R}')} [\phi(\vec{R}) - \phi(\vec{R}')]^2 + \sum_{\vec{R}} [ln y_0 m^2(\vec{R}) + 2\pi i K m(\vec{R}) \phi(\vec{R})] \right). \quad (4.3)$$

We have now converted the part of Z quadratic in $\phi(\vec{R})$ to exactly the spin-wave form of Appendix A by rescaling every $\phi(\vec{R})$ by K . The parameter y_0 controls fluctuations in $m(\vec{R})$. Although our original problem requires $y_0=1$, fluctuations become quite unlikely in the limit $y_0 \rightarrow 0$. We call the model represented by Eq. (4.3) the *generalized Villain model*.

It is easy to analyze Eq. (4.3) in the limit of small y_0 . In this limit, terms with $m_{\vec{R}}=0$ dominate, and the terms with $m_{\vec{R}}=\pm 1$ can be regarded as a small correction. Thus

$$\begin{aligned} \sum_{m(\vec{R})=0} \exp [ln y_0 m^2(\vec{R}) + 2\pi i K m(\vec{R}) \phi(\vec{R})] \\ \approx 1 + 2y_0 \cos[2\pi K \phi(\vec{R})] \\ \approx e^{2y_0 \cos[2\pi K \phi(\vec{R})]}, \end{aligned} \quad (4.4)$$

and (4.3) becomes in the small y_0 limit

$$\begin{aligned} Z(y_0) = \int d[\phi] \exp \left(-\frac{1}{2} K \sum_{(\vec{R}, \vec{R}')} [\phi(\vec{R}) - \phi(\vec{R}')]^2 \right) \\ \times \exp \left(2y_0 \sum_{\vec{R}} \cos 2\pi K \phi(\vec{R}) \right). \end{aligned} \quad (4.5)$$

But this is exactly the spin-wave problem we set for ourselves in Appendix A, in the presence of a "symmetry-breaking field" of the form $\cos(p_{\text{eff}} \theta)$, with

$$p_{\text{eff}} = 2\pi K. \quad (4.6)$$

As discussed in Sec. III and in the Appendix, the eigenvalue of such a perturbation is

$$\lambda_{p_{\text{eff}}} (T) = 2 - p_{\text{eff}}^2 / 4\pi K = 2 - \pi K. \quad (4.7)$$

We are lead to the conclusion that finite $m(\vec{R})$ or "vortex" excitations will alter the spin wave results at small y_0 only for

$$K^{-1} = K_B T/J > \frac{1}{2} \pi. \quad (4.8)$$

Above this temperature, the y_0 perturbation will break the symmetry. [The neglected terms in the sum (4.4) also produce symmetry-breaking couplings, but these break the symmetry only at tem-

peratures higher than (4.8).] But it is typical of dual models to be in a broken symmetry state when the original problem is in its disordered phase, and vice versa. This information is summarized in the "phase diagram" shown in Fig. 16(a). If we can use some renormalization technique to move from $y_0=0$ to $y_0=1$, we shall know the properties of the Villain model.

To control the size of fluctuations in $m(\vec{R})$, we introduce a new parameter y_0 in Eq. (4.2), writing

peratures higher than (4.8).] But it is typical of dual models to be in a broken symmetry state when the original problem is in its disordered phase, and vice versa. This information is summarized in the "phase diagram" shown in Fig. 16(a). If we can use some renormalization technique to move from $y_0=0$ to $y_0=1$, we shall know the properties of the Villain model.

B. Reduction to a Coulomb gas

Villain¹⁷ has shown that the model he proposed decomposes exactly into the decoupled spin-wave-vortex system treated by Kosterlitz.¹² We want to show that this representation also follows from the dual transformed Villain model (4.3), as a first step toward a systematic treatment of its low-temperature properties.

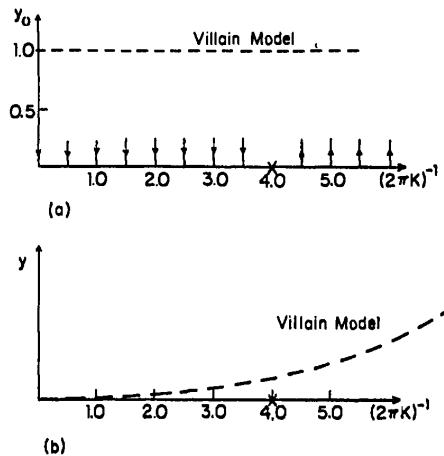


FIG. 16. (a) The Villain model (dashed line) in the space of couplings $2\pi K$ and y_0 . As suggested by the arrows, the variable y_0 appears to be an irrelevant perturbation to the fixed line at $y_0=0$ for $2\pi K < 4$, but is relevant for $2\pi K > 4$. (b) The Villain model (dashed line) in the space of couplings $2\pi K$ and y . In this representation, the Villain model comes exponentially close to the spin-wave-theory fixed line at low temperatures.

The spin-wave variables $\phi(\vec{R})$ may be eliminated entirely from (4.3) by the usual techniques of Gaussian integration. The result is

$$Z(y_0) = Z_{sw} Z_c(y_0), \quad (4.9)$$

where Z_{sw} is the spin-wave partition function calculated in Appendix A, and

$$Z_c(y_0) = \sum'_{\{m(\vec{R})\}} e^{A_c[m(\vec{R})]}, \quad (4.10)$$

with

$$\begin{aligned} A_c[m(\vec{R})] &= \sum_{\vec{R}} m_{\vec{R}}^2 \ln y_0 \\ &+ \sum_{\text{pairs}} 2\pi K m(\vec{R}) G'(\vec{R} - \vec{R}') m(\vec{R}'). \end{aligned} \quad (4.11)$$

The symbol \sum' in (4.10) is a sum over sets of $m(\vec{R})$ such that

$$\sum_{\vec{R}} m(\vec{R}) = 0, \quad (4.12)$$

while $G'(\vec{R} - \vec{R}')$ is a spin-wave lattice Green's function with a subtraction, defined in Appendix A. The sum over pairs in Eq. (4.11) counts each pair with $\vec{R} \neq \vec{R}'$ exactly once.

Following Kosterlitz and Thouless,¹⁰ we observe that $G'(\vec{R})$ is given to quite a good approximation by³⁰

$$G'(\vec{R}) \approx \ln(R/a_0) + \frac{1}{2} \ln(8e^{2y}) \quad (4.13a)$$

for all R , where y is Euler's constant and a_0 is the lattice space of a square lattice. Alternatively, we could approximate $G'(\vec{R})$ by

$$G'(\vec{R}) \approx \ln(R/a_0) + \frac{1}{2}\pi, \quad (4.13b)$$

which is exact at $R = a_0$ and off by a small additive constant as $R \rightarrow \infty$. On inserting either (4.13a) or (4.13b) into (4.11), the partition function (4.10) becomes equivalent to the partition function for a two-dimensional Coulomb gas, with action

$$\begin{aligned} A'_c[m(\vec{R})] &= \sum_{\vec{R}} m_{\vec{R}}^2 \ln y \\ &+ \sum_{\text{pairs}} (2\pi K)^{1/2} m(\vec{R}) \ln(|\vec{R} - \vec{R}'|/a_0) \\ &\times (2\pi K)^{1/2} m(\vec{R}'). \end{aligned} \quad (4.14)$$

The charges are $(2\pi K)^{1/2} \times (0, \pm 1, \pm 2, \dots)$ and the chemical potential for the production of a charge at a site is

$$y = y_0 e^{-r \ln(8e^{2y}) K/2} \quad (4.15a)$$

or

$$y = y_0 e^{-r^2 K/2}, \quad (4.15b)$$

depending on whether approximation (4.13a) or (4.13b) is used.

Clearly, the parameter y plays the role that y_0 played in our discussion of corrections to spin-wave theory in Sec. IV A. As y tends to zero, the Coulomb partition function Z_c goes to unity and we recover the spin wave results. Figure 16(a) can be redrawn in terms of y as Fig. 16(b), where the Villain model [as defined by (4.14)] becomes exponentially close to a simple spin wave theory at low temperatures.

For future reference, it is useful to display the vortex-vortex correlation which follows from (4.14) in the limit $y \rightarrow 0$. Because the dominant non-zero configuration in this limit consists of single excited vortex pair, we find, for $R \neq 0$,

$$\begin{aligned} \langle m(\vec{0}) m(\vec{R}) \rangle &= -2 y_0^2 e^{-2\pi K G'(\vec{R})} \\ &\approx -2 y^2 / (R/a_0)^{2\pi K} \quad (\text{large } R). \end{aligned} \quad (4.16a)$$

When $\vec{R} = \vec{0}$, we find

$$\begin{aligned} \langle m^2(\vec{0}) \rangle &= 2y_0^2 \sum_{\vec{R}} e^{-2\pi K G'(\vec{R})} \\ &\approx 2y^2 \sum_{\vec{R}} \left(\frac{R}{a_0} \right)^{-2\pi K}. \end{aligned} \quad (4.16b)$$

Physically, $m(\vec{R})$ represents the quantum number of vortex. Equations (4.16) express the fact that a pair of oppositely oriented vortices can appear in the system with a probability proportional to y^2 . They are attracted to each other with a logarithmic potential of strength $2\pi K$.

We are now in a position to develop a sort of "low-temperature series expansion" for the Villain model. To produce a low-temperature series for the Ising model in two or three dimensions, one first imagines a configuration of totally up or down spins. Corrections to this dominant configuration at low temperatures are calculated by overturning 1, 2, 3, ... spins at a time.³¹ Here, we expand about an ensemble of states taken into account by a simple spin-wave analysis. Corrections which form a power series in y correspond to the various possible vortex excitations. These ideas will be made explicit by the cumulant expansion described in Sec. IV D.

C. Correlation functions

Before developing a low-temperature cumulant expansion, we describe how to express the correlation function $g_p(\vec{R} - \vec{R}')$ between $e^{ip\phi(\vec{R})}$ and $e^{-ip\phi(\vec{R}')}$ in the Coulomb gas language. According to Eqs. (2.26) and (4.1), the relevant correlation in the Villain model is

$$g_p(\vec{r} - \vec{r}') = Z^{-1} \left(\sum_{\{\mathbf{m}(\vec{R})\}} \prod_{\vec{R}} \int_{-\infty}^{\infty} \frac{d\phi(\vec{R})}{2\pi K} \right) \exp \left(2\pi i \sum_{\vec{R}} m(\vec{R}) \phi(\vec{R}) - \frac{1}{2K} \sum_{(\vec{R}, \vec{R}')} [\phi(\vec{R}) - \phi(\vec{R}') - \eta_{\vec{R}, \vec{R}'} p]^2 \right), \quad (4.17)$$

where we remind the reader that the projector operators $\eta_{\vec{R}\vec{R}'}$ are only nonzero on bonds in the dual lattice which cross a previously chosen path from sites \vec{r} to \vec{r}' . It is convenient to rewrite (4.17) in terms of new functions $\eta'(\vec{R})$ and $\eta''(\vec{R})$:

$$\begin{aligned} g_p(\vec{r} - \vec{r}') &= Z^{-1} \sum_{\vec{R}} \int_{-\infty}^{\infty} \left(\frac{d\phi(\vec{R})}{2\pi K} \right) \sum_{\{\mathbf{m}(\vec{R})\}} \exp \left(2\pi i \sum_{\vec{R}} m(\vec{R}) \phi(\vec{R}) - \frac{1}{2K} \sum_{(\vec{R}, \vec{R}')} [\phi(\vec{R}) - \phi(\vec{R}')]^2 \right. \\ &\quad \left. - \frac{p^2}{2K} \sum_{\vec{R}} \eta_{\vec{R}\vec{R}}^2 + \frac{p}{K} \sum_{\vec{R}} \phi(\vec{R}) [\eta'(\vec{R}) - \eta''(\vec{R})] \right). \end{aligned} \quad (4.18)$$

Here, $\eta'(\vec{R})$ is a function which is ± 1 at all points on the left-hand vertex of a bond which crosses the path from left to right and zero everywhere else: $\eta''(\vec{R})$ equals unity on the right-hand edge of these bonds and is zero everywhere else (see Fig. 17).

The next to last term in (4.18) counts the number of dual lattice bonds crossed by the path. The mysterious functions $\eta'(\vec{R})$ and $\eta''(\vec{R})$ in the final term just give rise to the lattice version of the line integral along the path of the derivative of $\phi(\vec{R})$ perpendicular to that path.

As in the case of the partition function, the integral over the $\phi(\vec{R})$ is easily calculated, with the result

$$g_p(\vec{r} - \vec{r}') = g_p^{sw}(\vec{r} - \vec{r}') g_p^v(\vec{r} - \vec{r}'). \quad (4.19)$$

The "spin wave" contribution to g_p is,

$$g_p^{sw}(\vec{r} - \vec{r}') = \exp \left(- \left(\frac{p^2}{2K} \right) X(\vec{r} - \vec{r}') \right), \quad (4.20)$$

where

$$\begin{aligned} X(\vec{r} - \vec{r}') &= \sum_{\vec{R}} \eta_{\vec{R}, \vec{R}'}^2 - \sum_{\vec{R}, \vec{R}'} [\eta'(\vec{R}) - \eta''(\vec{R})] G(\vec{R} - \vec{R}') \\ &\quad \times [\eta'(\vec{R}') - \eta''(\vec{R}')]. \end{aligned} \quad (4.21)$$

The vortex contribution is

$$g_p^v(\vec{r} - \vec{r}') = \left\langle \exp \left(i \sum_{\vec{R}} m(\vec{R}) u(\vec{R}) \right) \right\rangle, \quad (4.22)$$

where the expectation is to be calculated in the vortex ensemble (4.11), and

$$u(\vec{R}) = \sum_{\vec{R}'} G'(\vec{R} - \vec{R}') [\eta'(\vec{R}') - \eta''(\vec{R}')]. \quad (4.23)$$

Although the expression (4.21) entering the "spin wave" part of g_p looks rather formidable, it is shown in Appendix C that (4.21) and (4.20) combine to give the standard spin-wave result (A5):

$$g_p^{sw}(r) = \exp \left[- \left(\frac{p^2}{2\pi K} \right) G'(r) \right]. \quad (4.24)$$

The vortex contribution is, of course, not so simple. However, if $|\vec{r} - \vec{R}|$ and $|\vec{r}' - \vec{R}'|$ are large compared to a lattice constant, it can be shown

(see Appendix C) that

$$u(\vec{R}) = \Theta(\vec{r} - \vec{R}) - \Theta(\vec{r}' - \vec{R}), \quad (4.25)$$

where $\Theta(\vec{r})$ is the shift in orientation of $\Theta(\vec{r})$ produced by a vortex at $\vec{R} = 0$:

$$\Theta(r) = \tan^{-1}(y/x), \quad \vec{r} = (x, y). \quad (4.26)$$

Note that if a single uncompensated vortex appears within a distance of order $|\vec{r} - \vec{r}'|$ or $|\vec{r}|$ and $|\vec{r}'|$, $u(\vec{R})$ will change by roughly π . As $|\vec{r} - \vec{r}'| \rightarrow \infty$, the probability of "destructive interference" of this sort increases, and the correlation function will tend to zero.

D. Fluctuation corrections to the correlations

As an example of the sort of low-temperature expansion possible within this reformulation of the planar model, we calculate the vortex correlation (4.22) to lowest nontrivial order. If the major contribution to (4.22) comes from pairs which are tightly bound, fluctuations in $\sum_{\vec{R}} m(\vec{R}) u(\vec{R})$ will be rather small. Consequently, we employ a cumulant expansion, which gives to lowest order

$$g_p^v(\vec{r} - \vec{r}') \simeq \exp \left(- \frac{1}{2} p^2 \sum_{\vec{R}, \vec{R}'} \langle m(\vec{R}) m(\vec{R}') \rangle \right. \\ \left. \times u(\vec{R}) u(\vec{R}') \right). \quad (4.27)$$

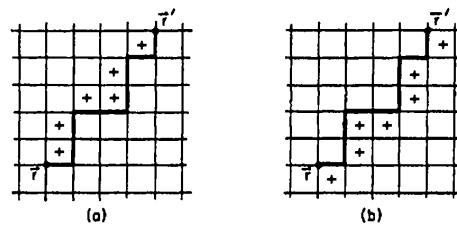


FIG. 17. Definition of the functions $\eta'(\vec{R})$ and $\eta''(\vec{R})$ for a particular path. The function $\eta'(\vec{R})$ is ± 1 on dual lattice points marked by a cross in lattice (a), and is zero everywhere else. Similarly, $\eta''(\vec{R})$ is nonzero only on the crosses shown in lattice (b).

To evaluate the sum in (4.27), take $\vec{R}' = \vec{R}_0 + \frac{1}{2} \vec{r}_0 a_0$, $\vec{R} = \vec{R}_0 - \frac{1}{2} \vec{r}_0 a_0$, and assume that $a_0 \vec{r}_0$ is small compared to $|\vec{R}_0 - \vec{r}|$ and $|\vec{R}_0 - \vec{r}'|$. This amounts to the assumption that tightly bound vortices dominate the sum for large r and r' . Expanding each $u(\vec{R})$ about \vec{R}_0 , and making use of the charge neutrality condition $\sum_{\vec{R}} m(\vec{R}) = 0$, we obtain

$$\ln g_p^V(\vec{r} - \vec{r}') = + \frac{1}{8} p^2 \sum_{\vec{R}_0, \vec{r}_0} \langle m(\vec{0}) m(a_0 \vec{r}_0) \rangle \\ \times a_0^2 [(\vec{r}_0 \cdot \nabla_{\vec{R}_0}) u(\vec{R})]^2. \quad (4.28)$$

But it follows from (4.25) and (4.26) that

$$\frac{\partial}{\partial x} u(\vec{R}) = \frac{y - Y}{|\vec{r} - \vec{R}|^2} - \frac{y' - Y}{|\vec{r}' - \vec{R}|^2}, \quad (4.29a)$$

$$\frac{\partial}{\partial y} u(\vec{R}) = \frac{x - X}{|\vec{r} - \vec{R}|^2} - \frac{x - X}{|\vec{r}' - \vec{R}'|^2} \quad (4.29b)$$

in this limit. Upon averaging over various orientations, (4.28) can be rewritten

$$\ln g_p^V(\vec{r} - \vec{r}') = \frac{1}{16} p^2 \sum \langle m(\vec{0}) m(a_0 \vec{r}_0) \rangle a_0^2 r_0^2 \sum_{\vec{R}_0} \nabla_{\vec{R}_0} [G'(\vec{R}_0 - \vec{r}) - G'(\vec{R}_0 - \vec{r}')] \nabla_{\vec{R}_0} [G'(R_0 - \vec{r}) - G'(\vec{R}_0 - \vec{r}')]. \quad (4.30)$$

We can evaluate the sum over R_0 immediately by integrating by parts and observing that

$$\nabla^2 G'(\vec{R}) = -2\pi \delta_{\vec{R}, 0}/a_0^2. \quad (4.31)$$

Our result is then that

$$g_p^V(r) = \exp \left(-\frac{1}{8} \pi p^2 G'(r) \sum_{\vec{r}_0} r_0^2 \langle m(\vec{0}) m(a_0 \vec{r}_0) \rangle \right). \quad (4.32)$$

This result for the vortex part of the correlation can be combined with the spin-wave contribution (4.24) to give finally

$$g_p(r) = e^{-p^2 G'(r)/2\pi K_{eff}}, \quad (4.33)$$

where

$$K_{eff}^{-1} = K^{-1} - \frac{1}{2} \pi^2 \sum_{\vec{r}_0} r_0^2 \langle m(\vec{0}) m(a_0 \vec{r}_0) \rangle. \quad (4.34)$$

Apparently, the fluctuations in $m(\vec{R})$ have produced a renormalization of K just as in the Migdal approximation of Sec. III. However, the nature of the renormalization is entirely different.

To see this let us look at the contributions from different ranges of \vec{r}_0 . The low-order calculation described at the end of Sec. IV B gave

$$\langle m(\vec{0}) m(a_0 \vec{r}_0) \rangle = -2y^2 e^{-2\pi K G'(a_0 \vec{r}_0)}. \quad (4.35)$$

Thus the nearest-neighbor part of (4.34) just gives a contribution to $K_{eff}^{-1} - K^{-1}$, which is

$$4\pi^2 y^2 e^{-\pi^2 K}. \quad (4.36)$$

However, other ranges of r_0 contribute with quite different weights. In fact, the contribution from higher range of r_0 takes the form

$$\sim \int_{a_0}^{\infty} dr_0 r_0^{2-2\pi K}. \quad (4.37)$$

In the Migdal approximation, all ranges of $\ln r_0$

contribute equally, in contrast to (4.37). Hence, it is inevitable that $K_{eff} \rightarrow 0$ after many interactions. From (4.37) we see that K_{eff} approaches a finite nonzero limit provided

$$2\pi K > 4. \quad (4.38)$$

The contribution from $r_0 \gtrsim a_0$ dominates in this case.

V. RECURSION RELATIONS AND DUALITY

A. Isotropic recursion relations

Our results and conclusions can be usefully summarized in terms of recursion relations, which are readily derived from the results of Sec. IV. Equation (4.34) for the effective coupling can be turned into a lattice integral equation by noting that, in an improved self-consistent theory, it is K_{eff} and not K which should enter the expression (4.35) for $\langle m(\vec{0}) m(a_0 \vec{r}_0) \rangle$. In an approximate continuum form, this integral equation takes the form³²

$$K_{eff}^{-1} = K^{-1} + 2\pi^3 y^2 \int_{a_0}^{\infty} \frac{dr}{a_0} \left(\frac{r}{a_0} \right)^{3-2\pi K_{eff}}. \quad (5.1)$$

For $K_{eff} < 2/\pi$, the integral diverges and our theory breaks down. To study this further, write out the perturbation series obtained by solving (5.1) iteratively,

$$K_{eff}^{-1} = K^{-1} + 2\pi^3 y^2 \int_{a_0}^{\infty} \frac{dr}{a_0} \left(\frac{r}{a_0} \right)^{3-2\pi K} + \dots \quad (5.2)$$

Now divide each integral into two parts,

$$\int_{a_0}^{\infty} dr = \int_{a_0}^{ba_0} dr + \int_{ba_0}^{\infty} dr, \quad (5.3)$$

with $0 < \ln b \ll 1$. One can combine the small- r parts of the integrals into a new bare coupling

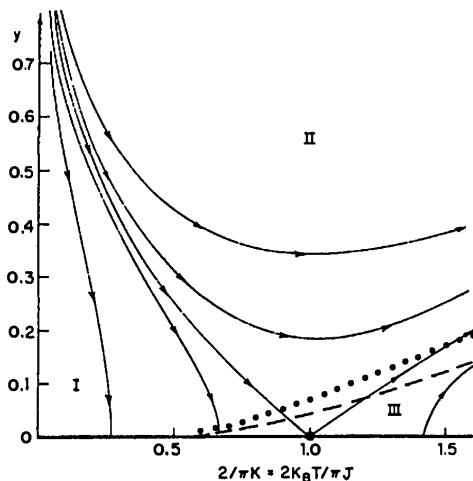


FIG. 18. Renormalization trajectories for the planar model at low temperatures. Two separatrices, which flow in and out of a fixed line at $y = 0$, divide the parameter space into three regions.

$(K^{-1})'$, and rescale the large- r integration variables so that the integrals again run from a_0 to ∞ . In the limit of small $\ln b$, the integral displayed in (5.2) makes the dominant contribution to $(K^{-1})'$. The rescalings can be absorbed into a redefinition of y .

On resumming the series obtained in this way, one obtains a new integral equation of precisely the same form:

$$K_{\text{eff}}^{-1} = (K^{-1})' + 2\pi^3 y'^2 \int_{a_0}^{\infty} \frac{dr}{r} \left(\frac{r}{a_0} \right)^{3-2\pi K_{\text{eff}}}, \quad (5.4)$$

where

$$(K^{-1})' = K^{-1} + 2\pi^3 y^2 \ln b, \quad (5.5)$$

$$y' = b^{2-\pi K} y \approx y + (2 - \pi K) y \ln b.$$

Apparently, elimination of the short-wavelength part of the integral equation has produced a Coulomb gas problem with parameters $(K^{-1})'$ and y' . A continuous family of such problems is obtained by iterating this transformation. The differential changes in K^{-1} and y are given by

$$\frac{dK^{-1}}{dl} = 2\pi^3 y^2, \quad (5.6a)$$

$$\frac{dy}{dl} = (2 - \pi K)y, \quad (5.6b)$$

where $l = \ln b$. Except for minor differences, these are precisely the equations obtained previously by Kosterlitz.¹²

Figure 18 shows the renormalization trajectories obtained from (5.6) (this is a low-temperature ver-

sion of Kosterlitz's Fig. 1). The spin-wave theory fixed line of Berezinskii is given by $y = 0$. The parameter space divides into three regions, partitioned by two separating lines (separatrices) which lead in and out of the fixed line. The fixed line is stable to vortex perturbations in region I, as was suggested by the arguments of Sec. IV A. Actions initially in regions II and III iterate toward large y , outside the range of our small- y theory. The locus of initial Hamiltonians for the Villain model is shown by the dashed curve in Fig. 18. Formula (4.33) for $g_s(r)$ applies to the Villain model only when it is in region I.

It is tempting to associate T_c with the intersection of the Villain locus and the left-hand separatrix of Fig. 18 as was done by Kosterlitz.¹² Certainly, a very plausible assumption is that both regions II and III ultimately flow into a high-temperature fixed point. Under this assumption, Kosterlitz showed that the correlation length, infinite below T_c , diverges as

$$\xi(T) \sim e^{\text{const}/|T - T_c|^{1/2}}, \quad (5.7)$$

as $T \rightarrow T_c$ from above.³³ A second consequence¹² is that the critical exponent η obtains a universal value

$$\eta = \frac{1}{4} \quad (5.8)$$

at T_c .

Unfortunately, Luther and Scalapino's recent solution of a planar model¹³ casts doubt on this simple picture. Their calculations suggest that the value of η at T_c is nonuniversal, depending on the details of the particular planar model. This would require another marginal operator (in addition to K^{-1}) in the theory. The only such operators we have found (other than trivial ones) are associated with symmetry-breaking fields.

However, there is one way out. We showed in Sec. IV A that the leading vortex perturbations to spin-wave theory could be viewed as a symmetry-breaking operator $\cos(p_{\text{eff}}\phi)$ with $p_{\text{eff}} = 2\pi K$.³⁴ The vortex perturbations become relevant at precisely $p_{\text{eff}} = 4$. One might speculate that, for large y in region II, the model goes over into a system with an infinitely strong symmetry-breaking field with $p_{\text{eff}} \approx 4$. It is not difficult to show that this would be an Ashkin-Teller model. The planar model could possibly have the continuously variable exponents of spin-wave theory in region I, the exponents of the Ashkin-Teller model in region II, and a high-temperature phase only in region III. Conceivably, this could happen in a way consistent with the Luther-Scalapino results.

In region I, where the physics is presumably well understood, it is of interest to calculate the eigenvalues of various symmetry-breaking fields.

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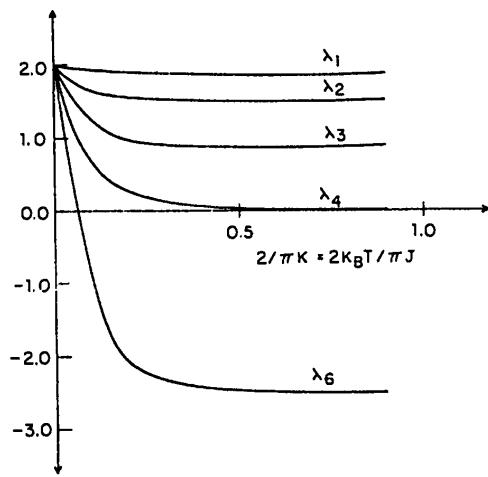


FIG. 19. Eigenvalues $\lambda_p(T)$ for symmetry-breaking fields applied to the Villain model obtained by taking vortex corrections to spin-wave theory. We cannot calculate the $\lambda_p(T)$ beyond $2k_B T \pi J = 0.9$, which may actually correspond to the critical temperature of the model.

This was done by Kosterlitz only for $p=1$. From Fig. 1, we see that these eigenvalues are determined simply by the mapping (5.6) of the Villain model onto spin-wave theory. According to (4.33),

$$g_p(r) \sim 1/r^{\eta_p(r)}, \quad \eta_p(T) = p^2/2\pi K_{\text{eff}}, \quad (5.9)$$

at large r . Because (see Appendix A)

$$\lambda_p(T) = 2 - \frac{1}{2}\eta_p(T), \quad (5.10)$$

$\lambda_p(T)$ follows from an approximate calculation of K_{eff} . These eigenvalues are shown in Fig. 19. They are calculable within this approach only up to the border of region II, where $2k_B T \pi J \approx 0.9$. Each $\lambda_p(T)$ varies smoothly from 2 to $2 - \frac{1}{2}p^2$. The important point is that $\lambda_6(T)$ goes negative at sufficiently high temperatures, above which h_6 is irrelevant. Above this temperature (but below the Kosterlitz-Thouless T_c), planar model behavior should be experimentally accessible in quasi-two-dimensional crystals dominated by hexagonal anisotropies. The eigenvalue $\lambda_4(T)$ goes to zero at precisely the transition temperature marking the border of regions I and II. In Sec. VC we show that cubic perturbations, which are marginal at this apparent T_c , actually sweep out a new (Baxter-like) line of fixed points. The critical behavior (if any) when the $\lambda_p(T)$ are relevant is impossible to ascertain except within the untrustworthy Migdal approach of Sec. III. Comparing Fig. 19 with the results displayed in Fig. 12, we see that the Migdal results may not be too bad for $p=1-3$.

B. Duality results

To proceed further, we quote a duality result which is proved in Appendix D. So far, we have considered the partition function of the Villain model with coupling K , and an extra parameter y_0 introduced into the dual model in Eq. (4.3). In addition, we have been interested in the effects of field terms, expressed as contributions to the exponentiated action of the form given in Eq. (1.1)

$$\prod_r e^{h_p \cos[p\theta(r)]} = \Lambda. \quad (5.11a)$$

It is only a small change to replace Λ by

$$\Lambda' = \prod_r \sum_{\{n(r)\}} \exp\{ip\theta(r)n(r) + \ln y_p[n(r)]^2\}. \quad (5.11b)$$

If $y_p = 0$, only the terms $n=0$ and ± 1 contribute, and Λ' goes into Λ provided

$$h_p = \frac{1}{2}y_p. \quad (5.12)$$

If $y_p = 1$, then $\theta(r)$ is forced to take on the values $(2\pi/p)q(r); q(r) = 0, 1, 2, \dots, p-1$,

appropriate to the p -state model. Hence $y_p = 1$ is just like $h_p = \infty$.

Imagine a problem which contains in the $\theta(r)$ picture a term like $\ln\Lambda'$ in its action and is otherwise identical to our generalized Villain model. This problem is defined more explicitly in Appendix D. There it is proven that the partition function of this model $Z(2\pi K, y_0, y_p)$ obeys the duality relation

$$Z(2\pi K, y_0, y_p) = Z(p^2/2\pi K, y_p, y_0)(p/2\pi K)^N. \quad (5.13)$$

We know that the generalized Villain model has a Kosterlitz-Thouless critical point at

$$2\pi K \approx 4, \quad (5.14a)$$

as $y_0 \rightarrow 0$ and $y_p \rightarrow 0$. Equation (5.13) then directly implies that this model also has another singularity at

$$2\pi K \approx \frac{1}{4}p^2, \quad (5.14b)$$

in the presence of a small- h_p (or y_p) type perturbation. And the singularities in the free energy must be identical! The transition (5.14b) is the change from behavior characteristic of the p -state model to planar model behavior. Thus the duality relation maps all these p -state to planar transitions into the Kosterlitz-Thouless "point." Since an infinite number of different transitions map into this "point," we have at least suggestive evidence that this "point" contains quite a bit of structure. It could conceivably represent a whole family of different universality classes, which would be consistent with the Luther-Scalapino picture.

For $y_0 = y_p = 1$, we have a p -state version of the Villain model. Villain¹⁷ estimated that a phase transition at $p = \infty$ took place when

$$K \approx 1/1.7.$$

Hence for large p , we expect the transition from the p -state Villain model to the planar behavior to occur at

$$K \approx [p^2/(2\pi)^2]1.7.$$

We expect this transition to occur provided $p \geq 4$.

C. Recursion relations with symmetry-breaking fields

The duality relation quoted in Sec. VB can be used to generalize Eqs. (5.6) to allow for symmetry-breaking fields. Setting $y = y_0 e^{-(1/2)\pi^2 K}$, we can rewrite (5.6) in the form

$$\frac{dK^{-1}}{dl} = 2\pi^3 y_0^2 e^{-\pi^2 K}, \quad (5.15a)$$

$$\frac{dy_0}{dl} = (2 - \pi K)y_0, \quad (5.15b)$$

where these equations are correct to leading order in y_0 . By exploiting the duality relation (5.13) with $y_p = 0$, these equations can be used to produce recursion relations for K^{-1} and y_p with $y_0 = 0$,

$$\frac{dK^{-1}}{dl} = -\frac{1}{2}\pi p^2 y_p^2 K^{-2} e^{-\pi^2 K^{-1}/4}, \quad (5.16a)$$

$$\frac{dy_p}{dl} = \left(2 - \frac{p^2}{4\pi} K^{-1}\right) y_p, \quad (5.16b)$$

correct to lowest order in y_p .

It is tempting to combine (5.15) and (5.16) into a set of recursion relations which might be valid for both y_p and y_0 nonzero:

$$\frac{dK^{-1}}{dl} = 2\pi^3 y_0^2 e^{-\pi^2 K} - \frac{1}{2}\pi p^2 y_p^2 K^{-2} e^{-\pi^2 K^{-1}/4}, \quad (5.17a)$$

$$\frac{dy_0}{dl} = (2 - \pi K)y_0, \quad (5.17b)$$

$$\frac{dy_p}{dl} = \left(2 - \frac{p^2}{4\pi} K^{-1}\right) y_p. \quad (5.17c)$$

By construction Eqs. (5.17) obey the duality relation (5.13) and reduce to the correct limits when either y_0 or y_p tends to zero. Furthermore, no additional terms can appear in (5.17) to lowest order in y_0 and y_p by symmetry. For example, a term proportional to $y_0 y_p$ cannot appear in (5.17a) because the equations must be invariant under $y_p \rightarrow -y_p$. Similarly, terms proportional to y_p or y_p^2 cannot appear into (5.17b): duality would demand y_0 and y_0^2 terms in (5.17c), again violating invariance under $y_p \rightarrow -y_p$. We are led to the conclusion that Eqs. (5.17) are correct as they stand

to lowest order in y_0 and y_p .

The differential equations (5.17) give strong evidence for the phase diagram in Fig. 1(a) for $p > 4$. As the initial temperature is varied for fixed $h_p = \frac{1}{2}y_p \neq 0$, we find from (5.17) that a segment of the Berezinskii fixed line is stable to both vortex and h_p perturbations. The vortex parameter y_0 becomes unstable and iterates toward large values for $T > T_1(h_p)$, while h_p becomes unstable and iterates toward large values for $T < T_2(h_p)$. We are led immediately to a phase diagram like that in Fig. 1(a), provided we associate the instability for $T > T_1(h_p)$ with a disordered phase, and the instability for $T < T_2(h_p)$ with an ordered p -state phase.

The critical properties for small y_0 and y_p with $p = 4$ are controlled by three fixed lines. In addition to the Berezinskii spin-wave fixed line ($y_4 = y_0 = 0$, K^{-1} arbitrary), we find two new fixed lines in (5.17) given by

$$K^{-1} = \frac{1}{2}\pi, \quad y_0 = \pm y_4. \quad (5.18)$$

Every point with $y_0 = \pm y_4 \neq 0$ along these lines is characterized by one marginal, one irrelevant, and one relevant eigenvalue. The two new fixed lines have two-dimensional domains of attraction in the $(K^{-1}, y_0 - y_4)$ -Hamiltonian space, and control the critical behavior for $y_4 \neq 0$. It is straightforward to show that this description in terms of three fixed lines leads to the phase diagram shown in Fig. 1(b). All three lines display continuously variable critical exponents with a conventional phase transition across $T_c(h_4)$.³⁵ Although the exponent $\eta(h_4)$ remains fixed at $\frac{1}{4}$ to lowest order in h_4 , we find that the correlation length exponent $\nu(h_4)$ diverges,

$$\nu(h_4) \sim 1/|h_4|,$$

as $h_4 \rightarrow 0$.

For $p < 4$ the entire spin-wave fixed line is unstable to either vortex or h_p perturbations, and we are unable to determine the critical behavior for small $h_p \neq 0$. Presumably, two Ising (Potts) critical lines are present in the (h_p, T) plane for $p = 2$ ($p = 3$). Further investigation is required to determine how these lines connect up to the phase diagram of the planar model for $h_p = 0$.

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APPENDIX A: SPIN-WAVE THEORY

In this appendix we review the standard source of low-temperature results for models with contin-

uous symmetry, spin-wave theory. The usual route to this approximation is to expand the interaction function in (1.1) to second order in $\theta(\vec{r}) - \theta(\vec{r}')$, so that it takes the form

$$A[\theta] = \frac{1}{2}K \sum_{\langle \vec{r}, \vec{r}' \rangle} [\theta(\vec{r}) - \theta(\vec{r}')]^2 + \sum_{\vec{r}, p} h_p \cos[p\theta(\vec{r})]. \quad (A1)$$

Then, the variables $\theta(\vec{r})$ (which can be chosen to take on values in the region $[-\pi, \pi]$) are replaced by variables $\phi(\vec{r})$ which run over all real values.^{7,8} In Sec. IV, it is shown that the dual representation of the Villain models involves an action of precisely this form. In the $h_p \rightarrow 0$ limit, all properties of the resulting Gaussian action can be evaluated quite explicitly.

As an approximation to (1.1), the spin-wave results are expected to be valid in the low-temperature limit. Neglected terms of order $K[\theta(\vec{r}) - \theta(\vec{r}')]$ ⁿ,

$$Z_{sw} = \left(\prod_{\vec{R}} \int_{-\infty}^{+\infty} \frac{d\phi(\vec{R})}{2\pi} \right) e^{A[\phi]} = \exp \left[-\frac{1}{2} \Omega \int_{-\pi}^{\pi} \frac{dq_x}{2\pi} \int_{-\pi}^{\pi} \frac{dq_y}{2\pi} \ln \left(\frac{K}{2\pi} (4 - 2 \cos q_x - 2 \cos q_y)^{2\Gamma} \right) \right], \quad (A4)$$

where Ω is the size of the system.

More interesting results obtainable within the spin-wave approximation are the correlation functions corresponding to the various h_p perturbations entering (A1). For example, it is straightforward to calculate

$$G_p^{sw}(\vec{r} - \vec{r}') = \langle e^{ip[\theta(\vec{r}) - \theta(\vec{r}')]}\rangle = e^{-(p^2/2\pi K)} G'(\vec{r} - \vec{r}'), \quad (A5)$$

where

$$G'(\vec{r}) = 2\pi[G(0) - G(\vec{r})]. \quad (A6)$$

Note that the infrared singularity in $G(\vec{r})$ produces an asymptotic form for $G'(\vec{r})$, which is

$$G'(\vec{r}) = \ln(r/a_0) + \text{const}, \quad (A7)$$

as $r \rightarrow \infty$. Thus, the spin-wave correlation function at large separations is

$$G_p^{sw}(\vec{r} - \vec{r}') \sim (|\vec{r} - \vec{r}'|/a_0)^{-p^2/2\pi K}. \quad (A8)$$

In a standard scaling theory of critical phenomena, we would interpret (A8) as a statement that the action (A2) is at a critical point, and that the perturbation $e^{ip\phi(r)}$ (or, equivalently, $\cos[p\phi(\vec{r})]$) had scaling index

$$\chi_p = p^2/4\pi K. \quad (A9)$$

The corresponding field h_p has a scaling index λ_p , which is $\lambda_p = d - \chi_p$, where d is the dimensionality. Consequently we have

$n = 4, 6, \dots$, produce interactions between spin waves and corrections of relative order K^{-1} . The extension of the range of integration to $\pm\infty$ eliminates vortex excitations, which are of relative order $e^{-p^2 K}$.^{36,37}

The action which produces the spin wave approximation can be written in the form

$$A[\phi] = -\frac{1}{2}K \sum_{\langle \vec{r}, \vec{r}' \rangle} \phi(\vec{r}) G^{-1}(\vec{r} - \vec{r}') \phi(\vec{r}'), \quad (A2)$$

where $G(\vec{r} - \vec{r}')$ is the lattice Green's function derived from (A1) for $h_p = 0$. This Green's function and its inverse may be written

$$G^{\pm 1}(\vec{r}) = \int_{-\pi}^{\pi} \frac{dq_x}{2\pi} \int_{-\pi}^{\pi} \frac{dq_y}{2\pi} \frac{e^{-i\vec{q} \cdot (\vec{r}-\vec{r}')/a_0}}{(4 - 2 \cos q_x - 2 \cos q_y)^{\pm 1}}. \quad (A3)$$

Using (A3), it is very easy to produce the spin-wave partition function, which is

$$\lambda_p = 2 - p^2/4\pi K. \quad (A10)$$

a result which is discussed in Sec. IIIC.

APPENDIX B: SYMMETRY-BREAKING FIELDS AND THE MIGDAL APPROXIMATION

The Migdal recursion scheme is fairly ambiguous in its treatment of symmetry-breaking fields. As shown in Fig. 20 one can imagine moving an arbitrary fraction α of the field on each site in the initial bond-moving step. A heuristic argument which suggests what fraction should be moved is summarized graphically in Fig. 21. One divides each on-site field symmetrically between the four connecting bonds, and then manipulates each bond-

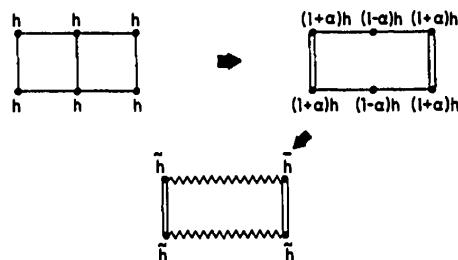


FIG. 20. Potential moving scheme for handling an on-site interaction within the Migdal approximation. The parameter α is, at present, arbitrary.

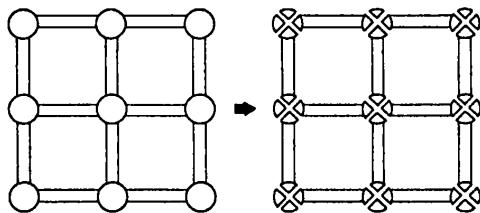


FIG. 21. Scheme for partitioning an onsite potential into four equal parts such that it can be treated by a bond-moving approach. The enlarged vertices represent the on-site potential.

plus-field component as before.³⁸ On a d -dimensional hypercubical lattice, this would lead to the requirement

$$\alpha = 1/d. \quad (\text{B1})$$

Once α is specified, our procedure for handling symmetry-breaking fields in the Migdal approach is straightforward and well defined. Because of the importance of choosing α properly, we now sketch an alternative argument which produces the results $\alpha = \frac{1}{2}$ in $d = 2$, in agreement with (B1).

It is well known that the Migdal approach¹⁴ gives results for the correlation length exponent ν which agree, to leading order, with the more complicated spin-wave theories^{15,16} in $2 + \epsilon$ dimensions for n -component isotropic fixed-length spin models. It does, however, produce $T_c(n, \epsilon)$ incorrectly, a quantity which should be universal to first order in ϵ .¹⁶ The competing results are, from the spin-wave analysis,

$$k_B T_c(n, \epsilon) / J = 2\pi\epsilon / (n - 2) + O(\epsilon^2), \quad (\text{B2a})$$

and from the Migdal approach,

$$k_B T_c(n, \epsilon) / J = 4\epsilon / (n - 2) + O(\epsilon^2). \quad (\text{B2b})$$

We can define a characteristic temperature scale T_0 for the case of interest here ($n = 2$, $\epsilon = 0$) by taking a limit:

$$\frac{k_B T_0}{J} = \lim_{\epsilon \rightarrow 0} \lim_{n \rightarrow 2} \frac{(n - 2) k_B T_c(n, \epsilon)}{\epsilon J} = \begin{cases} 2\pi \\ 4 \end{cases}. \quad (\text{B3a})$$

The Migdal approximation may be carried out analytically at low temperature on the "spin wave" action of Eq. (A1), with the result

$$\begin{aligned} \lambda_p(T) &= 2 - \frac{1}{2}(1 - \alpha)p^2 k_B T/J \\ &= 2 - (1 - \alpha)p^2(T/T_0), \end{aligned} \quad (\text{B4})$$

where we have expressed our results in terms of the temperature scale T_0 appropriate to the Migdal approach. The result (A10) from spin-wave theory may be rewritten in the form

$$\lambda_p = 2 - \frac{1}{2}p^2(T/T_0), \quad (\text{B5})$$

where T_0 is determined from the spin-wave result. The requirement that the coefficients of (T/T_0) in these expansions agree suggests that we take

$$\alpha = \frac{1}{2}. \quad (\text{B6})$$

The reader may view this particular route to the result $\alpha = \frac{1}{2}$ as somewhat capricious. Similar arguments, however, show that the choice $\alpha = \frac{1}{2}$ is necessary to get the eigenvalues of symmetry-breaking fields³⁶ correct for $n \geq 3$ and $d = 2 + \epsilon$. This choice of α enables the Migdal recursion scheme to get exponents correct, even though it underestimates $T_c(n, \epsilon)$.

APPENDIX C: MANIPULATIONS ON LATTICE PATH INTEGRALS

We wish to evaluate

$$\begin{aligned} X(\vec{r} - \vec{r}') &= \sum_{\vec{R}} \eta_{\vec{R}, \vec{R}'}^2 \\ &- \sum_{\vec{R}, \vec{R}'} [\eta'(\vec{R}) - \eta''(\vec{R})] G(\vec{r} - \vec{r}') \\ &\times [\eta'(\vec{R}') - \eta''(\vec{R}')]. \end{aligned} \quad (\text{C1})$$

The first term just gives the length of the path from \vec{r} to \vec{r}' [see Fig. 17(a)]. The definitions of $\eta'(\vec{R})$ and $\eta''(\vec{R}')$ restrict both sums in the second term to be in the neighborhood of this same path. The quantities $[\eta'(\vec{R}) - \eta''(\vec{R})]$ and $[\eta'(\vec{R}') - \eta''(\vec{R}')]$ are operators acting on $G(\vec{R} - \vec{R}')$ which generate the discrete analog of a perpendicular derivative along the path.

Equation (C1) can be rewritten in a convenient continuum notation

$$X(\vec{r} - \vec{r}') = \int_{\text{path}} dR - \int_{\text{path}} dR \int_{\text{path}} dR' \theta_{\perp} \theta'_{\perp} G(\vec{R} - \vec{R}'), \quad (\text{C2})$$

where θ_{\perp} and θ'_{\perp} are perpendicular derivatives with respect to \vec{R} and \vec{R}' , respectively. The scalar symbols dR and dR' represent line elements along the path. It is straightforward to transform this continuum notation back into the lattice language. The second term of (C2) can be simplified

$$\begin{aligned} &\int_{\text{path}} dR \int_{\text{path}} dR' \theta_{\perp} \theta'_{\perp} G(\vec{R} - \vec{R}') \\ &= - \int_{\text{path}} dR \int_{\text{path}} \theta'_{\perp} G(\vec{R} - \vec{R}') \\ &= - \int_{\text{path}} dR \int_{\text{path}} dR' [\nabla^2 G(\vec{R} - \vec{R}') - \theta_{\parallel}^2 G(\vec{R} - \vec{R}')], \end{aligned} \quad (\text{C3})$$

where θ_{\parallel} denotes a derivative along the path. Since $\nabla^2 G(\vec{R} - \vec{R}')$ is zero except at $\vec{R} = \vec{R}'$, the first term

of (C3) reduces to the path integral of unity and cancels the first term of (C2). We have finally

$$\begin{aligned} X(\vec{r} - \vec{r}') &= \int_{\text{path}} dR \int_{\text{path}} dR' \delta_{\parallel}^2 G(\vec{R} - \vec{R}') \\ &= - \int_{\text{path}} dR \int_{\text{path}} dR' \delta_{\parallel} \delta_{\parallel}^2 G(\vec{R} - \vec{R}') \\ &= -2[G(\vec{r}_1 - \vec{r}_2) - G(0)] = G'(|\vec{r} - \vec{r}'|)/\pi, \end{aligned} \quad (\text{C4})$$

which gives the desired spin-wave result.

The path integral

$$u(\vec{R}) = \sum_{\vec{R}} G'(\vec{R} - \vec{R}') [\eta^i(\vec{R}') - \eta^r(\vec{R}')] \quad (\text{C5})$$

can be handled in much the same way. For large separations $|\vec{R} - \vec{R}'|$ and $|\vec{R} - \vec{r}|$ this can be re-written (again in continuum notation)

$$u(\vec{R}) = \int_{\text{path}} dR' \delta_1' \ln(|\vec{R} - \vec{R}'|). \quad (\text{C6})$$

Let us regard $\ln(|\vec{R} - \vec{R}'|)$ as the real part of a complex function $\ln(z - z')$, $z = R_x + iR_y$, $z' = R'_x + iR'_y$, so that

$$\ln(|\vec{R} - \vec{R}'|) = \text{Re}[\ln(z - z')], \quad (\text{C7})$$

and consider the path integral as occurring in the complex z' plane:

$$u(z) = \int_{\text{path}} dz' \delta_1' \text{Re}[\ln(z - z')]. \quad (\text{C8})$$

This can be evaluated using the Cauchy-Riemann relation

$$\begin{aligned} u(z) &= - \int_{\text{path}} dz' \delta_{\parallel}^2 \text{Im}[\ln(z - z')] \\ &= \Theta(\vec{r} - \vec{R}) - \Theta(\vec{r}' - \vec{R}), \end{aligned} \quad (\text{C9})$$

$$Z(2\pi K, y_0, 0) = \sum_{\vec{m}(R)} \left(\prod_{\langle \vec{R}, \vec{R}' \rangle} \int_{-\infty}^{\infty} \frac{d\phi(\vec{R}, \vec{R}')}{2\pi} \right) \left(\prod_{\vec{R}} \bar{\Delta}(\vec{R}) \right) \exp \left(- \sum_{\langle \vec{R}, \vec{R}' \rangle} \frac{1}{2} [\phi(\vec{R}, \vec{R}')]^2 + \sum_{\vec{R}} (\ln y_0)[\bar{m}(R)]^2 \right). \quad (\text{D4})$$

In writing Eq. (D4), we have evaluated the Fourier transform in Eq. (D3). In (D4), $\bar{\Delta}(R)$ is a δ function essentially similar to the one in Eq. (2.15). In particular, for the arrangement of points shown in Fig. 22,

$$\begin{aligned} \bar{\Delta}(R) &= 2\pi \delta(\phi(R, R_1) + \phi(R, R_2) \\ &\quad - \phi(R'_1, R) - \phi(R'_2, R) + 2\pi m(R)). \end{aligned} \quad (\text{D5})$$

Just as before, one can "solve" the δ -function conditions (D5) by writing $\phi(R, R')$ in terms of quantities which refer to the dual lattice. In par-

where

$$\Theta(\vec{R}) = \tan^{-1}(x/y). \quad (\text{C10})$$

APPENDIX D: GENERALIZED MODELS AND DUALITY

For the sake of completeness and also to make contact with the gauge field literature,⁴⁰ we construct a rather general form of the duality relations for our type of model.

Start from our generalized version of the Villain model on the dual lattice, i.e., Eq. (2.19) with the extra $\ln y_0$ term of Eq. (4.3). Hence our expression for the partition function reads

$$Z(2\pi K, y_0, 0) = \sum_{\{\vec{m}(R)\}} \left(\prod_{\vec{R}} \int_{-\infty}^{\infty} \frac{d\bar{\phi}(R)}{2\pi K} \right) \exp \bar{A}[\bar{\phi}, \bar{m}], \quad (\text{D1})$$

with

$$\begin{aligned} \bar{A}[\bar{\phi}, \bar{m}] &= - \sum_{\langle \vec{R}, \vec{R}' \rangle} \frac{1}{2K} [\bar{\phi}(\vec{R}) - \bar{\phi}(\vec{R}')]^2 \\ &\quad + \sum_{\vec{R}} \{ 2\pi i \bar{\phi}(R) \bar{m}(R) + (\ln y_0)[\bar{m}(\vec{R})]^2 \}. \end{aligned} \quad (\text{D2})$$

For future convenience, in (D1) Z has been written as a function of three variables—one of which is set equal to zero. The "space" is being saved for a symmetry-breaking field, which is being held to zero at this point.

To understand this model, undo the dual transformation. Write $e^{\bar{v}} = e^{-(1/2K)(\bar{\phi}(\vec{R}) - \bar{\phi}(\vec{R}'))^2}$ as a Fourier integral

$$\begin{aligned} e^{\bar{v}(\bar{\phi}(\vec{R}) - \bar{\phi}(\vec{R}'))} &= \int_{-\infty}^{\infty} \frac{d\phi(\vec{R}, \vec{R}')}{2\pi} e^{v_0(\phi(\vec{R}, \vec{R}'))} \\ &\quad \times e^{i(\phi(\vec{R}, \vec{R}') - \bar{\phi}(\vec{R}) - \bar{\phi}(\vec{R}'))}, \end{aligned} \quad (\text{D3})$$

and substitute the result in Eq. (D1). Then the $\bar{\phi}(R)$ integrals can be calculated immediately to yield a result directly analogous to Eq. (2.16), namely

ticular, each nearest-neighbor bond on the dual lattice is cut by one and only one bond on the original lattice. Thus, we can relabel each $\phi(R, R')$ as a $\phi(r, r')$. For example, $\phi(R, R_1)$ in Fig. 22 can also be written $\phi(r_1, r_2)$. Given this relabeling we can rewrite the δ function (A6) as

$$\begin{aligned} \Delta(R) &= 2\pi \delta(\phi(r_1, r_2) + \phi(r_4, r_1) \\ &\quad - \phi(r_4, r_3) - \phi(r_3, r_2) + 2\pi m(R)). \end{aligned} \quad (\text{D6})$$

This δ -function condition can, in turn be satisfied by

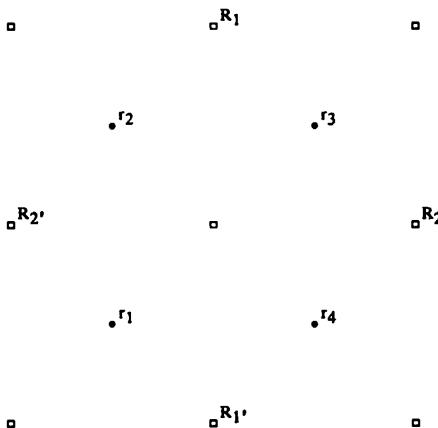


FIG. 22. Dual and original lattice points. Squares represent points of the dual lattice, dots sites in the original lattice.

$$\phi(r_1, r_2) = \theta(r_1) - \theta(r_2) - m(r_1, r_2). \quad (\text{D7})$$

Here, the θ 's are required to be in the interval $0 < \theta(r) \leq 2\pi$ and the integers $m(r_1, r_2)$ are adjusted to keep the θ 's in this range.

One further condition is required. Equation (D6) requires that the sum of the $m(r_1, r_2)$ around the loop, i.e.,

$$S_R(m) = m(r_4, r_1) + m(r_1, r_2) - m(r_3, r_2) - m(r_4, r_3), \quad (\text{D8})$$

be equal to $m(R)$. Equations (D7) and (D8) ensure that the δ function conditions are all properly satisfied. Then (D4) is seen to read

$$Z(2\pi K, y_0, 0) = \left(\prod_r \int_0^{2\pi} \frac{d\theta(r)}{2\pi} \right) \sum_{m(r, r')} e^{A[\theta, m]}, \quad (\text{D9})$$

where the new action is

$$A[\theta, m] = -\frac{1}{2}K \sum_{(r, r')} [\theta(\vec{r}) - \theta(\vec{r}') - 2\pi m(\vec{r}, \vec{r}')]^2 + \sum_R (\ln y_0) [S_R(m)]^2. \quad (\text{D10})$$

Notice how the periodicity in $\theta(r)$ is reflected in the action (D10). This action is invariant under the "gauge transformation"

$$\begin{aligned} \theta(\vec{r}) &\rightarrow \theta(\vec{r}) + 2\pi n(\vec{r}), \\ m(\vec{r}, \vec{r}') &\rightarrow m(\vec{r}, \vec{r}') + n(\vec{r}) - n(\vec{r}'). \end{aligned} \quad (\text{D11})$$

[Note that $S_R(m)$ is invariant under (D11).] Hence the result of the summations over m in Eq. (D9) is a completely periodic function of each $\theta(\vec{r})$.

The reason that our analysis gave a very simple $y_0 \rightarrow 0$ limit can also be seen from these equations. As $y_0 \rightarrow 0$, the only terms in the m sums which contribute are those with $S_R(m) = 0$ for all R . This condition will in turn be satisfied if

$$m(r_1, r_2) = n(r_1) - n(r_2). \quad (\text{D12})$$

Thence, the major contribution to Z as $y_0 \rightarrow 0$ is

$$\lim_{y_0 \rightarrow 0} Z(2\pi K, y_0, 0) = \prod_r \left(\int_0^{2\pi} \frac{d\theta(r)}{2\pi} \sum_{n(r)} \right) \exp - \sum_{(r, r')} \frac{1}{2}K[2\pi\phi(r) - 2\pi\phi(r')]^2. \quad (\text{D13})$$

where

$$2\pi\phi(r) = \theta(r) - 2\pi n(r). \quad (\text{D14})$$

But the sum over $n(r)$ and the integral over $\theta(r)$ combine to give a simple result

$$\int_0^{2\pi} \frac{d\theta(r)}{2\pi} \sum_{n(r)} = \int_{-\infty}^{\infty} d\phi(r).$$

Hence in the limit $y_0 \rightarrow 0$, all effects of periodicity in $\theta(r)$ completely vanish and we are left with a linear spin-wave problem.

One can also incorporate the symmetry-breaking terms with exactly the same analysis. Recall that the action (1.1) contained terms like

$$\sum_r \sum_p h_p \cos[p\theta(r)].$$

But, by suitably choosing a function $f_p(n)$ we can

always adjust a sum of the form

$$\sum_n e^{(1/y_0) f_p(n) + i\theta n p} \quad (\text{D15})$$

to be an exponential like

$$e^{h_p \cos \theta}. \quad (\text{D16})$$

For example, let us choose h_p to be very small, $h_p \ll 1$. Then take

$$y_p = \frac{1}{2}h_p \ll 1$$

and

$$f_p(n) = n^2. \quad (\text{D17})$$

With these choices (D15) and (D16) agree to first order in y_p .

Furthermore, if one chooses $y_p \rightarrow 1$, then the sum (D15) vanishes unless θ takes on one of the

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values appropriate to the p -state model. In this case, expression (D15) reduces to

$$\sum_{q=0}^{p-1} \delta\left(\frac{\theta}{2\pi} - \frac{q}{p}\right). \quad (\text{D18})$$

In short (D15) can represent symmetry-breaking fields as $y_p = 0$ and the p -state model as $y_p = 1$.

For this reason, we consider the generalization of Eq. (D9) which reads

$$\begin{aligned} Z(2\pi K, y_0, y_p) = & \left(\prod_{\vec{R}} \int_0^{2\pi} \frac{d\theta(\vec{R})}{2\pi} \right) \sum_{\{m(\vec{R}, \vec{R}')\}} \sum_{\{n(\vec{R})\}} \exp \left(\sum_{(r, r')} V_0(\theta(r) - \theta(r') - 2\pi m(r, r')) + \sum_{\vec{R}} (\ln y_0) f_0(S_{\vec{R}}(m)) \right. \\ & \left. + \sum_{\vec{R}} (\ln y_p) f_p(n(\vec{R})) + \sum_{\vec{R}} i n(\vec{R}) \theta(\vec{R}) p \right). \end{aligned} \quad (\text{D19})$$

This is a very general form of the action. For the case of interest to us here,

$$V_0(\theta) = -\frac{1}{2}K\theta^2, \quad f_p(x) = f_p(x) = x^2. \quad (\text{D20})$$

We have, in fact, calculated the dual of each and every term in Eq. (D19). Instead of recalculating, we simply present the result. After the dual transformation Eq. (D19) reads

$$\begin{aligned} Z(2\pi K, y_0, y_p) = & \left(\prod_{\vec{R}} \int_0^\phi d\bar{\phi}(\vec{R}) \right) \sum_{\{\vec{R}, \vec{R}'\}} \sum_{\vec{m}(\vec{R})} \exp \left(\sum_{(\vec{R}, \vec{R}')} \bar{V}(\bar{\phi}(\vec{R}) - \bar{\phi}(\vec{R}') - p\bar{n}(\vec{R}, \vec{R}')) + \sum_{\vec{R}} \ln y_0 f_0(\bar{m}(\vec{R})) \right. \\ & \left. + \sum_{\vec{R}} (\ln y_p) f_p(S_r(\vec{R})) + \sum_{\vec{R}} 2\pi i \bar{m}(\vec{R}) \bar{\phi}(\vec{R}) \right). \end{aligned} \quad (\text{D21})$$

The $\bar{\phi}$ integrals can, if one desires, be extended to infinity by making suitable gauge transforms of the form

$$\begin{aligned} \bar{\phi}(\vec{R}) &= \bar{\phi}(\vec{R}) + p\bar{n}(\vec{R}), \\ \bar{n}(\vec{R}, \vec{R}') &= \bar{n}(\vec{R}, \vec{R}') + \bar{n}(\vec{R}) - \bar{n}(\vec{R}'). \end{aligned} \quad (\text{D22})$$

But, Eq. (D21) is quite sufficient for our purposes. If one uses the Villain form for V_0 , i.e., that in Eq. (D20), then

$$\bar{V}(\bar{\phi}) = -(1/2K)\phi^2 - \frac{1}{2} \ln(2\pi K).$$

The difference in form between (D19) and (D21) will completely disappear if one defines a new integration variable in (D21), namely

$$\bar{\theta}(\vec{R}) = (2\pi/p)\phi(\vec{R}).$$

In this way, we conclude that

$$Z(2\pi K, y_0, y_p) = Z(p^2/2\pi K, y_p, y_0)(p/2\pi K)^N, \quad (\text{D23})$$

with N being the number of sites. Equation (D23) is the duality result which we sought.

Note added in proof. A superfluid layer provides a possible experimental realization of the pure planar model [see Doniach (Phys. Rev. Lett. 31, 1450 (1973)], and also private communications in which he kindly points out this omission in our thinking [an early theoretical calculation can be found in W. Kane and L. P. Kadanoff, Phys. Rev. 155, 80 (1967)]. See also the experiments by Reppy (to be published). In magnetic systems see the experiments by Y. S. Karimov and Y. N. Novikov [Zh. Eksp. Teor. Fiz. Pis'ma Red. 19, 268 (1974) Sov. Phys.-JETP Lett. 19, 159 (1974)]. We wish to thank V. Pokrovsky for pointing out this last reference to us.

The reader may want to compare the results of this Migdal style recursion calculation with that of Lublin [Phys. Rev. Lett. 34, 568 (1975)], who obtains a single nontrivial fixed point. Both calculations have similar defects in that they do not handle vortex pairs in an accurate fashion.

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