Thermodynamically, as we have mentioned, there is a relation between magnetic and gas–liquid systems. As we have just seen, this relationship takes the form of precise identities for the lattice gas and Ising magnet, but it goes without saying that these identities are not generally valid.

We conclude this section with a brief mention of the binary-alloy interpretation of the Ising model.

For a binary alloy we take the parameters t_P for the lattice gas to be

$$t_P = \begin{cases} 1 & \text{if site } P \text{ is occupied by an A atom} \\ 0 & \text{if site } P \text{ is occupied by a B atom.} \end{cases} \tag{2.22}$$

Then if ε_{AA}, ε_{BB}, and ε_{AB} denote the coupling (interaction) constants for nearest-neighbor A atoms, nearest-neighbor B atoms, and nearest-neighbor A and B atoms, respectively, the interaction energy is given by

$$E\{t\} = -\sum_{P,Q}{}^{*} \{\varepsilon_{AA} t_P t_Q + \varepsilon_{BB}(1 - t_P)(1 - t_Q) + \varepsilon_{AB}[t_P(1 - t_Q) + t_Q(1 - t_P)]\} \tag{2.23}$$

for a particular configuration $\{t\}$ of A and B atoms. It is left as an exercise for the reader to set up an isomorphism between the binary alloy and the magnet. It is almost obvious, for example, that the binary alloy with the same number of A and B atoms corresponds to a magnet with zero external field.

From this point on we shall mean the Ising magnet when we refer to the Ising model (or problem).

5-3 One-dimensional Model and Transfer Matrix

Let us consider first the one-dimensional open-chain model (Equation 1.3) with zero external field. The problem is to evaluate the partition function (Equation 1.8)

$$Z_N = \sum_{\mu_1 = \pm 1, \ldots, \mu_N = \pm 1} \exp\left(v \sum_{i=1}^{N-1} \mu_i \mu_{i+1} \right) \tag{3.1}$$

where $v = \beta J$. Because of the one-dimensional structure (cf. the Tonks gas) we can separate off and sum over the Nth spin μ_N to get

$$\begin{aligned} Z_N &= 2 \cosh v \sum_{\mu_1 = \pm 1, \ldots, \mu_{N-1} = \pm 1} \exp\left(v \sum_{i=1}^{N-2} \mu_i \mu_{i+1} \right) \\ &= (2 \cosh v) Z_{N-1}, \end{aligned} \tag{3.2}$$

where we have used the fact

$$\sum_{\mu_N = \pm 1} \exp(v \mu_{N-1} \mu_N) = e^{v}$$
$$= e^{v}$$
$$= 2$$

for either $\mu_{N-1} = +1$ or $-$ obvious fact that

$$Z_2 = \sum_{\mu_1 = \pm 1, \mu_2 = \pm 1} \exp(v\mu$$
$$= \sum_{\mu_1 = \pm 1} [\exp(v\mu_1) + e$$
$$= 4 \cosh v$$

gives

$$Z_N = 2(2 \cosh v)^{N-1}.$$

The free energy per spin

$$-\frac{\psi}{kT} = \lim_{N \to \infty} N^{-1} \log Z_N$$
$$= \log(2 \cosh v),$$

which is a completely a $(v = J/kT)$, for all positiv phase transition.

It is obvious that the el (3.2) will not work if the greater than one even with chain problem in an exte (closed) periodic chain (F identical results, and this, a

For the periodic chain problem is to evaluate

$$Z_N = \sum_{\{\mu\}} \exp\left(v \sum_{i=1}^{N} \mu_i \mu_{i+1} \right.$$

where $B = \beta H$. If we defir

$$L(\mu_i, \mu_{i+1}) = \exp\left[v \mu_i \mu \right.$$

where we have used the fact that since $\mu_{N-1} = \pm 1$,

$$\sum_{\mu_N = \pm 1} \exp(v\mu_{N-1}\,\mu_N) = \exp(v\mu_{N-1}) + \exp(-v\mu_{N-1}) = \exp(v) + \exp(-v) = 2\cosh v \tag{3.3}$$

for either $\mu_{N-1} = +1$ or -1. The recurrence relation (3.2) together with the obvious fact that

$$Z_2 = \sum_{\mu_1 = \pm 1,\, \mu_2 = \pm 1} \exp(v\mu_1\,\mu_2) = \sum_{\mu_1 = \pm 1} [\exp(v\mu_1) + \exp(-v\mu_1)] = 4\cosh v \tag{3.4}$$

gives

$$Z_N = 2(2\cosh v)^{N-1}. \tag{3.5}$$

The free energy per spin ψ in the thermodynamic limit is given by

$$-\frac{\psi}{kT} = \lim_{N\to\infty} N^{-1}\log Z_N = \log(2\cosh v), \tag{3.6}$$

which is a completely analytic function of v, and hence temperature ($v = J/kT$), for all positive temperatures. Hence, as expected, there is no phase transition.

It is obvious that the elementary device leading to the recurrence relation (3.2) will not work if there is an external magnetic field, or in dimensions greater than one even with $H = 0$. Although it is possible to solve the open-chain problem in an external field, it is considerably easier to consider the (closed) periodic chain (Figure 5.3). In the limit $N \to \infty$ we would expect identical results, and this, as we will see, is the case.

For the periodic chain ($\mu_{N+1} = \mu_1$) in an external magnetic field H the problem is to evaluate

$$Z_N = \sum_{\{\mu\}} \exp\left(v\sum_{i=1}^{N} \mu_i\,\mu_{i+1} + B\sum_{i=1}^{N} \mu_i \right), \tag{3.7}$$

where $B = \beta H$. If we define

$$L(\mu_i, \mu_{i+1}) = \exp\left[v\mu_i\,\mu_{i+1} + \frac{B}{2}(\mu_i + \mu_{i+1}) \right] \tag{3.8}$$

we can write

$$Z_N = \sum_{\{\mu\}} L(\mu_1, \mu_2)L(\mu_2, \mu_3)\cdots L(\mu_{N-1}, \mu_N)L(\mu_N, \mu_1), \tag{3.9}$$

which has the form of a matrix product. Indeed, if $\mathbf{L}$ is the 2 by 2 *transfer matrix* with elements $L(\mu, \mu')$ defined by Equation 3.8, i.e.,

$$\begin{aligned}\mathbf{L} &= \begin{pmatrix} L(+1,+1) & L(+1,-1) \\ L(-1,+1) & L(-1,-1) \end{pmatrix} \\ &= \begin{pmatrix} \exp(v+B) & \exp(-v) \\ \exp(-v) & \exp(v-B) \end{pmatrix},\end{aligned} \tag{3.10}$$

we have, after summing in Equation 3.9 over $\mu_2 = \pm 1, \ldots, \mu_N = \pm 1$, that

$$Z_N = \sum_{\mu_1 = \pm 1} L^N(\mu_1, \mu_1), \tag{3.11}$$

where $L^N(\mu, \mu')$ denotes the (μ, μ') elements of the matrix $\mathbf{L}$ raised to the Nth power. Z_N (Equation 3.11) is therefore the sum of the diagonal elements of L^N, i.e., the trace of L^N. Now since the trace of a matrix is the sum of its eigenvalues and the eigenvalues of $\mathbf{L}^N$ are the eigenvalues of $\mathbf{L}$ raised to the Nth power, we have that

$$\begin{aligned} Z_N &= \mathrm{Tr}(\mathbf{L}^N) \\ &= \lambda_1^N + \lambda_2^N, \end{aligned} \tag{3.12}$$

where λ_1 and λ_2 are the eigenvalues of the matrix $\mathbf{L}$ (Equation 3.10). The eigenvalue equation is

$$\mathrm{Det}\begin{pmatrix} \exp(v+B)-\lambda & \exp(-v) \\ \exp(-v) & \exp(v-B)-\lambda \end{pmatrix} = \lambda^2 - 2\lambda e^v \cosh B + 2\sinh 2v = 0, \tag{3.13}$$

which gives

$$\left.\begin{matrix}\lambda_1 \\ \lambda_2\end{matrix}\right\} = e^v \cosh B \pm (e^{2v}\sinh^2 B + e^{-2v})^{1/2} \tag{3.14}$$

for the eigenvalues of $\mathbf{L}$.

Noting that λ_2/λ_1 is str

$$\begin{aligned} -\frac{\psi}{kT} &= \lim_{N\to\infty} N^{-1}\log Z \\ &= \lim_{N\to\infty} N^{-1}\log\{ \\ &= \log\lambda_1 + \lim_{N\to\infty} \\ &= \log\lambda_1 \\ &= \log[e^v \cosh B \end{aligned}$$

When $B = 0$ the right-h precisely the expression Equation 3.14 with $B =$

$$\lambda_1 = 2\cosh v,$$

$$\lambda_2 = 2\sinh v,$$

so, from Equation 3.12,

$$Z_N = (2\cosh v)^N + (2$$

which obviously differs thermodynamic limit, butes. We will see that t matrix method.

Note that the magn is given by

$$m = \frac{\partial}{\partial B}\left(-\frac{\psi}{kT}\right)$$

$$= \sinh B(\sinh^2 B +$$

In zero field ($B = 0$) t for all finite temperatu

5-4 Transfer Matrix

The advantage of the m or more dimensions. L square lattice wrapped

Noting that λ_2/λ_1 is strictly less than unity for all $v > 0$ we have that

$$
\begin{aligned}
-\frac{\psi}{kT} &= \lim_{N\to\infty} N^{-1} \log Z_N \\
&= \lim_{N\to\infty} N^{-1} \log\{\lambda_1^N [1 + (\lambda_2/\lambda_1)^N]\} \\
&= \log \lambda_1 + \lim_{N\to\infty} N^{-1} \log[1 + (\lambda_2/\lambda_1)^N] \\
&= \log \lambda_1 \\
&= \log[e^v \cosh B + (e^{2v} \sinh^2 B + e^{-2v})^{1/2}].
\end{aligned}
\tag{3.15}
$$

When $B = 0$ the right-hand side of Equation 3.15 is $\log(2 \cosh v)$, which is precisely the expression (Equation 3.6) for the open chain. Further, from Equation 3.14 with $B = 0$,

$$
\begin{aligned}
\lambda_1 &= 2 \cosh v, \\
\lambda_2 &= 2 \sinh v,
\end{aligned}
\tag{3.16}
$$

so, from Equation 3.12, the partition function for the finite chain is given by

$$Z_N = (2 \cosh v)^N + (2 \sinh v)^N, \tag{3.17}$$

which obviously differs from the open-chain-result, Equation 3.5. In the thermodynamic limit, however, only the maximum eigenvalue (λ_1) contributes. We will see that this is generally the case in applications of the transfer-matrix method.

Note that the magnetization per spin computed from Equation 3.15 is is given by

$$
\begin{aligned}
m &= \frac{\partial}{\partial B}\left(-\frac{\psi}{kT}\right) \\
&= \sinh B(\sinh^2 B + e^{-4v})^{-1/2}.
\end{aligned}
\tag{3.18}
$$

In zero field ($B = 0$) the (spontaneous) magnetization is zero, as expected, for all finite temperatures ($v > 0$).

5-4 Transfer Matrix for the Two- and Higher-dimensional Models

The advantage of the matrix method is that it can be easily generalized to two or more dimensions. Let us consider first the two-dimensional problem on a square lattice wrapped on a cylinder (i.e., periodic in columns but not rows),

as shown in Figure 5.4. The interaction energy is given by (Equation 1.2 with $\mu_{i,n+1} = \mu_{i,1}$)

$$E\{\mu\} = -J\sum_{i=1}^{m-1}\sum_{j=1}^{n}\mu_{i,j}\mu_{i+1,j} - J\sum_{i=1}^{m}\sum_{j=1}^{n}\mu_{i,j}\mu_{i,j+1} - H\sum_{i=1}^{m}\sum_{j=1}^{n}\mu_{i,j}. \qquad (4.1)$$

If we now denote a column configuration by σ_j, i.e.,

$$\sigma_j = (\mu_{1,j}, \mu_{2,j}, \ldots, \mu_{m,j}) \qquad (4.2)$$

(there are a total of 2^m possible configurations for each column), we can write $E\{\mu\}$ as a sum of two terms—the interaction energy of columns and the interaction energy between nearest-neighbor columns—i.e., if we define

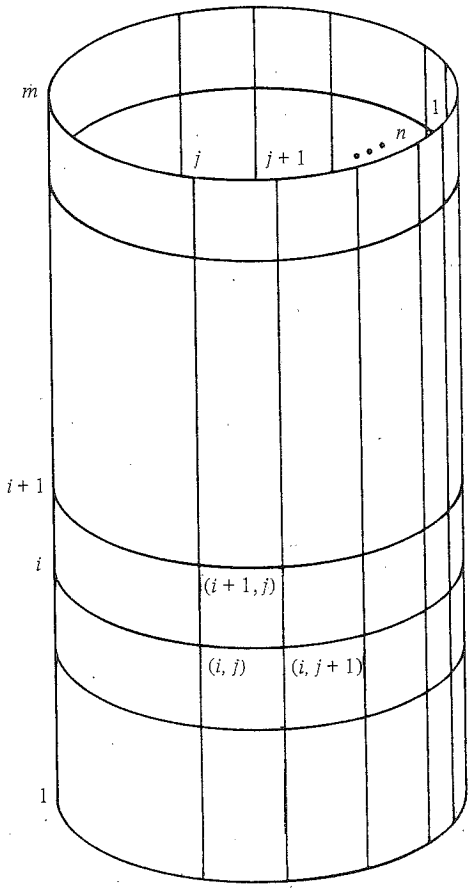

FIGURE 5.4. Two-dimensional Ising lattice wrapped on a cylinder.

$$V_1(\sigma_j) = -J\sum_{i=1}^{m-1}\mu_{i,j}\mu_{i+}$$

to be the interaction ener

$$V_2(\sigma_j, \sigma_{j+1}) = -J\sum_{i=1}^{m}$$

to be the interaction ene
write $(\sigma_{n+1} = \sigma_1)$

$$E\{\mu\} = E\{\sigma_1, \sigma_2, \ldots, \sigma$$

$$= \sum_{j=1}^{n}[V_1(\sigma_j) + V_2$$

The partition function c

$$Z_{n,m} = \sum_{\{\mu\}}\exp(-\beta E\{\mu\}$$

$$= \sum_{\sigma_1,\ldots,\sigma_n}\exp\Big[-\beta$$

$$= \sum_{\sigma_1,\ldots,\sigma_n}L(\sigma_1, \sigma_2$$

$$= \sum_{\sigma_1}L^n(\sigma_1, \sigma_1),$$

where from Equations
$(\mu'_1, \mu'_2, \ldots, \mu'_m)$,

$$L(\sigma, \sigma') = \exp[-\beta V_1($$

$$= \exp\Big(\nu\sum_{i=1}^{m-1}\mu_i$$

with

$$\nu = \beta J \quad \text{and} \quad B$$

Alternatively, we can
dimensional model)

$$L'(\sigma, \sigma') = \exp\Big[-\frac{\beta}{2}$$

$$= \exp\Big(\frac{\nu}{2}\sum_{i=1}^{m-1}$$

$$\times \exp\Big(\frac{\nu}{2}$$

is given by (Equation 1.2

$$+1 - H\sum_{i=1}^{m}\sum_{j=1}^{n}\mu_{i,j}. \qquad (4.1)$$

.,

(4.2)

each column), we can write
nergy of columns and the
ıns—i.e., if we define

rapped on a cylinder.

$$V_1(\sigma_j) = -J\sum_{i=1}^{m-1}\mu_{i,j}\mu_{i+1,j} - H\sum_{i=1}^{m}\mu_{i,j} \qquad (4.3)$$

to be the interaction energy of the jth column, and

$$V_2(\sigma_j, \sigma_{j+1}) = -J\sum_{i=1}^{m}\mu_{i,j}\mu_{i,j+1} \qquad (4.4)$$

to be the interaction energy between the jth and $(j+1)$th columns, we can write $(\sigma_{n+1} = \sigma_1)$

$$\begin{aligned} E\{\mu\} &= E\{\sigma_1, \sigma_2, \ldots, \sigma_n\} \\ &= \sum_{j=1}^{n}[V_1(\sigma_j) + V_2(\sigma_j, \sigma_{j+1})]. \end{aligned} \qquad (4.5)$$

The partition function can then be written as

$$\begin{aligned} Z_{n,m} &= \sum_{\{\mu\}}\exp(-\beta E\{\mu\}) \\ &= \sum_{\sigma_1,\ldots,\sigma_n}\exp\left[-\beta\left(\sum_{j=1}^{n}\{V_1(\sigma_j) + V_2(\sigma_j,\sigma_{j+1})\}\right)\right] \\ &= \sum_{\sigma_1,\ldots,\sigma_n}L(\sigma_1,\sigma_2)L(\sigma_2,\sigma_3)\cdots L(\sigma_{n-1},\sigma_n)L(\sigma_n,\sigma_1) \\ &= \sum_{\sigma_1}L^n(\sigma_1,\sigma_1), \end{aligned} \qquad (4.6)$$

where from Equations 4.3 and 4.4 with $\sigma = (\mu_1, \mu_2, \ldots, \mu_m)$ and $\sigma' = (\mu_1', \mu_2', \ldots, \mu_m')$,

$$\begin{aligned} L(\sigma,\sigma') &= \exp[-\beta V_1(\sigma)]\exp[-\beta V_2(\sigma,\sigma')] \\ &= \exp\left(\nu\sum_{i=1}^{m-1}\mu_i\mu_{i+1} + B\sum_{i=1}^{m}\mu_i\right)\exp\left(\nu\sum_{i=1}^{m}\mu_i\mu_i'\right) \end{aligned} \qquad (4.7)$$

with

$$\nu = \beta J \qquad \text{and} \qquad B = \beta H. \qquad (4.8)$$

Alternatively, we can take the symmetric matrix (as we did for the one-dimensional model)

$$\begin{aligned} L'(\sigma,\sigma') &= \exp\left[-\frac{\beta}{2}V_1(\sigma)\right]\exp[-\beta V_2(\sigma,\sigma')]\exp\left[-\frac{\beta}{2}V_1(\sigma')\right] \\ &= \exp\left(\frac{\nu}{2}\sum_{i=1}^{m-1}\mu_i\mu_{i+1} + \frac{B}{2}\sum_{i=1}^{m}\mu_i\right)\exp\left(\nu\sum_{i=1}^{m}\mu_i\mu_i'\right) \\ &\quad\times\exp\left(\frac{\nu}{2}\sum_{i=1}^{m-1}\mu_i'\mu_{i+1}' + \frac{B}{2}\sum_{i=1}^{m}\mu_i'\right). \end{aligned} \qquad (4.9)$$

The final result is, of course, the same. $L^n(\sigma, \sigma)$ in Equation 4.6 denotes the (σ, σ) component of the 2^m by 2^m matrix $\mathbf{L}$ with elements 4.7, raised to the nth power, i.e., by analogy with Equation 3.12,

$$\begin{aligned} Z_{n,m} &= \mathrm{Tr}(\mathbf{L}^n) \\ &= \sum_{j=1}^{2^m} \lambda_j^n, \end{aligned} \tag{4.10}$$

where $\lambda_1 > \lambda_2 \geq \cdots \geq \lambda_{2^m}$ are the eigenvalues of the 2^m by 2^m matrix $\mathbf{L}$. If now, in the thermodynamic limit, we allow n to approach infinity before m (this is convenient rather than necessary), we have for the free energy per spin ψ,

$$\begin{aligned} -\frac{\psi}{kT} &= \lim_{m\to\infty} \lim_{n\to\infty} (mn)^{-1} \log Z_{n,m} \\ &= \lim_{m\to\infty} m^{-1} \log \lambda_1 + \lim_{m\to\infty} \left[\lim_{n\to\infty} (mn)^{-1} \log\left(1 + \sum_{j=2}^{2^m} (\lambda_j/\lambda_1)^n\right)\right] \\ &= \lim_{m\to\infty} m^{-1} \log \lambda_1. \end{aligned} \tag{4.11}$$

So the problem has again been reduced to finding the largest eigenvalue of a matrix, but notice the dramatic effect of dimensionality: In one dimension we had only to find the largest eigenvalue of a 2 by 2 matrix, but in two dimensions we have to find the largest eigenvalue of a 2^m by 2^m matrix and then let m approach infinity!

The manipulation leading to Equation 4.11 can be repeated essentially word for word in three and higher dimensions. Thus in three dimensions, for example, we define σ_j to be the configuration of the jth (two-dimensional) plane and build the lattice up by planes. $V_1(\sigma_j)$ then represents the interaction energy of a plane and $V_2(\sigma_j, \sigma_{j+1})$ the interaction energy of nearest-neighbor jth and $(j+1)$th planes, and so forth. The interested reader can fill in the details for himself.

The two-dimensional problem with $H = 0$ was solved by Onsager (1944) in one of the most celebrated articles of modern times. The corresponding problem in three dimensions and the two-dimensional problem with $H \neq 0$ are unsolved.

There have been many simplifications in the derivation of the Onsager result since 1944, but even the simplest are rather complicated. We shall present in the following section only a statement and discussion of Onsager's result. A detailed derivation based on Equation 4.11 is given in Appendix D.

5-5 The Onsager Solu

By a masterly applicati
found the largest eigen
to be

$$\lambda_1 = (2 \sinh 2v)^{m/2} e^{}$$

where γ_k is defined by

$$\cosh \gamma_k = \cosh 2v \cos$$

and

$$v = \frac{J}{kT}.$$

A derivation of this res

The free energy per
Equations 4.11 and 5.1

$$-\frac{\psi}{kT} = \lim_{m\to\infty} m^{-1} \log$$

$$= \tfrac{1}{2} \log(2 \sinh 2v$$

In the limit $m \to \infty$ t
Equation 5.2), so that

$$-\frac{\psi}{kT} = \tfrac{1}{2} \log(2 \sinh$$

Use of the identity

$$\cosh^{-1}|z| = \pi^{-1} \int_0^{\pi}$$

allows us to write

$$-\frac{\psi}{kT} = \frac{1}{2} \log(2 \sinh$$

$$+ \frac{1}{2\pi^2} \iint_0^{\pi}$$

Equation 4.6 denotes the
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(4.10)

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$$\left(1+\sum_{j=2}^{2^m}(\lambda_j/\lambda_1)^n\right)\Bigg] \quad (4.11)$$

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derivation of the Onsager
her complicated. We shall
nd discussion of Onsager's
11 is given in Appendix D.

5-5 The Onsager Solution of the Two-dimensional Model

By a masterly application of Lie algebras and group representations, Onsager found the largest eigenvalue of the transfer matrix, Equation 4.7, with $H = 0$, to be

$$\lambda_1 = (2\sinh 2v)^{m/2}\exp[\tfrac{1}{2}(\gamma_1+\gamma_3+\cdots+\gamma_{2m-1})], \quad (5.1)$$

where γ_k is defined by

$$\cosh\gamma_k = \cosh 2v\coth 2v - \cos\left(\frac{\pi k}{m}\right) \quad (5.2)$$

and

$$v = \frac{J}{kT}. \quad (5.3)$$

A derivation of this result is given in Appendix D.

The free energy per spin ψ in the thermodynamic limit is then given, from Equations 4.11 and 5.1, by

$$\begin{aligned} -\frac{\psi}{kT} &= \lim_{m\to\infty} m^{-1}\log\lambda_1 \\ &= \tfrac{1}{2}\log(2\sinh 2v) + \lim_{m\to\infty}(2m)^{-1}\sum_{k=0}^{m-1}\gamma_{2k+1}. \end{aligned} \quad (5.4)$$

In the limit $m\to\infty$ the sum in Equation 5.4 approaches an integral (see Equation 5.2), so that

$$-\frac{\psi}{kT} = \tfrac{1}{2}\log(2\sinh 2v) + (2\pi)^{-1}\int_0^{\pi}\cosh^{-1}(\cosh 2v\coth 2v - \cos\theta)\,d\theta. \quad (5.5)$$

Use of the identity

$$\cosh^{-1}|z| = \pi^{-1}\int_0^{\pi}\log[2(z-\cos\phi)]\,d\phi \quad (5.6)$$

allows us to write

$$\begin{aligned} -\frac{\psi}{kT} &= \frac{1}{2}\log(2\sinh 2v) + \frac{1}{2}\log 2 \\ &\quad + \frac{1}{2\pi^2}\iint_0^{\pi}\log(\cosh 2v\coth 2v - \cos\theta - \cos\phi)\,d\theta\,d\phi, \end{aligned} \quad (5.7)$$

which gives the symmetric Onsager formula

$$-\frac{\psi}{kT} = \log 2 + \frac{1}{2\pi^2}\int_0^{\pi}\int \log[\cosh^2 2v - \sinh 2v(\cos\theta_1 + \cos\theta_2)]\, d\theta_1\, d\theta_2 . \tag{5.8}$$

From Equation 5.8 the internal energy U is given by

$$\begin{aligned} U &= -kT^2 \frac{\partial}{\partial T}\frac{\psi}{kT} \\ &= J\frac{\partial}{\partial v}\frac{\psi}{kT} \\ &= -J\coth 2v \\ &\quad \times \left[1 + (\sinh^2 2v - 1)\frac{1}{\pi^2}\int_0^{\pi}\int \frac{d\theta_1\, d\theta_2}{\cosh^2 2v - \sinh 2v(\cos\theta_1 + \cos\theta_2)}\right]. \end{aligned} \tag{5.9}$$

The integral in Equation 5.9 diverges logarithmically (at the origin $\theta_1 = \theta_2 = 0$) when $\cosh^2 2v = 2\sinh 2v$. To see this, note that in the neighborhood of the origin

$$\cos\theta_1 + \cos\theta_2 \sim 2 - \tfrac{1}{2}(\theta_1^2 + \theta_2^2) + \cdots,$$

so when $\delta = \cosh^2 2v - 2\sinh 2v \sim 0$,

$$\begin{aligned} \frac{1}{\pi^2}\int_0^{\pi}\int \frac{d\theta_1\, d\theta_2}{\cosh^2 2v - \sinh 2v(\cos\theta_1 + \cos\theta_2)} &\sim \frac{1}{\pi^2}\int_0^{\pi}\int \frac{d\theta_1\, d\theta_2}{\delta + \frac{1}{2}\sinh 2v(\theta_1^2 + \theta_2^2)} \\ &= \frac{2}{\pi}\int_0 \frac{r\, dr}{\delta + \frac{1}{2}\sinh 2v\, r^2} \\ &\sim -\frac{2}{\pi\sinh 2v}\log|\delta|, \end{aligned} \tag{5.10}$$

where in the last step we have transformed to polar coordinates ($\theta_1^2 + \theta_2^2 = r^2$, etc.).

There is a singularity, or phase-transition point, therefore, when

$$\delta = \cosh^2 2v - 2\sinh 2v = 0, \tag{5.11}$$

i.e., when $v = v_c = J/kT_c$

$$\sinh 2v_c = 1.$$

In Equation 5.9 for the
multiplied by $(\sinh^2 2v$ -
follows that the internal
borhood of v_c,

$$U \sim -J\coth 2v_c[1 +$$

where A is a constant.
defined by

$$C = \frac{\partial U}{\partial T},$$

has a symmetrical loga
critical point v_c, as show

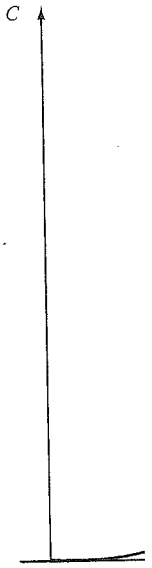

FIGURE 5.5. Zerc
Ising model. C di

i.e., when $v = v_c = J/kT_c$, given by

$$\sinh 2v_c = 1. \tag{5.12}$$

In Equation 5.9 for the internal energy U, the integral, Equation 5.10, is multiplied by $(\sinh^2 2v - 1)$, which is zero at the critical point $v = v_c$. It follows that the internal energy is continuous at $v = v_c$ and that in the neighborhood of v_c,

$$U \sim -J \coth 2v_c[1 + A(v - v_c) \log|v - v_c|], \tag{5.13}$$

where A is a constant. From this result it follows that the specific heat, defined by

$$C = \frac{\partial U}{\partial T}, \tag{5.14}$$

has a symmetrical logarithmic divergence (i.e., $C \sim B \log|v - v_c|$) at the critical point v_c, as shown in Figure 5.5.

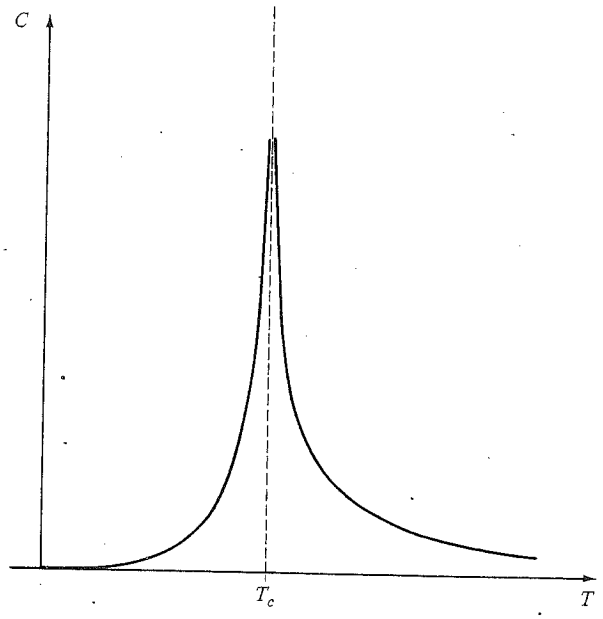

FIGURE 5.5. Zero-field specific heat C of the two-dimensional square Ising model. C diverges logarithmically on both sides of the critical point T_c.

To obtain the "Onsager logarithm" it is not necessary, as shown above, to evaluate the integrals exactly. The integral 5.9 can, however, be evaluated exactly and one finds that

$$U = -J \coth 2v \left[1 + (2 \tanh^2 2v - 1)\frac{2}{\pi} K(k_1)\right], \tag{5.15}$$

where

$$k_1 = \frac{2 \sinh 2v}{\cosh^2 2v}, \tag{5.16}$$

and $K(k_1)$ is the complete elliptic integral of the first kind defined by

$$K(k_1) = \int_0^{\pi/2} (1 - k_1^2 \sin^2 \theta)^{-1/2}\, d\theta. \tag{5.17}$$

The analysis required for Equation 5.15 is straightforward and is left as an exercise for the reader (see Problem 5). The specific heat is obtained from the definition 5.14 and the properties of elliptic integrals (see Problem 6). It is given by

$$C = \frac{2k}{\pi} (v \coth 2v)^2 \left\{2K(k_1) - 2E(k_1) - 2(1 - \tanh^2 2v) \left[\frac{\pi}{2} + (2 \tanh^2 2v - 1)K(k_1)\right]\right\}, \tag{5.18}$$

where $E(k_1)$ is the complete elliptic integral of the second kind, defined by

$$E(k_1) = \int_0^{\pi/2} (1 - k_1^2 \sin^2 \theta)^{1/2}\, d\theta. \tag{5.19}$$

In the neighborhood of $k_1 = 1-$ (see Problem 7)

$$K(k_1) \sim \log[4(1 - k_1^2)^{-1/2}], \tag{5.20}$$

so from the exact result (Equation 5.18) we obtain a logarithmically divergent specific heat.

As remarked previously, the two-dimensional model in an external field is an unsolved problem. Nevertheless, by various indirect means a number of people have obtained an expression for the spontaneous magnetization, or what is thought to be the spontaneous magnetization. Thermodynamically the spontaneous magnetization is defined by

$$m_0 = \lim_{H \to 0+} \frac{\partial}{\partial(\beta H)} \Big(-$$

with the limit $H \to 0+$
evaluation of m_0, therefc
Indirect methods based
tion, which we shall not

$$m_0 = \begin{cases} [1 - (\sinh 2v)^- \\ 0 \end{cases}$$

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$$m_0 = \lim_{H\to 0+} \frac{\partial}{\partial(\beta H)}\left(-\frac{\psi}{kT}\right) \tag{5.21}$$

with the limit $H \to 0+$ taken after the thermodynamic limit. An exact evaluation of m_0, therefore, really requires the solution of the $H \neq 0$ problem. Indirect methods based on alternative definitions of spontaneous magnetization, which we shall not go into here, suggest that

$$m_0 = \begin{cases} [1-(\sinh 2v)^{-4}]^{1/8} & T < T_c \\ 0 & T \geq T_c, \end{cases} \tag{5.22}$$

but we stress that nobody has actually proved that this expression agrees with the definition (Equation 5.21).

The expression 5.22 was first derived by Onsager in the middle 1940s, but in true Onsager fashion he has not to this day published his derivation. He tantalized numerous people by writing down Equation 5.22 in various places [Onsager (1949)], and it was not until 1952 that C. N. Yang [Yang (1952a)] gave the first published derivation. Yang's derivation and others given recently [e.g., Montroll et al. (1963)] are extremely complicated. In view of the simplicity of the final result, this fact is both surprising and frustrating.

The two-dimensional problem has been reformulated and solved by many people in a variety of ways, in the hope that a new derivation would light the way for a solution to the three-dimensional problem. This hope has unfortunately not materialized as yet, although many interesting results and interrelations between mathematics and other branches of physics have emerged. Most notable among these is the relation between the Ising problem and combinatorial mathematics. Some new results in combinatorics have been obtained by this pursuit, but unfortunately little has been added to our knowledge of the Ising model. We shall devote Chapter 6 to the combinatorial approach to the Ising problem.

In conclusion we remark that all methods to date can be applied with only mild variations to other two-dimensional lattices (e.g., triangular and hexagonal) and to lattices with different coupling constants in different directions. Although the critical points are different in each case, the critical behavior is the same—a logarithmically divergent specific heat and a $\frac{1}{8}$ power law for the spontaneous magnetization. We shall have more to say about this lattice invariance of critical behavior in Chapter 6.

5-6 Correlation Functions, Eigenvalue Degeneracy, and Long-range Order

The pair-correlation function $\langle \mu_k \mu_l \rangle$ is defined in general by

$$\langle \mu_k \mu_l \rangle = Z_N^{-1} \sum_{\{\mu\}} \mu_k \mu_l \exp(-\beta E\{\mu\}), \tag{6.1}$$

where $E\{\mu\}$, Equation 1.1, is the interaction energy, i.e.,

$$E\{\mu\} = -J \sum_{P,Q}^{*} \mu_P \mu_Q - H \sum_{P} \mu_P . \tag{6.2}$$

Similarly, one defines three spin-correlation functions $\langle \mu_k \mu_l \mu_m \rangle$, etc.

The one spin-correlation function $\langle \mu_k \rangle$ is essentially the magnetization $\left(= N^{-1} \sum_k \langle \mu_k \rangle = \langle \mu_k \rangle \text{ for periodic lattices}\right)$, which vanishes for finite N when $H = 0$ because of the symmetry of the interaction energy under the transformation $\mu_P \to -\mu_P$, all lattice points P.

In zero field the pair-correlation function is of particular interest since it in a sense measures the "degree of order" of the lattice. Thus if r_{kl} denotes the distance between lattice points k and l and

$$\rho = \lim_{r_{kl} \to \infty} \lim_{N \to \infty} \langle \mu_k \mu_l \rangle \tag{6.3}$$

exists and is nonzero, we say that there is long-range order, which is to say that spins μ_k and μ_l are not independent of one another when separated by an infinite distance.

It seems reasonable that if long-range order exists, there will be a phase transition (i.e., a nonanalytic point of the free energy). This, in fact, must be the case if there is long-range order at (sufficiently) low temperatures and zero long-range order at (sufficiently) high temperatures, since an analytic function cannot be nonzero in one region and identically zero in another region. On the other hand, if there is a nonanalytic point of the free energy, it is conceivable that there will be no long-range order at any temperature. This is indeed the case for an antiferromagnet, where $\langle \mu_k \mu_l \rangle$ oscillates in sign, but for a ferromagnet the question is still open. There is a suggestion that one can have a ferromagnetic transition (divergent susceptibility as $T \to T_c+$ for the two-dimensional Heisenberg model) with zero long-range order at all temperatures. There is also a suggestion that one can have a nonzero spontaneous magnetization without long-range order, but at the moment there is no proof of either statement. Since most of the recent work

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Summing over all $\mu_j =$

$$\langle \mu_k \mu_l \rangle = Z_N^{-1} \sum_{\substack{\mu_k = \pm 1 \\ \mu_l = \pm 1}}$$

where $L^s(\mu, \mu')$ denot
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$$L^s(\mu, \mu') = \sum_{j=1}^{2} \lambda_j^s \phi_j($$

where λ_j and ϕ_j are,
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3.16),

$$\lambda_1 = 2 \cosh v,$$

and

$$\phi_1 = \begin{pmatrix} \phi_1(+1) \\ \phi_1(-1) \end{pmatrix} =$$

on the existence and nonexistence of phase transitions in lattice models is based on long-range-order considerations, it would be extremely valuable to settle these questions. The interested reader is referred to the article by Griffiths (1966), where the problems are stated most clearly.

For the one-dimensional model the evaluation of $\langle \mu_k \mu_l \rangle$ is straightforward, particularly for the open chain (see Problem 8). We shall consider here the slightly more complicated closed-chain problem in order to facilitate the discussion of the two-dimensional problem.

In one dimension with periodic boundary conditions (i.e., a closed chain of N spins with $\mu_{N+1} = \mu_1$)

$$\langle \mu_k \mu_l \rangle = Z_N^{-1} \sum_{\{\mu\}} \mu_k \mu_l \exp\left(v \sum_{j=1}^{N} \mu_j \mu_{j+1} + B \sum_{j=1}^{N} \mu_j \right), \tag{6.4}$$

where $v = J/kT$ and $B = H/kT$. Defining as before (Equation 3.8) the transfer matrix $\mathbf{L}$ with components

$$L(\mu, \mu') = \exp\left[v\mu\mu' + \frac{B}{2}(\mu + \mu') \right], \tag{6.5}$$

Equation 6.4 can be written, assuming $l > k$, as

$$\langle \mu_k \mu_l \rangle = Z_N^{-1} \sum_{\{\mu\}} L(\mu_1, \mu_2) \cdots L(\mu_{k-1}, \mu_k) \mu_k L(\mu_k, \mu_{k+1}) \cdots L(\mu_{l-1}, \mu_l) \mu_l L(\mu_l, \mu_{l+1}) \cdots L(\mu_N, \mu_1). \tag{6.6}$$

Summing over all $\mu_j = \pm 1$ in Equation 6.6 except μ_k and μ_l gives

$$\langle \mu_k \mu_l \rangle = Z_N^{-1} \sum_{\substack{\mu_k = \pm 1 \\ \mu_l = \pm 1}} \mu_k L^{N-l+k}(\mu_k, \mu_l) \mu_l L^{l-k}(\mu_l, \mu_k), \tag{6.7}$$

where $L^s(\mu, \mu')$ denotes the (μ, μ') component of the matrix $\mathbf{L}$ raised to the sth power. Now

$$L^s(\mu, \mu') = \sum_{j=1}^{2} \lambda_j^s \phi_j(\mu) \phi_j(\mu'), \tag{6.8}$$

where λ_j and ϕ_j are, respectively, the eigenvalues and corresponding eigenvectors of the matrix $\mathbf{L}$. For example, when $H = 0$ (see Equations 3.10 and 3.16),

$$\lambda_1 = 2 \cosh v, \qquad \lambda_2 = 2 \sinh v, \tag{6.9}$$

and

$$\phi_1 = \begin{pmatrix} \phi_1(+1) \\ \phi_1(-1) \end{pmatrix} = 2^{-1/2} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad \phi_2 = \begin{pmatrix} \phi_2(+1) \\ \phi_2(-1) \end{pmatrix} = 2^{-1/2} \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \tag{6.10}$$

In general, from Equations 6.7 and 6.8 and the fact that (Equation 3.12)

$$Z_N = \lambda_1^N + \lambda_2^N, \tag{6.11}$$

we have

$$\langle \mu_k \mu_l \rangle = (\lambda_1^N + \lambda_2^N)^{-1} \sum_{\substack{\mu_k = \pm 1 \\ \mu_l = \pm 1}} \sum_{i,\, j=1}^{2} \lambda_i^{N-l+k} \mu_k \phi_i(\mu_k) \phi_i(\mu_l) \lambda_j^{l-k} \mu_l \phi_j(\mu_k) \phi_j(\mu_l)$$

$$= [1 + (\lambda_2/\lambda_1)^N]^{-1} \sum_{i,\, j=1}^{2} \left(\frac{\lambda_i}{\lambda_1}\right)^{N-l+k} \left(\frac{\lambda_j}{\lambda_1}\right)^{l-k} (\phi_i, \mu\phi_j)^2, \tag{6.12}$$

where

$$(\phi_i, \mu\phi_j) = \sum_{\mu = \pm 1} \mu \phi_i(\mu) \phi_j(\mu). \tag{6.13}$$

Now for fixed k and l, since $\lambda_2 < \lambda_1$,

$$\lim_{N \to \infty} \left(\frac{\lambda_i}{\lambda_1}\right)^{N-l+k} = \delta_{i,\,1}. \tag{6.14}$$

Also, since $\lim_{N \to \infty} (\lambda_2/\lambda_1)^N = 0$,

$$\rho_{kl} = \lim_{N \to \infty} \langle \mu_k \mu_l \rangle = \sum_{j=1}^{2} \left(\frac{\lambda_j}{\lambda_1}\right)^{l-k} (\phi_1, \mu\phi_j)^2. \tag{6.15}$$

In zero field, from Equation 6.10,

$$(\phi_1, \mu\phi_j) = \delta_{j,\,2}. \tag{6.16}$$

Hence, from Equations 6.9 and 6.15,

$$\rho_{kl} = \left(\frac{\lambda_2}{\lambda_1}\right)^{l-k} = (\tanh v)^{l-k} \qquad (l > k). \tag{6.17}$$

For finite N and $H = 0$ it is easily verified from Equations 6.9, 6.10, and 6.12 that $(l > k)$

$$\langle \mu_k \mu_l \rangle = [1 + (\tanh v)^N]^{-1} [(\tanh v)^{l-k} + (\tanh v)^{N-l+k}]. \tag{6.18}$$

As expected, from Equation 6.17,

$$\lim_{|k-l| \to \infty} \rho_{kl} = \lim_{|k-l| \to \infty} (\tanh v)^{|k-l|} = 0 \tag{6.19}$$

for all $v > 0$; i.e., there is no long-range order in one dimension for any

finite temperature. (At z
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In two dimensions the
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$$Z_{n,\,m} = \sum_{j=1}^{2m} \lambda_j^n$$

we have in the limit $n \to$

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$$= \sum_{j=1}^{2m} \left(\frac{\lambda_j}{\lambda_1}\right)^r (\phi_1$$

Since the principal eig
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finite temperature. (At zero temperature corresponding to $v \to \infty$ there is, of course, long-range order; in fact, there is complete order.)

In two dimensions the above derivation can be repeated essentially word for word with only slight changes in notation. Thus consider the pair-correlation function $\langle \mu_{k,l}\mu_{k,l+r}\rangle$ of two spins in the kth row and the lth and $(l+r)$th columns, respectively. Since the 2^m by 2^m transfer matrix $L(\sigma, \sigma')$ (Equation 4.7) transfers from one column with configuration $\sigma = (\mu_1, \ldots, \mu_m)$ to the neighboring column with configuration $\sigma' = (\mu_1', \ldots, \mu_m')$ we can write, by analogy with Equations 6.6 and 6.7,

$$\begin{aligned}\langle \mu_{k,l}\mu_{k,l+r}\rangle &= Z_{n,m}^{-1}\sum_{\{\mu\}}\mu_{k,l}\mu_{k,l+r}\exp(-\beta E\{\mu\}) \\ &= Z_{n,m}^{-1}\sum_{\sigma,\sigma'}\mu_k L^r(\sigma,\sigma')\mu_k' L^{n-r}(\sigma',\sigma),\end{aligned} \tag{6.20}$$

where σ and σ' denote, respectively, the configurations of the lth and $(l+r)$th colums. Using (see Equation 6.8)

$$L^s(\sigma,\sigma') = \sum_{j=1}^{2^m}\lambda_j^s\phi_j(\sigma)\phi_j(\sigma'), \tag{6.21}$$

where λ_j and ϕ_j are, respectively, the eigenvalues and corresponding eigenvectors of the matrix $\mathbf{L}$, enables us to write

$$\langle \mu_{k,l}\mu_{k,l+r}\rangle = Z_{n,m}^{-1}\sum_{i,j=1}^{2^m}\lambda_i^{n-r}\lambda_j^r(\phi_i, \mu_k\phi_j)^2, \tag{6.22}$$

where it is to be noted from periodicity that the scalar product does not depend on k. Now since (Equation 4.10)

$$Z_{n,m} = \sum_{j=1}^{2^m}\lambda_j^n \tag{6.23}$$

we have in the limit $n \to \infty$ with r and m fixed,

$$\begin{aligned}C_m(r) &= \lim_{n\to\infty}\langle \mu_{k,l}\mu_{k,l+r}\rangle \\ &= \sum_{j=1}^{2^m}\left(\frac{\lambda_j}{\lambda_1}\right)^r(\phi_1, \mu_k\phi_j)^2.\end{aligned} \tag{6.24}$$

Since the principal eigenvector ϕ_1 in zero field is symmetric [i.e., $\phi_1(\sigma) = \phi_1(-\sigma)$], the $j = 1$ term in Equation 6.24 vanishes, so the question of the existence of long-range order is now a question of the degeneracy of the maximum eigenvalue λ_1 of $\mathbf{L}$. For finite m we can appeal to a theorem of

Frobenius [see Gantmacher (B1964)], which states that the maximum eigenvalue of a finite matrix whose components are all positive (see Equation 4.7) is strictly nondegenerate. It then follows that there is no long-range order for an infinite ($n \to \infty$) by finite (m) lattice. That is, from Equation 6.24, since the $j = 1$ term vanishes and $(\lambda_j/\lambda_1) < 1$ for all $j \geq 2$,

$$\lim_{\substack{r\to\infty \\ (m \text{ fixed})}} C_m(r) = 0. \tag{6.25}$$

In the limit $m \to \infty$, however, as shown in Appendix D, λ_1 becomes asymptotically degenerate for $T < T_c$ (i.e., for temperatures below the critical temperature). Precisely, we have

$$\begin{aligned} \frac{\lambda_2}{\lambda_1} &< 1 && \text{for all } m \text{ and } T > T_c \\ &= 1 - 0(e^{-cm}) && \text{as } m \to \infty \text{ and } T < T_c. \end{aligned} \tag{6.26}$$

It follows from Equation 6.24 that

$$\lim_{r\to\infty}\lim_{m\to\infty} C_m(r) = \begin{cases} \lim_{m\to\infty} (\phi_1, \mu_k \phi_2)^2 > 0 & \text{for } T < T_c \\ 0 & \text{for } T > T_c; \end{cases} \tag{6.27}$$

i.e., there is long-range order below T_c and zero long-range order above T_c, as one might have expected.

It is clear that, in general, whenever one has a formula such as Equation 6.24 that long-range order exists if and only if the maximum eigenvalue λ_1 is asymptotically degenerate [i.e., $\lim_{m\to\infty} (\lambda_2/\lambda_1) = 1$ and $(\phi_1, \mu\phi_2) \neq 0$ for all m]. Thus from Equation 6.24

$$\begin{aligned} C_m(r) &\leq \left(\frac{\lambda_2}{\lambda_1}\right)^r \sum_{j=1}^{2m} (\phi_1, \mu\phi_j)^2 \\ &= \left(\frac{\lambda_2}{\lambda_1}\right)^r (\phi_1, \mu^2\phi_1)^2 \\ &= \left(\frac{\lambda_2}{\lambda_1}\right)^r, \end{aligned} \tag{6.28}$$

where in the second step we have made use of Parseval's theorem. It follows from Equation 6.28 that if λ_1 is not asymptotically degenerate, there is zero long-range order. Similarly, from Equation 6.24),

$$C_m(r) \geq \left(\frac{\lambda_2}{\lambda_1}\right)^r (\phi_1, \mu\phi_2)^2, \tag{6.29}$$

it follows that there is l
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$$P(\sigma) = \frac{L^n(\sigma, \sigma)}{\mathrm{Tr}(\mathbf{L}^n)},$$

and in view of Equati

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(6.29)

it follows that there is long-range order if λ_1 is asymptotically degenerate and $\lim_{m\to\infty}(\phi_1, \mu\phi_2) \neq 0$, which proves the assertion.

It has been suggested by Kac (1968) that the phenomenon of eigenvalue degeneracy may well be a general mathematical mechanism for a phase transition to long-range order. The idea is to construct from the Hamiltonian of the system under consideration an operator whose largest eigenvalue gives the (limiting) free energy of the systems, such that a phase transition occurs if and only if the largest eigenvalue is asymptotically degenerate. This program has been carried through for a number of model systems [e.g., Kac (1968) and Thompson (1968a)], so it may well turn out that eigenvalue degeneracy provides a general mathematical mechanism for phase transitions.

To conclude this section we present a physical interpretation of the principal eigenvector ϕ_1.

Consider a particular column of the lattice and denote by $P(\sigma)$ the probability that the column is in a particular configuration σ. By definition

$$P(\sigma) = Z_{n,m}^{-1} \sum_{\{\mu\}}{}' \exp(-\beta E\{\mu\}), \tag{6.30}$$

where the primed sum is over all configurations of the lattice with the column configuration σ held fixed. In terms of the transfer matrix (see Equation 4.6) we can write

$$P(\sigma) = \frac{L^n(\sigma, \sigma)}{\mathrm{Tr}(\mathbf{L}^n)}, \tag{6.31}$$

and in view of Equations 4.10 and 6.21 (with $\sigma' = \sigma$) we have

$$\lim_{n\to\infty} P(\sigma) = \phi_1^2(\sigma). \tag{6.32}$$

$\phi_1^2(\sigma)$, therefore, provides us with another measure of the degree of order of the lattice. Physically one would expect $\phi_1^2(\sigma)$ to be concentrated around "ordered configurations" at low temperatures ($T < T_c$) and equally spread among all configurations at high temperatures ($T > T_c$).

One final point to note is that we have considered above only pair-correlation functions for two spins in the same row. We could equally well have considered the pair-correlation function for two spins in the same column. The final result for this situation (see Problem 9) is

$$\lim_{n\to\infty} \langle \mu_{k,l}\mu_{k+r,l}\rangle = \sum_{\sigma} \phi_1(\sigma)\mu_k\mu_{k+r}\phi_1(\sigma), \tag{6.33}$$

where $\sigma = (\mu_1, \ldots, \mu_m)$ denotes the configuration of the lth column. Eigenvalue degeneracy now does not seem to play any role in the discussion of long-range column order. It does, however, appear in a devious way through the ordered–disordered form of $\phi_1^2(\sigma)$ described above. Note also that by symmetry, Equations 6.33 and 6.24 are identical in the limit $m, n \to \infty$. This rather peculiar identity seems to be extremely difficult to prove directly.

PROBLEMS

1. Consider the lattice shown in Figure 5.6 with spins $\mu_P = \pm 1$ on the (six) vertices. What is the minimum (i.e., antiferromagnetic ground state) of the expression $\sum_{P,Q}^{*} \mu_P \mu_Q$, where the sum is over nearest-neighbor lattice points P and Q, and for what configurations is the minimum achieved?

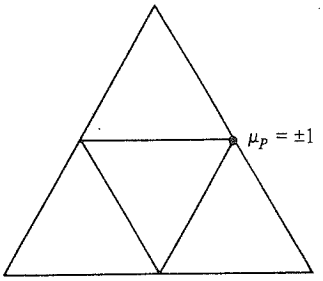


FIGURE 5.6. Six-spin antiferromagnetic Ising lattice.

2. Derive the relations between susceptibility and compressibility, Equation 2.20, and between specific heats, Equation 2.21 for the Ising magnet and the lattice gas.

3. Compute the grand-canonical partition function $Z_G(z, V, T)$ for the one-dimensional lattice gas with interaction energy

$$E\{t\} = -J \sum_{i=1}^{V} t_i t_{i+1},$$

where $t_i = 1$ or 0, $t_{V+1} = t_1$, and $\sum_{i=1}^{V} t_i = N$, and

(a) show that for $J > 0$ the zeros of $Z_G(z, V, T)$ lie on the unit circle in the complex z plane.
(b) Compute the pressure as a function of z.

4. Consider a 2 by N l
with interaction energy

$$E\{\mu, \mu'\} = -J \sum_{i=1}^{N} \mu_i \mu_i' \cdot$$

($\mu_{N+1} = \mu_1$ and $\mu_{N+1}' =$
transferring from one c
$Z_{2,N}$ can be written as

$$Z_{2,N} = \sum_{\{\mu, \mu'\}} \exp(-\beta E$$

where

$$\mathbf{A} = \begin{pmatrix} e^{3v} & 1 & 1 \\ 1 & e^{v} & e^{-} \\ 1 & e^{-3v} & e^{v} \\ e^{-v} & 1 & 1 \end{pmatrix}$$

F

5. By performing one
energy U of the two-d
in terms of the complet

$$K(k) = \int_0^{\pi/2} (1 - k^2 \mathrm{s}$$

6. Derive the result,

$$k \frac{d}{dk} K(k) = (1 - k^2$$

4. Consider a 2 by N lattice with the Nth column coupled to the first and with interaction energy

$$E\{\mu, \mu'\} = -J\sum_{i=1}^{N} \mu_i \mu_i' - J\sum_{i=1}^{N} (\mu_i \mu_{i+1} + \mu_i' \mu_{i+1}')$$

($\mu_{N+1} = \mu_1$ and $\mu_{N+1}' = \mu_1'$) for the configuration shown in Figure 5.7. By transferring from one column to the next, show that the partition function $Z_{2,N}$ can be written as

$$Z_{2,N} = \sum_{\{\mu, \mu'\}} \exp(-\beta E\{\mu, \mu'\}) = \mathrm{Tr}(\mathbf{A}^N),$$

where

$$\mathbf{A} = \begin{pmatrix} e^{3v} & 1 & 1 & e^{-v} \\ 1 & e^{v} & e^{-3v} & 1 \\ 1 & e^{-3v} & e^{v} & 1 \\ e^{-v} & 1 & 1 & e^{3v} \end{pmatrix}, \qquad v = \beta J.$$

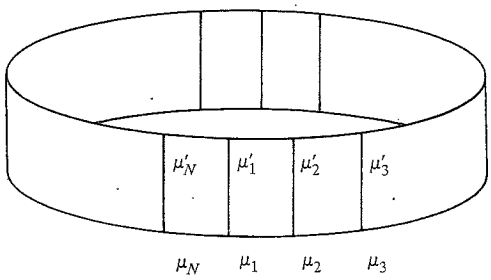


FIGURE 5.7. A 2 by N Ising model.

5. By performing one of the θ_i integrations in Equation 5.9 for the internal energy U of the two-dimensional Ising model, derive Equation 5.15 for U in terms of the complete elliptic integral of the first kind,

$$K(k) = \int_0^{\pi/2} (1 - k^2 \sin^2 \theta)^{-1/2}\, d\theta.$$

6. Derive the result,

$$k\frac{d}{dk}K(k) = (1 - k^2)^{-1}E(k) - K(k),$$

where

$$E(k) = \int_0^{\pi/2} (1 - k^2 \sin^2 \theta)^{1/2}\, d\theta$$

is the complete elliptic integral of the second kind.

7. By writing

$$K(k) = \int_0^{\pi/2} (1 - k \sin\theta)(1 - k^2 \sin^2\theta)^{-1/2}\, d\theta + \int_0^{\pi/2} k \sin\theta (1 - k^2 \sin^2\theta)^{-1/2}\, d\theta,$$

show that

$$K(k) \sim \log[4(1 - k^2)^{-1/2}] \qquad \text{as } k \to 1-.$$

8. By summing successively over the Nth, $(N-1)$th, etc., spins ($\mu_N = \pm 1$, $\mu_{N-1} = \pm 1$, etc.), show that

$$Z(J_1, J_2, \ldots, J_{N-1}) = \sum_{\{\mu\}} \exp\left(\sum_{i=1}^{N-1} J_i \mu_i \mu_{i+1}\right) = 2 \prod_{i=1}^{N-1} (2 \cosh J_i).$$

By differentiating with respect to J_k, J_{k+1}, ..., J_{k+r} and setting $J_i = J$ all $i = 1, 2, \ldots, N-1$, show that the two-spin correlation function for the open chain is given by

$$\langle \mu_k \mu_{k+r} \rangle = [Z(J, \ldots, J)]^{-1} \sum_{\{\mu\}} \mu_k \mu_{k+r} \exp\left(J \sum_{i=1}^{N-1} \mu_i \mu_{i+1}\right) = (\tanh J)^r \qquad \text{for all } N > 1.$$

9. Derive Equation 6.33 for the pair-correlation function of two spins in a column.

CHAPTER 6

The Ising Mod

6-1 Formulation

The basic idea behind t
was noted many years a
evaluate the partition fu
written in the form

$$Z_N = \sum_{\{\mu\}} \prod_{P,Q}^{*} \exp(v \mu_P \mu$$

where the starred prod
$v = J/kT$, and the sum
Expanding the exponen

$$(\mu_P \mu_Q)^n = \begin{cases} 1 \\ \mu_P \mu_Q \end{cases}$$

we have

$$\exp(v \mu_P \mu_Q) = \cosh v$$
$$= \cosh v$$

where

$$\omega = \tanh v.$$

CHAPTER 6

The Ising Model: Combinatorial Approach

6-1 Formulation

The basic idea behind the combinational approach is extremely simple and was noted many years ago by Van der Waerden (1941). The problem is to evaluate the partition function Z_N (Equation 1.7 of Chapter 5), which can be written in the form

$$Z_N = \sum_{\{\mu\}} \prod_{P,Q}{}^{*} \exp(v\mu_P \mu_Q), \tag{1.1}$$

where the starred product is over nearest-neighbor lattice points P and Q, $v = J/kT$, and the sum is over all configurations of the lattice ($\mu_P = \pm 1$). Expanding the exponential in Equation 1.1 and noting, since $\mu_P^2 = +1$, that

$$(\mu_P \mu_Q)^n = \begin{cases} 1 & \text{if } n \text{ is even} \\ \mu_P \mu_Q & \text{if } n \text{ is odd,} \end{cases} \tag{1.2}$$

we have

$$\begin{aligned} \exp(v\mu_P \mu_Q) &= \cosh v + \mu_P \mu_Q \sinh v \\ &= \cosh v(1 + \omega \mu_P \mu_Q), \end{aligned} \tag{1.3}$$

where

$$\omega = \tanh v. \tag{1.4}$$

We can then write the partition function, Equation 1.1, in the form

$$Z_N = (\cosh v)^{Nq/2} \sum_{\{\mu\}} \prod_{P,Q}^{*} (1 + \omega \mu_P \mu_Q), \tag{1.5}$$

where q is the lattice coordination number and N is the number of lattice sites (so that $\sum_{P,Q}^{*} = Nq/2$ is the total number of nearest neighbor bonds). We now expand the product in Equation 1.5,

$$\prod_{P,Q}^{*} (1 + \omega \mu_P \mu_Q) = 1 + \omega \sum_{P,Q}^{*} \mu_P \mu_Q + \omega^2 \sum_{\substack{P_1,Q_1 \\ (P_1,Q_1)\neq(P_2,Q_2)}}^{*} \sum_{P_2,Q_2}^{*} \mu_{P_1} \mu_{Q_1} \mu_{P_2} \mu_{Q_2} + \cdots \tag{1.6}$$

and represent each product $\mu_P \mu_Q$ corresponding to a nearest-neighbor pair of lattice points P and Q by a bond on the lattice connecting P and Q. For example, each term in the coefficient of ω has the representation shown in Figure 6.1 and each term in the coefficient of ω^2 has either the representation (a) or (b) shown in Figure 6.2. In case (a),

$$\mu_{P_1} \mu_{Q_1} \mu_{P_2} \mu_{Q_2} = \mu_{P_1} (\mu_{Q_1})^2 \mu_{Q_2} = \mu_{P_1} \mu_{Q_2} \tag{1.7}$$

and in general any point that appears an even number of times in a product of μ's has its μ^n replaced by 1. Similarly, any point that appears an odd number of times has a μ remaining. Since

$$\sum_{\mu=\pm 1} \mu = 0 \quad \text{and} \quad \sum_{\mu=\pm 1} \mu^2 = 2, \tag{1.8}$$

it then follows from Equations 1.5 and 1.6 that

$$Z_N = 2^N (\cosh v)^{Nq/2} \sum_{r=0}^{\infty} n(r) \omega^r, \tag{1.9}$$

where $n(0) = 1$ and $n(r)$ is the number of graphs that can be constructed from r bonds on the lattice with the restrictions that (1) no bond can occur more

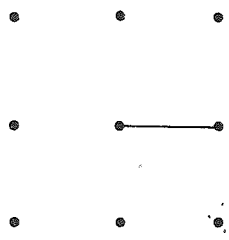
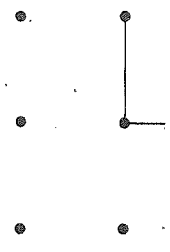


FIGURE 6.1. Possible one-bond graphs for the two-dimensional Ising model.



(a)

FIGURE 6.2. Po

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reduced to counting gra
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This approach is clea
one has merely to cou
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Nevertheless, a relativ
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Section 6-5.

To illustrate the cou
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Figure 6.3 is the only
places,

$$n(4) = N;$$

in other words, there is
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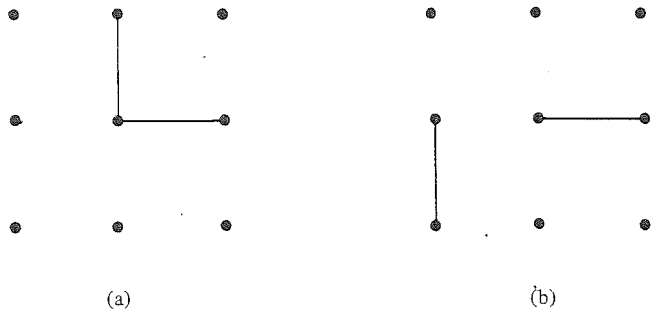
himself that

$$n(r) = 0 \quad \text{for } r \text{ odd}$$

When $r = 6$ there are
there are N of each,

$$n(6) = 2N;$$



(a) (b)

FIGURE 6.2. Possible two-bond graphs for the two-dimensional Ising model.

than once in a given graph, and (2) only an even number of bonds can meet at a lattice point (e.g., 0, 2, or 4 for the square lattice). The problem is therefore reduced to counting graphs on a lattice. For simplicity we shall refer to graphs satisfying conditions (1) and (2) as closed graphs.

This approach is clearly ideally suited to generating series expansions since one has merely to count graphs. The number of graphs $n(r)$, of course, becomes enormous as r increased, particular for three-dimensional lattices. Nevertheless, a relatively large number of terms have been calculated (15 or so in three dimensions). These expansions are our only real source of exact information in three dimensions. We shall have more to say about this in Section 6-5.

To illustrate the counting procedure let us consider the two-dimensional square lattice wrapped on a torus. Clearly, there can be no graphs satisfying conditions (1) and (2) for $r = 1$, 2, or 3. For $r = 4$ the unit square shown in Figure 6.3 is the only possible graph, and since it can be in any one of N places,

$$n(4) = N; \tag{1.10}$$

in other words, there is one square per site. When $r = 5$ there are no graphs satisfying the required conditions, and in fact the reader can easily convince himself that

$$n(r) = 0 \qquad \text{for } r \text{ odd.} \tag{1.11}$$

When $r = 6$ there are two possible graphs shown in Figure 6.4 and since there are N of each,

$$n(6) = 2N; \tag{1.12}$$

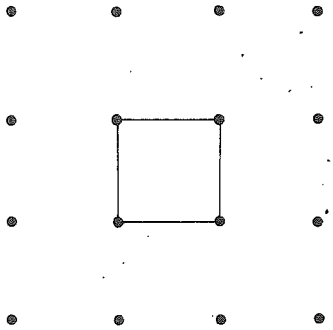
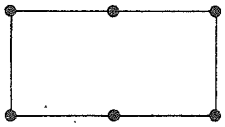


FIGURE 6.3. Only contributing four-bond graph.



or

FIGURE 6.4. Contributing six-bond graphs.

in other words, there are two hexagons per site. When $r = 8$ we can have the connected graphs shown in Figure 6.5, giving a total or $7N$ graphs, or a disconnected graph consisting of two disjoint squares. With one square fixed there are $N - 5$ possible positions for the other square, giving a total contribution of $\frac{1}{2}N(N-5)$. It follows that

$$\begin{aligned} n(8) &= 7N + \tfrac{1}{2}N(N-5) \\ &= \tfrac{1}{2}N^2 + \tfrac{9}{2}N. \end{aligned} \tag{1.13}$$

For larger r the problem rapidly becomes complicated, so we shall stop at this point.

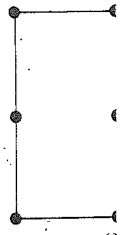


FIGURE 6.5.

From Equation 1.9

$Z_N = (2\cosh^2 \dot{v})^N[1 -$

For large N, $\log Z_N$ sho
5 that $\lim_{N\to\infty} N^{-1} \log$
1.14 we take logarithm
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ω^8 we obtain

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$$Z_N \sim \left(1 + \sum_{n=1}^{\infty} a_n \omega^n\right)$$

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In general, if r is les

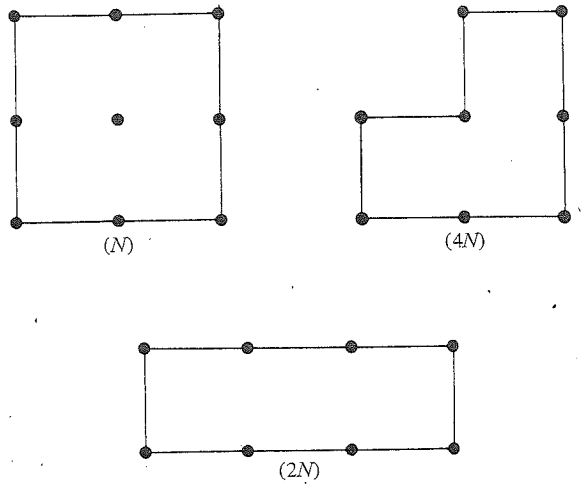

FIGURE 6.5. Contributing connected eight-bond graphs.

From Equation 1.9 to 1.13 we have that ($q = 4$)

$$Z_N = (2\cosh^2 v)^N[1 + N\omega^4 + 2N\omega^6 + (\tfrac{1}{2}N^2 + \tfrac{9}{2}N)\omega^8 + \cdots]. \tag{1.14}$$

For large N, $\log Z_N$ should be proportional to N (since we know from Chapter 5 that $\lim_{N\to\infty} N^{-1} \log Z_N$ exists). To see how this comes about from Equation 1.14 we take logarithms of both sides of Equation 1.14 and formally expand the logarithm of the bracketed term. If we do this and retain only terms up to ω^8 we obtain

$$\begin{aligned} \log Z_N &= N \log 2\cosh^2 v + N\omega^4 + 2N\omega^6 + (\tfrac{1}{2}N^2 + \tfrac{9}{2}N)\omega^8 - \tfrac{1}{2}(N\omega^4)^2 + \cdots \\ &= N(\log 2\cosh^2 v + \omega^4 + 2\omega^6 + \tfrac{9}{2}\omega^8 + \cdots), \end{aligned} \tag{1.15}$$

which has the required form. The important point to note is that the N^2 term in Equation 1.14 cancels when one computes the free energy. The expansion of the logarithm of Equation 1.14 is not legitimate, since the series diverges for sufficiently large N. One obtains the same result, however, by taking

$$Z_N \sim \left(1 + \sum_{n=1}^{\infty} a_n \omega^n\right)^N, \tag{1.16}$$

expanding the right-hand side in a binomial series and equating coefficients with those in Equation 1.14. This process can be made perfectly rigorous.

In general, if r is less than the circumference of the torus (i.e., $r < N^{1/d}$ in d

dimensions), $n(r)$ is a polynomial of degree $m \leq r/4$ (or $\leq r/3$ if triangles can occur), i.e.,

$$n(r) = Na_r^{(1)} + N^2 a_r^{(2)} + \cdots + N^m a_r^{(m)}. \tag{1.17}$$

Taking logarithms as above, the coefficients of $N^2, \ldots, N^m$ vanish and we are left with

$$\begin{aligned} -\frac{\psi}{kT} &= \lim_{N\to\infty} N^{-1} \log Z_N \\ &= \log 2 + \frac{q}{2} \log \cosh v + \sum_{r=0}^{\infty} a_r^{(1)} \omega^r. \end{aligned} \tag{1.18}$$

The problem then is to compute $a_r^{(1)}$ in Equation 1.17. More detailed discussions of the counting problem can be found in the review articles by Domb (1960) and Fisher (1965, 1967).

An exact evaluation of Z_N in two dimensions based on the combinational formula 1.9 was first attempted by Kac and Ward (1952). Their idea was to express the generating function for the graph-counting problem (i.e., the partition function 1.9) as a determinant of a matrix. They succeeded in constructing a matrix to give the Onsager result, but they were unable to prove that all graphs were counted correctly (although clearly "most" graphs must have been counted correctly). Sherman (1960) showed that not all graphs were counted correctly by the Kac–Ward matrix, but with the aid of a conjecture of Feynmann, which Sherman himself proved, he was able to make the Kac–Ward argument completely rigorous.

A variant of the Kac–Ward method emerged in the early 1960s when a number of Ising-model enthusiasts became aware of Pfaffians, which were known to mathematicians last century but were subsequently forgotten. This method will be discussed in Section 6-3, where the Ising problem is related to a dimer problem that can be solved by Pfaffians.

6-2 Low-temperature Expansions and Lattice Duality in Two Dimensions

Since $\omega = \tanh(J/kT)$ is small when T is large, the combinational formula 1.9 gives a high-temperature expansion for the partition function. Low-temperature expansions can be developed in a similar manner if we start from the completely ordered state (corresponding to zero temperature), i.e., when all