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On the Theory of the Ising Model of Ferromagnetism*

GORDON F. NEWELL AND ELLIOTT W. MONTROLL

Institute for Fluid Dynamics and Applied Mathematics, University of Maryland, College Park, Maryland

1. INTRODUCTION

IN his doctors dissertation of 1925, Ising[1]† proposed a simple model of ferromagnetism which has been the subject of considerable investigation during the past fifteen years. The model is based upon the view that ferromagnetism is caused by an interaction between the spins of certain electrons in the atoms making up a crystal.

We must therefore associate with each particle of the crystal, a spin coordinate σ. We imagine the particles to be rigidly fixed in the lattice, either neglecting the vibrations of the crystal or assuming that they act independently of the spin configuration and can therefore be considered separately. Instead of adopting the accepted model and considering σ as a vector spin, we consider σ as a scalar quantity which can achieve either of two values $\sigma=\pm 1$. The value $\sigma=1$ corresponds to a spin state with the spin in some preassigned direction, and $\sigma=-1$ corresponds to a spin in the opposite direction. The spin is considered to be either "up or down."

The interaction energy between two particles located at the jth and kth lattice points and having spins σ_j and σ_k, respectively, is postulated to be

$$E_{jk}=\begin{cases}-J\sigma_j\sigma_k & \text{if } j \text{ and } k \text{ are nearest neighbors}\\ 0 & \text{otherwise.}\end{cases} \tag{1.1}$$

Thus, we postulate that only particles on nearest neighbor lattice points interact; that the energy is $-J$ if the nearest neighbors have the same spin and $+J$ if they have unlike spins. The zero of energy has been conveniently chosen as the average of these two. The constant J, which appears as a parameter, is a measure of the strength of this coupling and must be determined from the physical properties of the system. J will be positive for a ferromagnetic system and negative for an antiferromagnetic system.

In addition to this energy, we postulate that the particles can interact with an external magnetic field. A magnetic moment μ is assigned to each lattice point, and the energy of interaction of the jth particle with the field is chosen to be

$$E_H=-\mu H\sigma_j. \tag{1.2}$$

The thermodynamic and magnetic properties of a crystal which contains N lattice points can be determined from the partition function

$$Z=\sum_{\sigma_1=\pm 1}\cdots\sum_{\sigma_N=\pm 1}\exp\{\tfrac{1}{2}K\sum_{j,k=1}^{N}a_{jk}\sigma_j\sigma_k+\mu\mathfrak{H}\sum_{j=1}^{N}\sigma_j\}, \tag{1.3}$$

where

$$a_{jk}=\begin{cases}1 & \text{if } j \text{ and } k \text{ are nearest neighbors}\\ 0 & \text{otherwise,}\end{cases} \tag{1.4}$$

$$K=J/kT,\quad \mathfrak{H}=H/kT. \tag{1.5}$$

For example, the internal energy per particle is given by

$$\bar{E}=N^{-1}kT^2\partial\log Z/\partial T \tag{1.6}$$

and the magnetization per particle by

$$M=N^{-1}\partial\log Z/\partial\mathfrak{H}. \tag{1.7}$$

If the only reason for studying the Ising partition function (1.3) is to advance the theory of ferromagnetism, then undue attention has been paid to this problem considering that the spin interaction used is a scalar one and that the lattice distances are fixed and do not depend on spin orientation. Actually the widespread interest in the model is primarily derived from

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† References will be found under Bibliography at end of article.

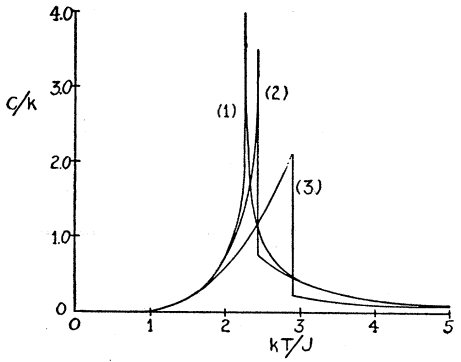

FIG. 1. The exact specific heat curve of the two-dimensional Ising lattice (curve 1) is compared with approximate curves of Kramer-Wannier (curve 2), and Bethe (curve 3) (see reference 3).

the fact that it is one of the simplest examples of a system of interacting particles which still has some features of physical reality in it. The model forms an excellent test case for any new approximate method of investigating systems of interacting particles. If a proposed method cannot deal with the Ising model, it can hardly be expected to be powerful enough to give reliable results in more complicated cases.

Underlying the interest in this problem as a study of some physical model, there rests the more fundamental question. Does the formalism of statistical mechanics predict phase transitions and, if so, how? We can hardly give satisfactory answers to these questions without examples. Even an artificial example is better than none. So far only a few examples have been successfully studied. One of these is the famous Einstein-Bose gas condensation and another is Onsager's brilliant analysis of the two-dimensional Ising model. A third is the spherical model of cooperative phenomena. The model and not some mathematical approximation is in each case the sole cause of the phase transition represented mathematically by a singularity in some of the thermodynamic quantities.

Even though the Ising model is not considered to be a very realistic model of ferromagnetism, it is equivalent to a very good model of a binary substitutional alloy and an interesting model of a gas or liquid.

It can easily be shown (see Appendix 1) that the grand partition function used to describe the order-disorder phenomenon in binary alloys has exactly the same mathematical form as that of an Ising ferromagnet in a magnetic field. An alloy with equal numbers of two atomic species is equivalent to the Ising model in the absence of an external field. The coordinate σ_j no longer represents a spin, but rather represents the two possible states of the jth lattice point. $\sigma_j=+1$ or -1 accordingly as the jth point is occupied by an atom of type 1 or type 2.

The "lattice" model of a gas or liquid is formed by dividing a given volume into a large number of cells of equal size, with each cell being occupied by either one or no molecules. An empty cell is represented by $\sigma=-1$ and a filled one by $\sigma=+1$. It is shown in Appendix 1 that the specific volume of a lattice gas is related to the magnetization of the Ising model.

The Ising model can also be related to a theory of adsorption of gases on surfaces.

This paper is a review of the work done on the Ising problem (and its equivalents) since the appearance of the comprehensive review of order-disorder phenomenon by Nix and Shockley.[2] Much of the emphasis in this period (and hence in this review) has been on the development of exact analytical expressions for thermodynamic quantities. It has been shown that critical phenomenon are not always accurately described by approximate theories.[3] For example, the critical temperature of the two-dimensional Ising problem is incorrectly given by approximate theories, as is the nature of the specific heat singularity. The exact specific heat curve derived by Onsager[4] is compared with the corresponding curves of various other theories in Fig. 1. It is to be noted that the form of the approximate curves at temperatures above the critical temperature are especially poor.

The thermodynamic properties of two-dimensional lattices of various sorts (with nearest neighbors interaction only) can now be derived by either of two methods. In the first, that used by Onsager, the partition function is expressed as the largest characteristic value of a certain matrix. This characteristic value was determined by Onsager using a complicated algebraic development. Through the use of spinors and the theory of Lie algebras, Kaufman[5,6] and van der Waerden (in an unpublished letter to Onsager, 1946) have simplified the Onsager analysis considerably and have given more motivation to the individual steps in his work. The second method, which has been developed recently by Kac and Ward[7] is based on the van der Waerden[8] combinational formulation of the partition function. The partition function is expressed in terms of the number of ways closed graphs with a given number of bonds can be constructed on a lattice. Finally a determinant is constructed such that each term in its expansion (by the definition of a determinant) corresponds to a closed graph. We shall discuss both of these methods in parts 2 and 4 of this paper.

To date no one has found exact expressions for (a) the partition function of a three-dimensional Ising lattice; (b) that of a two-dimensional lattice in a magnetic field; or (c) a two-dimensional lattice with interactions between next nearest neighbors as well as nearest neighbors. The first few terms in high and low temperature series for the partition functions of (a) and (b) will be reviewed in Sec. 7.

2. MATHEMATICAL FORMULATION OF PROBLEM

In this section we express the partition function (1.3) in several alternative forms so that we can proceed with both the matrix and combinational analysis of the two-dimensional lattices.

2.1 Matrix Formulation

Here we relate the partition function of the Ising model to the largest characteristic value of a certain matrix whose elements are functions of T and the coupling constants.[9–12] We first derive the required relations for a more general class of system than the Ising model and finally specialize to it.

We consider a lattice consisting of m "layers" of particles. We represent the possible states of the jth layer by ν_j. For a one-dimensional nearest neighbor system such as the Ising problem, the "layers" will be individual particles and ν_j will be described by the internal coordinates σ_j of these particles. For a two-dimensional lattice the "layers" will be rows of particle and ν_j will be given by the set of internal coordinates σ_k of all lattice points in the jth row. For a three-dimensional lattice, the "layer" will be a layer in the usual sense and ν_j will be given by the set of all internal coordinates of that layer.

In general the word "layer" will be used to describe any subdivision of the lattice into small (usually identical) parts but in such a way that the jth layer interacts only with the $j-1$th and $j+1$th layers. If there are interactions between nearest and next nearest lattice points, we choose a layer, in the one-dimensional case for example, to be a pair of particles which interacts only with a neighboring pair of particles. If the lattice has forces of finite range, we can still consider it a type of nearest neighbor system but with interacting units containing more than one lattice points.

The energy of such a system we assume to be of the form

$$V=\sum_{j=1}^{m-1} V(\nu_j, \nu_{j+1})+\sum_{j=1}^{m} V(\nu_j), \tag{2.1}$$

where $V(\nu_j, \nu_{j+1})$ is the interaction energy between the jth and $j+1$th layers, and $V(\nu_j)$ is the internal energy of the jth layer.

It is mathematically convenient to assign periodic boundary conditions by inserting an additional interaction $V(\nu_m, \nu_1)$ between the mth and first layers. Physically this is equivalent to bending the lattice into a ring, but, as one takes a larger and larger system, such surface effects become negligible.

The partition function of a system in which the mth layer is connected to the first is

$$Z=\sum_{\nu_1}\cdots\sum_{\nu_m}\prod_{j=1}^{m} P(\nu_j, \nu_{j+1}), \tag{2.2}$$

where

$$P(\nu_j, \nu_{j+1})=\exp\{-[V(\nu_j, \nu_{j+1})+\tfrac{1}{2}V(\nu_j)+\tfrac{1}{2}V(\nu_{j+1})]/kT\}. \tag{2.2a}$$

Notice that P is a function of a two-parameter set of numbers ν_j and ν_{j+1}, which we shall assume to be discrete. We may consider $\mathbf{P}$ as a matrix with matrix elements $P(\nu_j, \nu_{j+1})$ between the states ν_j and ν_{j+1}. Because of the particular choice of $\mathbf{P}$ with $\frac{1}{2}V(\nu_j)$ and $\frac{1}{2}V(\nu_{j+1})$, $\mathbf{P}$ is a symmetric matrix. It is sometimes convenient but not necessary to make $\mathbf{P}$ symmetric. We could have defined a matrix

$$P'(\nu_j, \nu_{j+1})=\exp\{-[V(\nu_j, \nu_{j+1})+V(\nu_j)]/kT\} \tag{2.2b}$$

which would substitute for $\mathbf{P}$ in (2.2).

One recognizes that the sum over ν_j in (2.2) yields simply the conventional matrix product. Indeed considering $\mathbf{P}$ as a matrix

$$Z=\text{trace}\,(\mathbf{P}^m)=\sum_j \lambda_j{}^m, \tag{2.3}$$

where $\{\lambda_j\}$ is the set of characteristic values of the matrix $\mathbf{P}$.

We are not usually interested in knowing Z exactly for arbitrary m but only

$$\lim_{m\to\infty} m^{-1}\log Z=\log\lambda_{\max}+\lim_{m\to\infty} m^{-1}\log[1+\sum_{j\geq 2}(\lambda_j/\lambda_{\max})^m].$$

Here we have factored out the largest eigenvalue $\lambda_{\max}$ and numbered the λ_j so that $\lambda_{\max}$ is λ_1. If $\lambda_{\max}$ is nondegenerate then $\lambda_j/\lambda_{\max}<1$ and $(\lambda_j/\lambda_{\max})^m\to 0$. Thus, the second term above does not contribute. Even if $\lambda_{\max}$ is degenerate or asymptotically degenerate as $m\to\infty$, the second term will not contribute unless the number of degenerate states or asymptotically degenerate states increase exponentially with m. To our knowledge such a situation has, however, not arisen in any applications; thus

$$\lim_{m\to\infty} m^{-1}\log Z=\log\lambda_{\max}. \tag{2.4}$$

Let us now find explicitly the matrix $\mathbf{P}$ for the one- and two-dimensional Ising lattice (without a magnetic field).

In the one-dimensional case ν_j is simply σ_j and

$$V(\sigma, \sigma')=-J\sigma\sigma', \quad V(\sigma)=0.$$

Hence (since $\sigma^2=1$),

$$P(\sigma, \sigma')=\exp(K\sigma\sigma')=(1+u\sigma\sigma')\cosh K,$$
$$u=\tanh K,$$

so that

$$\mathbf{P}=\begin{pmatrix} e^K & e^{-K} \\ e^{-K} & e^K \end{pmatrix}=e^K\mathbf{I}+e^{-K}\mathbf{C}, \tag{2.5}$$

where $\mathbf{I}$ is the identity matrix and

$$\mathbf{C}=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{C}^2=\mathbf{I}.$$

Another form for $\mathbf{P}$ is

$$\mathbf{P}=(2\sinh 2K)^{\frac{1}{2}}\exp(K^*\mathbf{C}), \tag{2.6a}$$

where K^* is defined by

$$\tanh K^* = e^{-2K}, \quad \sinh 2K^* \sinh 2K = 1. \tag{2.6b}$$

Since the characteristic vectors of $\mathbf{C}$ are

$$\psi_1 = 2^{-\frac{1}{2}}\begin{pmatrix}1\\1\end{pmatrix} \quad \text{and} \quad \psi_2 = 2^{-\frac{1}{2}}\begin{pmatrix}1\\-1\end{pmatrix},$$

and every vector is a characteristic vector of the identity matrix

$$\lambda_1 = 2\cosh K, \quad \lambda_2 = 2\sinh K,$$
$$Z = (2\cosh K)^m + (2\sinh K)^m \sim (2\cosh K)^m. \tag{2.7}$$

The thermodynamic and magnetic properties of a one-dimensional Ising lattice are discussed in Appendix 2.

The matrix associated with the two-dimensional Ising lattice is much more complex. In the absence of a magnetic field, the potential energy $V(\nu)$ is the potential energy of interaction between neighboring particles in the same row. If n is the number of particles per row,

$$V(\nu) = -J' \sum_{j=1}^{n} \sigma_j \sigma_{j+1}.$$

This includes an interaction $\sigma_n \sigma_{n+1}$. For the purposes of obtaining greater symmetry, we impose periodic boundary conditions also in the rows by defining $\sigma_{n+1} \equiv \sigma_1$. Physically this means that the lattice is wrapped on a torus; it is periodic along both the rows and columns. We again anticipate that this device should have a negligible effect upon the physical properties of the system.

The potential energy between two neighboring rows is

$$V(\nu, \nu') = -J \sum_{j=1}^{n} \sigma_j \sigma_j'.$$

We have introduced here two different coupling constants J and J'. We thus consider the possibility that the lattice will have stronger couplings in one direction than the other. Wherever no additional complications arise from such a generalization we shall continue to consider $J \neq J'$ even though this generalization leads to no very interesting physical effects that $J = J'$ does not show.

Using (2.2b), we obtain

$$P'(\nu, \nu') = \exp\left(K \sum_{j=1}^{n} \sigma_j \sigma_{j+1} + K' \sum_{j=1}^{n} \sigma_j \sigma_j'\right); \tag{2.8}$$

$\mathbf{P}'$ is a matrix of dimension 2^n. A state ν is described by the values of $\sigma_1, \sigma_2, \cdots, \sigma_n$ with $\sigma_j = \pm 1$.

$\mathbf{P}'$ can be put into a more convenient form by factoring it into the product of simpler matrices.[3] We first make use of the following simple fact. If $(V_2)_{\nu\nu''}$ is a diagonal matrix with diagonal elements $(V_2)_\nu$,

$$(V_2)_{\nu\nu''} = (V_2)_\nu \delta_{\nu\nu''}$$

and $(V_1')_{\nu\nu'}$ any arbitrary matrix, then

$$(V_2 V_1')_{\nu\nu'} = \sum_{\nu''} (V_2)_\nu \delta_{\nu\nu''} (V_1')_{\nu''\nu'} = (V_2)_\nu (V_1')_{\nu\nu'}.$$

Notice that $\mathbf{P}'$ is of this form if we write

$$\mathbf{P}' = \mathbf{V}_2 \mathbf{V}_1',$$

$$(V_2)_{\nu\nu'} = \delta_{\sigma_1\sigma_1'} \delta_{\sigma_2\sigma_2'} \cdots \delta_{\sigma_n\sigma_n'} \exp\left(K' \sum_{j=1}^{n} \sigma_j \sigma_{j+1}\right), \tag{2.9}$$

$$(V_1')_{\nu\nu'} = \exp\left(K \sum_{j=1}^{n} \sigma_j \sigma_j'\right) = \prod_{j=1}^{n} \exp(K \sigma_j \sigma_j').$$

Each of these two matrices can also be simplified. We notice that $\mathbf{V}_1$ is simply the nth direct product of the 2×2 matrices for the one-dimensional problem [Eq. (2.5)]. For some remarks about direct products see Appendix 3.

$$\mathbf{V}_1' = (e^K \mathbf{I} + e^{-K}\mathbf{C}) \times (e^K \mathbf{I} + e^{-K}\mathbf{C}) \times \cdots \times (e^K \mathbf{I} + e^{-K}\mathbf{C})$$
$$= (2\sinh 2K)^{n/2} \exp(K^*\mathbf{C}) \times \exp(K^*\mathbf{C}) \times \cdots \times \exp(K^*\mathbf{C}).$$

If we define

$$\mathbf{C}_j = \mathbf{I} \times \mathbf{I} \times \cdots \times \mathbf{I} \times \mathbf{C} \times \mathbf{I} \times \cdots \times \mathbf{I} \tag{2.10}$$

with $\mathbf{C}$ in the jth factor, then

$$\mathbf{V}_1' = (2\sinh 2K)^{n/2} \prod_{j=1}^{n} \exp(K^* \mathbf{C}_j).$$

To simplify $\mathbf{V}_2$ we define a matrix

$$\mathbf{s} = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix} \tag{2.11}$$

and

$$\mathbf{s}_j = \mathbf{I} \times \mathbf{I} \times \cdots \times \mathbf{I} \times \mathbf{s} \times \mathbf{I} \times \cdots.$$

$\mathbf{s}_j$ is also a diagonal matrix with diagonal elements $+1$ if the state ν has $\sigma_j = +1$ and -1 if $\sigma_j = -1$. In terms of these matrices $\mathbf{s}_j$, we may write

$$\mathbf{V}_2 = \exp\left(K' \sum_{j=1}^{n} \mathbf{s}_j \mathbf{s}_{j+1}\right). \tag{2.12}$$

If we define

$$\mathbf{V}_1 = \exp\left(K^* \sum_{j=1}^{n} \mathbf{C}_j\right), \tag{2.13}$$

then

$$\mathbf{P}' = (2\sinh 2K)^{n/2} \mathbf{V}_2 \mathbf{V}_1.$$

The symmetric matrix $\mathbf{P}$ of (2.2a) can be deduced in the same manner to be

$$\mathbf{P} = (2\sinh 2K)^{n/2} \mathbf{V}_2^{\frac{1}{2}} \mathbf{V}_1 \mathbf{V}_2^{\frac{1}{2}}.$$

This differs from $\mathbf{P}'$ only by a similarity transformation by $\mathbf{V}_2^{\frac{1}{2}}$. Since neither the eigenvalues nor $Z = \text{trace } \mathbf{P}^m$ are altered by a similarity transformation to $\mathbf{P}$, we again confirm that we can use either $\mathbf{P}$ or $\mathbf{P}'$.

It is easy to generalize the form of $\mathbf{P}'$ to include an interaction with a magnetic field. In this case

$$\mathbf{P}'=(2\sinh 2K)^{n/2}\mathbf{V}_3\mathbf{V}_2\mathbf{V}_1, \tag{2.14}$$

$$\mathbf{V}_3=\exp(\mu\mathfrak{H}\sum_{j=1}^{n}\mathbf{s}_j).$$

We shall return to this matrix method again in Secs. 3.2 and 4.

By imposing slightly different boundary conditions, Kramers and Wannier[9] showed that one could also formulate this problem with a different matrix. Whereas the matrix $\mathbf{P}$ represents the contribution to Z of an entire row of the lattice, we can define a matrix $\mathbf{M}$ which represents the contribution of only a single particle.

To do this we must choose "screw" boundary conditions. Instead of imposing an interaction between the nth and first particles of the same row (periodic boundary conditions), we let the nth particle of one row interact with the first particle of the next row. Thus the rows are connected to each other as on a screw. To eliminate any loose ends on the lattice, we connect the nth particle of the last (mth) row to the first particle of the first row. The rows of the lattice thus have the geometry of a helix with its ends connected to form a torus.

With this geometry, it is natural to number the particles consecutively from 1 to $n\times m$. The interaction between particles in the same column appears then as

$$-J\sigma_j\sigma_{j+n}$$

and that in the rows as

$$-J'\sigma_j\sigma_{j+1}.$$

The partition function for this system is

$$Z=\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_{nm}=\pm1}\exp[K'\sum_{j=1}^{nm}\sigma_j\sigma_{j+1}+K\sum_{j=1}^{nm}\sigma_j\sigma_{j+n}] \tag{2.15}$$

with

$$\sigma_{nm+j}\equiv\sigma_j.$$

We wish to represent this as a matrix product in such a way that the jth factor contributes the terms depending upon σ_j. Since the contribution of σ_j depends upon the state of the $j-n$th particle, it is still necessary to have a matrix of dimension 2^n. The physical significance of this matrix will be more apparent after the discussions of Sec. 3.2.

The appropriate matrix is defined by

$$M_{\sigma_n'\cdots\sigma_1',\sigma_n\cdots\sigma_1}$$
$$\equiv\exp(K'\sigma_n'\sigma_n)\exp(K\sigma_n'\sigma_1)\prod_{j=1}^{n-1}\delta(\sigma_j'-\sigma_{j+1}). \tag{2.16}$$

The matrix connects the state $\sigma_1,\cdots,\sigma_n$ to the state $\sigma_n',\cdots,\sigma_1'$. Most of the matrix elements, however, are zero. They are nonzero only if $\sigma_1'=\sigma_2$, $\sigma_2'=\sigma_3$, $\cdots$, $\sigma_{n-1}'=\sigma_n$. σ_n' is the only "free" index and may be interpreted to be σ_{n+1}. The matrix thus may be considered to connect the states $\sigma_1,\cdots,\sigma_n$ to the state $\sigma_2,\cdots,\sigma_{n+1}$ and to produce a factor appropriate to describe the energy of interaction between σ_{n+1} and $\sigma_1,\cdots,\sigma_n$. Since the indices are dummy indices, we can also interpret it as connecting the state $\sigma_{j+1},\cdots,\sigma_{j+n}$ to the states $\sigma_{j+2},\cdots,\sigma_{j+n+1}$.

Regardless of how one interprets the matrix $\mathbf{M}$ one observes from (2.15) and (2.16) that

$$Z=\mathrm{trace}\mathbf{M}^{nm}=\sum_{j=1}^{2^n}\lambda_j{}^{nm}. \tag{2.17}$$

One can also express the matrix $\mathbf{M}$ in terms of simpler matrices. In addition to the matrices already defined by Eqs. (2.5), (2.10), and (2.11), we define a matrix

$$R_{\sigma_1'\cdots\sigma_n',\sigma_1\cdots\sigma_n}\equiv\delta(\sigma_1'-\sigma_2)\delta(\sigma_2'-\sigma_3)\cdots$$
$$\times\delta(\sigma_{n-1}'-\sigma_n)\delta(\sigma_n'-\sigma_1). \tag{2.18}$$

This matrix merely cyclically permutes the n particles of one row. Thus, $\mathbf{R}^n=\mathbf{I}$. One easily deduces that[13]

$$\mathbf{M}=(2\sinh 2K)^{\frac{1}{2}}\exp(K'\mathbf{s}_n\mathbf{s}_{n-1})\exp(K^*\mathbf{C}_n)\mathbf{R}. \tag{2.19}$$

Loosely speaking one can say that the operator $\mathbf{R}$ turns the lattice from one point to the next, and the other factors introduce the appropriate Boltzmann factor for the new point.

Following the procedure above, one can also easily construct matrices appropriate for the three-dimensional lattice. One can in fact do this in at least three ways. By appropriate choice of boundary conditions, one can form matrices which represent the contribution to Z of an entire layer, a single row or a single particle in a manner analogous to that used in deducing $\mathbf{P}$ and $\mathbf{M}$ for the two-dimensional lattice. The matrices will in each case be of dimension 2^{lm} if the layers are l particles wide and m particles deep.

The reader may wish to try this as an exercise. Since there has been little progress toward solution of these matrices, we shall not discuss them in any detail.

2.2 Combinational Formulation

At high temperatures and zero magnetic field, an expansion of the partition function in powers of $\tanh^2 K$ can be constructed by counting the number of ways of forming closed paths of given length along the bonds of the lattice. This formulation of the problem was suggested by van der Waerden.[8] (Kirkwood[14] gave the first systematic approach to the order-disorder problem.)

We modify (1.3) slightly to read

$$Z=\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_N=\pm1}\prod_{n.n.}\exp(K\sigma_j\sigma_k).$$

The product over "*n.n.*" denotes the product over values of j and k corresponding to nearest neighbor

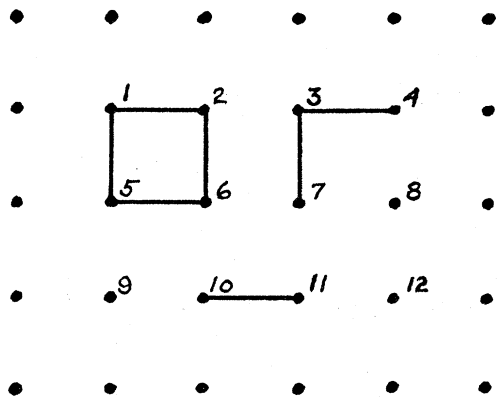

FIG. 2. An example of a graph connecting points of the lattice with no bond repeated.

points of the lattice. We next write[15]

$$\exp K\sigma_j\sigma_k = (1+u\sigma_j\sigma_k)\cosh K \qquad u=\tanh K \tag{2.20}$$

to give

$$Z=(\cosh K)^{cN/2}\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_N=\pm1}\prod_{n.n.}(1+u\sigma_j\sigma_k),$$

where c is the number of nearest neighbors of a given particle and $Nc/2$ is the total number of interactions. For the square lattice $c=4$. The formalism to this point, however, is also applicable to other lattices. For three-dimensional simple cubic lattices $c=6$.

We next expand the product

$$Z=(\cosh K)^{cN/2}\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_N=\pm1}\{1+u\sum_{n.n.}\sigma_i\sigma_j + u^2\sum_{n.n.}(\sigma_i\sigma_j)\sum_{n.n.}(\sigma_k\sigma_l)+\cdots\}. \tag{2.21}$$

The coefficient of u^l is the sum of products of $2l$ σ's. The σ's occur in pairs corresponding to nearest neighbors, and no such pair is to occur twice in the same product (by the simple rules of the expansion).

To obtain a convenient geometrical picture, we can associate with a pair $\sigma_i\sigma_j$, a bond connecting the neighbors i and j, and with the pair $\sigma_k\sigma_l$ another bond connecting k and l, etc. With each product of $2l$ σ's, we associate a "graph" or set of l bonds. Since pairs occur at most once in a given product, no bond is to appear more than once in the same graph. In Fig. 2 we have drawn the graph associated with the term

$$(\sigma_1\sigma_2)(\sigma_3\sigma_4)(\sigma_1\sigma_5)(\sigma_2\sigma_6)(\sigma_3\sigma_7)(\sigma_5\sigma_6)(\sigma_{10}\sigma_{11}).$$

Since

$$\sum_{\sigma=\pm1}\sigma=0, \qquad \sum_{\sigma=\pm1}\sigma^2=2, \tag{2.22}$$

the only terms of (2.21) which contribute to Z are those in which each σ_i occurs to an even power. Since a bond can appear only once in a term, σ_i can occur at most c times or 4 times for the square lattice. This also means that the only graphs of interest are those in which each lattice point is connected by an even number of bonds (0, 2, or 4 for the square net). We conclude from this that all contributing graphs must be the superposition of simple closed polygons (polygons with no loops) having no common sides. Also the converse is true; there is a nonzero term in Z for each such superposition of simple closed polygons. (Such polygons may have common points however.) For simplicity we shall call such graphs, "closed graphs" (Fig. 3).

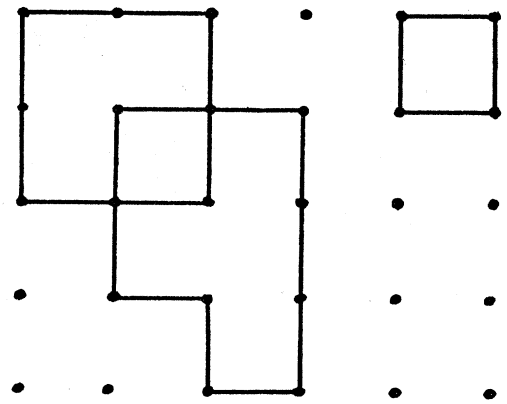

FIG. 3. An example of a closed graph in which each point is connected by 0, 2, or 4 bonds.

Each closed graph of m bonds contributes to Z a term $2^N u^m$ after summing over σ_1 to σ_N. Hence, the partition can be written as

$$Z=2^N(\cosh K)^{Nc/2}\sum_r n(r)\tanh^r K, \tag{2.23}$$

where $n(r)$ is the number of closed graphs of r bonds which can be constructed on the lattice. $n(0)=1$ and in a square or cubic lattice $n(r)=0$ unless r is even.

Equation (2.23) can be generalized to include more complex interactions. If, for example, K represents the interaction between lattice points of a square lattice which lie in the same row and K' that between pairs in the same column, then

$$Z=(\cosh K\cosh K')^N 2^N\sum_{r,s}n(r,s)\tanh^r K\tanh^s K', \tag{2.24}$$

where $n(r,s)$ is the number of closed graphs with $r+s$ bonds, r in the horizontal and s in the vertical direction.

Equation (2.24) is the starting point of the combinational derivation of the two-dimensional Onsager formulas by Kac and Ward.[7]

It is also possible to obtain a low temperature expansion of Z which involves a somewhat different combinational problem (except in the two-dimensional square lattice in which, as we shall see in the next section, both high and low temperature counting procedures are equivalent).

For any given state of the system, let

N_1 = number of σ's that are $+1$,

N_{12} = number of unlike pairs of nearest neighbors.

Since $Nc/2$ is the total number of nearest neighbor pairs (as before, c is the number of nearest neighbors for one lattice point),

$$\sum_{n.n.} \sigma_i\sigma_j = (Nc/2-N_{12})(+1)+N_{12}(-1) = Nc/2-2N_{12},$$

$$\sum_{i=1}^{N} \sigma_i = N_1(+1)+(N-N_1)(-1) = N-2N_1.$$

If $g(N, N_1, N_{12})$ is the number of ways a given N_1 and N_{12} can be chosen on a lattice of N points, then

$$Z = \exp(N\mathfrak{H}\mu)\exp(NcK/2)\sum_{N_1,N_{12}} g(N, N_1, N_{12}) \times \exp(-2KN_{12}-2\mathfrak{H}\mu N_1). \quad (2.25)$$

In the absence of a magnetic field

$$Z = e^{NcK/2}\sum_r m(r)e^{-2Kr}, \quad (2.26)$$

where $m(r)$ is the number of ways r pairs of unlike neighbors can be arranged on a lattice.

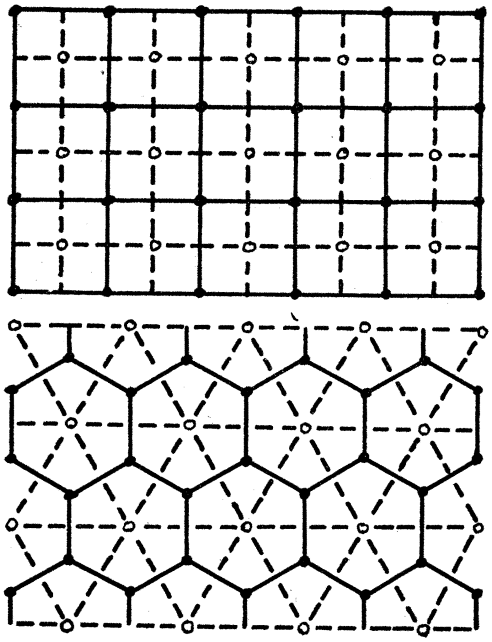

FIG. 4. A square lattice (above) hexagonal lattice (below) are illustrated by solid lines along the bonds joining nearest neighbors. The dual lattice, formed by bisecting the bonds of the original lattice, is similarly illustrated by the broken lines.

High and low temperature expansions based upon (2.24) and (2.25) will be discussed further in Sec. 7.

3. PHASE TRANSITIONS

3.1 Duality Theorems

Through certain symmetries in the matrix approach to the Ising problem, Kramers and Wannier[9] derived an interesting relation between the high and low temperature expansions for the partition function of a square lattice. Although this relation was not powerful enough to yield an analytic expression for the partition function, it was sufficient to locate the Curie point if we assume one existed. Onsager (see Wannier[3]) generalized this relation by a topological argument to a wider class of two-dimensional lattices.

Onsager constructed a "dual lattice" to a given lattice by drawing a bond through each bond of the original lattice and connecting these new bonds at points in the center of each unit cell of the original lattice. In Fig. 4 is shown the square lattice (solid line) and its dual (dotted lines) also a hexagonal lattice and its dual which is a triangular lattice. Since the dual of the square is also a square lattice, we describe it as self-dual.

To derive Wannier's duality theorem between the high and low temperature behavior by geometrical arguments, we consider the square lattice of Fig. 5. We represent lattice points with $\sigma=+1$ by dots and those with $\sigma=-1$ by $\times$. Each bond joining unlike spins is bisected by a bond of the dual lattice. It is clear that (except perhaps for points near the boundary of the lattice) this set of bonds on the dual lattice forms a closed graph of the type described in the preceeding section and that the number of bonds of the dual lattice is exactly the number of unlike pairs of the original lattice. Indeed there is a one-to-one correspondence between arrangements of bonds connecting unlike σ's on the original lattice and closed graphs of the same number of bonds on the dual lattice.

By comparing the definitions of $n(r)$ (2.23) and $m(r)$ (2.26), we notice that

$$\begin{aligned} m(r) &= n_D(r), \\ m_D(r) &= n(r), \end{aligned} \quad (3.1)$$

where the subscript D refers to functions on the dual lattice. These relations hold for other two-dimensional lattices as well as the square lattice used in the illustration. In the case of the square lattice, we can discard the subscript D because the dual lattice is the same as the original lattice.

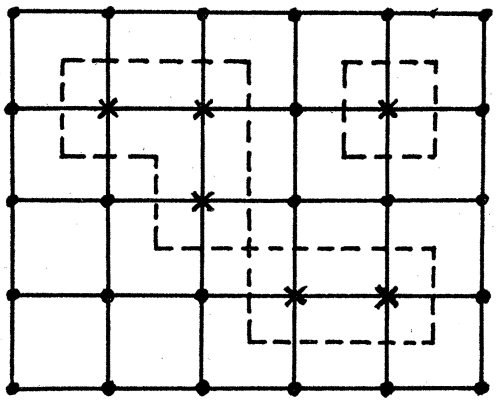

FIG. 5. An example to show that each configuration of "up spins" denoted by dots and "down spins" denoted by x can be described by a closed graph on the dual lattice. The bonds of the closed graph bisect bonds of the original lattice joining unlike pairs of spins.

Using the definition of K^* given in (2.6b) and the relations (3.1), we see that the expressions (2.26) and (2.23) for Z are related as follows:

$$\begin{aligned} Z(K)e^{-NcK/2} &= \sum_r m(r)e^{-2Kr} \\ &= \sum_r n_D(r)\tanh^r K^* \\ &= Z_D(K^*)[2^{N_D}(\cosh K^*)^{N_D c_D/2}]^{-1}. \end{aligned}$$

Since there is a bond of the dual lattice to each bond of the original lattice, $N_D c_D/2 = Nc/2$. The above can be simplified somewhat to read

$$Z(K) = Z_D(K^*)2^{-N_D}(2\sinh 2K)^{Nc/4}. \tag{3.2}$$

A large value of K^* is associated with a small value of K by (2.6b). Hence the partition function of one lattice at a high temperature is related to the partition function of its dual at a low temperature and vice versa.

In a self-dual lattice such as the square lattice, (3.2) implies that if a singularity exists at a temperature $T = J/kK$, then another singularity exists at a temperature $T^* = J/kK^*(K)$. If, however, as is intuitively expected, only one singularity exists, it must occur at $T = T^*$. From (2.6b) we see that this critical point is given by

$$|\sinh 2K_c| = 1, \quad K_c = \pm 0.4407$$

(K_c will be positive if J is positive, negative if J is negative). Substituting $T = T_c$ into (3.2), we see that (3.2) is identically satisfied so that we know the singularity is not a discontinuity of Z.

The above arguments cannot be directly applied to either the triangular or hexagonal lattices since these lattices are not self-dual. It is possible, however, to locate the Curie point. Onsager (see Wannier[3]) found another quite different relation between the triangular and hexagonal lattices, the so-called star-triangle transformation derived in Appendix 4. This relates the low temperature behavior of the triangular lattice to the low temperature behavior of the hexagonal lattice. Using both the star triangle and the dual transformations, one obtains a relation between the low and high temperature behaviors of the triangular lattice (also the hexagonal lattice). Thus, we can use the same arguments as above to deduce the Curie points of each of these lattices, assuming that one such exists.

3.2 Long-Range Order

The Ising lattice has many very interesting properties that would not generally be classified as thermodynamics. If, in the lattice, we should fix the spin configuration of part of the system, we might ask what effect this has upon the system as a whole. If when we fix the spin of one particle, particles far away from the fixed spin show a preference for some definite spin direction, we say that the system has a long-range order. We describe a system as ordered if the spins show a strong tendency toward some organized pattern. In a ferromagnet, for example, the spins of an ordered state are predominantly in the same direction.

Ashkin and Lamb[16] showed that long-range order in a nearest neighbor system is associated with a degeneracy or asymptotic degeneracy of the largest eigenvalue of the matrix $\mathbf{P}$ defined in Sec. 2.1.

Imagine that we build a large crystal by starting with a single layer and add new layers one at a time to the existing configuration. Suppose we should fix the state ν_0 of the original layer or, to be more general, suppose we assign a probability distribution $p_0(\nu_0)$ to the states ν_0.

We next add to the zero layer, the first layer of particles. Let $p_1(\nu_1)$ be the probability that the first layer is in the state ν_1 if the zero layer is distributed according to $p_0(\nu_0)$. We see that the equilibrium distribution is given by

$$p_1(\nu_1) = \frac{\sum_{\nu_0} \exp\{-[V(\nu_1,\nu_0)+V(\nu_1)]/kT\}p_0(\nu_0)}{\sum_{\nu_0,\nu_1} \exp\{-[V(\nu_1,\nu_0)+V(\nu_1)]/kT\}p_0(\nu_0)}. \tag{3.3a}$$

The denominator is a normalization factor chosen so that $\sum_{\nu_1} p_1(\nu_1) = 1$. The numerator is the sum over all ν_0 of the Boltzmann factor of the state ν_1 if the neighboring state is ν_0 times $p_0(\nu_0)$. In a similar manner, we see that since $p_2(\nu_2)$ depends only upon the state ν_1,

$$p_2(\nu_2) = \frac{\sum_{\nu_1} \exp\{-[V(\nu_2,\nu_1)+V(\nu_2)]/kT\}p_1(\nu_1)}{\sum_{\nu_2,\nu_1} \exp\{-[V(\nu_2,\nu_1)+V(\nu_2)]/kT\}p_1(\nu_1)}$$

$$= \frac{\sum_{\nu_1,\nu_0} \exp\{-[V(\nu_2,\nu_1)+V(\nu_1,\nu_0)+V(\nu_2)+V(\nu_1)]/kT\}p_0(\nu_0)}{\sum_{\nu_2,\nu_1,\nu_0} \exp\{-[V(\nu_2,\nu_1)+V(\nu_1,\nu_0)+V(\nu_2)+V(\nu_1)]/kT\}p_0(\nu_0)}. \tag{3.4a}$$

In general, we find

$$p_m(\nu_m) = \frac{\sum_{\nu_{m-1}}\cdots\sum_{\nu_0} \exp\{-\sum_{j=1}^{m}[V(\nu_j)+V(\nu_j,\nu_{j-1})]/kT\}p_0(\nu_0)}{\sum_{\nu_m}\cdots\sum_{\nu_0} \exp\{-\sum_{j=1}^{m}[V(\nu_j)+V(\nu_j,\nu_{j-1})]/kT\}p_0(\nu_0)}. \tag{3.5a}$$

This procedure of adding one layer of particles at a time describes a Markov process. The probability distribution of the mth layer depends only upon the state of the $m-1$th layer. The usual theory of Markov processes is ideally suited to the analysis of this type of system.

We can simplify considerably the notation of Eqs. (3.3a) to (3.5a) by considering $\mathbf{p}_j$ to be a vector with components $p_j(\nu_j)$, $\mathbf{I}$ a vector with unit component for each state ν, and $\mathbf{P}'$ the matrix defined in Eq. (2.2b). The above equations can then be written in the usual matrix notation

$$\mathbf{p}_1=\frac{\mathbf{P}'\cdot\mathbf{p}_0}{\mathbf{I}\cdot\mathbf{P}'\cdot\mathbf{p}_0}, \tag{3.3b}$$

$$\mathbf{p}_2=\frac{\mathbf{P}'\cdot\mathbf{p}_1}{\mathbf{I}\cdot\mathbf{P}'\cdot\mathbf{p}_1}=\frac{(\mathbf{P}')^2\cdot\mathbf{p}_0}{\mathbf{I}\cdot(\mathbf{P}')^2\cdot\mathbf{p}_0}, \tag{3.4b}$$

$$\mathbf{p}_m=\frac{\mathbf{P}'\cdot\mathbf{p}_{m-1}}{\mathbf{I}\cdot\mathbf{P}'\cdot\mathbf{p}_{m-1}}=\frac{(\mathbf{P}')^m\cdot\mathbf{p}_0}{\mathbf{I}\cdot(\mathbf{P}')^m\cdot\mathbf{p}_0}. \tag{3.5b}$$

The matrix $\mathbf{P}'$ is similar to the symmetric matrix $\mathbf{P}$ and thus has a set of eigenvalues λ_j and complete set of eigenfunctions ψ_j. We can expand $\mathbf{p}_0$ in a series of these ψ_j,

$$\mathbf{p}_0=\sum_j c_j\psi_j. \tag{3.6}$$

By definition of the λ_j and ψ_j,

$$\mathbf{P}'\psi_j=\lambda_j\psi_j.$$

Therefore, (3.5b) becomes

$$\mathbf{p}_m=[\textstyle\sum_j c_j\lambda_j{}^m\psi_j]/[\sum_j c_j\lambda_j{}^m(\mathbf{I}\cdot\psi_j)]. \tag{3.7}$$

We again order the eigenvalues so that $\lambda_1\geq\lambda_2\geq\lambda_3\cdots$, so that if $c_1\neq 0$,

$$\mathbf{p}_m=\frac{\psi_1+\sum_{j\geq 2}(\lambda_j/\lambda_1)^m c_j\psi_j/c_1}{(\mathbf{I}\cdot\psi_1)+\sum_{j\geq 2}(\lambda_j/\lambda_1)^m c_j(\mathbf{I}\cdot\psi_j)/c_1}. \tag{3.8}$$

If λ_1 is neither degenerate nor asymptotically degenerate as $m\to\infty$, $(\lambda_j/\lambda_1)^m\to 0$ and

$$\mathbf{p}_m\to\psi_1/(\mathbf{I}\cdot\psi_1) \quad \text{as} \quad m\to\infty.$$

This means that the distribution of layers far from the original layer are independent of the coefficients c_j which describe the distribution of the zero layer. $\mathbf{p}_m$ is independent of $\mathbf{p}_0$. If there is no degeneracy, there is no long-range order.

If, on the other hand, the largest eigenvalue were degenerate, for example if $\lambda_1=\lambda_2>\lambda_3\cdots$, then

$$\mathbf{p}_m\to[c_1\psi_1+c_2\psi_2]/[c_1(\mathbf{I}\cdot\psi_1)+c_2(\mathbf{I}\cdot\psi_2)].$$

The distribution of a layer arbitrarily far from the original layer still depends upon c_2 and c_1 which in turn depend upon $\mathbf{p}_0$. A degeneracy of the largest eigenvalue therefore implies the existance of long-range order.

The question of what matrices have degenerate largest eigenvalues becomes a significant one. There is in some cases a definite answer to this question. Frobenius proved that if all the matrix elements of a finite matrix are positive and nonzero, then the largest eigenvalue is nondegenerate.

The matrix elements of $\mathbf{P}'$ are indeed positive and nonzero. It follows then that if we are to have long-range order, it is necessary that the number of states ν be infinite or become infinite as $m\to\infty$. In a two-dimensional lattice such as the Ising lattice, we are interested in the properties of lattices in which the number of particles per row is of the same order of magnitude as the number of rows. If we let $m\to\infty$, we must also let the number of particles per row $n\to\infty$, and the λ_j will depend upon m in the sense that as we add new layers (rows) we also wish to add new particles to the layers. As $m\to\infty$, the number of states per row also becomes infinite. Frobenius' theorem thus does not apply to a lattice infinite in two or more directions but it does forbid long-range order in most (if not all) systems of interest which are infinite in only one direction.[11,17]

Just as the matrix $\mathbf{P}$ describes a Markov process that gives the distribution of the mth layer in terms of the distribution of the $m-1$th layer, the matrix $\mathbf{M}$ discussed near the end of Sec. 2.1 described a Markov process giving the distribution of the particles $j+1$ to $j+n$ in terms of the distribution of the particles j to $j+n-1$. Notice that the "screw" boundary conditions make it possible to generate a lattice by iterating the procedure of adding a single particle at a time. This is not true of the periodic boundary conditions because one must change this procedure of adding single particles when one has filled a row and starts a new row. One can also build a three-dimensional lattice by an iterative procedure of adding single particles.

Frobenius' theorem does not directly apply to the matrix $\mathbf{M}$ because not all matrix elements of $\mathbf{M}$ are nonzero. There are equivalent theorems which do apply, however.

4. THE TWO-DIMENSIONAL SQUARE LATTICE

The solution of the two-dimensional square Ising lattice in zero magnetic field has been obtained in several ways. No one has found a short cut to success. All these methods are quite lengthy and very tricky. It would hardly be appropriate to describe in detail here all the various procedures. We shall discuss only one combinational method and one algebraic method.

Although the original solution by Onsager[4] could be easily followed from step to step, the motivations and over-all plan were obscure. In Sec. 4.2, we shall attempt to give some of the key steps in this original formulation and to describe, as we see it, the motivations that lead from one step to the next. We have

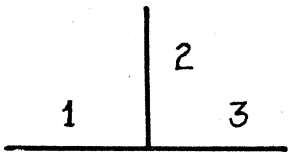

FIG. 6. Polygons containing the above type of connecting bonds are not to be counted.

chosen to discuss this method as the one example of an algebraic procedure not because we consider it the best, but because it affords an opportunity to present some ideas about it that have circulated privately but have never been published.

Interest in this problem reached a climax several years after Onsager's publication when Kaufman[5] described a simplified procedure based upon the theory of spinor representations of the rotation group. Her analysis was not only elegant but very clearly presented even to those not disciplined in the mathematical techniques employed. We shall have little to say about this procedure here for we see no way to add to or improve upon her analysis of the problem. For the details of this method, which in many ways still seems the most elegant despite more recent developments, we refer the reader to her original presentation.

Nambu[18] also independently discovered a method which was in principle very similar to Kaufman's.

Following these papers came a rapid sequence of minor refinements and applications. The method was also applied[13] to the matrix **M** discussed in Sec. 2 instead of the matrix **P** originally considered by Kaufman. It was also applied to other lattice types than the square lattice. Some of these supplementary calculations are discussed in Secs. 5 and 6.

In Sec. 4.1 we discuss one of the most recent techniques based upon the combinational procedure described in Sec. 2.2. This technique was discovered by Kac and Ward.[7] Domb has also solved the problem by obtaining recursion formulas for the $n(r)$ of Eq. (2.23). The method has not been published but has been described as being very lengthy.

The thermodynamic properties of the square lattice, based upon the results of Secs. 4.1 and 4.2, are summarized in Sec. 4.3.

4.1 Combinatorial Method

In this section we shall obtain an expression for the partition function of a two-dimensional square lattice by employing a combinatorial method, recently developed by Kac and Ward. This method is "elementary" in the sense that no spinors, Lie algebras, or other specialized algebraic techniques of the type used in the matrix method solution are required; however, it introduces some problems in topology that have not been rigorously solved. The starting point is the formula (2.24)

$$Z_{n,m}=(2\cosh K\cosh K')^{mn}\sum_{r,s}n(r,s)\tanh^{r}K\tanh^{s}K' \tag{4.1}$$

for the partition function of a square lattice of nm lattice points. Here $n(r,s)$ is the number of closed graphs with $r+s$ bonds, r in the horizontal and s in the vertical directions, which can be constructed on the lattice. The aim is to construct a matrix **A** whose determinant generates terms which are in a one-to-one correspondence with closed graphs on the lattice. We seek an **A** such that

$$Z_{n,m}=(2\cosh K\cosh K')^{mn}\det\mathbf{A}. \tag{4.2}$$

To see that there is a relation between determinants and closed graphs formed by connecting points on a lattice, let us examine the defining equation of the determinant of an Nth order matrix whose elements are A_{ij}

$$\det\mathbf{A}=\sum\pm A_{1k_1}A_{2k_2}\cdots A_{Nk_N}. \tag{4.3}$$

The set of indices $k_1, k_2, \cdots, k_N$ is some permutation of the indices $1, 2, \cdots, N$: the sum extends over all permutations, and the sign is $+$ or $-$ accordingly as the permutation is odd or even (it is even if an even number of interchanges of the indices $k_1, k_2, \cdots, k_N$ are required to put them in the order $1, 2, \cdots, N$).

It is well known in the theory of permutations that a given permutation can be expressed as a product of cyclic (see Carmichael, *Theory of Finite Groups*, Ginn and Company, 1937, p. 6) permutations, no two of which have a letter in common. Hence, the product of the A_{ik}'s in any term of (4.3) can be rearranged in the form

$$\pm(A_{i_1i_2}A_{i_2i_3}\cdots A_{i_{s(1)}i_1})(A_{j_1j_2}A_{j_2j_3}\cdots A_{j_{s(2)}j_1})\cdots\times(A_{l_1l_2}A_{l_2l_3}\cdots A_{l_{s(r)}l_1}). \tag{4.4}$$

The permutation $1, 2, 3\cdots N\rightarrow k_1, k_2, \cdots, k_N$ is thus described as a cyclic permutation of $i_1, i_2, i_3, \cdots, i_{s(1)}$ times a cyclic permutation of $j_1, j_2, j_3, \cdots, j_{s(2)}$, etc. The sign is $+$ or $-$ accordingly as the second indices

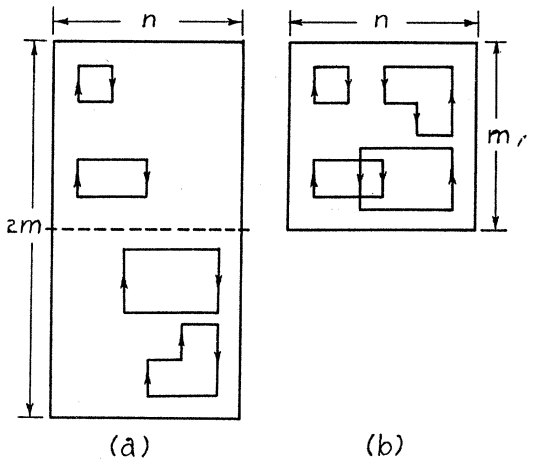

FIG. 7. Diagram (a) illustrates a closed graph on an $n\times 2m$ lattice, whereas (b) illustrates the corresponding oriented closed graph on an $n\times m$ lattice as described in the text.

$i_2, i_3, \cdots, i_{s(1)}, i_1; j_2 \cdots j_{s(2)}, j_1; \cdots$ represent an even or odd permutation of the first indices $i_1, i_2, \cdots i_{s(1)}$; $j_1, j_2 \cdots$. The number of interchanges necessary to bring $i_2, i_3, \cdots, i_{s(1)}, i_1$ into the order $i_1, i_2, i_3, \cdots, i_{s(1)}$ is $s(1)-1$ as one can easily see by interchanging successively the last and next to last numbers, the next to last and second from the last, etc. Thus, the sign is

$$(-1)^{s(1)-1}(-1)^{s(2)-1}(-1)^{s(3)-1}\cdots(-1)^{s(r)-1}. \quad (4.5)$$

We now ask in what way are the terms (4.4) similar to terms of the expansion of Z? First, we note that the cycles of (4.4) can be pictured as simple closed polygons. If the indices $i_1, i_2, \cdots$ represent points of a lattice and the matrix element $A_{i_1 i_2}$ represents a connection (bond) joining i_1 and i_2, then (4.4) is associated with the superposition of r simple closed polygons, one connecting the points $i_1, i_2, \cdots, i_{s(1)}$ another connecting $j_1, j_2, \cdots, j_{s(2)}$, etc.

This association is not quite what is required, for these polygons are somewhat different from the closed graphs of Z. The polygon $i_1, i_2, \cdots, i_{s(1)}$ has no point in common with $j_1, \cdots, j_{s(2)}$; they are *disjoint* polygons. As we saw in Sec. 2.2, the closed graphs of Z were not restricted to be the superposition of disjoint simple closed polygons but rather the superposition of simple closed polygons with no common sides.

This restriction on the polygons which generate Z suggests that perhaps we can establish a correspondence between the *sides* of these polygons and the indices of (4.4). Indeed, we can in this way come one step closer to success because the bonds of the simple closed polygons which generate the closed graphs are such that each bond joins another bond in a sequence which forms a cycle, but the same bond can appear in only one cycle. These are just the properties of the indices of (4.4).

In (4.4) we see that each bond is so represented as both a first and a last index of some A_{jk}, i.e., each bond is part of some polygon. In Z, however, not all points are parts of a graph. This can be remedied in a rather trivial manner. We interpret a cycle of order 1, an element A_{jj}, as indicating the absence of the jth bond in any polygon; the jth bond does not connect with anything except itself.

We have now established at least a one way correspondence between closed graphs of Z and terms of det **A**. There is for every closed graph a corresponding term in det **A**. There are many terms of det **A** which must be eliminated. The only nonzero matrix elements of $A_{jj'}$ would be those between two bonds j and j' having an end point in common; thus, most of the matrix elements would be zero.

There remain some very troublesome barriers to establishing a one-to-one correspondence between terms of Z and the terms of det **A**. The cycles $A_{i_1 i_2} A_{i_2 i_3} \cdots A_{i_{s(1)} i_1}$ and $A_{i_1 i_{s(1)}} \cdots A_{i_3 i_2} A_{i_2 i_1}$, which are inverses of each other, correspond to the same polygon. Also terms in the expansion of the determinant which correspond to cycles such as $A_{12}A_{21}$ or $A_{12}A_{23}A_{31}$ (see Fig. 6) are not related to any closed graphs on our lattice. The difficulty here seems to be rather fundamental. The terms of the determinant expansion seems to be more closely associated with oriented polygons, those traversed in a given direction. We must be able to distinguish between the two ends of a bond so that we can connect a new bond only to the "loose end" of its predecessor.

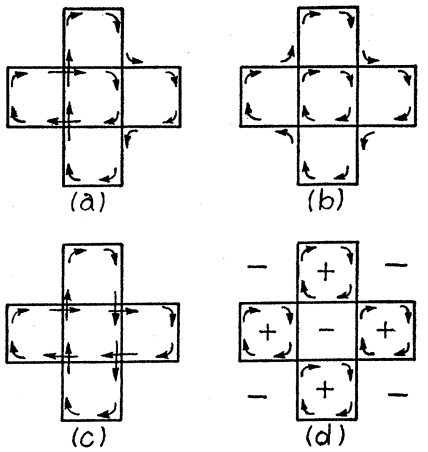

FIG. 8. The closed graph illustrated above can be oriented in many ways of which four examples are shown. Each is associated with a superposition of simple clockwise oriented polygons. If we first separate the space into two regions designated in (d) by + and −, then one can assign the unique orientation (d) to the closed graph by always choosing the bond orientation so that the + region is to the right of this direction.

Kac and Ward[7] overcame this hurdle by showing that the expansion of the partition function of an $n\times 2m$ lattice could be discussed in terms of oriented polygons on an $n\times m$ lattice. This correspondence is illustrated in Fig. 7. In the $n\times 2m$ lattice (a) upon which we draw the closed graphs that generate Z, we disregard those polygons which cross the center line. We are therefore really considering an $n\times 2m$ lattice consisting of two independent $n\times m$ lattices so that

$$Z_{n,2m} = Z_{nm}{}^2.$$

For any closed graph on the $n\times 2m$ lattice (7a), we construct oriented graphs on the $n\times m$ lattice (7b) in the following manner. We first adapt a rule for uniquely orienting the bonds of all graphs in Fig. 7a, a rule which is the same for both the upper and lower parts of Fig. 7a. Those graphs or parts of graphs in the upper half of (a) are transcribed on to (b). Those in the lower half of (a) are reflected across the center line and then transcribed on to (b). Kac and Ward suggested that the graphs in 7a be oriented "clockwise." This is a rule which is unambiguous if the graphs are simple closed polygons. It is also easily applied to the superposition of disjoint simple closed polygons each of which would be oriented clockwise.

Even though any closed graph is a superposition of simply closed polygons with no common sides, each of which would be oriented clockwise, the decomposition

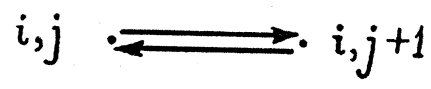

FIG. 9. An oriented polygon is not to contain this bond connection in which a right bond follows a left bond (or vice versa).

of a complex graph into its component polygons is not always unique (see, for example, Fig. 8). Since we want to count different graphs and not all ways of decomposing them, we must adapt some rule for extracting a unique decomposition.

Such a rule can be given for the graphs of interest by recalling the basis of the dual theorem in Sec. 3.1. This theorem is based upon the observation that the closed graphs on the dual lattice uniquely separate the lattice into two parts, one having spins in one direction (up or down) and the other part having the opposite spin (down or up). For any closed graph, it is possible to separate the space into two such parts which we desig- by + and − (see Fig. 8). One can then uniquely assign a direction of the bonds to be such that a + region is always to the right of the bond direction. The unique decomposition into simple closed polygons is achieved by choosing those polygons surrounding + regions and orienting them clockwise.

The problem of calculating Z has been described now as a problem of counting oriented closed graphs of the above type. The plan to write

$$Z_{n,2m}=Z_{n,m}{}^2=(2\cosh K\cosh K')^{2mn}\det\mathbf{A} \quad (4.6)$$

has been aided by the fact that det **A** does count oriented polygons, but we have achieved this goal at the expense of complicating the type of oriented graphs to be counted.

A bond in Fig. 7b can now appear at most twice, which means that it can no longer be associated in a one-to-one manner with the indices of (4.4). It will now be necessary to establish a two-to-one correspondence. Although the correspondence is not as elegant as one might have hoped, the scheme that finally leads to success is to associate directed bonds with the indices of (4.4).

A directed bond can be characterized by its direction and the lattice point toward which it is directed. Instead of numbering the bonds consecutively with a single index as in (4.4), it is convenient to replace these indices by a set of three parameters. The pair of variables (i, j) will be used to represent the row and column which locate the lattice point toward which the bond of interest is directed. The letter Γ will be used to represent the direction of the bond. Γ will have one of four values R, L, D, or U depending on whether the bond is directed to the right, left, up or down. The symbol

$$A(i, j, \Gamma; i', j', \Gamma') \quad (4.7)$$

will replace the matrix element $A_{j,k}$ of (4.4). This symbol will be associated with an ordered pair of bonds, the first of which is in the direction Γ, directed toward the lattice point (i, j) and the second, which will be interpreted to start at (i, j), proceeds in the direction Γ' toward the lattice point (i', j'). The matrix (4.7) will be of dimension 4 nm with 4 values of Γ for each of the nm lattice points.

Even though we have not yet completely established the desired one-to-one correspondence between unoriented graphs of Fig. 7a and the terms of det **A**, let us consider some properties that should be required of the matrix **A**.

As was indicated earlier in this section, in order to make the terms in the expansion of det **A** correspond only to oriented polygons on our lattice, we must set all matrix elements $A(i, j, \Gamma; i', j', \Gamma')$ equal to zero unless the point (i, j) can be connected by a bond in the direction Γ' to the point (i', j'). (The only exceptions to this are the diagonal elements which represent the bonds that are absent.) Of these possibilities we also wish to rule out those situations illustrated by Fig. 9 in which one step on a directed polygon is followed by a retracing of itself in the opposite direction. These rules can be summarized by the condition $A(i, j, \Gamma; i', j', \Gamma')=0$ unless

$$i=i', \quad j=j' \quad \text{and} \quad \Gamma=\Gamma', \quad (4.8a)$$
$$i=i', \quad j=j'+1, \quad \Gamma'=L, \quad \text{and} \quad \Gamma\neq R, \quad (4.8b)$$
$$i=i', \quad j=j'-1, \quad \Gamma'=R, \quad \text{and} \quad \Gamma\neq L, \quad (4.8c)$$
$$i=i'+1, \quad j=j', \quad \Gamma'=D, \quad \text{and} \quad \Gamma\neq U, \quad (4.8d)$$

or

$$i=i'-1, \quad j=j', \quad \Gamma'=U, \quad \text{and} \quad \Gamma\neq D. \quad (4.8e)$$

To make these conditions also valid at the boundary, we introduce periodic boundary conditions as in Sec. 2.1 by wrapping the lattice on a torus. We see then that the above conditions are invariant to rotations of the torus about either of its axes, i.e., to cyclic permutations of the indices $i\to i+1(m\to m+1=1)$ or $j\to j+1(n\to n+1=1)$. Indeed, we expect that the matrix elements themselves must be invariant to such transformations since these transformations leave the geometry of the lattice invariant.

In order to take advantage of the periodicity of the lattice, it is convenient to imagine the $4m\times n$th order matrix as consisting 4×4 blocks or as an $m\times n$th order matrix, the matrix elements of which are themselves 4×4 matrices. We use the convention that $\mathbf{A}(i, j; i', j')$ is for each i, j, i' and j' a 4×4 matrix with matrix elements $A(i, j, \Gamma; i', j', \Gamma')$. We realize that the matrices $\mathbf{A}(i, j; i', j')$ should be invariant to the cyclic transformations of the lattice, therefore

$$\mathbf{A}(i, j; i', j')=\mathbf{A}(0, 0; i'-i, j'-j). \quad (4.9)$$

In view of the conditions (4.8), the only independent matrices (4.9) that are not null matrices are $\mathbf{A}(0, 0; 0, 0)$, $\mathbf{A}(0, 0; 0, +1)$, $\mathbf{A}(0, 0; 0, -1)$, $\mathbf{A}(0, 0; +1, 0)$, and $\mathbf{A}(0, 0; -1, 0)$.

According to (4.8), $\mathbf{A}(0, 0, 0, 0)$ is a diagonal matrix, the diagonal elements of which correspond to the absence of a bond in a closed graph. All graphs are not weighted equally as seen by (4.1). The weight is assigned according to the number of vertical and horizontal bonds in the graph. Since the total number of possible bonds of a graph is fixed at $4nm$, this unequal weighting can be introduced either into the off diagonal matrices $\mathbf{A}(0, 0, 0; -1)$, etc., which in a certain sense count the number of such bonds or into $\mathbf{A}(0, 0, 0, 0)$ which counts the number of such bonds that are missing.

Another way of describing this freedom is to recall that multiplication of any row or column of a matrix by some constant changes the determinant into this constant times the original determinant. Thus, we can always replace a determinant, by a known multiple of another determinant all of whose diagonal elements are one.

We may, without any loss of flexibility, set

$$\mathbf{A}(0, 0, 0, 0) = \mathbf{I}_4, \tag{4.10a}$$

$\mathbf{I}_4$ being the 4×4 identity matrix, and then choose the other matrices so as to give the desired weights.

We know that for every horizontal bond that appears in a graph, (4.4) must contain a factor $x=\tanh K$. The number of such bonds will be equal to the number of times a matrix element from $\mathbf{A}(0, 0, 0, \pm1)$ appears in (4.4). To simplify notation we write

$$\mathbf{A}(0, 0, 0, \pm1) \equiv x\mathbf{A}(0, \pm1), \quad x=\tanh K, \tag{4.10b}$$

similarly

$$\mathbf{A}(0, 0, \pm1, 0) \equiv y\mathbf{A}(\pm1, 0), \quad y=\tanh K'. \tag{4.10c}$$

$\mathbf{A}(0, \pm1)$ and $\mathbf{A}(\pm1, 0)$ will now be matrices independent of x and y. They will depend only upon the geometry of the lattice.

Most of the matrix elements of these matrices will also vanish as a result of (4.8). $\mathbf{A}(0, 1)$ must in fact be of the form

$$\mathbf{A}(0, +1) = \begin{pmatrix} \gamma & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \beta & 0 & 0 & 0 \\ \alpha & 0 & 0 & 0 \end{pmatrix}, \tag{4.11a}$$

in which the matrix indices are taken in the order R, L, U, and D and γ, β, and α are as yet unspecified. Thus, γ corresponds to an element with $\Gamma=R$, $\Gamma'=R$; β corresponds to the element $\Gamma=U$, $\Gamma'=R$ and α to the element $\Gamma=D$, $\Gamma'=R$.

From $\mathbf{A}(0, -1)$, one uniquely determines also $\mathbf{A}(0, +1)$ and $\mathbf{A}(\pm1, 0)$. We ask that the matrix (4.7) be invariant to the interchange of x and y along with the transformation which rotates the positive horizontal direction into the positive vertical direction (a 90° rotation if the lattice were on a flat surface). Such a transformation preserves the topology of the graphs. Thus $A(i, j, \Gamma; i', j', \Gamma')$ must remain invariant if we simultaneously send $i\to j$, $j\to -i$, $i'\to j'$, $j'\to -i'$, $R\to U$, $U\to L$, $L\to D$, $D\to R$ and $x\leftrightarrow y$. It follows from this that

$$\mathbf{A}(+1, 0) = \begin{pmatrix} 0 & 0 & \alpha & 0 \\ 0 & 0 & \beta & 0 \\ 0 & 0 & \gamma & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{4.11b}$$

$$\mathbf{A}(0, -1) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \gamma & 0 & 0 \\ 0 & \alpha & 0 & 0 \\ 0 & \beta & 0 & 0 \end{pmatrix}, \tag{4.11c}$$

$$\mathbf{A}(-1, 0) = \begin{pmatrix} 0 & 0 & 0 & \beta \\ 0 & 0 & 0 & \alpha \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma \end{pmatrix}. \tag{4.11d}$$

One might be tempted to also make $\mathbf{A}$ invariant to reflections. Although it is true that Z is invariant to reflections, the topology of the oriented polygons is not invariant; a reflection takes a clockwise polygon into a counterclockwise polygon. $\mathbf{A}$ will in fact not be invariant to reflections. α corresponds to a counterclockwise turn of $\pi/2$, β to a clockwise turn, and γ to no turn of connecting bonds (see Fig. 10).

The values of α, β, and γ are now to be chosen so that any term of the expansion of $\det \mathbf{A}$ corresponding to a superposition of simple closed polygons of the prescribed type contributes $1\times\tanh^r K \tanh^s K' = x^r y^s$ in accordance with (4.1). The substitution (4.10) assures that a term of the expansion will have the correct power of x and y but (4.5) indicates that we must choose α, β, and γ to give a positive sign.

Each simple closed polygon on a square lattice has an even number of bonds, therefore $s(j)-1$ in Eq. (4.5) will be an odd number and the sign (4.5) will be $(-1)^r$. To make the terms positive, α, β, and γ must be chosen so that an additional factor of (-1) appears with each cycle in the expansion. A simple closed polygon directed in a clockwise direction has four more clockwise turns then counterclockwise turns. Thus, in (4.4) there will be 4 more powers of β than α for each clockwise cycle and 4 more powers of α than β for each counterclockwise cycle. There is for each cycle a factor of the form $(\alpha\beta)^n\beta^4$ or $(\alpha\beta)^n\alpha^4$ for some n. We can obtain the desired factor $(-1)^r$ if we choose $\alpha=\beta^{-1}$, $\alpha^4=\beta^4=-1$, and $\gamma=1$. Thus,

$$\alpha=\exp(i\pi/4), \quad \beta=\exp(-i\pi/4), \quad \gamma=1. \tag{4.12}$$

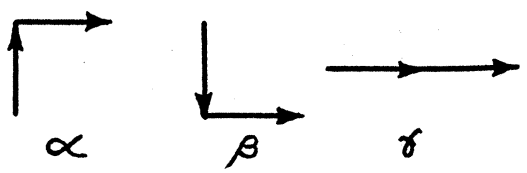

FIG. 10. The three types of bonds connections illustrated above correspond to the elements α, β, and γ in Eq. (4.11).

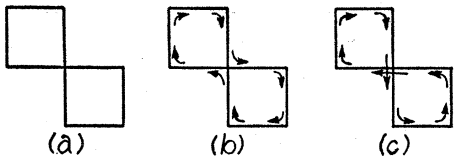

FIG. 11. The unoriented closed graph (a) corresponds to many oriented graphs. Among these are the unicursal paths (b) and (c) in which both polygons of (a) are traversed in a single cycle.

The matrix **A** has been completely specified on the basis of a few simple requirements which do, however, guarantee that det **A** will count correctly at least the simple closed polygons and superpositions of disjoint polygons on the lattice of Fig. 7b. The terms in det **A** which are associated with the bonds appearing in such graphs, consist of one term for each possible combination of clockwise and counterclockwise orientation of the disjoint polygons and each such combination does appear once in a figure such as 7b.

Det **A** also correctly counts many other types of graphs but there is as yet no proof that it correctly counts *all* possible graphs. Actually we know that there are some which are not counted correctly, namely those which "loop" the torus. Such failures would not be considered serious however since one would attribute them to the selection of periodic boundary conditions.

Kac and Ward considered a few simple cases of overlapping polygons and showed that they also are counted correctly.

One class of configurations which they considered was the graphs consisting of simple closed polygons on the lattice 7b which touch each other at single points only (no overlapping bonds). A simple example is given in Fig. 11a. A troublesome feature of such graphs is that det **A** includes terms corresponding to unicursal paths, i.e., those which traverse more than one polygon in a single cycle as illustrated in Figs. 11b and 11c. One readily sees that Fig. 11b has an excess of 4 clockwise turns and therefore is counted as a positive term, whereas 11c has an equal number of clockwise and counterclockwise turns and therefore contributes a negative term to det **A**. One can easily check that the net contribution of all unicursal paths of Fig. 11a is zero. Kac and Ward claim that this is true of the entire class of graphs which are composed of more than one polygon and in which each polygon has a point in common with at least one other polygon.

It is apparent that after the elimination of the unicursal paths, det **A** properly counts all possible graphs at least for the simple cases such as in Fig. 11 or disjoint superpositions of these. One might still question the count on a graph such as Fig. 8 which proved to be an annoyance earlier.

Perhaps even a more troublesome category of graphs is that in which bonds from the upper and lower parts of Fig. 7a overlap when transcribed onto Fig. 7b. Because of the choice of clockwise orientations in Fig. 7a, these double bonds may consist of either two bonds directed the same or two bonds directed oppositely. Since indices in (4.4) are never repeated in the same term, det **A** will not contain terms corresponding to graphs having an identical pair of bonds such as in Fig. 12a or Fig. 13a.

On the other hand, det **A** will count some superpositions of clockwise oriented polygons which have common sides forming a pair of oppositely directed bonds such as Figs. 12b and 13b, and even single polygons which loop back on themselves to form an oppositely directed pair as also illustrated within Fig. 13b and in Fig. 14. None of these graphs appear on the lattice of Fig. 7b because the graphs of Fig. 7a do not contain double bonds.

Kac and Ward did resolve the difficulties presented by the cases illustrated by Figs. 12 and 14. The contributions of Figs. 14a and 14b cancel as do all terms corresponding to similar type graphs. Regarding the situation in Figs. 12a and 12b, they pointed out that there is a one-to-one correspondence between graphs of type 12a and those of type 12b. Instead of counting the "allowed" polygons 12a, the determinant counts the "forbidden" polygons 12b.

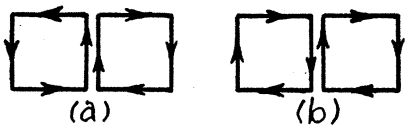

FIG. 12. (a) illustrates a superposition of simple closed polygons forming an identical pair of bonds. (b) illustrates a superposition of polygons forming an oppositely directed pair of bonds. Det **A** counts only type (b), whereas Fig. 7b contains only graphs of type (a).

A graph such as in Fig. 13 which contains both an identical pair and an oppositely directed pair of bonds was not considered. One cannot establish a one-to-one correspondence between allowed and forbidden paths by merely reversing the direction of one of the polygons as in Fig. 12.

It is certain that det **A** does correctly count all closed graphs since the partition function derived below checks (at least for large lattices) with that obtained by other methods. The manner in which some complicated graphs are counted is still uncertain, however. Although the analysis is as yet logically incomplete, the ideas presented are very praiseworthy.

It is worth pointing out here that this method of counting cannot be generalized in any obvious way to the three-dimensional problem nor to the two-dimensional problems with a magnetic field or longer-range interactions. The magnetic field problem involves a much more complicated counting procedure. One must keep account not only of the number of bonds in the polygon but also the area. The crossing of diagonal bonds in the next nearest neighbor problem causes

trouble, whereas in three dimensions, one encounters polygons with knots. Perhaps even more serious is the fact that a polygon in three dimensions does not divide the space into an "inside and outside." The solution above, thus, rests heavily upon the peculiar topological properties of this particular problem.

In view of the evidence presented above, we shall accept as correct the postulate that det **A** correctly counts closed graphs and proceed to obtain an explicit expression for Z based upon (4.6).

There would be little advantage in expressing Z in terms of det **A** if it were not for the fact that det **A** is invariant to any similarity transformation of **A**. In particular det **A** is equal to the product of the eigenvalues of **A**.

The matrix **A** is defined by Eqs. (4.7), (4.9), (4.10), (4.11), and (4.12), of which Eq. (4.10) represents the key to the simplification of det **A**. This equation expresses the cyclic character of **A** and immediately suggests that one transform the matrix **A** by a double Fourier expansion, thus transforming to a set of base vectors that are eigenfunctions of the two cyclic permutation operators (one for the vertical symmetry and one for the horizontal symmetry) that leave the lattice invariant.

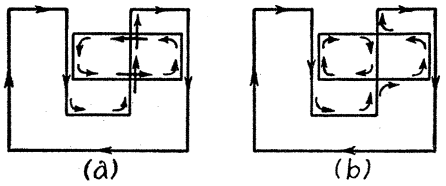

FIG. 13. A graphs such as (a) can appear as a graph in Fig. 7b but will not by counted by det **A** because it contains an identical pair of bonds. It also contains an oppositely directed pair. (b) illustrates another orientation of the same graph with no identical bond pairs.

We define a unitary matrix **R** of dimension $4nm$ with matrix elements

$$\mathbf{R}(k,l;k',l')=(nm)^{-\frac{1}{2}}\mathbf{I}_4\exp(2\pi ikk'/m+2\pi ill'/n). \quad (4.13)$$

The convention here is consistent with that used in Eq. (4.10). $\mathbf{I}_4$ is the 4×4 identity and $\mathbf{R}(k,l;k',l')$ is a 4×4 matrix. If we define **B**

$$\mathbf{B}\equiv\mathbf{RAR}^{-1}, \quad (4.14)$$

then det **A**=det **B**. One easily finds by using the orthogonality properties of the Fourier exponentials that

$$\mathbf{B}(k,l;k',l')=\delta_{kk'}\delta_{ll'}\sum_{s=1}^{n}\sum_{t=1}^{m}\mathbf{A}(0,0;t,s)\times\exp(-2\pi ikt/m-2\pi ils/n). \quad (4.15)$$

All elements of **B** vanish except those for which $k=k'$ and $l=l'$. Substituting Eq. (4.10) into (4.15), we find

$$\mathbf{B}(k,l;k,l)\equiv\mathbf{B}(k,l)=\mathbf{I}_4+y\mathbf{A}(1,0)\times\exp(-2\pi ik/m)+y\mathbf{A}(-1,0)\exp(2\pi ik/m)+x\mathbf{A}(0,1)\exp(-2\pi il/n)+x\mathbf{A}(0,-1)\exp(2\pi il/n)$$

$$=\begin{pmatrix}1+x\epsilon_l^{-1} & 0 & y\delta_k^{-1}\alpha & y\delta_k\alpha^{-1}\\ 0 & 1+x\epsilon_l & y\delta_k^{-1}\alpha^{-1} & y\delta_k\alpha\\ x\epsilon_l^{-1}\alpha^{-1} & x\epsilon_l\alpha & 1+y\delta_k^{-1} & 0\\ x\epsilon_l^{-1}\alpha & x\epsilon_l\alpha^{-1} & 0 & 1+y\delta_k\end{pmatrix}, \quad (4.16)$$

where

$$\epsilon=\exp(2\pi il/n),\quad \delta=\exp(2\pi ik/m),\quad \alpha=\exp(i\pi/4).$$

Since the eigenvalues of **A** are the eigenvalues of the $\mathbf{B}(k,l)$

$$\det\mathbf{A}=\prod_{k=1}^{m}\prod_{l=1}^{n}\det\mathbf{B}(k,l)$$

$$=\prod_{k=1}^{m}\prod_{l=1}^{n}\{(1+x^2)(1+y^2)-y(1-x^2)(\epsilon_l+\epsilon_l^{-1})-x(1-y^2)(\delta_k+\delta_k^{-1})\},$$

$$Z_{n,m}{}^2=2^{2nm}\prod_{k=1}^{m}\prod_{l=1}^{n}\{\cosh2K\cosh2K'-\sinh2K'\cos(2\pi l/n)-\sinh2K\cos(2\pi k/m). \quad (4.17)$$

The quantity of particular interest is

$$\lim_{n,m\to\infty}(nm)^{-1}\log Z$$

$$=\log2+\tfrac{1}{2}(mn)^{-1}\sum_{k=1}^{m}\sum_{l=1}^{n}\log[\cosh2K\cosh2K-\sinh2K'\cos(2\pi l/n)-\sinh2K\cos(2\pi k/m)]$$

$$=\log2+\tfrac{1}{2}\pi^{-2}\int_0^{\pi}\int_0^{\pi}\log(\cosh2K\cosh2K'-\sinh2K\cos w-\sinh2K'\cos w')dwdw'. \quad (4.18)$$

An attempt has been made by F. J. Murray[19] to apply a combinatorial approach to a three-dimensional lattice. The calculations have not yet been developed far enough to yield analytical results.

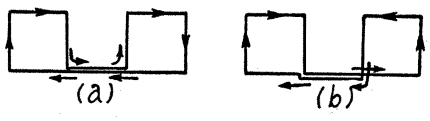

FIG. 14. Det **A** has terms corresponding to oriented polygons that "loop back on themselves" as illustrated by the two examples above. The terms corresponding to (a) and (b) cancel.

4.2 Algebraic Method

We now consider an algebraic procedure for finding the eigenvalue associated with the partition function for the two-dimensional square Ising lattice in zero magnetic field. We shall briefly outline Onsager's original solution with special emphasis on the method and motivations rather than the detailed algebra. For a more extensive discussion of the latter the reader is referred to Onsager's original presentation.[4]

As was shown in Sec. 2, the operator to be investigated is $\mathbf{V}_2\mathbf{V}_1$ [see Eqs. (2.12) and (2.13) for definitions]. It is convenient to express this in terms of two operators $\mathbf{A}_0$ and $\mathbf{A}_1$ defined by

$$\mathbf{A}_0=-\sum_{j=1}^{n}\mathbf{C}_j, \quad \mathbf{A}_1=\sum_{j=1}^{n}\mathbf{s}_j\mathbf{s}_{j+1} \tag{4.19}$$

with $\mathbf{s}_{n+j}\equiv\mathbf{s}_j$. (In the following we shall also have occasion to use the convention $\mathbf{C}_{n+j}\equiv\mathbf{C}_j$.) The matrices of interest are

$$\mathbf{V}_1=e^{-H^*\mathbf{A}_0} \quad \text{and} \quad \mathbf{V}_2=e^{H'\mathbf{A}_1}. \tag{4.20}$$

The general plan for solving this problem is to first perform some algebraic transformations. Starting from $\mathbf{A}_0$ and $\mathbf{A}_1$, we generate a Lie algebra (see Appendix 5) by forming the commutator $[\mathbf{A}_0, \mathbf{A}_1]$, then forming the commutators of this with $\mathbf{A}_0$ and $\mathbf{A}_1$. We continue to generate commutators of commutators until we obtain a set of operators such that the commutator of any two is a linear combination of operators already in the set.‡

One can, of course, generate a Lie algebra starting with any set of operators. Matrices of dimension 2^n will in many cases lead to a Lie algebra of 4^n elements, i.e., an algebra which contains as many independent elements as there are matrix elements in the matrix of dimension 2^n. The first fortunate feature of the operators $\mathbf{A}_0$ and $\mathbf{A}_1$ is that they generate a Lie algebra of only $3n-1$ linearly independent elements.

We next notice certain very convenient symmetries in the structure constants of the Lie algebra. Because of these symmetries we can, by applying linear transformations in the Lie algebra, decompose the Lie algebra into subalgebras of very simple structure. By expressing $\mathbf{A}_0$ and $\mathbf{A}_1$ in terms of these subalgebras we obtain a form of $\mathbf{V}_2\mathbf{V}_1$ which is readily factored into commuting matrices which can be diagonalized separately.

Attempts to apply this procedure to the three-dimensional problem or even the two-dimensional problem with a magnetic field are seriously hindered at an early stage because the operators of interest generate a much larger Lie algebra, so large in fact that it would seem to be of little value. All the various algebraic methods take advantage of very special properties of the operators, and it has not been possible to generalize them in any very interesting way.

The first step of the procedure is to generate a Lie algebra from $\mathbf{A}_0$ and $\mathbf{A}_1$. Rather than generate this element by element, we shall anticipate the results and write them in the most convenient form.

We define a set of operators

$$\begin{aligned}&\mathbf{P}_{a,a}=-\mathbf{C}_a,\\ &\mathbf{P}_{a,b}=\mathbf{s}_a\mathbf{C}_{a+1}\mathbf{C}_{a+2}\cdots\mathbf{C}_{b-1}\mathbf{s}_b \quad a\neq b,\end{aligned} \tag{4.21}$$

using the convention that $\mathbf{s}_{n+j}\equiv\mathbf{s}_j$ and $\mathbf{C}_{n+j}\equiv\mathbf{C}_j$. Thus,

$$\mathbf{A}_0=\sum_{a=1}^{n}\mathbf{P}_{a,a}, \quad \mathbf{A}_1=\sum_{a=1}^{n}\mathbf{P}_{a,a+1}. \tag{4.22}$$

These are but two operators of a set $\mathbf{A}_k$ which we define by

$$\mathbf{A}_k\equiv\sum_{a=1}^{n}\mathbf{P}_{a,a+k}. \tag{4.23}$$

There are $2n$ linearly independent $\mathbf{A}_k$. From (4.21) we see that

$$\begin{aligned}&\mathbf{P}_{a,a+k+n}=-\mathbf{U}\mathbf{P}_{a,a+k},\\ &\mathbf{U}\equiv\mathbf{C}_1\mathbf{C}_2\cdots\mathbf{C}_n.\end{aligned} \tag{4.24}$$

(The minus sign appears because $\mathbf{s}_j$ anticommutes with $\mathbf{C}_j$, as one readily observes from the definitions [(2.6a), (2.10), and (2.11)].) Thus

$$\mathbf{A}_{k+n}=-\mathbf{U}\mathbf{A}_k \quad \text{and} \quad \mathbf{A}_{k+2n}=\mathbf{A}_k. \tag{4.25}$$

(Note that $\mathbf{A}_k$ commutes with $\mathbf{U}$ and $\mathbf{U}^2=\mathbf{I}$.)

With the addition of a set of elements

$$\mathbf{G}_k=\tfrac{1}{4}[\mathbf{A}_k, \mathbf{A}_0], \tag{4.26}$$

we can define a complete Lie algebra containing the elements $\mathbf{A}_k$ and $\mathbf{G}_k$. The commutation rules for this algebra are (see reference 4, p. 127)

$$\begin{aligned}&[\mathbf{A}_j, \mathbf{A}_k]=4\mathbf{G}_{j-k},\\ &[\mathbf{A}_l, \mathbf{G}_{j-k}]=2(\mathbf{A}_{l+j-k}-\mathbf{A}_{l-j+k}),\\ &[\mathbf{G}_j, \mathbf{G}_k]=0.\end{aligned} \tag{4.27}$$

We have defined $2n$ operators $\mathbf{G}_k$ but actually only $n-1$ are linearly independent. Since $[\mathbf{A}_k, \mathbf{A}_j]=-[\mathbf{A}_j, \mathbf{A}_k]$, we see from (4.27) that $\mathbf{G}_m=-\mathbf{G}_{-m}=-\mathbf{G}_{2n-m}$. $\mathbf{G}_0=[\mathbf{A}_j, \mathbf{A}_j]=0$ because an operator always commutes with itself. $\mathbf{G}_n=[\mathbf{A}_{j+n}, \mathbf{A}_j]=[-\mathbf{U}\mathbf{A}_j, \mathbf{A}_j]=0$ because $\mathbf{U}$ also commutes with $\mathbf{A}_j$. We, therefore, have only $\mathbf{G}_1, \mathbf{G}_2, \cdots, \mathbf{G}_{n-1}$ as linearly independent operators.

We have seen so far that $\mathbf{A}_0$ and $\mathbf{A}_1$ generate a Lie algebra of only $3n-1$ elements ($2n$ $\mathbf{A}_k$'s and $n-1$ $\mathbf{G}_k$'s). We also observe that the structure of this Lie algebra is rather unique. Notice that if in (4.27) we replace $\mathbf{A}_j$ by $\mathbf{A}_{j+x}$, the commutation relations remain un-

‡ van der Waerden is credited with the observation that the algebra so generated and the transformations that follow belong to the theory of Lie algebras. The authors are indebted to Dr. Bruria Kaufman for describing this connection.

changed. From (4.27) alone there is no "preferred" $\mathbf{A}_j$; there is no way to single out one $\mathbf{A}_k$ as being different from all the others. The symmetry here is formally very similar to the symmetry of the cyclic matrix in Sec. 4.1, the cause of which could be traced to the fact that the crystal has cyclic symmetry, i.e., all particles in a row of the lattice are equivalent (with the periodic boundary conditions). The cyclic symmetry in (4.27) arises, however, from a different source. The periodicity in the lattice has already been incorporated into the $\mathbf{A}_j$ and $\mathbf{G}_k$ which are themselves invariant to a cyclic transformation of the lattice points. The cause of the cyclic symmetry in (4.27) is not obvious physically.

The existence of this symmetry, however, suggests the next step. From general properties of the group of cyclic permutations, one is assured that a Fourier transformation of the operators $\mathbf{A}_k$ and $\mathbf{G}_k$ will give an even simpler description of the Lie algebra. Just as a Fourier transformation of a cyclic matrix makes most of the matrix elements vanish, so also does a Fourier transformation to this cyclic Lie algebra make most of the structure constants vanish.

The Fourier transformation is achieved by introducing the operators

$$\begin{aligned}\mathbf{X}_r &= (2n)^{-1}\sum_{m=1}^{2n}\mathbf{A}_m\cos(\pi rm/n),\\ \mathbf{Y}_r &= -(2n)^{-1}\sum_{m=1}^{2n}\mathbf{A}_m\sin(\pi mr/n),\\ \mathbf{Z}_r &= i(2n)^{-1}\sum_{m=1}^{2n}\mathbf{G}_m\sin(m\pi r/n).\end{aligned}\tag{4.28}$$

We notice that

$$\begin{aligned}\mathbf{X}_r &= \mathbf{X}_{-r} = \mathbf{X}_{2n-r},\\ \mathbf{Y}_r &= -\mathbf{Y}_{-r} = -\mathbf{Y}_{2n-r},\\ \mathbf{Z}_r &= -\mathbf{Z}_{-r} = -\mathbf{Z}_{2n-r}.\end{aligned}\tag{4.29}$$

A check on the number of independent operators shows that there are $n-1$ independent $\mathbf{Y}_r$, $n-1$ independent $\mathbf{Z}_r$, but $n+1$ independent $\mathbf{X}_r$.

The commutation rules for these operators are easily calculated from (4.27) to be

$$\begin{aligned}[\mathbf{X}_r, \mathbf{Y}_r] &= -2i\mathbf{Z}_r,\\ [\mathbf{Y}_r, \mathbf{Z}_r] &= -2i\mathbf{X}_r \quad 1\leqslant r\leqslant n-1,\\ [\mathbf{Z}_r, \mathbf{X}_r] &= -2i\mathbf{Y}_r.\end{aligned}\tag{4.30}$$

All operators (including $\mathbf{X}_0$ and $\mathbf{X}_n$) commute with any other operator with a different subscript; thus, for $r\neq s$, $[\mathbf{X}_r, \mathbf{X}_s]=0$, $[\mathbf{X}_r, \mathbf{Y}_s]=0$, etc. The three operators $\mathbf{X}_r$, $\mathbf{Y}_r$, and $\mathbf{Z}_r$ (for each r) themselves form a Lie algebra which is a subalgebra of the complete set. We have, as predicted, decomposed the original Lie algebra into small subalgebras of very simple structure. The subalgebras are in fact very similar to those associated with the three-dimensional infinitesimal rotation group (see Appendix 5).

Our aim now is to express $\mathbf{V}_2\mathbf{V}_1$ in terms of this new set of operators and to take advantage of the simple structure (4.30). The relation (4.28) can be easily inverted by the usual rules of Fourier transforms to give $\mathbf{A}_m$ and $\mathbf{G}_m$ in terms of $\mathbf{X}_r$, $\mathbf{Y}_r$, and $\mathbf{Z}_r$. The result of this is

$$\begin{aligned}\mathbf{A}_m &= \sum_{r=1}^{2n}[\mathbf{X}_r\cos(m\pi r/n)-\mathbf{Y}_r\sin(m\pi r/n)],\\ \mathbf{G}_m &= -i\sum_{r=1}^{2n}\mathbf{Z}_r\sin(mr\pi/n).\end{aligned}\tag{4.31}$$

In particular,

$$\mathbf{A}_0=\sum_{r=1}^{2n}\mathbf{X}_r=\mathbf{X}_0+2\mathbf{X}_1+2\mathbf{X}_2+\cdots+2\mathbf{X}_{n-1}+\mathbf{X}_n,$$

$$\begin{aligned}\mathbf{A}_1&=\sum_{r=1}^{2n}[\mathbf{X}_r\cos(r\pi/n)-\mathbf{Y}_r\sin(\pi r/n)]\\ &=\mathbf{X}_0+2[\mathbf{X}_1\cos(\pi/n)-\mathbf{Y}_1\sin(\pi/n)]+\cdots\\ &\quad+2[\mathbf{X}_{n-1}\cos((n-1)\pi/n)\\ &\qquad-\mathbf{Y}_{n-1}\sin((n-1)\pi/n)]-\mathbf{X}_n.\end{aligned}\tag{4.32}$$

Substitution of (4.32) into (4.20) gives

$$\begin{aligned}\mathbf{V}_2\mathbf{V}_1=\exp\{K'\sum_{r=1}^{2n}&[\mathbf{X}_r\cos(\pi r/n)\\ &-\mathbf{Y}_r\sin(\pi r/n)]\}\exp\{-K^*\sum_{r=1}^{2n}\mathbf{X}_r\}.\end{aligned}\tag{4.33}$$

We can make valuable use of the commutation rules (4.30) by noting that if two operators $\mathbf{A}$ and $\mathbf{B}$ commute, then $e^{\mathbf{A}+\mathbf{B}}=e^{\mathbf{A}}e^{\mathbf{B}}=e^{\mathbf{B}}e^{\mathbf{A}}$. It is therefore possible to factor (4.33) into the product of commuting matrices:

$$\begin{aligned}\mathbf{V}_2\mathbf{V}_1&=\prod_{r=0}^{n}\mathbf{U}_r,\\ \mathbf{U}_r&=\exp\{2K'[\mathbf{X}_r\cos(\pi r/n)\\ &\quad-\mathbf{Y}_r\sin(\pi r/n)]\}\exp\{-2K^*\mathbf{X}_r\}\quad r\neq 0, n,\\ \mathbf{U}_0&=\exp\{(K'-K^*)\mathbf{X}_0\},\\ \mathbf{U}_n&=\exp\{-(K'+K^*)\mathbf{X}_n\}.\end{aligned}\tag{4.34}$$

The fact that the $\mathbf{U}_r$ commute with each other also implies that they can all be simultaneously diagonalized and that the eigenvalues of $\mathbf{V}_2\mathbf{V}_1$ are products of eigenvalues of the $\mathbf{U}_r$.

We can find the eigenvalues of the $\mathbf{U}_r$ by a somewhat indirect procedure. It is not wise to try to determine explicitly the matrices $\mathbf{X}_r$, $\mathbf{Y}_r$, and $\mathbf{Z}_r$ in the original

representation. The multiplication table of the $\mathbf{X}_r$, $\mathbf{Y}_r$, and $\mathbf{Z}_r$ is independent of representation as are also the eigenvalues. The latter are, with the help of a few rather simple bits of knowledge such as the dimension of the matrices, etc., determined by the former.

We have so far given only the commutation rules of the $\mathbf{X}_r$, $\mathbf{Y}_r$, and $\mathbf{Z}_r$. To proceed further we must also know $\mathbf{X}_r^2$, $\mathbf{Y}_r^2$, $\mathbf{Z}_r^2$, $\mathbf{X}_r\mathbf{Y}_r$, etc., which can be found by direct evaluation using the abstract properties of the $\mathbf{P}_{ab}$ (see reference 4, p. 129). The complete multiplication table is given below (the operators $\mathbf{R}_r$ are defined by the expressions below):

$$\left.\begin{aligned}&\mathbf{X}_r^2=\mathbf{Y}_r^2=\mathbf{Z}_r^2=\mathbf{R}_r=\mathbf{R}_r^2,\\&\mathbf{X}_r=\mathbf{R}_r\mathbf{X}_r=\mathbf{X}_r\mathbf{R}_r=i\mathbf{Y}_r\mathbf{Z}_r=-i\mathbf{Z}_r\mathbf{Y}_r\\&\mathbf{Y}_r=\mathbf{R}_r\mathbf{Y}_r=\mathbf{Y}_r\mathbf{R}_r=i\mathbf{Z}_r\mathbf{X}_r=-i\mathbf{X}_r\mathbf{Z}_r\\&\mathbf{Z}_r=\mathbf{R}_r\mathbf{Z}_r=\mathbf{Z}_r\mathbf{R}_r=i\mathbf{X}_r\mathbf{Y}_r=-i\mathbf{Y}_r\mathbf{X}_r\end{aligned}\right\}\ 1\leqslant r\leqslant n-1,$$
$$\left.\begin{aligned}&\mathbf{X}_r^2=\mathbf{R}_r=\mathbf{R}_r^2\\&\mathbf{X}_r=\mathbf{R}_r\mathbf{X}_r=\mathbf{X}_r\mathbf{R}_r\end{aligned}\right\} r=0,\ n. \tag{4.35}$$

From this table one can calculate any combination of products of $\mathbf{X}_r$, $\mathbf{Y}_r$, and $\mathbf{Z}_r$. The important features of the table are the following. The operators $\mathbf{X}_r$, $\mathbf{Y}_r$, and $\mathbf{Z}_r$ anticommute with each other and $\mathbf{X}_r^2$, $\mathbf{Y}_r^2$, and $\mathbf{Z}_r^2$ are all projection operators ($\mathbf{R}_r^2=\mathbf{R}_r$), i.e., they have eigenvalues either zero or one.

We can very easily establish that $\mathbf{R}_r$ is not the unit matrix and is truly a projection operator with some zero eigenvalues. From (4.28) we notice that since $\mathbf{A}_{m+n}=-\mathbf{U}\mathbf{A}_m$,

$$\mathbf{X}_r=(2n)^{-1}[\mathbf{I}-(-1)^r\mathbf{U}]\sum_{m=1}^{n}\mathbf{A}_m\cos(m\pi r/n).$$

Similarly $\mathbf{Y}_r$ and $\mathbf{Z}_r$ contain a factor $[\mathbf{I}-(-)^r\mathbf{U}]$.

The operator $\mathbf{U}$ defined in (4.24) plays a rather important role in this problem. $\mathbf{U}$ is the operator which changes all spins σ_j to $-\sigma_j$.

The eigenvalues and eigenfunctions of $\mathbf{U}$ are very simple. Since $\mathbf{U}^2=\mathbf{I}$, the eigenvalues are ±1. $\mathbf{U}$ operating on any state given by ν: $(\sigma_1, \sigma_2, \cdots, \sigma_n)$ changes it to a new state $\mathbf{U}\nu$: $(-\sigma_1, -\sigma_2, \cdots, -\sigma_n)$. For each pair of states ν and $\mathbf{U}\nu$ as described above, there is an "even" and an "odd" state given, respectively, by $\nu+\mathbf{U}\nu$ and $\nu-\mathbf{U}\nu$. In the "even space" $\mathbf{U}=\mathbf{I}'$ and in the "odd space" $\mathbf{U}=-\mathbf{I}'$. Each subspace is of dimension 2^{n-1}. In this representation $\mathbf{U}$ has the form

$$\begin{pmatrix}\mathbf{I}' & \mathbf{O}\\ \mathbf{O} & -\mathbf{I}'\end{pmatrix},$$

where $\mathbf{I}'$ is the 2^{n-1} identity matrix and $\mathbf{O}$ is the 2^{n-1} dimensional null matrix. In this same representation $\frac{1}{2}(\mathbf{I}+\mathbf{U})$ and $\frac{1}{2}(\mathbf{I}-\mathbf{U})$ are, respectively, the projection operators

$$\begin{pmatrix}\mathbf{I}' & \mathbf{O}\\ \mathbf{O} & \mathbf{O}\end{pmatrix}\quad\text{and}\quad\begin{pmatrix}\mathbf{O} & \mathbf{O}\\ \mathbf{O} & \mathbf{I}'\end{pmatrix}.$$

$\mathbf{V}_2$, $\mathbf{V}_1$, and all the operators used in describing them, including the $\{\mathbf{X}_r\}$, $\{\mathbf{Y}_r\}$, and $\{\mathbf{Z}_r\}$, commute with $\mathbf{U}$. This means that in the representation above, all these matrices must be of the general type

$$\begin{pmatrix}\mathbf{X} & \mathbf{O}\\ \mathbf{O} & \mathbf{X}'\end{pmatrix},$$

where $\mathbf{X}$ denotes some 2^{n-1} dimensional matrix. In particular, since $\mathbf{X}_r$, $\mathbf{Y}_r$, and $\mathbf{Z}_r$ contain $[\mathbf{I}-(-1)^r\mathbf{U}]$ as a factor, these operators must be of the type

$$\begin{pmatrix}\mathbf{X} & \mathbf{O}\\ \mathbf{O} & \mathbf{O}\end{pmatrix}\quad\text{for } r \text{ odd}$$

and

$$\begin{pmatrix}\mathbf{O} & \mathbf{O}\\ \mathbf{O} & \mathbf{X}'\end{pmatrix}\quad\text{for } r \text{ even}.$$

The nonsingular part of the projection operator $\mathbf{R}_r$ is at most of dimension 2^{n-1}.

Equipped with the multiplication table (4.35) and some simple properties of the $\mathbf{X}_r$, $\mathbf{Y}_r$, and $\mathbf{Z}_r$, we return again to the eigenvalue problem (4.34). Matrices such as (4.35) have been studied extensively, particularly in connection with representations of the rotation group and the Lie algebra discussed in Appendix 5. One need not be an expert on such things, however, to solve this problem.

We first observe that a transformation with $\exp(iz_r\mathbf{Z}_r)$, with z_r a constant, produces the following transformation of the $\mathbf{X}_r$, $\mathbf{Y}_r$, and $\mathbf{Z}_r$ ($r\neq0, n$):

$$\begin{aligned}&\exp(iz_r\mathbf{Z}_r)\mathbf{X}_r\exp(-iz_r\mathbf{Z}_r)=\mathbf{X}_r\cos2z_r+\mathbf{Y}_r\sin2z_r,\\&\exp(iz_r\mathbf{Z}_r)\mathbf{Y}_r\exp(-iz_r\mathbf{Z}_r)\\&\qquad=-\mathbf{X}_r\sin2z_r+\mathbf{Y}_r\cos2z_r,\\&\exp(iz_r\mathbf{Z}_r)\mathbf{Z}_r\exp(-iz_r\mathbf{Z}_r)=\mathbf{Z}_r.\end{aligned}\tag{4.36}$$

If we imagine the $\mathbf{X}_r$, $\mathbf{Y}_r$, and $\mathbf{Z}_r$ to be orthogonal vectors, then the above similarity transformation also produces an orthogonal transformation of the vectors $\mathbf{X}_r$, $\mathbf{Y}_r$, and $\mathbf{Z}_r$. In general any orthogonal transformation of the $\mathbf{X}_r$, $\mathbf{Y}_r$, and $\mathbf{Z}_r$ can be produced by a similarity transformation of the type

$$\exp(z_r\mathbf{Z}_r+y_r\mathbf{Y}_r+x_r\mathbf{X}_r). \tag{4.37}$$

This correspondence between orthogonal transformations and similarity transformations is the basis for the theory of representations of the rotation group and also underlies the Dirac theory of the electron. A generalization of this is also the basis of Kaufman's scheme for solving the Ising problem.

If now we should expand the exponentials in (4.34) using the rules (4.35), we can express $\mathbf{U}_r$ as a constant plus a linear combination in $\mathbf{R}_r$, $\mathbf{X}_r$, $\mathbf{Y}_r$, and $\mathbf{Z}_r$. Note that any power of $\mathbf{X}_r$, for example, is either $\mathbf{X}_r$ or $\mathbf{R}_r$.

By using a transformation of the type (4.37), which leaves $\mathbf{R}_r$ invariant, we can eliminate $\mathbf{Z}_r$ and $\mathbf{Y}_r$. If we considered the linear expression in $\mathbf{X}_r$, $\mathbf{Y}_r$, and $\mathbf{Z}_r$ as a vector, then this procedure is identical to the rotation of coordinates so that the vector is along the "X axis."

It will not be necessary to find this transformation explicitly. We can easily show that $\mathbf{U}_r$ is transformed into the form

$$\mathbf{U}_r\sim(\mathbf{I}-\mathbf{R}_r)+\mathbf{R}_r\cosh\gamma_r+\mathbf{X}_r\sinh\gamma_r=\exp(\gamma_r\mathbf{X}_r) \quad (4.38)$$

($\sim$ indicates similarity). We already have argued that this expression will be linear in $\mathbf{R}_r$ and $\mathbf{X}_r$. In addition, we know from (4.34) that the projection $\frac{1}{2}(\mathbf{I}-\mathbf{R}_r)\mathbf{U}_r$ is a unit matrix (since $\mathbf{X}_r$, $\mathbf{Y}_r$, $\mathbf{Z}_r$, and $\mathbf{R}_r$ all vanish in this space) and is unaffected by the transformation (4.37). Furthermore, we see that transformation of (4.34) by $\exp(\frac{1}{2}\pi i\mathbf{Z}_r)$ changes both factors of $\mathbf{U}_r$ into their reciprocals, $\mathbf{X}_r\rightarrow-\mathbf{X}_r$ and $\mathbf{Y}_r\rightarrow-\mathbf{Y}_r$. $\mathbf{U}_r$ and $\mathbf{U}_r^{-1}$ are therefore similar and $|\det\mathbf{U}_r|=1$. Since this property also must be preserved by a similarity transformation, the coefficients of $\mathbf{R}_r$ and $\mathbf{X}_r$ are restricted in the manner indicated.

The problem of finding γ_r is very easy because the similarity transformation affects only the coefficients of $\mathbf{X}_r$, $\mathbf{Y}_r$, and $\mathbf{Z}_r$ leaving the coefficient of $\mathbf{R}_r$ unaltered. $\cosh\gamma_r$ is therefore the coefficient of $\mathbf{R}_r$ in the original expansion of $\mathbf{U}_r$:

$$\cosh\gamma_r=\cosh2K'\cosh2K^*-\sinh2K'\sinh2K^*\cos(r\pi/n). \quad (4.39)$$

Since $\mathbf{X}_r$, $\mathbf{Y}_r$, and $\mathbf{Z}_r$ commute with operators of a different index, we can apply the appropriate transformations for each r to $\mathbf{V}_2\mathbf{V}_1$ and bring all $\mathbf{U}_r$ simultaneous into the form (4.38).

We have thus established

$$\mathbf{V}_2\mathbf{V}_1\sim\exp[-\tfrac{1}{2}(\gamma_0\mathbf{X}_0+2\gamma_1\mathbf{X}_1+\cdots+2\gamma_{n-1}\mathbf{X}_{n-1}+\gamma_n\mathbf{X}_n)], \quad (4.40)$$

where

$$\gamma_0=K^*-K' \quad \text{and} \quad \gamma_n=K'+K^* \quad (4.41)$$

are also consistent with (4.39).

We have not as yet commented on the sign of the γ_j. The signs of γ_0 and γ_n are defined by (4.41) but except for $j=0$ and n, only $|\gamma_j|$ are defined by (4.39). This is all that is necessary, however, because the transformation $\exp(\frac{1}{2}i\pi\boldsymbol{Z}_r)$ sends $\boldsymbol{X}_r$ into $-\boldsymbol{X}_r$ [Eq. (4.36)]. Equation (4.40) is thus valid if we replace $\boldsymbol{X}_j$ by $-\boldsymbol{X}_j$ or γ_r by $-\gamma_r$, $(j\neq0, n)$. For convenience we shall hereafter choose all γ_r, $(j\neq0, n)$ as the positive solution of (4.39).

Since the $\mathbf{X}_r$ commute, they can all be simultaneously diagonalized. The $\mathbf{X}_r$ satisfy the equation

$$\mathbf{X}_r(\mathbf{X}_r^2-\mathbf{I})=0; \quad (4.42)$$

therefore they have eigenvalues $X_r=0$ or ±1.

All eigenvalues of $\mathbf{V}_2\mathbf{V}_1$ must be of the type

$$\lambda=\prod_{r=0}^{n}\lambda_r,$$

$$\lambda_r=e^{\frac{1}{2}\gamma_r},\quad e^{-\frac{1}{2}\gamma_r}\quad\text{or}\quad 1\quad\text{for}\quad r=0,n, \quad (4.43)$$

$$\lambda_r=e^{\gamma_r},\quad e^{-\gamma_r}\quad\text{or}\quad 1\quad\text{for}\quad r\neq0,n.$$

Unfortunately, the converse of this is not true; not all λ of the type (4.43) are eigenvalues of $\mathbf{V}_2\mathbf{V}_1$ (there are 3^{n+1} possible combinations of (4.43) but only 2^n eigenvalues). Even though the $\mathbf{X}_r$ can be simultaneously diagonalized, the subspace in which X_0 is $+1$ might be a space in which, for example, X_1 could be only $+1$. We are still confronted with the task of determining which combinations in (4.43) are allowed.

We can very easily eliminate a large number of the solutions of (4.43) by recalling that in the even space ($\mathbf{U}=+\mathbf{I}'$), $\mathbf{X}_r=0$ for all odd r, whereas in the odd space ($\mathbf{U}=-\mathbf{I}'$), $\mathbf{X}_r=0$ for all even r. We therefore know that either the λ_r with r odd are 1 (in the even space) or λ_r with r even are 1 (in the odd space),

$$\lambda=\lambda_1\lambda_3\lambda_5\cdots \quad\text{or}\quad \lambda=\lambda_0\lambda_2\lambda_4\cdots. \quad (4.44)$$

Whereas the spinor analysis method automatically gives all the eigenvalues and their degeneracies, the problem of completely disentangling the proper combinations of the above is at this state a rather tedious operation (although not a difficult one). Fortunately, we are interested only in the largest eigenvalue of $\mathbf{V}_2\mathbf{V}_1$ and perhaps also in any that are asymptotically degenerate with the largest.

The problem is to determine the simultaneous eigenvalues of the $\mathbf{X}_r$. To find at least some of these we consider

$$\mathbf{A}_0=-\sum_{j=1}^{n}\mathbf{C}_j=\sum_{r=0}^{2n-1}\mathbf{X}_r. \quad (4.45)$$

The $\mathbf{C}_j$ all commute and are very easily diagonalized simultaneously. Since $\mathbf{C}_j^2=\mathbf{I}$, the eigenvalues of $\mathbf{C}_j$ are ±1 and since the $\mathbf{C}_j$ are direct product matrices, the eigenvalues of $\mathbf{C}_j$ do not depend in any way on the eigenvalues of other $\mathbf{C}_k$. The 2^n eigenvalues of $\mathbf{A}_0$ are given by

$$-A_0=\pm1\pm1\pm1\pm\cdots\pm1. \quad (4.46)$$

There are n terms in (4.46) and the 2^n solutions are obtained by selecting all possible combinations of the $\pm$ signs. If the $\mathbf{C}_j$ are all diagonalized, then $\mathbf{U}=\mathbf{C}_1\mathbf{C}_2\cdots\mathbf{C}_n$ is also diagonal and has the value ±1 accordingly as the right side of (4.46) has an even or odd number of minus signs. In particular we note that the lowest eigenvalue of $\mathbf{A}_0$ is nondegenerate, belongs in the even space, and has the value

$$A_0=-n. \quad (4.47)$$

The next lowest eigenvalue of $\mathbf{A}_0$ is degenerate, belongs

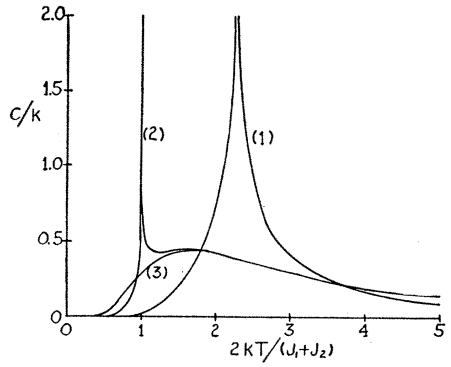

FIG. 15. The specific heat of the two-dimensional Ising lattice with (1) $J=J'$ (isotropic), (2) $J=100J'$, and (3) $J'=0$ (linear chain) (see reference 4).

in the odd space, and has the value

$$A_0=-n+2. \tag{4.48}$$

Returning to (4.45), we also recall that for $\mathbf{U}=+I'$, all $\mathbf{X}_r$ for r even vanish. There is one eigenfunction of the $\mathbf{X}_r$ which gives

$$A_0=-n=X_1+X_3+\cdots+X_{2n-1}$$
$$=\begin{cases}2X_1+2X_3+\cdots+2X_{n-2}+X_n & \text{for } n \text{ odd}\\ 2X_1+2X_3+\cdots+2X_{n-1} & \text{for } n \text{ even.}\end{cases}$$

Since the $\mathbf{X}_r$ can be only ±1 or 0, there is only one way that this equation can be satisfied, namely for all $\mathbf{X}_r$ (r odd) to have the value $\mathbf{X}_r=-1$.

This simple argument tells us that $\mathbf{V}_2\mathbf{V}_1$ has an eigenvalue

$$\lambda_+=\begin{cases}\exp[\tfrac{1}{2}(2\gamma_1+2\gamma_3+\cdots+2\gamma_{n-2}+\gamma_n)] & \text{for } n \text{ odd}\\ \exp[\tfrac{1}{2}(2\gamma_1+2\gamma_3+\cdots+2\gamma_{n-1})] & \text{for } n \text{ even}\end{cases} \tag{4.49}$$

or by extending the definition (4.39) of γ_j for $j>n$

$$\lambda_+=\exp[\tfrac{1}{2}(\gamma_1+\gamma_3+\cdots+\gamma_{2n-1})]. \tag{4.50}$$

By comparing this with other expressions in (4.44), we see that this is certainly the largest eigenvalue in the even space. The next largest in this space is smaller by at least a factor $e^{-\gamma_1}$. Comparison with the possible eigenvalues of the odd space shows that this is also larger than any of these but one of the possible eigenvalues of the odd space is asymptotically equal to the above, namely the solution with all positive exponentials.

There is one final question to be answered. Is the solution of (4.44)

$$\lambda=\exp[\tfrac{1}{2}(|\gamma_0|+\gamma_2+\gamma_4+\cdots+\gamma_{2n-2})]$$

really an eigenvalue of $\mathbf{V}_2\mathbf{V}_1$? To obtain a partial answer to this question we notice again (4.48) and observe that in the odd space, the smallest eigenvalue of $\mathbf{A}_0$ is

$$A_0=-n+2=X_0+X_2+\cdots+X_{2n-2}$$
$$=\begin{cases}X_0+2X_2+2X_4+\cdots+2X_{n-2}+X_n & \text{for } n \text{ even}\\ X_0+2X_2+2X_4+\cdots+2X_{n-1} & \text{for } n \text{ odd.}\end{cases}$$

The X_r cannot all simultaneously be -1 for this would contradict the above being the lowest eigenvalue of $\mathbf{A}_0$. The only possible solutions of the above are $X_0=+1$ and all other $X_j=-1$, $X_n=+1$ (for n even) and all other $X_j=-1$ or some $X_j=0$ ($j\neq0, n$) and all other $X_j=-1$. We shall not pursue further the question of which of these possibilities are really solutions (it turns out that they all are). The solution of particular interest is the case $X_0=+1$ all other $X_j=-1$, for this leads to the largest eigenvalue of $\mathbf{V}_2\mathbf{V}_1$ in the odd space:

$$\lambda_-=\exp[\tfrac{1}{2}(-\gamma_0+\gamma_2+\gamma_4+\cdots+\gamma_{2n-2})]. \tag{4.51}$$

If $K^*<K'$, $\gamma_0=K^*-K'$ is negative and for large n approaches the value of $-\gamma_1$. If $K^*<K'$, λ_- and λ_+ are asymptotically degenerate. At $K^*=K'$, γ_0 changes sign and for $K^*>K'$ the degeneracy no longer exists.

The situation here illustrates very nicely the predictions made in Sec. 3. There we predicted that if a phase transition exists, at least in the case $K'=K$, it occurs at $K'=K^*$, the point where this degeneracy disappears. We also saw that a degeneracy of the largest eigenvalue is associated with long-range order, thus the critical temperature truly represents a transition from an ordered to a disordered state.

To complete the analysis of this section, we find an asymptotic expression for Z. As shown by Eq. (2.4) a degeneracy of the above nature has no effect upon the thermodynamic properties derived from Z

$$\lim_{n,m\to\infty}(nm)^{-1}\log Z-\tfrac{1}{2}\log(2\sinh2K)$$
$$=\lim_{n\to\infty}(2n)^{-1}(\gamma_1+\gamma_3+\cdots+\gamma_{2n-1})$$
$$=\lim_{n\to\infty}(2n)^{-1}\sum_{r=1}^{n}\cosh^{-1}[\cosh2K'\cosh2K^*$$
$$-\sinh2K'\sinh2K^*\cos((2r-1)\pi/n)]$$
$$=(4\pi)^{-1}\int_0^{2\pi}d\omega\gamma(\omega), \tag{4.52}$$

$$\gamma(\omega)=\cosh^{-1}(\cosh2K'\cosh2K^*$$
$$-\sinh2K'\sinh2K^*\cos\omega).$$

This expression does not show the symmetry in K and K'. We can obtain a more symmetric form by converting (4.52) into a double integral using the relation

$$\int_0^{2\pi}\log(2\cosh x-2\cos\omega)d\omega=2\pi x.$$

This yields

$$\lim_{n,m\to\infty}(nm)^{-1}\log Z=\log 2$$
$$+\tfrac{1}{2}\pi^{-2}\int_0^\pi d\omega\int_0^\pi d\omega'\log(\cosh 2K\cosh 2K'$$
$$-\sinh 2K\cos\omega-\sinh 2K'\cos\omega'). \quad (4.53)$$

4.3 Thermodynamic Properties

In Secs. 4.1 and 4.2, we have derived by two quite different procedures the partition function of the two-dimensional square Ising lattice. The result of this calculation was

$$\lim_{n,m\to\infty}(nm)^{-1}\log Z=\log 2$$
$$+\tfrac{1}{2}\pi^{-2}\int_0^\pi\int_0^\pi\log(\cosh 2K\cosh 2K$$
$$-\sinh 2K\cos\omega-\sinh 2K'\cos\omega')d\omega d\omega'. \quad (4.18)$$

This expression shows the symmetry with respect to interchange of K and K'. One of the integrals is easily performed using the identity

$$\int_0^\pi\log(2\cosh x-2\cos\omega)d\omega=\pi x$$

to give the less symmetric form

$$\lim_{n,m\to\infty}(nm)^{-1}\log Z$$
$$=\tfrac{1}{2}\log(2\sinh 2K)+(2\pi)^{-1}\int_0^\pi\gamma(\omega)d\omega, \quad (4.52)$$

where

$$\cosh\gamma(\omega)=\cosh 2K'\cosh 2K^*$$
$$-\sinh 2K'\sinh 2K^*\cos\omega.$$

Although the above integrals are not of a common type, the thermodynamic functions involving derivatives of these integrals can be expressed in terms of elliptic functions. The analysis of these integrals for arbitrary K and K' is given in Onsager's paper. This analysis is considerably simplified if we let $K=K'$ as we shall do in the following. $\gamma(\omega)$ is then given by

$$\cosh\gamma(\omega)=\cosh 2K\,\mathrm{ctnh}2K-\cos\omega.$$

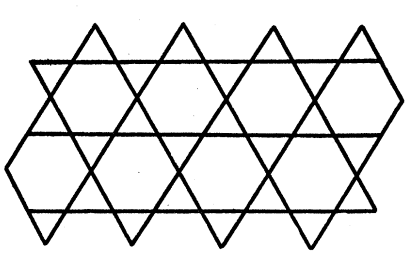

FIG. 16. The Kagomé lattice.

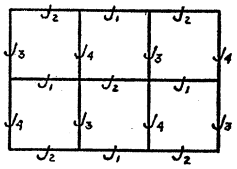

FIG. 17. A square lattice with four independent coupling constants denoted by J_1, J_2, J_3, and J_4.

The internal energy per particle is found from

$$\bar{E}=kT^2\partial[(nm)^{-1}\log Z]/\partial T \quad (1.6)$$
$$=-J\partial[(nm)^{-1}\log Z]/\partial K$$
$$=-J\coth 2K[1+2\pi^{-1}(2\tanh^2 2K-1)K_1(k_1)], \quad (4.54)$$

where

$$k_1=2\sinh 2K\cosh^{-2}2K$$

and $K_1(k_1)$ is the complete elliptic integral of the first kind,

$$K_1(k_1)=\int_0^{\pi/2}(1-k_1^2\sin^2\varphi)^{-\frac{1}{2}}d\varphi.$$

The critical point for this system has already been predicted in Sec. 3.1 as the point where $|\sinh 2K_c|=1$. For $K=K_c$, $k_1=1$ and $2\tanh^2 2K=1$. Even though $K_1(k_1)$ has a logarithmic singularity at $k_1=1$, the coefficient of $K_1(k_1)$ vanishes linearly with the result that $\bar{E}$ is continuous at T_c. There is no latent heat.

The specific heat is, however, given by

$$C=\partial\bar{E}/\partial T.$$

Since one of the terms of $\bar{E}$ is proportional to $|T-T_c|\times\log|T-T_c|$ near $T=T_c$, there is a term in C which is proportional to $\log|T-T_c|$. The specific heat has a logarithmic singularity at $T=T_c$.

The more complicated analysis of the general case $K\neq K'$ shows that the specific heat still has a logarithmic singularity at a temperature given by

$$\sinh 2K\sinh 2K'=1. \quad (4.55)$$

If we fix $J+J'$, the spin-spin internal energy at 0° Kelvin, and let J' become small. The critical temperature becomes smaller. If $J'=0$, the two-dimensional lattice degenerates into a system of independent one-dimensional chains which, as already seen, has no critical temperature. As $J'\to 0$, the critical point tends toward $T=0$ and finally disappears for $J'=0$. (See Fig. 15.)

5. OTHER LATTICES

The detailed analysis in the previous sections has been primarily restricted to properties of the square lattice. Other lattice types have been considered by several authors.[20–25] However, when these types have been successfully treated, the results have not differed in any very interesting way from the properties of the square net. We shall therefore only briefly summarize the calculations that have been done.

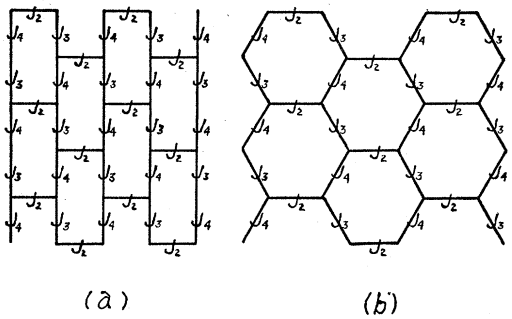

FIG. 18. (a) is obtained from Fig. 17 by setting $J_1=0$, thus eliminating the bond so designated. (a) can then be deformed into the hexagonal lattice (b). The partition function depends only upon the J's and the topology of the lattice.

The triangular and hexagonal lattices which have already been described in Sec. 3.1 can be solved exactly by essentially the same technique used for the square lattice. Another lattice that has been treated in the same way is the Kagomé lattice,[26] a woven bamboo pattern as shown in Fig. 16.

All these lattice types can be considered as special cases of a generalized square lattice.[27] In this generalized square lattice we introduce several interaction constants. For example, we may use four different constants, one for each of the four nearest neighbors as shown in Fig. 17. Each bond is labeled with its coupling constant.

The techniques used for solving the usual square net, particularly the method of spinor analysis, can with minor modifications solve this more complex lattice. It is in fact possible to solve exactly a square net with even more complex arrangements of coupling constants. The details of such will however not be given here.

We shall notice that from the solution of this lattice we obtain as special cases, the solution for both the triangular and hexagonal lattices. If we set $J_1=0$ we eliminate the bonds so designated. The resulting lattice shown in Fig. 18 is then deformable into the hexagonal lattice.

If, on the other hand, we take the limit $J\to\infty$, the spin pairs so coupled must take the same values. They therefore act as a single particle. The lattice resulting from bringing the particles joined by J_1 into a single particle gives the triangular lattice.

The Kagomé lattice is a special case of a more complex square lattice. The specialization is illustrated in Fig. 19 where we have designated by ∞ and 0 those bonds of the square lattice whose coupling constants are ∞ and 0, respectively.

With but a few special exceptions mentioned below, the properties of these lattices are of the same general type as the regular square lattice discussed in Sec. 4.3. They all exhibit a logarithmic singularity in the specific heat corresponding to a transition from an ordered to a disordered state. The critical temperature depends upon the values of the various coupling constants, for example, the critical temperature of the triangular lattice is given by the solution of

$$(\cosh 2K_2\cosh 2K_3\cosh 2K_4+\sinh 2K_2\sinh 2K_3\sinh 2K_4)^2=2+\sinh^2 2K_2+\sinh^2 2K_3+\sinh^2 2K_4 \tag{5.1}$$

$$K_j=J_j/kT.$$

The exceptions to this type of behavior are furnished by special antiferromagnetic lattices which have no "perfectly ordered" state. An example of such is the triangular lattice for which the three coupling constants are all exactly equal and negative $J_1=J_2=J_3<0$. Each particle tries to have its spin opposite to that of all its neighbors. One readily sees that it is not possible to arrange positive and negative spins so that each spin in the lattice is different than all its neighbors. There is no ordered state as for example in the rectangular and hexagonal lattices illustrated by Fig. 20.

This triangular lattice fails to have a transition if and only if one or three J_i's are negative and the two weakest $|J_i|$ are exactly equal. All these cases lack an ordered state. It is interesting that, if one or three J_i are negative and we let the two weakest $|J_i|$ approach equal values, the value of T_c becomes smaller and smaller until it finally disappears at $T_c=0$ much as the singularity in the two-dimensional square lattice vanished as we let one of the couplings go to zero.

Even in the general case $J_1\neq J_2\neq J_3$, it is possible to obtain both a dual transformation and a star-triangle transformation as in Sec. 2. These are obtained in the same manner as before but the algebra becomes more cumbersome. The fact that certain triangular lattices have no transition does not imply, however, that the hexagonal lattice has any such solutions of physical interest. By applying the star-triangle transformation to these special triangular lattices one finds that they correspond to hexagonal lattices with imaginary couplings. All hexagonal lattices with nonzero real coupling constants have phase transitions.

The triangular lattice may be considered as a first step toward the solution of a nearest and next nearest neighbor square net problem. We can deform the triangular lattice as shown in Fig. 21. It is then apparent

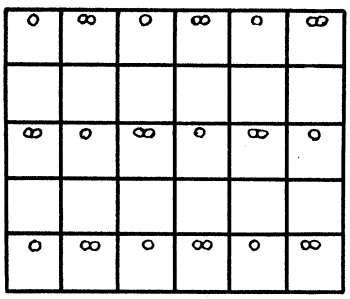

FIG. 19. By eliminating those bonds designated by 0 and joining points connected by the bonds ∞, one can deform the above lattice into the Kagomé lattice of Fig. 16.

that the triangular net is a square net with an additional interaction along one of the diagonals. Unfortunately, it has not been possible to solve the case of interactions along both diagonals. Indeed none of the cases considered involve interactions that "cross." The difficulties here are remindful of those in the three-dimensional lattice where the topology of closed paths involve knots. It would appear that this also may be a very difficult problem.

The partition function per particle Z_H, of a hexagonal lattice is given by[20]

$$\log(\tfrac{1}{2}Z_H)=\frac{1}{16\pi^2}\int_0^{2\pi}\int_0^{2\pi}\log\tfrac{1}{2}\{\cosh 2K_1\cosh 2K_2\times\cosh 2K_3+1-\sinh 2K_2\sinh 2K_3\cos\omega_1-\sinh 2K_3\sinh 2K_1\cos\omega_2-\sinh 2K_1\sinh 2K_2\cos(\omega_1+\omega_2)\}d\omega_1 d\omega_2.$$

That of a triangular lattice Z_T is given by

$$\log(\tfrac{1}{2}Z_T)=\frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{2\pi}\log\{\cosh 2K_1\cosh 2K_2\times\cosh 2K_3+\sinh 2K_1\sinh 2K_2\sinh 2K_3-\sinh 2K_1\cos\omega_1-\sinh 2K_2\cos\omega_2-\sinh 2K_3\cos(\omega_1+\omega_2)\}d\omega_1 d\omega_2.$$

6. SPECIAL PROPERTIES OF THE TWO-DIMENSIONAL ISING LATTICE

6.1 Ferromagnetism

Perhaps the most interesting feature of the Ising lattice is its spontaneous magnetization, a necessary feature of any ferromagnet. Peierls[28] was the first to show that the Ising model was ferromagnetic and series expansions for the spontaneous magnetization were long ago given for low temperatures by van der Waerden[8] and Ashkin and Lamb.[16]

The magnetization per particle has already been defined as

$$M=N^{-1}\mu\sum_{j=1}^{N}\bar{\sigma}_j=N^{-1}\partial\log Z/\partial\mathfrak{H}. \tag{6.1}$$

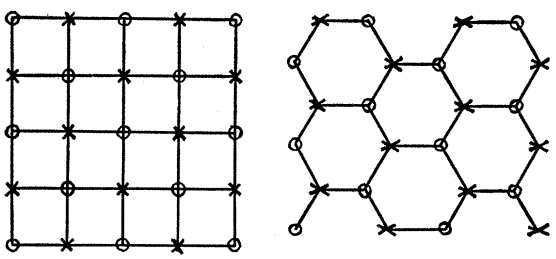

FIG. 20. For an antiferromagnetic square or hexagonal lattice, a state of "perfect order" exists. This state is illustrated with circle describing up (or down) spins and x describing down (or up) spins. Such a state does not exist for the triangular lattice.

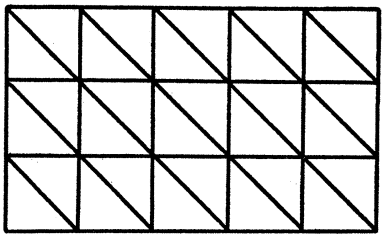

FIG. 21. A triangular lattice can be deformed into the above form which can be interpreted as a square lattice with interactions along one of the diagonal directions.

To be ferromagnetic, a system must have a discontinuity in $M(H, T)$ as a function of H at $H=0$ and T less than some critical temperature T_c. If we take the limit $M(H, T)$ as $H\to 0$ from positive values of H, then $M(0_+, T)>0$. The ferromagnet retains its magnetization in the direction of H even after the magnetic field is turned off. If, on the other hand, we let $H\to 0$ from the negative side, then $M(0_-, T)<0$.

The energy levels of the Ising lattice are given by

$$-J\sum_{n.n.}\sigma_i\sigma_j-\mu H\sum_{j=1}^{N}\sigma_j.$$

If we change the direction of the magnetic field ($H\to -H$) and all the spins ($\sigma_j\to-\sigma_j$), the energy remains unchanged. Since Z involves the sum over all $\sigma_j=\pm 1$ or $-\sigma_j=\pm 1$,

$$\begin{aligned}Z(H)&=Z(-H),\\ M(H)&=-M(-H).\end{aligned} \tag{6.2}$$

For any finite lattice $M(0)=0$. This is apparent since, for a finite lattice Z is a sum of a finite number of functions each analytic in H. Z and M must therefore be analytic in H, and $M(H)=-M(-H)$ implies $M(0)=0$. If, however, we allow the system to be infinite, Z becomes the limit of a sequence of analytic functions which is not necessary analytic. To calculate a spontaneous magnetization, it is necessary to first let $N\to\infty$, then let $H\to 0$. If we put $H=0$ first, we shall always obtain $M(0)=0$.

Although we do not have a solution of the Ising problem for arbitrary H, the spontaneous magnetization depends only upon the behavior of $Z(H, T)$ for small H to terms linear in H.

The existence of a spontaneous magnetization was first proved on the basis of the low temperature expansion of Z. Regarding Eq. (2.25), we note that because of the symmetry with respect to changing σ to $-\sigma$,

$$g(N, N_1, N_{12})=g(N, N-N_1, N_{12}),$$

where N_1 is the number of σ's that are $+1$ and $N-N_1$ the number that are -1. We combine the terms of (2.25) with $N>N/2$ and those with $N\equiv N/2$ to obtain

$$Z=2e^{NcK/2}\sum_{N_{12}}\sum_{N_1\le N/2}g(N, N_1, N_{12})\times\exp(-2KN_{12})\cosh[(N-2N_1)\mu\mathfrak{H}]. \tag{6.3}$$

(The one term with $N_1=N/2$ for N even is incorrect by a factor of 2 but this error is negligible for large N.)

For N is finite, (6.3) is a function only of $\mathfrak{H}^2$ and therefore gives $M(0)=0$. For low temperatures and positive K, the main contribution to Z comes from terms with $N_{12}\ll Nc/2$.

The existence or nonexistence of a spontaneous magnetization hinges on the dependence of N_1 on N_{12}. These two are certainly not independent quantities for example $N_{12}=0$ implies $N_1=0$ or N. In a one-dimensional lattice, there is, however, very little correlation between N_1 and N_{12} for $N_{12}>0$ because each unfavorable bond (joining unlike spins) gives a boundary between regions of $\sigma=+1$ and $\sigma=-1$. One can shift these boundaries almost at will. Such a shift leaves N_{12} unchanged but N_1 depends upon the length of the regions with $\sigma=+1$. One can make all regions with $\sigma=+1$ small to give a small N_1 or make them all large to give a large N_1.

In two or three dimensions, the situation is quite different. The correlation between N_1 and N_{12} is much stronger. The feature we will want to exploit is that small N_{12} implies small N_1 (or small $N-N_1$); if there are few unlike pairs, then most particles must have the same spin. This difference between the one-dimensional lattice and those of higher dimension is the cause of most of the marked dissimilarity of the thermodynamic and magnetic properties of the one-dimensional lattice.

The dependence of Z on H is contained in the factor $\cosh[(N-2N_1)\mu\mathfrak{H}]$ and the spontaneous magnetization comes from first allowing N to become infinite and then letting $\mu\mathfrak{H}\to 0$. The behavior of Z for small $\mathfrak{H}$ depends strongly on whether or not for most states $N-2N_1\to\infty$ as $N\to\infty$. Such is the case in two or three dimensions at sufficiently low temperatures because a low temperature implies that N_{12} is small for most states and therefore N_1/N is also small. (In one dimension such is not true.)

If $N_1/N\ll 1$ for most states as $N\to\infty$, then for any nonzero $\mu\mathfrak{H}$,

$$\cosh[(N-2N_1)\mu\mathfrak{H}]\to\tfrac{1}{2}\exp[(N-2N_1)|\mu\mathfrak{H}|]$$

for most states. Here lies the source of the spontaneous magnetization, for if we now let $|\mu\mathfrak{H}|\to 0$. Z contains terms linear in $|\mu\mathfrak{H}|$ leading to a nonzero magnetization for $\mathfrak{H}\to 0$ and a discontinuity. For very low temperature and small $\mathfrak{H}$,

$$\begin{aligned} &Z(H)\sim Z(0)\cosh(N\mu\mathfrak{H})\\ &M(H)\sim\mu\lim_{N\to\infty}\tanh(N\mu\mathfrak{H})=\begin{cases}\mu & \text{for } H>0\\ -\mu & \text{for } H<0\end{cases}\end{aligned}\tag{6.4}$$

(except in one dimension).

A closed expression for $M(0)$ as a function of T has not been derived by combinatorial methods although rather lengthy series expansions have been calculated (see Sec. 7). The spontaneous magnetization of the two-dimensional Ising lattice has been derived, however, using algebraic methods. This was done by Yang[29] (it was reported but never published by Onsager at the Cornell Phase Transition Conference, 1948) using a first-order perturbation of the solution of the Ising problem in zero field. We shall only indicate here the preliminary steps to this calculation. Although the basis for the method is quite obvious, the detailed calculations are both tricky and tedious.

In Eq. (2.14), the partition function is written as

$$\begin{aligned} Z&=(2\sinh 2K)^{nm/2}\,\mathrm{trace}\,(\mathbf{V}_3\mathbf{V}_2\mathbf{V}_1)^m\\ &\sim(2\sinh 2K)^{mn/2}\lambda^m{}_{\max},\end{aligned}$$

where $\lambda_{\max}$ is the largest eigenvalue of

$$\mathbf{V}_3\mathbf{V}_2\mathbf{V}_1=\mathbf{V}_2\mathbf{V}_1+\mu\mathfrak{H}(\sum_{j=1}^{n}\mathbf{s}_j)\mathbf{V}_2\mathbf{V}_1+\cdots.$$

We write $\lambda_{\max}=\lambda^0{}_{\max}+\mu\mathfrak{H}\lambda'_{\max}$ with $\lambda^0{}_{\max}$ the largest eigenvalue of $\mathbf{V}_2\mathbf{V}_1$ and we determine $\lambda'_{\max}$ by the usual first-order perturbation theory.

Perturbation theory is somewhat more elegant if the matrices are symmetric because then the eigenfunction are orthogonal. Instead of treating the matrix $\mathbf{V}_3\mathbf{V}_2\mathbf{V}_1$, Yang considers matrix $\mathbf{V}_1^{\frac{1}{2}}\mathbf{V}_3\mathbf{V}_2\mathbf{V}_1^{\frac{1}{2}}$ which is similar to the above but also symmetric. This is not a generalization of the symmetric matrix $\mathbf{P}$ of Sec. 2. Such a matrix would be $\mathbf{V}_2^{\frac{1}{2}}\mathbf{V}_3^{\frac{1}{2}}\mathbf{V}_1\mathbf{V}_3^{\frac{1}{2}}\mathbf{V}_2^{\frac{1}{2}}$. All three of these matrices are similar and therefore have the same eigenvalues. One should be able to carry through all the analysis irrespective of representation but to avoid confusion we use here the same matrix as Yang. We therefore write

$$\mathbf{V}_1^{\frac{1}{2}}\mathbf{V}_3\mathbf{V}_2\mathbf{V}_1^{\frac{1}{2}}=\mathbf{V}_1^{\frac{1}{2}}\mathbf{V}_2\mathbf{V}_1^{\frac{1}{2}}+\mu\mathfrak{H}\mathbf{V}_1^{\frac{1}{2}}\sum_{j=1}^{n}\mathbf{s}_j\mathbf{V}_2\mathbf{V}_1^{\frac{1}{2}}.$$

Perturbation theory warns us that we must distinguish between cases where $\lambda^0{}_{\max}$ is degenerate and cases where it is nondegenerate. We therefore consider separately the cases $T>T_c$ and $T<T_c$.

We have seen (Sec. 3.2) that for $T>T_c$, the largest eigenvalue of $\mathbf{V}_1^{\frac{1}{2}}\mathbf{V}_2\mathbf{V}_1^{\frac{1}{2}}$ is nondegenerate and its eigenfunction ψ_+ belongs to the space of even functions. Each of the matrices $\mathbf{V}_2$ and $\mathbf{V}_1$ commutes with $\mathbf{U}$, thus they send even functions into even functions and odd functions into odd functions. $\mathbf{s}_j$, however, anticommutes with $\mathbf{U}$, it sends even functions into odd functions and vice versa. The perturbing term above therefore has no diagonal elements in the representation in which $\mathbf{V}_1^{\frac{1}{2}}\mathbf{V}_2\mathbf{V}_1^{\frac{1}{2}}$ is diagonal and

$$\lambda'_{\max}=(\psi_+,\,\mathbf{V}_1^{\frac{1}{2}}\sum_{j=1}^{n}\mathbf{s}_j\mathbf{V}_2\mathbf{V}_1^{\frac{1}{2}}\psi_+)=0.$$

For $T>T_c$ there is no correction to λ linear in $\mathfrak{H}$, thus no spontaneous magnetization.

For $T<T_c$, the situation is quite different. We have seen that $\lambda^0{}_{\max}$ is then twofold degenerate in the limit $n\to\infty$. There is an eigenfunction ψ_+ in the even space and an eigenfunction ψ_- in the odd space. The perturba-

tion "splits" the degeneracy, and we have a situation quite analogous to the anomalous Zeeman effect in the quantum theory of the hydrogen atom.

The first step in a perturbation procedure is to consider separately those parts of the matrices corresponding to the space in which $\lambda^0_{\max}$ is degenerate. In this case we consider the 2×2 section of the matrices corresponding to the space ψ_+ and ψ_-. We wish to choose a representation in which the 2×2 part of both the zero-order and first-order matrices $\mathbf{V}_1^{\frac{1}{2}}\mathbf{V}_2\mathbf{V}_1^{\frac{1}{2}}$ and

$$\mathbf{V}_1^{\frac{1}{2}}\sum_{j=1}^{n}\mathbf{s}_j\mathbf{V}_2\mathbf{V}_1^{\frac{1}{2}},$$

respectively, are diagonal. This portion of the matrix $\mathbf{V}_1^{\frac{1}{2}}\mathbf{V}_2\mathbf{V}_1^{\frac{1}{2}}$ is simply $\lambda^0_{\max}$ times the 2×2 identity matrix and is invariant to any transformation of ψ_+ and ψ_-. It will be diagonal in any representation including that in which this part of the first-order matrix is diagonal. The 2×2 portion of the first-order matrix is symmetric and has zero diagonal elements in the representation ψ_+ and ψ_-. The first-order eigenfunctions are therefore $2^{\frac{1}{2}}(\psi_+\pm\psi_-)$ and

$$\lambda'_{\max}=[2^{-\frac{1}{2}}(\psi_++\psi_-),\ \mathbf{V}_1^{\frac{1}{2}}\sum_{j=1}^{n}\mathbf{s}_j\mathbf{V}_2\mathbf{V}_1^{\frac{1}{2}}2^{-\frac{1}{2}}(\psi_++\psi_-)].$$

Since $\mathbf{V}_1^{\frac{1}{2}}\mathbf{V}_2\mathbf{V}_1^{\frac{1}{2}}(\psi_++\psi_-)=\lambda^0_{\max}(\psi_++\psi_-)$,

$$\lambda'_{\max}=\tfrac{1}{2}\lambda^0_{\max}[(\psi_++\psi_-),\ \mathbf{V}_1^{\frac{1}{2}}\sum_{j=1}^{n}\mathbf{s}_j\mathbf{V}_1^{-\frac{1}{2}}(\psi_++\psi_-)]$$

$$=\lambda^0_{\max}(\psi_-,\ \mathbf{V}_1^{\frac{1}{2}}\sum_{j=1}^{n}\mathbf{s}_j\mathbf{V}_1^{-\frac{1}{2}}\psi_+)$$

because $\mathbf{s}_j$ has no matrix elements connecting ψ_+ to ψ_+ or ψ_- to ψ_- but $\mathbf{s}_j$ is symmetric.

Using (6.1), we see that to order $\mathfrak{H}$,

$$M=n^{-1}\partial\log\lambda_{\max}/\partial\mathfrak{H}=n^{-1}\mu\lambda'_{\max}/\lambda^0_{\max}$$

$$=n^{-1}\mu(\psi_-,\ \mathbf{V}_1^{\frac{1}{2}}\sum_{j=1}^{n}\mathbf{s}_j\mathbf{V}_1^{-\frac{1}{2}}\psi_+).$$

Since each point in the row is equivalent to any other point, each of the n values of j give the same contribution; therefore,

$$M=\mu(\psi_-,\ \mathbf{V}_1^{\frac{1}{2}}\mathbf{s}_1\mathbf{V}_1^{-\frac{1}{2}}\psi_+).$$

The magnetization is thus described by a single matrix element which formally looks quite simple. The evaluation of it is, however, rather complicated even though the answer is relatively simple. Yang[29] found for $K=K'$

$$|M(0)|=\mu(1+z^2)^{\frac{1}{4}}(1-z^2)^{-\frac{1}{4}}(1-6z^2+z^4)^{1/8}$$
$$z=e^{-2K}. \tag{6.5}$$

Near the critical point $z=z_c=\sqrt{2}-1$, $M(0)$ has a branch point

$$M(0)\simeq\mu[4(\sqrt{2}+2)(z_c-z)]^{1/8}.$$

The magnetization $M(0, T)$ is shown in Fig. 22.§

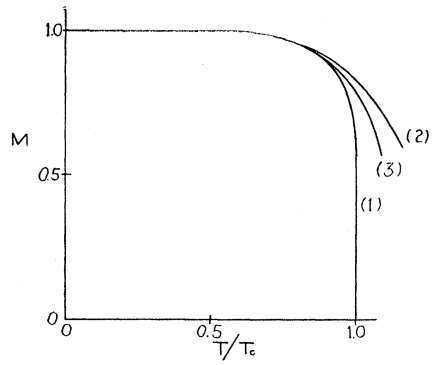

FIG. 22. The spontaneous magnetization of the two-dimensional Ising lattice is plotted *vs* the temperature (curve 1) (see reference 29). Curve (2) is an extrapolation of the low temperature series expansion in powers of $z=e^{-2K}$, including terms of order z^{12} [deduced by van der Waerden (see reference 8) and Ashkin and Lamb (see reference 16)]. Curve (3) is the expansion to terms of order z^{18} as given by Domb (see reference 34), the longest series known prior to Yang's exact treatment.

6.2 Correlations

Aside from the usual thermodynamic quantities, one is also interested in the correlations between spins at different lattice sites. Such correlations are observed experimentally in x-ray diffraction effects.

A great deal of literature exists on approximate theories of ferromagnetism and binary alloys based upon short-range and long-range correlations. A review of such work would carry us far away from our purpose here. This voluminous literature has been reviewed elsewhere.

Exact expressions for correlations have been calculated only for the two-dimensional square Ising lattice.[30] The correlation of the ith spin to the jth spin is defined as the average of σ_i if $\sigma_j=+1$. We may re-express this in many ways. It is also the average of σ_j if $\sigma_i=+1$, or the negative of the average of σ_i if $\sigma_j=-1$. The most convenient expression is the average of $\sigma_i\sigma_j$ written below as $\langle\sigma_i\sigma_j\rangle$. The equivalence of these definitions is apparent since $\sigma_i=+1$ with equal *a priori* probabilities.

$\langle\sigma_i\sigma_j\rangle$ is calculated from

$$\langle\sigma_i\sigma_j\rangle=Z^{-1}\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_N=\pm1}\sigma_i\sigma_j\exp(-E/kT). \tag{6.6}$$

These averages are evaluated by again using matrix expressions. For a two-dimensional lattice, let σ_{jk} be the spin of the particle in the jth row and kth column.

§ *Note added in proof:* Formulas for the magnetization of the asymmetric square and triangular lattices have been presented by R. B. Potts [Phys. Rev. 88, 352 (1952)]. The formulas of the former were also given by C. H. Chang [Phys. Rev. 88, 1422 (1952)].

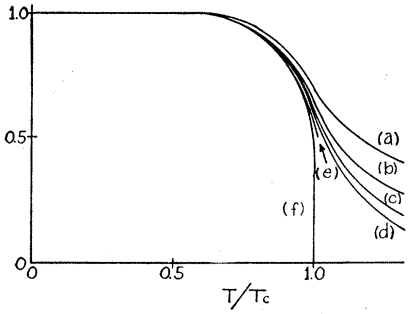

FIG. 23. Correlation coefficients of the two-dimensional square Ising lattice as a function of temperature (see reference 30); (a) $\langle\sigma_{11}\sigma_{12}\rangle$, (b) $\langle\sigma_{11}\sigma_{22}\rangle$, (c) $\langle\sigma_{11}\sigma_{13}\rangle$, (d) $\langle\sigma_{11}\sigma_{23}\rangle$, (e) $\langle\sigma_{11}\sigma_{14}\rangle$, and (f) M^2. Since, as one observes from the figure, these averages are monotone functions of the distance between the points, the long-range correlations approach a limit M^2 independent of direction on the lattice.

If ν_k represents the state of the kth row as in Sec. 2.1, then (6.6) can be written in the form

$$\langle\sigma_{jk}\sigma_{ab}\rangle=Z^{-1}\sum_{\nu_1=1}^{2^n}\cdots\sum_{\nu_m=1}^{2^n}P_{\nu_1\nu_2}\times\cdots\times P_{\nu_{j-1}\nu_j}(s_k)_{\nu_j\nu_j}P_{\nu_j\nu_{j+1}}\times\cdots\times P_{\nu_{a-1}\nu_a}(s_b)_{\nu_a\nu_a}P_{\nu_a\nu_{a+1}}\times\cdots\times P_{\nu_m\nu_1},$$

where $P_{\nu\nu'}$ is the matrix defined in Sec. 2.1. The above is again expressible as the trace of a matrix product,

$$\langle\sigma_{jk}\sigma_{ab}\rangle=Z^{-1}\text{ trace }(\mathbf{P}^{j-1}\mathbf{s}_k\mathbf{P}^{a-j}\mathbf{s}_b\mathbf{P}^{m-a+1})=Z^{-1}\text{ trace }(\mathbf{s}_k\mathbf{P}^{a-j}\mathbf{s}_b\mathbf{P}^{m-a+j}).\qquad(6.7)$$

The right side depends upon a and j only through the combination of $j-a$ as is to be expected physically as a result of the periodic boundary conditions. Also it depends upon k and a only through $k-a$ because the matrix $\mathbf{P}$ is invariant to a cyclic permutation of the particles in a row. One needs only consider $\langle\sigma_{11}\sigma_{ab}\rangle$. Also the correlations are independent of reflections about vertical or horizontal lines, they depend only upon $|a-1|$ and $|b-1|$, thus we need only consider $1<a\leq\frac{1}{2}m+1$ and $1<b\leq\frac{1}{2}n+1$.

Since the trace is invariant to a similarity transformation, we apply the transformation which diagonalizes $\mathbf{P}$. Let $\mathbf{\Psi}$ be this transformation matrix,

$$\langle\sigma_{11}\sigma_{ab}\rangle=(\sum_{l=1}^{2^n}\lambda_l{}^m)^{-1}\sum_{l=1}^{2^n}\lambda_l{}^{m-a+1}(\mathbf{\Psi}^{-1}\mathbf{s}_1\mathbf{P}^{a-1}\mathbf{s}_b\mathbf{\Psi})_{ll}.\qquad(6.8)$$

Since $a-1\leq m/2$, $m-a+1$ will be large for m large and we need only consider the values of l corresponding to the largest eigenvalue. For $T>T_c$, the largest eigenvalue is nondegenerate and we neglect all l but one:

$$\langle\sigma_{11}\sigma_{ab}\rangle\simeq\lambda_{\max}{}^{-a+1}(\psi_+,\ \mathbf{s}_1\mathbf{P}^{a-1}\mathbf{s}_b\psi_+).\qquad(6.8a)$$

For $T<T_c$ the largest eigenvalue is doubly degenerate, in which case

$$\langle\sigma_{11}\sigma_{ab}\rangle\simeq\tfrac{1}{2}\lambda_{\max}{}^{-a+1}[(\psi_+,\ \mathbf{s}_1\mathbf{P}^{a-1}\mathbf{s}_b\psi_+)+(\psi_-,\ \mathbf{s}_1\mathbf{P}^{a-1}\mathbf{s}_b\psi_-)].\qquad(6.8b)$$

The correlations between nearby point (a and b small) in an infinite lattice (m and $n\to\infty$) are used to describe "short-range order." Long-range order already discussed in Sec. 3.2 is described by the limit of $\langle\sigma_{11}\sigma_{ab}\rangle$ as a and $b\to\infty$ (after m and $n\to\infty$).

The correlations have been calculated by Kaufman and Onsager for several of the nearby pairs of points. The detailed evaluation of the matrix elements (6.8a,b) is again a rather tedious operation. The results of these calculations are plotted in Fig. 23.

Long-range order and spontaneous magnetization describe essentially the same thing as we shall see below. One can very easily see from (6.8) and (6.8a) that no long-range order exists for $T>T_c$. If we let $l=1$ correspond to the largest eigenvalue (it is nondegenerate), then

$$\langle\sigma_{11}\sigma_{ab}\rangle\to\lambda_1{}^{-a+1}(\mathbf{\Psi}^{-1}\mathbf{s}_1\mathbf{\Psi}\mathbf{\Psi}^{-1}\mathbf{P}^{a-1}\mathbf{\Psi}\mathbf{\Psi}^{-1}\mathbf{s}_b\mathbf{\Psi})_{11}$$

as $m\to\infty$

$$=\lambda_1{}^{-a+1}\sum_{j=1}^{2^n}(\mathbf{\Psi}^{-1}\mathbf{s}_1\mathbf{\Psi})_{1j}\lambda_j{}^{a-1}(\mathbf{\Psi}^{-1}\mathbf{s}_b\mathbf{\Psi})_{j1}$$

$$\to(\mathbf{\Psi}^{-1}\mathbf{s}_1\mathbf{\Psi})_{11}(\mathbf{\Psi}^{-1}\mathbf{s}_b\mathbf{\Psi})_{11}$$

as $a\to\infty$

$$=\langle\sigma_{11}\rangle\langle\sigma_{1b}\rangle=0$$

because both σ_{11} and σ_{1b} are zero. Thus, we again prove that long-range order cannot exist unless the largest eigenvalue is degenerate.

We might look at this from a slightly different point of view. Suppose $|M|=M(0_+,T)=-M(0_-,T)$ is the spontaneous magnetization per particle, N_1 the number of "up" spins and N_2 the number of "down" spins, then

$$|M|=|N_1-N_2|/N=\pm(N_1-N_2)/N,\quad N=N_1+N_2.$$

The $\pm$ is chosen accordingly as the magnetization is in the positive or negative direction (up or down). This gives

$$N_1/N=\tfrac{1}{2}(1\pm|M|),\quad N_2/N_1=\tfrac{1}{2}(1\mp|M|).$$

We now ask what is the average magnetization if one spin (call it σ_{11}) is positive? We use the symbol $Pr\{a\}$ to denote the probability of the event a. We have just deduced that

$$Pr\{\sigma_{11}>0\quad\text{if}\quad M=\pm|M|\}=\tfrac{1}{2}(1\pm|M|).$$

However,

$$Pr\{\sigma_{11}>0\quad\text{and}\quad M=\pm|M|\}=Pr\{\sigma_{11}>0\quad\text{if}\quad M=\pm|M|\}Pr\{M=\pm|M|\}=Pr\{M=\pm|M|\quad\text{if}\quad\sigma_{11}>0\}Pr\{\sigma_{11}>0\}.$$

In the absence of a magnetic field $Pr\{M=\pm|M|\}$ and $Pr\{\sigma_{11}=\pm 1\}$ are all $\frac{1}{2}$. Thus,

$$Pr\{M=\pm|M| \quad \text{if} \quad \sigma_{11}>0\} = Pr\{\sigma_{11}>0 \quad \text{if} \quad M=\pm|M|\}=\tfrac{1}{2}(1\pm|M|).$$

We find that the average magnetization if $\sigma_{11}>0$ to be

$$|M|Pr\{M=|M| \quad \text{if} \quad \sigma_{11}>0\} - |M|Pr\{M=-|M| \quad \text{if} \quad \sigma_{11}>0\} = \tfrac{1}{2}|M|(1+|M|)-\tfrac{1}{2}|M|(1-|M|)=M^2.$$

M^2 is the conditional average of all spins if $\sigma_{11}>0$. It can also be expressed in terms of the correlations above

$$M^2=\lim_{m,n\to\infty}(nm)^{-1}\sum_{a=1}^{m}\sum_{b=1}^{n}\langle\sigma_{11}\sigma_{ab}\rangle.$$

As n and $m\to\infty$, no finite set of a, b contribute to this sum. We obtain a nonzero M^2 if and only if $\langle\sigma_{11}\sigma_{ab}\rangle$ is nonzero for arbitrarily large a and b. Thus, we see that the existence of long-range order is equivalent to the existence of a spontaneous magnetization.

7. THREE-DIMENSIONAL LATTICES

It has already been mentioned that the methods used in finding exact expressions for properties of two-dimensional lattices break down when they are applied to the investigation of three-dimensional lattices. However, the first few terms have been calculated in certain power series expansions for the partition function of three-dimensional Ising lattices. Expansions exist which are valid in the high and low temperature ranges. These have been obtained by both the matrix and combinatorial methods. Although it is impossible to base a rigorous discussion of critical phenomenon on these series, they give accurate results at temperatures not too close to the critical point and are useful for the estimation of the range of validity of approximate expressions for thermodynamic properties.

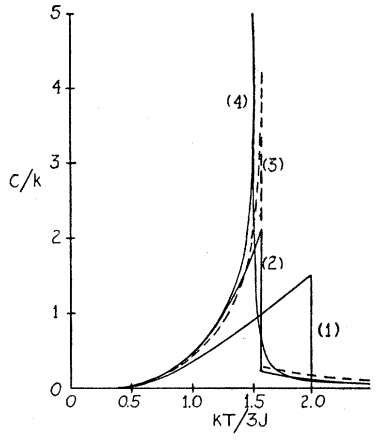

FIG. 24. Approximate specific heat curves for the three-dimensional cubic Ising lattice (see references 2, 31). In order of their apparent accuracy they are (1) Bragg-Williams approximation, (2) Bethe second approximation, (3) Kirkwood approximation, and (4) and extrapolation of high and low temperature expansions by Wakefield known to be accurate everywhere except near the critical point.

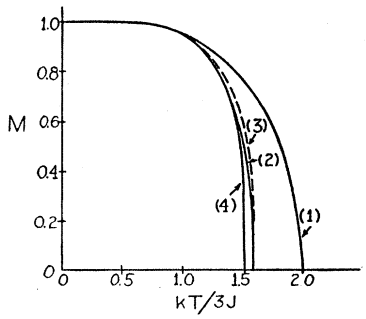

FIG. 25. Approximate spontaneous magnetization curves for the cubic lattice corresponding to the curves of Fig. 24.

Since Rushbrook[31] recently published a detailed review of the status of these series, we shall merely state the best available results for the simple, body-centered and face-centered cubic lattices and present specific heat and spontaneous magnetization curves (see Figs. 24 and 25) for the simple cubic lattice. These curves are compared with those computed on the basis of the Bragg-Williams and Bethe formulas.

A large number of articles have been written about series expansions. Some of the more recent ones are those of Rushbrook[32] and Wakefield;[33] Domb;[34] Trefftz;[35] Somers;[36] Ter Haar;[37] Oguchi;[38] Tanaka, Katsumori, and Toshima;[39] and Kikuchi.[40]

We shall consider only the case in which the interaction parameters in all directions are equal. We let

$$x=\tanh K. \tag{7.1}$$

Then the high temperature expansions for the Nth root of the partition function (in a lattice of N particles) are

a. simple cubic lattice

$$Z^{1/N}=2\cosh^3 K(1+3x^4+22x^6+192x^8+2070x^{10}+24\,943x^{12}+\cdots); \tag{7.2}$$

b. body-centered cubic

$$Z^{1/N}=2\cosh^4 K(1+12x^4+148x^6+1860x^8+\cdots); \tag{7.3}$$

c. face-centered cubic

$$Z^{1/N}=2\cosh^6 K(1+8x^3+33x^4+168x^5+962x^6+5928x^7+\cdots). \tag{7.4}$$

The low temperature series for $N^{-1}\log Z$ are expressed in powers of $z=\exp(-2J/kT)$,

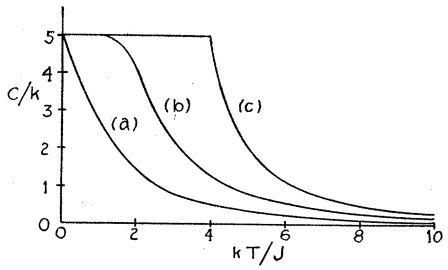

FIG. 26. Specific heat *vs* temperature for the spherical model in (a) one dimension, (b) two dimensions, and (c) three dimensions.

a. simple cubic lattice

$$z^{-3}\Big(z^6+3z^{10}-\frac{7}{2}z^{12}+15z^{14}-33z^{16}+\frac{313}{3}z^{18}-\frac{561}{2}z^{20}+849z^{22}-\frac{9847}{4}z^{24}+7485z^{26}-\frac{45\,069}{2}z^{28}+\cdots\Big); \quad (7.5)$$

b. body-centered cubic

$$z^{-2}\Big(z^8+4z^{14}-\frac{9}{2}z^{16}+28z^{20}-64z^{22}+\frac{145}{3}z^{24}+204z^{26}-786z^{28}+1164z^{30}+\frac{3691}{4}z^{32}-8760z^{34}+\cdots\Big); \quad (7.6)$$

c. face-centered cubic

$$z^{-3}\Big(z^{12}+6z^{22}-\frac{13}{2}z^{24}+8z^{30}+42z^{32}-120z^{34}+\frac{217}{3}z^{36}+24z^{28}+123z^{40}+126z^{42}-1623z^{44}+2418z^{46}+\cdots\Big). \quad (7.7)$$

The formulas for spontaneous magnetization are

a. simple cubic[11]

$$M/\mu=1-2z^6-12z^{10}+14z^{12}-90z^{14}+192z^{16}-792z^{18}+2148z^{20}-7716z^{22}+23\,262z^{24}-79\,512z^{26}+252\,054z^{28}+\cdots;$$

b. body-centered

$$M/\mu=1-2z^8-16z^{14}+18z^{16}-168z^{20}+384z^{22}-314z^{24}-1184z^{26}+6248z^{28}-9744z^{30}-10\,174z^{32}+\cdots;$$

[11] *Note added in proof:* The coefficient of z^{26} is that given in reference 39, Wakefield (reference 33), however, gives 79530.

c. face-centered

$$M/\mu=1-2z^{12}-24z^{22}+26z^{24}-48z^{30}-252z^{32}+720z^{34}-438z^{36}-192z^{36}-984z^{40}-1008z^{42}-\cdots.$$

It has frequently been conjectured that the partition function Z for a three-dimensional lattice is the simple generalization of the Onsager formula

$$\log\tfrac{1}{2}Z^{1/N}=\frac{1}{2(2\pi)^3}\int_0^{2\pi}\!\!\int\!\!\int \times\log(\cosh 2K_1\cosh 2K_2\cosh 2K_3-\sinh 2K_1\cos\omega_1-\sinh 2K_2\cos\omega_2-\sinh 2K_3\cos\omega_3)\,d\omega_1 d\omega_2 d\omega_3.$$

When the interaction constant in the z direction, K_3, vanishes this expression reduces to the correct two-dimensional formula (4.53). Unfortunately, if one sets $K_1=K_2=K_3=K$ the high temperature power series in $x=\tanh K$ is not the same as the exact series (7.2).

8. SPHERICAL MODEL

The partition function (1.3) of the Ising model (in the absence of a magnetic field, $\mathfrak{H}=0$) is a multiple sum whose summand is the exponential of a quadratic form in the σ's. The infinite integral over an exponential of a quadratic form whose real part is negative definite can be evaluated much easier than the sum by employing the formula

$$\int_{-\infty}^{\infty}\cdots\int \exp\Big(-\sum_{i,j=1}^{N}a_{ij}\sigma_i\sigma_j\Big)d\sigma_1\cdots d\sigma_N = \pi^{N/2}\,(\det|a_{jk}|)^{-\frac{1}{2}}. \quad (8.1)$$

This suggests that if one could replace the summation operation in (1.3) by an integration, it might be possible to evaluate the resulting partition function rather easily.

With this motivation Kac proposed the spherical model of cooperative phenomenon in which the spin variables $\{\sigma_j\}$ are considered to be continuous rather than discrete. The σ's of the Ising model satisfy the relations

$$\sigma_j^2=1, \quad j=1, 2, \cdots, N \quad (8.2)$$

$$\sum_{j=1}^{N}\sigma_j^2=N. \quad (8.3)$$

The spherical model is characterized by the relaxation of the strong conditions (8.2) and the postulation that the σ's can simultaneously have any real values which lie on the hypersphere (8.3).

There are certain properties of the spherical model which are physically unrealistic. For example, the fact

that the σ's are continuous suggests that the thermodynamic behavior should be classical at low temperatures (for example, the specific heat does not approach zero as $T\to 0$). On the other hand, the magnetic properties of the spherical model may resemble those of a real ferromagnetic more closely than does the Ising model. The two-dimensional spherical model has no transition while the corresponding Ising does. There is considerable evidence[41] that a real two-dimensional ferromagnet does not have a transition either; it has been suggested that the magnetic anisotropy of the Ising model induces the transition in two dimensions.

The attractive feature of the spherical model is that all its thermodynamic and magnetic properties can be calculated exactly in one, two, and three dimensions for any common type of lattice. Also the interaction of a particle with other than nearest neighbors can be introduced into the spherical model without causing any significant mathematical difficulties. In three dimensions a phase transition exists with long-range order below the critical temperature. The thermodynamic properties have been calculated by Berlin and Kac[42] and one of the authors.[43] Since the recent paper of Berlin and Kac is quite complete in all the details, we shall merely outline the methods used and summarize the results.

The partition function (normalized to unity as $T\to\infty$) of the spherical model in the absence of a magnetic field is

$$Z=A_N^{-1}\int\cdots\int_{\sum_{j=1}^{N}\sigma_j^2=N} d\sigma_1\cdots d\sigma_N \exp(\tfrac{1}{2}K\textstyle\sum a_{ij}\sigma_i\sigma_j), \quad (8.4)$$

where

$$A_N=\int\cdots\int_{\sum_{j=1}^{N}\sigma_j^2=N} d\sigma_1\cdots d\sigma_N=2\pi^{\frac{1}{2}N}N^{\frac{1}{2}(N-1)}/\Gamma(\tfrac{1}{2}N). \quad (8.5)$$

All other symbols have the meaning given to them in Sec. 1. One way of evaluating the partition function is to introduce the δ-function,

$$\delta(N-\sum_{j=1}^{N}\sigma_j^2)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp\{iy(N-\sum_{j=1}^{N}\sigma_j^2)\}dy \quad (8.6)$$

into the integrands of (8.4) and (8.5). Since $\delta(N-\sum_{j=1}^{N}\sigma_j^2)$ vanishes, unless the sphericalization condition (8.3) is satisfied, the integration over the σ's can be allowed to extend over all real values, $-\infty<\sigma_j<\infty$ for all j. The integration over the σ's is then easily carried out by applying (8.1). The integration over the new variable y is performed by the method of steepest descents.

The final expression for the partition function of an s dimensional-simple cubic lattice is

$$\lim_{N\to\infty}\frac{1}{N}\log Z=-\tfrac{1}{2}-\tfrac{1}{2}\log 2K-\tfrac{1}{2}f(z_s)+Kz_s, \quad (8.7)$$

and the specific heat per particle is

$$C=\frac{k}{2}[1+2K^2dz_s/dK] \quad (8.8)$$

when a real position solution z_s exists for the equation

$$2K=\frac{1}{(2\pi)}\int_0^{2\pi}\cdots\int\frac{d\omega_1\cdots d\omega_s}{z_s-\cos\omega_1-\cdots-\cos\omega_s}. \quad (8.9)$$

The function $f(z_s)$ is defined by

$$f(z_s)=\frac{1}{(2\pi)^s}\int_0^{2\pi}\cdots\int\ln[z_s-\sum_{j=1}^{s}\cos\omega_j]d\omega_1\cdots d\omega_s. \quad (8.10)$$

When $s=1$ or 2, Eq. (8.9) has a solution z_s for all $0\leq K\leq\infty$; that is for all temperatures. Indeed, in these two cases z_s is an analytic function of K, as is the specific heat (8.8). No phase transitions occur.

In the three-dimensional case Eq. (8.9) has a real positive root z_s (which is ≥ 3) only when

$$T\geq T_c=3.9568J/k. \quad (8.11)$$

For $T<T_c$, it can be shown that the specific heat per particle is given by

$$C=\tfrac{1}{2}k, \quad T<T_c. \quad (8.12)$$

The function C/k is not analytic in this case. It has a singularity at $T=T_c$. The specific heat is plotted in Fig. 26. Notice that as $T\to 0$ it has a finite limit rather than zero, the corresponding limit in the Ising model. Berlin and Kac showed that the long-range correlation coefficient vanished at temperatures above T_c, while

$$\langle\sigma_j/\sigma_k\rangle_{\text{Av}}/\langle\sigma_j^2\rangle_{\text{Av}}^{\frac{1}{2}}\langle\sigma_k^2\rangle_{\text{Av}}^{\frac{1}{2}}\to 1-(T/T_c), \quad T<T_c \quad (8.13)$$

as $|r_j-r_k|\to\infty$. The spontaneous magnetization is proportional to $(1-T/T_c)^{\frac{1}{2}}$ for $T<T_c$.

One might argue that the critical phenomenon discussed above are caused by a small number of excessively large spins [such are possible according to (8.3)]. However, the statistical weight of such spins is very small. It can be shown that

$$\langle\sigma_j^4\rangle_{\text{Av}}=\begin{cases}3 & T>T_c\\ 3-2(1-T/T_c)^2 & \text{for } T\leq T_c.\end{cases} \quad (8.14)$$

(Of course, $\sigma_j^4=1$ in the Ising model.) If on the average only one spin was abnormally large, say $\simeq\frac{1}{2}N^{\frac{1}{2}}$, and the rest small and equal, we would have $\langle\sigma_j^4\rangle$

$\sim N(1+9N^{-1})/16$ which is in contradiction to (8.14). Hence, we can say that the existance of even one very large spin is such an improbable event that it could hardly be responsible for the critical properties of the model.

The magnetic susceptibility of the spherical model in the presence of a homogeneous magnetic field $\mathfrak{H}$ is very similar to that given by the Curie-Weiss phenomenological theory of ferromagnetism. In the Curie-Weiss theory the susceptibility per particle is

$$\chi=T_c^*/\alpha^*[T-T_c^*],$$

where T_c^* is the transition temperature and α^* an empirical parameter. The spherical model with a simple cubic lattice yields

$$\chi=T_c/\alpha[Th(T)-T_c],$$

where $T_c\simeq 4J/k$ rather than the Curie-Weiss value $T_c^*=6J/k$. The parameter $\alpha=6J/\mu^2$ is to be identified with α^*. The quantity $h(T)$ is defined by

$$h(T)=T_c z_3(\mathfrak{H})/3T,$$

where $z_3(\mathfrak{H})$ is a positive real root of

$$2K=\frac{1}{(2\pi)^3}\int_0^{2\pi}\!\!\int\!\!\int \frac{d\omega_1 d\omega_2 d\omega_3}{z_3(\mathfrak{H})-\cos\omega_1-\cos\omega_2-\cos\omega_3}+\frac{\mu^2\mathfrak{H}^2}{2k^2T^2K[z_3(\mathfrak{H})-3]}.$$

Berlin and Kac have shown that if one sets $T_c^*=\gamma T_c$,

$$\chi=(T_c^*/\alpha)/[T\gamma h(T)-T_c^*]. \tag{8.15}$$

The combination $\gamma h(T)$ is, in the entire temperature range $T_c\leq T<\infty$, restricted by the inequality

$$3/2\geq\gamma h(T)\geq 1.$$

Hence, Eq. (8.15) differs very slightly from the phenomenological Curie-Weiss law.

Interesting results have been obtained by Berlin and Thomsen[44] and Lax[45] by applying the sphericalization technique to the theory of electric dipole-dipole interaction in crystals. It can also be applied to a classical vector spin model of a ferromagnet.

APPENDIX 1

We stated in Sec. 1 that a very satisfactory model of a binary substitution alloy or a binary mixture is mathematically equivalent to the Ising model of a ferromagnet.[28] Also the Ising model is equivalent to a simplified model of a gas and liquid.[46] We shall here describe these models in more detail and show their relation to the Ising problem.

Let us first consider a binary system of N molecules of which on the average N_1 are of type 1 and N_2 are of type 2. These particles are distributed on lattice sights and the state of the system is described by giving the type of particle on each lattice sight. The energy of the system is chosen to be the sum of the energies of interacting pairs of nearest neighbors. The energy between pairs is written as $E_{ij}=E_{ji}$, if one member of the pairs is of the ith species and the other is of the jth species. Furthermore, we let the chemical potential of the jth species be μ_j.

The grand partition function of our system is

$$Z_A=\sum_{n_1+n_2=N}\sum_m \exp[(\mu_1 n_1+\mu_2 n_2-E_m)/kT]. \tag{A1.1}$$

n_i has the significance of being the number of i type particles; m numbers the states of the system for fixed n_i; and E_m is the total energy of the system in the state m. The chemical potentials must be chosen in such a way that the system gives the preassigned composition.

$$N_i=\langle n_i\rangle=Z^{-1}\sum_{n_1+n_2=N}\sum_m n_i \times\exp[(\mu_1 n_1+\mu_2 n_2-E_m)/kT] =kT\partial\log Z/\partial\mu_i. \tag{A1.2}$$

We again represent the "state" of the jth lattice point by $\sigma_j=\pm 1$. $\sigma_j=+1$ if the jth lattice point is occupied by a particle of type 1, and $\sigma=-1$ if it is occupied by a particle of type 2. $(1+\sigma_j)/2$ is 1 if the jth point has an atom of type 1 and zero if it has no atom of type 1. Thus,

$$n_1=\tfrac{1}{2}\sum_{j=1}^{N}(1+\sigma_j),\qquad n_2=\tfrac{1}{2}\sum_{j=1}^{N}(1-\sigma_j). \tag{A1.3}$$

If i and j are a pair of nearest neighbors on the lattice, the expression

$$v(\sigma_i,\sigma_j)=\tfrac{1}{4}E_{11}(1+\sigma_i)(1+\sigma_j)+\tfrac{1}{4}E_{22}(1-\sigma_i)(1-\sigma_j)+\tfrac{1}{2}E_{12}(1-\sigma_i\sigma_j) \tag{A1.4}$$

is E_{11}, E_{22}, or E_{12} accordingly as the i and j lattice points are occupied by two particles of type 1, two particles of type 2, or a mixed pair. $v(\sigma_i,\sigma_j)$ thus represents the energy between the pairs i and j. The total energy is given by

$$E_m=\sum_{i,j=1}^{N}\tfrac{1}{2}a_{ij}v(\sigma_i,\sigma_j), \tag{A1.5}$$

where a_{ij} is as defined in 1.4. If we rewrite (A1.1) in the new notation of the σ_j, the sums over $n_1+n_2=N$ and m is equivalent to the multiple sum over all $\sigma_j=\pm 1$,

$$Z_A=\sum_{\sigma_1=\pm 1}\cdots\sum_{\sigma_N=\pm 1}\exp[(\mu_1 n_1+\mu_2 n_2-E_m)/kT],$$

where in view of (A1.3) to (A1.5)

$$\begin{aligned}\mu_1 n_1+\mu_2 n_2-E_m &= \tfrac{1}{2}\sum_{j=1}^{N}[\mu_1(1+\sigma_j)+\mu_2(1-\sigma_j)] \\ &\quad -\tfrac{1}{2}\sum_{i,j=1}^{N} a_{ij}[\tfrac{1}{4}E_{11}(1+\sigma_i)(1+\sigma_j) \\ &\quad +\tfrac{1}{4}E_{22}(1-\sigma_i)(1-\sigma_j)+\tfrac{1}{2}E_{12}(1-\sigma_i\sigma_j)] \\ &= (N/8)[4\mu_1+4\mu_2-c(E_{11}+E_{22}+2E_{12})] \\ &\quad +\tfrac{1}{4}[2\mu_1-2\mu_2-c(E_{11}-E_{22})]\sum_{j=1}^{N}\sigma_j \\ &\quad -(1/8)(E_{11}+E_{22}-2E_{12})\sum_{i,j=1}^{N} a_{ij}\sigma_i\sigma_j. \qquad \text{(A1.6)}\end{aligned}$$

c designates the number of nearest neighbors for a given particle

$$(\sum_{j=1}^{N} a_{ij}=c).$$

To finally transcribe this into the notation of the Ising problem, we define

$$\begin{aligned}\mu H &= \tfrac{1}{4}[2\mu_1-2\mu_2-c(E_{11}-E_{22})]=\mu\mathfrak{H}kT \\ J &= -\tfrac{1}{4}(E_{11}+E_{22}-2E_{12})=KkT \qquad \text{(A1.7)} \\ \alpha &= (1/8)[4\mu_1+4\mu_2-c(E_{11}+E_{22}+2E_{12})],\end{aligned}$$

so that

$$\begin{aligned}Z_A &= \exp(N\alpha/kT)\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_N=\pm1} \\ &\quad \times\exp\{K\sum_{i,j=1}^{N}\tfrac{1}{2}a_{ij}\sigma_i\sigma_j+\mu\mathfrak{H}\sum_{j=1}^{N}\sigma_j\} \qquad \text{(A1.8)} \\ &= \exp(N\alpha/kT)Z_I.\end{aligned}$$

Z_I denotes the partition function for the Ising problem. We have thus established a simple relation between the Ising problem and the binary alloy.

The important thermodynamic functions of each are also related. For example, in the alloy

$$N_1=\langle n_1\rangle_{\text{Av}}=\tfrac{1}{2}\sum_{j=1}^{N}\langle(1+\sigma_j)\rangle_{\text{Av}}=(N/2)(1+\langle\sigma\rangle_{\text{Av}}).$$

The constant α has no effect upon any average so that $\langle\sigma\rangle_{\text{Av}}$ is the same as in the Ising problem, where the magnetization per particle is given by

$$M=\mu\langle\sigma\rangle_{\text{Av}},$$

thus,

$$N_1=(N/2)(1+M/\mu), \quad N_2=(N/2)(1-M/\mu). \qquad \text{(A1.9)}$$

If $H=0$, the Boltzmann factor is invariant to the transformation $\sigma_j=-\sigma_j$. Therefore, $M=-M=0$. The Ising lattice with $H=0$ thus corresponds to a binary alloy with $N_1=N_2=N/2$.

If J is positive, the Ising model is a model of a ferromagnet, if J is negative an antiferromagnet. In the binary alloy, J positive corresponds to a binary mixture which at low temperatures separates into two phases. J negative corresponds to a substitutional alloy, and a phase transition would be described as an order-disorder transition with the ordered state having type 1 and 2 particles on alternating lattice sites.

It will be shown in Sec. 6 that the Ising ferromagnet in two dimensions has a spontaneous magnetization (also in three dimensions), i.e., M as a function of H has a discontinuity at $H=0$ from $M=|M(0)|$ for $H=0_+$ to $M=-|M(0)|$ at $H=0_-$. Knowing the value of $M(0)$ for $H=0$, one deduces the critical composition from (A1.9).

The mathematical formulation of the "lattice gas" model is very similar to the above. As a starting point we choose the familiar expression for the grand partition function of a gas enclosed in a volume V,

$$Z_G(V,\mu,T)=\sum_{N=1}^{\infty} y^N Q_N/N!,$$

$$y=(2\pi mkT/h^2)^{\frac{3}{2}}\exp(\mu/kT), \qquad \text{(A1.10)}$$

$$Q_N=\int_V\cdots\int d\tau_1 d\tau_2\cdots d\tau_N\exp(-U_N/kT).$$

y is known as the fugacity, μ is the chemical potential and U_N is the potential energy of a system with N particles. The other symbols have their customary meaning.

From the evaluation of Z, one deduces the pressure from

$$p=kT\lim_{V\to\infty} V^{-1}\log Z_G(V), \qquad \text{(A1.11)}$$

and the density is given by

$$\rho=\lim_{V\to\infty}\partial(V^{-1}\log Z_G)/\partial\log y. \qquad \text{(A1.12)}$$

Since either ρ or p in addition to V and T is usually known, one uses one of the above equations to select the value of μ which appears as a parameter in Z.

The lattice gas[47] is described by dividing V into cells of uniform size. For convenience we shall choose the units of V such that these cells are of unit size. U_N is expressed as a sum of the potential energies u between pairs of particles. u in turn is described in this model by

$$\begin{aligned}u&=+\infty && \text{if the two atoms occupy the same lattice sight,} \\ u&=-4J && \text{if the two atoms are nearest neighbors,} \qquad \text{(A1.13)} \\ u&=0 && \text{otherwise.}\end{aligned}$$

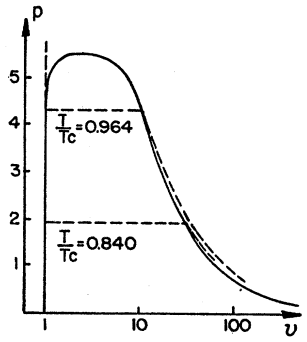

FIG. 27. $p-v$ diagram for the two-dimensional lattice gas (see reference 47). The solid curve is the exact boundary of the two-phase region. The dotted curves are the isotherms.

This interaction has the desirable feature of being very repulsive (infinitely so) at very short distances, attractive at intermediate distances, and zero at larger distances. It qualitatively represents the true interaction between gas molecules.

The infinite repulsion between particles in the same cell prohibits the occupation of a cell by more than one particle. The energy of the system can be described by giving for each cell the value of a set of coordinates σ_j, $1\leq j\leq V$. $\sigma_j=+1$ if the jth cell is occupied and -1 if unoccupied. In terms of the σ_j, U_N becomes

$$U_N=-J\sum_{i,j=1}^{V}\tfrac{1}{2}a_{ij}(\sigma_i+1)(\sigma_j+1). \qquad \text{(A1.14)}$$

Since the integrand of Q_N is a constant over-all cell, we can replace it by a multiple sum. There will be a term corresponding to each possible allocation of the N particles among the cells. For any choice of the σ_j there will be just $N!$ equal terms of the sum corresponding to the $N!$ permutation of the particles among each other which leave U_N invariant.

Since $\frac{1}{2}\sum(\sigma_j+1)$ is the number of particles in the lattice, we write

$$Q_N=N!\sum\cdots\sum\exp[(J/2kT)\sum_{i,j=1}^{V}a_{ij}(\sigma_i+1)(\sigma_j+1)],$$

where the multiple sum is over all $\sigma_j=\pm1$ with the restriction $\frac{1}{2}\sum(\sigma_j+1)=N$. When we substitute this into Z, the summation over N eliminates the restriction on the above sum, and we write

$$Z_G=\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_V=\pm1}y^{\frac{1}{2}\sum_j(\sigma_j+1)}\times\exp[\tfrac{1}{2}K\sum_{i,j=1}^{V}a_{ij}(\sigma_i+1)(\sigma_j+1)]$$

$$=\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_V=\pm1}\exp[\tfrac{1}{2}K\sum_{i,j=1}^{V}a_{ij}\sigma_i\sigma_j]\times\exp[(cK+\tfrac{1}{2}\log y)\sum_{j=1}^{V}\sigma_j]\exp[\tfrac{1}{2}(cK+\log y)V],$$

$$K\equiv J/kT,$$

where c is again the number of nearest neighbors of a particle and V is not only the volume but also the number of cells.

The formal similarity between Z_G and the partition function for the Ising problem is quite apparent. If we write

$$\log y=2(\mu H-Jc)/kT=2(\mu\mathfrak{H}-cK),$$

then

$$Z_G=\exp[(\mu\mathfrak{H}-\tfrac{1}{2}cK)V]\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_V=\pm1}\times\exp[\tfrac{1}{2}K\sum_{i,j=1}^{V}a_{ij}\sigma_i\sigma_j+\mu\mathfrak{H}\sum_{j=1}^{V}\sigma_j]$$

$$=\exp[(\mu\mathfrak{H}-\tfrac{1}{2}cK)V]Z_I. \qquad \text{(A1.15)}$$

From this, we can establish relationships between the thermodynamic properties of the Ising lattice and of the lattice gas. Since V is the number of lattice cells, the free energy per particle F of the Ising problem is

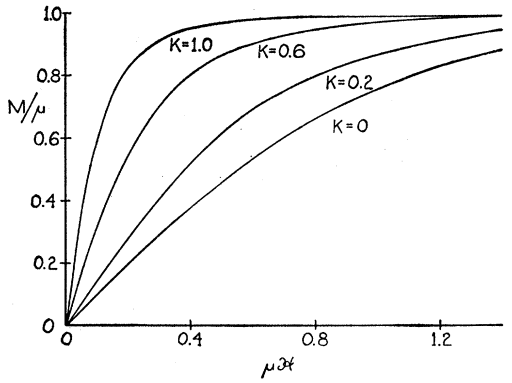

FIG. 28. Magnetization of the one-dimensional Ising chain as a function of the magnetic field $\mu\mathfrak{H}=\mu H/kT$ for several values of $K=J/kT$.

given by

$$Z_I=\exp(FV/kT),$$

and we find

$$p=kTV^{-1}\log Z_G=\mu H-\tfrac{1}{2}Jc+F. \qquad \text{(A1.16)}$$

The density is given by

$$\rho=\partial V^{-1}\log Z/\partial\log y=\tfrac{1}{2}V^{-1}\sum_{j=1}^{V}(\langle\sigma_j\rangle_{Av}+1)=\tfrac{1}{2}(1+M/\mu).$$

The specific volume v is given by

$$v=\rho^{-1}=2(1+M/\mu)^{-1}. \qquad \text{(A1.17)}$$

As was pointed out by Lee and Yang,[47] the $p-v$ isotherms of the lattice gas are closely related to the M, H isotherms of the Ising lattice. In particular a discontinuity in M gives a discontinuity in v. As has already been noted, the Ising lattice has a spontaneous magnetization or a discontinuity in M at $H=0$ for temperatures below the ferromagnetic Curie temperature T_c.

Although the two-dimensional Ising problem for arbitrary fields has not been evaluated, it is indeed

fortunate that the interesting part of the diagram for the two-dimensional lattice gas, namely the condensation curve, corresponds to $H=0$ for which we know all the necessary data. We know the magnetization has a jump from $|M|$ to $-|M|$ at $H=0$. We know both M and F as a function of T. The Curie temperature corresponds to the critical temperature above which no condensation occurs. The two-phase boundary is obtained by evaluating p and v for $H=0$ and is shown in Fig. 27.

In conjunction with their study of the lattice gas Yang and Lee have also proved many interesting theorems regarding the general properties of gases. They also announce the solution of the Ising problem in a magnetic field $\mathfrak{H}=i\pi/2$ or $H=i\pi kT/2$.

APPENDIX 2

Some of the properties of the one-dimensional Ising lattice were derived in Sec. 2. One must be an optimist to expect a one-dimensional system to behave like its two- or three-dimensional analog. If one is hopeful that techniques used to solve a one-dimensional problem will help solve a two- or three-dimensional problem, his optimism quickly subsides when he tries to apply them to the Ising lattice.

Despite this, we shall summarize here a few other properties of the one-dimensional Ising lattice. Although they may be rather useless, they are at least simple.

There is no difficulty in extending the analysis of Sec. 2 to include a magnetic field interaction. For such a system

$$P=\begin{pmatrix} e^{K+\mu\mathfrak{H}} & e^{-K} \\ e^{-K} & e^{K-\mu\mathfrak{H}} \end{pmatrix}, \tag{A2.1}$$

and

$$\lambda_1=e^K\cosh\mu\mathfrak{H}+[e^{2K}\sinh^2\mu\mathfrak{H}+e^{-2K}]^{\frac{1}{2}}. \tag{A2.2}$$

λ_1 is analytic in T for $0<T<\infty$, thus there is no transition (see Sec. 3.2). It has no spontaneous magnetization since

$$M=kT\partial\log\lambda_1/\partial\mathfrak{H} =(\mu\sinh\mu\mathfrak{H})[\sinh^2\mu\mathfrak{H}+e^{-2K}]^{\frac{1}{2}} \tag{A2.3}$$

goes to zero as H goes to zero. M as a function of $\mathfrak{H}$ is shown in Fig. 28.

We note that for $\mathfrak{H}=0$

$$\lambda_1=2\cosh K,$$

and for $K=0$

$$\lambda_1=2\cosh\mu\mathfrak{H};$$

thus, the usual thermodynamic properties (excluding of course the magnetization) for a system of noninteracting particles ($J=0$) in a magnetic field are similar to those of a system of interacting particles with $H=0$. (This is not true in higher dimensions.)

Even though the system is well behaved, the properties of the system are quite sensitive to small magnetiz fields. If H is small compared with K, the term $e^{2K}\sinh^2\mu\mathfrak{H}$ in (A2.2) may not be small compared with e^{-2K}. We certainly anticipate even a small H to have a considerable effect at sufficiently low temperatures since it forces the spins to be all the same as $T\to 0$, but it turns out that H has an appreciable effect up to temperatures of the order

$$T\sim 2J[k\log(J/\mu\mathfrak{H})]^{-1},$$

a temperature which is rather insensitive to H. Figure 29 shows the specific heat *vs* temperature for some small values of H/J. In view of the spontaneous magnetization for two- or three-dimensional systems, they are also sensitive to small fields though in a quite different manner.

As a final remark on this problem, we note that for $H=0$, the partition function can be evaluated quite simply without appeal to the matrix method of Sec. 2.1 or without imposing the periodic boundary conditions.

$$Z(N)=\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_N=\pm1}\prod_{j=1}^{N-1}\exp(K\sigma_j\sigma_{j+1}).$$

Only one of the above factors involves σ_N, so we can first sum $\sigma_N=\pm1$.

$$Z(N)=\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_{N-1}=\pm1}[\prod_{j=1}^{N-2}\exp(K\sigma_j\sigma_{j+1})]2\cosh K\sigma_{N-1}.$$

σ_{N-1}, however, has only values ±1, and $\cosh K\sigma_{N-1}=\cosh K$.

$$Z(N)=2\cosh K\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_{N-1}=\pm1}[\prod_{j=1}^{N-2}\exp(K\sigma_j\sigma_{j+1})]$$

$$=2\,(\cosh K)Z(N-1).$$

By iterating this and noting that $Z(1)=2$, we obtain

$$Z(N)=2^N\cosh^{N-1}K.$$

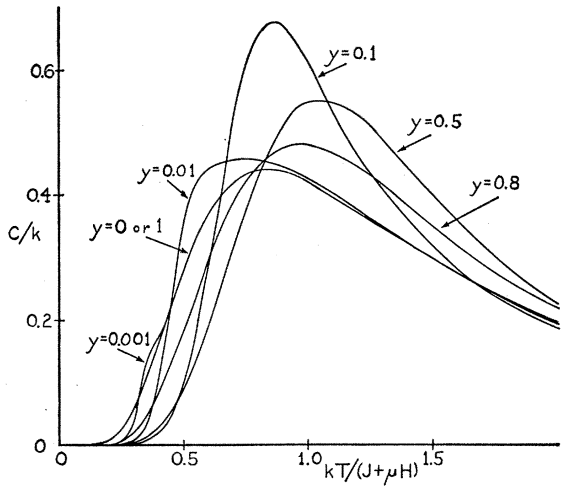

FIG. 29. Specific heat *vs* temperature for the one-dimensional Ising chain for several values of $y=\mu H/(J+\mu H)$. Temperature is measured in units $(J+\mu H)/k$ so that all curves have the same normalization.

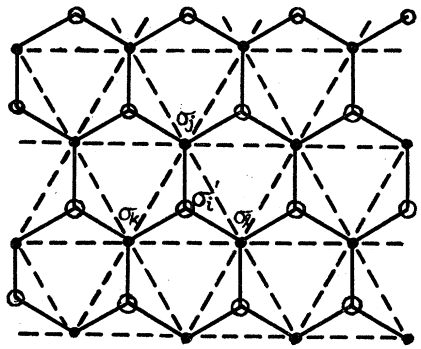

FIG. 30. Star-triangle transformation. The hexagonal lattice is shown by the solid line and its corresponding triangular lattice by the broken lines.

APPENDIX 3

We present here a brief review of the properties of direct product matrices used in Secs. 2.1 and 4.1.

Consider two matrices A and B of dimension n and m, respectively, with matrix elements A_{ij} and B_{kl}. The direct product $A\times B$ of A and B is defined as a matrix of dimension $m\times n$ with matrix elements,

$$(A\times B)_{ik,\,jl}=A_{ij}B_{kl}. \tag{A3.1}$$

The first index of $A\times B$ is the pair of first indices i and k of A and B usually considered to be ordered in dictionary order. For example, let n and m both be two

$$A=\begin{pmatrix}A_{11} & A_{12}\\ A_{21} & A_{22}\end{pmatrix},\quad B=\begin{pmatrix}B_{11} & B_{12}\\ B_{21} & B_{22}\end{pmatrix},$$

then

$$A\times B=\left(\begin{array}{cc:cc} A_{11}B_{11} & A_{11}B_{12} & A_{12}B_{11} & A_{12}B_{12}\\ A_{11}B_{21} & A_{11}B_{22} & A_{12}B_{21} & A_{12}B_{22}\\ \hdashline A_{21}B_{11} & A_{21}B_{12} & A_{22}B_{11} & A_{22}B_{12}\\ A_{21}B_{21} & A_{21}B_{22} & A_{22}B_{21} & A_{22}B_{22}\end{array}\right).$$

Direct product matrices are used extensively (disguised perhaps) in physical problems particularly in quantum mechanics. If x_j represent vector components in the n dimensional space in which A operates and y_l components in an m dimensional space in which B operates, we can define an $n\times m$ dimensional vector with components x_jy_l ordered according to the index pair (j, l) upon which $A\times B$ can operate.

Since

$$\sum_{j,\,l}(A\times B)_{ik,\,jl}x_jy_l=\sum_{j,\,l}A_{ij}B_{kl}x_jy_l$$

$$=(\sum_j A_{ij}x_j)(\sum_l B_{kl}y_l),$$

the direct product operating on a vector xy carries xy into the vector (Ax) (By). $A\times B$ is thus the matrix representation of the product of an operation A which affects only the x_j components and an operation B which effects only the y_l components. In quantum mechanics the direct matrix product could be used, for example, to represent the product of an operation that affects only particle one-wave functions and an operator that affects only particle two-wave functions.

The most important property of direct product matrices is the manner in which they multiply. Let $A_1\times B_1$ and $A_2\times B_2$ be two direct product matrices. Then according to the usual rules of matrix multiplication,

$$[(A_1\times B_1)(A_2\times B_2)]_{ik,\,jl}$$

$$=\sum_{m,\,n}(A_1\times B_1)_{ik,\,mn}(A_2\times B_2)_{mn,\,jl}$$

$$=\sum_{m,\,n}(A_1)_{im}(B_1)_{kn}(A_2)_{mj}(B_2)_{nl}$$

$$=(A_1A_2)_{ij}(B_1B_2)_{kl}=(A_1A_2\times B_1B_2)_{ik,\,jl},$$

or

$$(A_1\times B_1)(A_2\times B_2)=A_1A_2\times B_1B_2. \tag{A3.2}$$

This relation is the key to almost all the theorems regarding direct products. We can immediately conclude that if T and T^* are transformations which diagonalize A and B, respectively, then $T\times T^*$ diagonalizes $A\times B$.

$$(T^{-1}\times T^{*-1})(A\times B)(T\times T^*)=(T^{-1}AT)\times(T^{*-1}BT)$$

is the direct product of two diagonal matrices which is also diagonal. If the eigenvalues of A are λ_j and those of B, $\lambda_k{}^*$, then $A\times B$ has eigenvalues $\lambda_j\lambda_k{}^*$.

APPENDIX 4

In Sec. 3.1, it was shown that one could locate the Curie point of a self-dual lattice by using the dual transformation (3.2). We stated that although the hexagonal lattice is not self-dual, one could find the Curie point by using the dual transformation in conjunction with the star-triangle transformation to be derived here.[3]

To derive the star-triangle transformation, we first divide the lattice into two sublattices with equal numbers of particles in the manner shown in Fig. 30. One sublattice is represented by dots, the other by circles. We shall represent the coordinates of the former by σ_k, $1\leq k\leq N/2$ and the latter by $\sigma_k{}'$. It is important to notice that a point of one lattice interacts only with points of the other lattice.

We write Z in the form

$$Z_H=\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_{N/2}=\pm1}\{\sum_{\sigma_1'=\pm1}\cdots\sum_{\sigma'_{N/2}=\pm1}$$

$$\times\exp(\sum_{n.n.}K_H\sigma_i\sigma_j')\}, \tag{A4.1}$$

where $K_H=J_H/kT$; J_H is the coupling constant for the hexagonal lattice.

Consider now only the quantity in braces, which we shall denote by $Z'(\sigma_1, \cdots, \sigma_{N/2})$. A σ_j' does not interact with other σ_k' and for any set of values of $\sigma_1, \sigma_2, \cdots, \sigma_{N/2}$, the σ_j' behave as independent particles. The summation over σ_j' are easily performed. If we let σ_j, σ_k, and σ_l be the three nearest neighbors of a point σ_i', then

$$Z'(\sigma_1, \cdots, \sigma_{N/2}) = \sum_{\sigma_1'=\pm 1} \cdots \sum_{\sigma'_{N/2}=\pm 1} \times \exp\Big[\sum_{i=1}^{N/2} K_H(\sigma_i'\sigma_j + \sigma_i'\sigma_k + \sigma_i'\sigma_l)\Big]$$

$$= \prod_{i=1}^{N/2} \Big\{ \sum_{\sigma_i'=\pm 1} \exp[K_H(\sigma_i'\sigma_j + \sigma_i'\sigma_k + \sigma_i'\sigma_l)] \Big\}$$

$$= \prod_{i=1}^{N/2} \Big\{ \sum_{\sigma_i'=\pm 1} (c_H + \sigma_i'\sigma_j s_H)(c_H + \sigma_i'\sigma_j s_H)(c_H + \sigma_i'\sigma_j s_H) \Big\}$$

$$= \prod_{i=1}^{N/2} \{2c_H{}^3 + 2s_H{}^2 c_H(\sigma_j\sigma_k + \sigma_j\sigma_l + \sigma_k\sigma_l)\},$$

where

$$c_H \equiv \cosh K_H, \quad s_H \equiv \sinh K_H.$$

Thus,

$$Z_H = 2^{N/2} \cosh^{3N/2} K_H \sum_{\sigma_1=\pm 1} \cdots \sum_{\sigma_{N/2}=\pm 1} \prod_{i=1}^{N/2} \times [1 + \tanh^2 K_H(\sigma_j\sigma_k + \sigma_j\sigma_l + \sigma_k\sigma_l)]. \quad \text{(A4.2)}$$

The manner in which the σ_k appear in (A4.2) suggests that we compare Z_H with the partition function for the triangular lattice represented in Fig. 30 by the dashed lines. We again use the index i to number the circles in Fig. 30 or the centers of alternating triangles. The partition function for this lattice can be written in the form

$$Z_T = \sum_{\sigma_1=\pm 1} \cdots \sum_{\sigma_{N/1}=\pm 1} \prod_{i=1}^{N/2} \exp[K_T(\sigma_j\sigma_k + \sigma_j\sigma_l + \sigma_k\sigma_l)].$$

However,

$$\exp[K_T(\sigma_j\sigma_k + \sigma_j\sigma_l + \sigma_k\sigma_l)] = (c_T + \sigma_j\sigma_k s_T)(c_T + \sigma_j\sigma_l s_T)(c_T + \sigma_k\sigma_l s_T) = c_T{}^3 + s_T{}^3 + c_T s_T(c_T + s_T)(\sigma_j\sigma_k + \sigma_j\sigma_l + \sigma_k\sigma_l)$$

with

$$c_T \equiv \cosh K_T, \quad s_T \equiv \sinh K_T.$$

Thus,

$$Z_T = (c_T{}^3 + s_T{}^3)^{N/2} \sum_{\sigma_1=\pm 1} \cdots \sum_{\sigma_{N/2}=\pm 1} \prod_{i=1}^{N/2} \times [1 + (\sigma_j\sigma_k + \sigma_j\sigma_l + \sigma_k\sigma_l) \times c_T s_T(c_T + s_T)/(c_T{}^3 + s_T{}^3)] \quad \text{(A4.3)}$$

comparing (A4.2) and (A4.3), we see that Z_T and Z_H will differ only by a known factor if we choose

$$c_T s_T(c_T + s_T)/(c_T{}^3 + s_T{}^3) = \tanh^2 K_H.$$

A somewhat neater version of this relation is

$$\exp 4K_T = 2\cosh 2K_H - 1. \quad \text{(A4.4)}$$

Under condition (A4.4), the partition function (A4.2) and (A4.3) are related by

$$Z_H(K_H)[2\sinh 2K_H]^{-N_H/2} = Z_T(K_T)[2\sinh 2K_T]^{-N_T/2}, \quad \text{(A4.5)}$$

where $N_H = N$ is the number of particles on the hexagonal lattice and $N_T = N/2$ is the number of particles on the triangular lattice.

Equations (A4.4) and (A4.5) give the results of the star-triangle transformation. We see from (A4.4) that a small K_T gives a small K_H and a large K_T a large K_H.

To also apply the dual-transformation we write (3.2) in the more symmetric form

$$Z_H(K_H)[2\sinh 2K_H]^{-N_H/2} = Z_T(K_H{}^*)[2\sinh 2K_H{}^*]^{-N_T/2}. \quad \text{(A4.6)}$$

Equations (A4.6) and (A4.5) together give

$$Z_T(K_T)[2\sinh 2K_T]^{-N_T/2} = Z_T(K_H{}^*)[2\sinh 2K_H{}^*]^{-N_T/2}. \quad \text{(A4.7)}$$

If we use (2.6b) to eliminate K_H from (A4.4), we obtain

$$[\exp(4K_T - 1][\exp(4K_H{}^*) - 1] = 4. \quad \text{(A4.8)}$$

Equations (A4.7) and (A4.8) describe a relation between the high and low temperature behavior of the triangular lattice. If a Curie point exists, it must occur $K_T = K_H{}^*$ or for $4K_T = \log 3$.

Similar relations for the hexagonal lattice give

$$Z_H(K_H)[2\sinh 2K_H]^{-N_H/2} = Z_H(K_T{}^*)[2\sinh 2K_T{}^*]^{-N_H/2}$$

with

$$\sinh K_H \sinh K_T{}^* = \tfrac{1}{2}.$$

The Curie point is at $\sinh^2 K_H = \tfrac{1}{2}$.

It is interesting to notice that in the triangular lattice $4K_T = \log 3$ has a solution only for $K > 0$. The antiferromagnetic triangular lattice ($K < 0$) has no Curie point (see Sec. 5). The properties of the hexagonal lattice are however invariant to $K_H \longrightarrow -K_H$.

APPENDIX 5

A Lie algebra is a set of elements $x_1, x_2, x_3, \cdots$ (nondenumerable, however) upon which the usual rules of addition and multiplication by any complex number apply. The algebra includes $ax + by$ if x and y are ele-

ments, and a and b are any complex numbers. There is also defined another operation $[x, y]$ which satisfies the conditions

(a) $[x, y]+[y, x]=0$; (A5.1)

(b) $[[x, y], z]+[[y, z], x]+[[z, x], y]=0$; (Lie–Jacobi equation) (A5.2)

(c) if x and y are elements, then $[x, y]$ is also an element. The Lie algebra is in every respect the same as the usual abstract algebra except that the multiplication operation is replaced by the operation $[x, y]$ having the above properties. If x, y, and z are square matrices, a Lie algebra can be defined with the usual rules of addition of matrices and an operation $[x, y]=xy-yx$ the commutator of x and y. One readily checks that the commutator satisfies conditions (a) and (b).

A set of elements $x_1, x_2, \cdots, x_r$ are said to form a basis for a finite Lie algebra if there exists a set of numbers $\{c_{jk}{}^t\}$ which have the property

$$[x_j, x_k]=\sum_{t=1}^{r} c_{jk}{}^t x_t. \tag{A5.3}$$

These constants are called the structure constants of the algebra. The abstract properties of the algebra are completely described by the structure constants.

An important example of a Lie algebra is that associated with the three-dimensional rotations. According to Euler's theorem, any rotation in three dimensions can be decomposed into three successive rotations, one about the z axis, followed by one about the rotated x axis, and then one about the new z axis. A general rotation can also be considered as a vector (really a pseudovector) with components in the x, y, and z directions.

Let us consider an infinitesimal rotation through an angle γ about the z axis. The matrix for such a rotation is

$$\begin{pmatrix} \cos\gamma & -\sin\gamma & 0 \\ \sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix} \sim \mathbf{I}_3+\gamma\mathbf{Z}+0(\gamma^2),$$

where

$$\mathbf{Z}=\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

$\mathbf{I}_3$ is the identity matrix, and $0(\gamma^2)$ indicates order γ^2. Note that

$$\mathbf{Z}^{2n}=\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{Z}^{2n+1}=\mathbf{Z};$$

hence, the direct expansion of $\exp\gamma\mathbf{Z}$ yields

$$\exp\gamma\mathbf{Z}=\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}+\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}\cos\gamma+\mathbf{Z}\sin\gamma$$
$$=\begin{pmatrix} \cos\gamma & -\sin\gamma & 0 \\ \sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

which is a rotation through a finite angle γ about the z axis.

In a similar way, we can show that an infinitesimal rotation by an angle β about the y axis is given by

$$\mathbf{I}_3+\beta\mathbf{Y} \quad \text{with} \quad \mathbf{Y}=\begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

and a rotation through a finite angle β by $\exp(\beta\mathbf{Y})$. An infinitesimal rotation α about the x axis is given by

$$\mathbf{I}_3+\alpha\mathbf{X} \quad \text{with} \quad \mathbf{X}=\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix},$$

and a finite rotation by $\exp(\alpha\mathbf{X})$.

Euler's theorem implies that any general rotation can be written as

$$\exp(\alpha\mathbf{Z})\exp(\beta\mathbf{Y})\exp(\gamma\mathbf{Z}).$$

It can also be written in the form

$$\exp[(\alpha\mathbf{X}+\beta\mathbf{Y}+\gamma\mathbf{Z})]$$

which is a rotation through an angle $(\alpha^2+\beta^2+\gamma^2)^{\frac{1}{2}}$.

The operators $\mathbf{X}$, $\mathbf{Y}$, $\mathbf{Z}$ take vectors into new vectors which are normal to the original one. For example,

$$\mathbf{Z}\cdot\begin{pmatrix} x \\ y \\ z \end{pmatrix}=\begin{pmatrix} -y \\ x \\ 0 \end{pmatrix}.$$

If we let $x_1=\mathbf{Z}$, $x_2=\mathbf{Y}$, and $x_3=\mathbf{X}$, the commutators of these operators generate a Lie algebra with the three base elements x_1, x_2, and x_3. We obtain

$$\begin{aligned} [x_1, x_2]&=x_3 \\ [x_3, x_1]&=x_2 \\ [x_2, x_3]&=x_1. \end{aligned} \tag{A5.4}$$

This structure constants of the algebra are

$$c_{ik}{}^t=0 \quad \text{except} \quad c_{12}{}^3=c_{31}{}^2=c_{23}{}^1=1.$$

There is also another representation of the Lie algebra defined by (A5.4). Consider the Pauli spin matrices

$$\mathbf{C}=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{s}=\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \text{and} \quad \mathbf{sC}=\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

It is easy to see that the three operators $x_1=i\mathbf{s}/2$, $x_2=-i\mathbf{C}/2$, and $x_3=\mathbf{sC}/2$ have the same commutation rules as $\mathbf{X}$, $\mathbf{Y}$, and $\mathbf{Z}$.

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