

and universality, forms the subject matter of Chapter 7.

## 6.1 Ising Model in Two Dimensions

In a landmark paper, Onsager [222] exactly calculated the free energy of the two-dimensional ferromagnetic Ising model in zero magnetic field on the rectangular lattice. This calculation provided the first exact solution of a model that displays a phase transition. Onsager's original derivation is mathematically complex. Since his original paper, a number of more transparent solutions of the problem have appeared. Below, we present a brief account of one of these, namely that of Schultz *et al.* [270]. Our motivation for including this calculation is twofold. Most of this book is concerned with approximation techniques, but we feel that it is worthwhile to exhibit an exact calculation in statistical physics as a counterpoint to the examples of mean field theory and approximate renormalization group calculations. Second, we frequently quote the exact results of Onsager for the specific heat and order parameter and feel that some readers may not feel comfortable with these results without the evidence of a derivation. Those readers not interested in the technical details may skip ahead to Section 6.1.4.

### 6.1.1 Transfer matrix

We have already solved the one-dimensional Ising model in Section 3.6 by use of the transfer matrix approach and will also apply this method in two dimensions. We first formulate the one-dimensional problem in a slightly different way. Consider, again, the Hamiltonian

$$H = -J \sum_{i=1}^N \sigma_i \sigma_{i+1} - h \sum_i \sigma_i. \quad (6.1)$$

The partition function is

$$Z = \sum_{\{\sigma\}} (e^{\beta h \sigma_1} e^{K \sigma_1 \sigma_2}) (e^{\beta h \sigma_2} e^{K \sigma_2 \sigma_3}) \dots (e^{\beta h \sigma_N} e^{K \sigma_N \sigma_1}) \quad (6.2)$$

where we have grouped the factors somewhat differently from (3.36) and where  $K = \beta J$ .

We now introduce two orthonormal basis states  $|+1\rangle$  and  $|-1\rangle$  and Pauli

operators, which in this basis have the representation

$$\sigma_Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad (6.3)$$

with  $\sigma_X = \sigma^+ + \sigma^-$  and  $\sigma_Y = -i(\sigma^+ - \sigma^-)$ . It is now easy to see that the Boltzmann weight  $\exp\{\beta h \sigma_i\}$  can be expressed as a diagonal matrix,  $\mathbf{V}_1$ , in this basis:

$$\langle +1 | \mathbf{V}_1 | +1 \rangle = e^{\beta h}, \quad \langle -1 | \mathbf{V}_1 | -1 \rangle = e^{-\beta h}$$

or

$$\mathbf{V}_1 = \exp\{\beta h \sigma_Z\}. \quad (6.4)$$

Similarly, we define the operator  $\mathbf{V}_2$  corresponding to the nearest-neighbor coupling by its matrix elements in this basis:

$$\langle +1 | \mathbf{V}_2 | +1 \rangle = \langle -1 | \mathbf{V}_2 | -1 \rangle = e^K$$

$$\langle +1 | \mathbf{V}_2 | -1 \rangle = \langle -1 | \mathbf{V}_2 | +1 \rangle = e^{-K}.$$

Therefore,

$$\mathbf{V}_2 = e^K \mathbf{1} + e^{-K} \sigma_X = A(K) \exp\{K^* \sigma_X\} \quad (6.5)$$

where in the second step we have used the fact that  $(\sigma_X)^{2n} = \mathbf{1}$ . The constants  $A(K)$  and  $K^*$  are determined from the equations

$$\begin{aligned} A \cosh K^* &= e^K \\ A \sinh K^* &= e^{-K} \end{aligned} \quad (6.6)$$

or  $\tanh K^* = \exp\{-2K\}$ ,  $A = \sqrt{2 \sinh 2K}$ . Using these results, we write the partition function as follows:

$$\begin{aligned} Z &= \sum_{\{\mu=+1,-1\}} \langle \mu_1 | \mathbf{V}_1 | \mu_2 \rangle \langle \mu_2 | \mathbf{V}_2 | \mu_3 \rangle \langle \mu_3 | \mathbf{V}_1 | \mu_4 \rangle \dots \langle \mu_N | \mathbf{V}_2 | \mu_1 \rangle \\ &= \text{Tr}(\mathbf{V}_1 \mathbf{V}_2)^N = \text{Tr}(\mathbf{V}_2^{1/2} \mathbf{V}_1 \mathbf{V}_2^{1/2})^N = \lambda_1^N + \lambda_2^N \end{aligned} \quad (6.7)$$

where  $\lambda_1$  and  $\lambda_2$  are the two eigenvalues of the Hermitian operator

$$\mathbf{V} = (\mathbf{V}_2^{1/2} \mathbf{V}_1 \mathbf{V}_2^{1/2}) = \sqrt{2 \sinh 2K} e^{K^* \sigma_X / 2} e^{\beta h \sigma_Z} e^{K^* \sigma_X / 2}. \quad (6.8)$$

In arriving at this symmetric form of the transfer matrix  $\mathbf{V}$  we have used the invariance of the trace of a product of matrices under a cyclic permutation

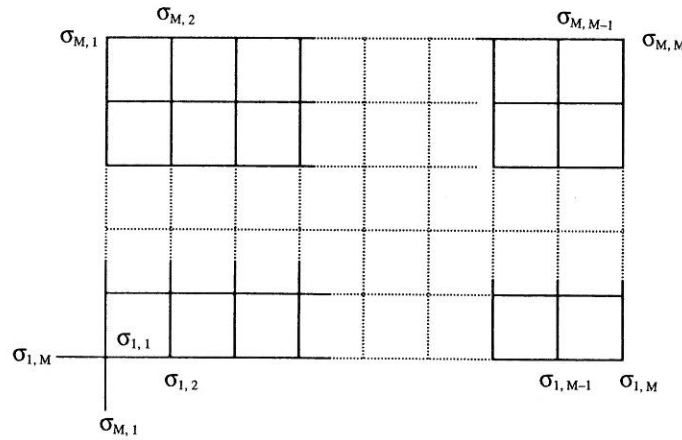


Figure 6.1:  $M \times M$  square lattice with periodic boundary conditions.

of the factors. Clearly, in the case  $h = 0$ , the two eigenvalues are given by  $\lambda_1 = A \exp \{K^*\}$ ,  $\lambda_2 = A \exp \{-K^*\}$  and we recover our previous result (3.37).

We note, in passing, that in this procedure a one-dimensional problem in classical statistics has been transformed into a zero-dimensional (only one "site") quantum-mechanical ground-state problem (largest eigenvalue). This result is quite general. There exists a correspondence between the ground state of quantum Hamiltonians in  $d - 1$  dimensions and classical partition functions in  $d$  dimensions which can sometimes be exploited, for example in numerical simulations of quantum-statistical models [296], [297].

We now generalize this procedure to the two-dimensional Ising model and consider an  $M \times M$  square lattice with periodic boundary conditions (see Figure 6.1) and the Hamiltonian

$$H = -J \sum_{r,c} \sigma_{r,c} \sigma_{r+1,c} - J \sum_{r,c} \sigma_{r,c} \sigma_{r,c+1} \quad (6.9)$$

where the label  $r$  refers to rows,  $c$  to columns, and  $\sigma_{r+M,c} = \sigma_{r,c+M} = \sigma_{r,c}$ .

The first term in (6.9) contains only interactions in column  $c$  and is, in this sense, analogous to the magnetic field term in (6.1). The second term in (6.9) is the coupling between neighboring columns and will lead to a non-diagonal factor in the complete transfer matrix.

In analogy with the one-dimensional case, we now introduce the  $2^M$  basis states

$$|\mu\rangle \equiv |\mu_1, \mu_2, \dots, \mu_M\rangle \equiv |\mu_1\rangle |\mu_2\rangle \cdots |\mu_M\rangle \quad (6.10)$$

with  $\mu_j = \pm 1$  and  $M$  sets of Pauli operators ( $\sigma_{jX}, \sigma_{jY}, \sigma_{jZ}$ ) which act on the  $j$ th state in the product (6.10), that is,

$$\begin{aligned} \sigma_{jZ} |\mu_1, \mu_2, \dots, \mu_j, \dots, \mu_M\rangle &= \mu_j |\mu_1, \mu_2, \dots, \mu_j, \dots, \mu_M\rangle \\ \sigma_j^+ |\mu_1, \mu_2, \dots, \mu_j, \dots, \mu_M\rangle &= \delta_{\mu_j, -1} |\mu_1, \mu_2, \dots, \mu_j + 2, \dots, \mu_M\rangle \\ \sigma_j^- |\mu_1, \mu_2, \dots, \mu_j, \dots, \mu_M\rangle &= \delta_{\mu_j, 1} |\mu_1, \mu_2, \dots, \mu_j - 2, \dots, \mu_M\rangle. \end{aligned} \quad (6.11)$$

Moreover, we impose the commutation relations  $[\sigma_{j\alpha}, \sigma_{m\beta}] = 0$  for  $j \neq m$ . For  $j = m$  the usual Pauli matrix commutation relations apply.

If we think of the index  $\mu_i$  as the orientation of the  $i$ th spin in a given column, we see immediately that the Boltzmann factors  $\exp \{K \sum_r \sigma_{r,c} \sigma_{r+1,c}\}$  are given by the matrix elements of the operator  $\mathbf{V}_1 = \exp \{K \sum_j \sigma_{jZ} \sigma_{j+1,Z}\}$ . Similarly, the matrix element

$$\begin{aligned} \langle \{\mu\} | \mathbf{V}_2 | \{\mu'\} \rangle &= \langle \mu_M, \mu_{M-1}, \dots, \mu_1 | \prod_{j=1}^M (e^{K\mathbf{1}} + e^{-K} \sigma_{jX}) | \mu'_1, \mu'_2, \dots, \mu'_M \rangle \\ &= \exp \{(M - 2n)K\} \end{aligned} \quad (6.12)$$

where  $n$  of the indices  $\{\mu'\}$  differ from the corresponding entries in  $\{\mu\}$ . Thus the partition function of the two-dimensional Ising model, in zero magnetic field, is, as can easily be verified, given by

$$\begin{aligned} Z &= \sum_{\{\mu_1\}, \{\mu_2\}, \dots, \{\mu_M\}} \langle \mu_1 | \mathbf{V}_1 | \mu_2 \rangle \langle \mu_2 | \mathbf{V}_2 | \mu_3 \rangle \langle \mu_3 | \mathbf{V}_1 | \mu_4 \rangle \cdots \langle \mu_M | \mathbf{V}_2 | \mu_1 \rangle \\ &= \text{Tr}(\mathbf{V}_1 \mathbf{V}_2)^M = \text{Tr}(\mathbf{V}_2^{1/2} \mathbf{V}_1 \mathbf{V}_2^{1/2})^M. \end{aligned} \quad (6.13)$$

In (6.13) the sum over each  $\{\mu_j\}$  is, of course, over the entire set of  $2^M$  basis states. Using (6.5) and (6.6), we may write

$$\mathbf{V}_2 = (2 \sinh 2K)^{M/2} \exp \left\{ K^* \sum_{j=1}^M \sigma_{jX} \right\} \quad (6.14)$$

and we have reduced the calculation of the partition function to the determination of the largest eigenvalue of the Hermitian operator

$$\begin{aligned} \mathbf{V} &= \mathbf{V}_2^{1/2} \mathbf{V}_1 \mathbf{V}_2^{1/2} \\ &= (2 \sinh 2K)^{M/2} \exp \left\{ \frac{K^*}{2} \sum_{j=1}^M \sigma_{jX} \right\} \end{aligned}$$

$$\times \exp \left\{ K \sum_{j=1}^M \sigma_{jZ} \sigma_{j+1,Z} \right\} \exp \left\{ \frac{K^*}{2} \sum_{j=1}^M \sigma_{jX} \right\} \quad (6.15)$$

which is still a nontrivial task since the factors in (6.15) do not commute with each other and, since the matrix  $\mathbf{V}$  becomes infinite dimensional in the thermodynamic limit.

### 6.1.2 Transformation to an interacting fermion problem

It is convenient for what follows to perform a rotation of the spin operators and to let  $\sigma_{jZ} \rightarrow -\sigma_{jX}$ ,  $\sigma_{jX} \rightarrow \sigma_{jZ}$  for all  $j$ . These rotations, of course, leave the eigenvalues invariant. Using  $\sigma_{jZ} = 2\sigma_j^+ \sigma_j^- - 1$  and  $\sigma_{jX} = \sigma_j^+ + \sigma_j^-$ , we arrive at the forms

$$\begin{aligned} \mathbf{V}_1 &= \exp \left\{ K \sum_{j=1}^M (\sigma_j^+ + \sigma_j^-) (\sigma_{j+1}^+ + \sigma_{j+1}^-) \right\} \\ \mathbf{V}_2 &= (2 \sinh 2K)^{M/2} \exp \left\{ 2K^* \sum_{j=1}^M (\sigma_j^+ \sigma_j^- - \frac{1}{2} \mathbf{1}) \right\}. \end{aligned} \quad (6.16)$$

Schultz *et al.* [270] showed that these operators can be simplified by a series of transformations. The first of these is the Jordan–Wigner transformation which converts the Pauli operators to fermion operators (see the Appendix for a discussion of second quantization). This step is useful because of subsequent canonical transformations that are not possible for angular momentum operators. One writes

$$\begin{aligned} \sigma_j^+ &= \exp \left\{ \pi i \sum_{m=1}^{j-1} c_m^\dagger c_m \right\} c_j^\dagger \\ \sigma_j^- &= c_j \exp \left\{ -\pi i \sum_{m=1}^{j-1} c_m^\dagger c_m \right\} = \exp \left\{ \pi i \sum_{m=1}^{j-1} c_m^\dagger c_m \right\} c_j \end{aligned} \quad (6.17)$$

where the operators  $c, c^\dagger$  obey the commutation relations

$$\begin{aligned} [c_j, c_m^\dagger]_+ &\equiv c_j c_m^\dagger + c_m^\dagger c_j = \delta_{jm} \\ [c_j, c_m]_+ &= [c_j^\dagger, c_m^\dagger]_+ = 0. \end{aligned}$$

The operator  $c_m^\dagger c_m$  is the fermion number operator for site  $m$  with integer eigenvalues 0 and 1. Since  $e^{i\pi n} = e^{-i\pi n}$  the last step of (6.17) follows. To see

that the spin commutation relations are preserved under this transformation consider, for  $n > j$ ,

$$[\sigma_j^-, \sigma_n^+] = \exp \left\{ \pi i \sum_{m=j+1}^{n-1} c_m^\dagger c_m \right\} \left( c_j e^{\pi i c_j^\dagger c_j} c_n^\dagger - c_n^\dagger e^{\pi i c_j^\dagger c_j} c_j \right).$$

Noting that  $\exp \left\{ \pi i c_j^\dagger c_j \right\} c_j = c_j$  and  $c_j \exp \left\{ \pi i c_j^\dagger c_j \right\} = -c_j$ , we have  $[\sigma_j^-, \sigma_n^+] = 0$  for  $n \neq j$ . We also immediately see that the on-site anticommutator

$$[\sigma_j^-, \sigma_j^+]_+ = [c_j, c_j^\dagger]_+ = 1.$$

The verification of further commutation relations and the derivation of the inverse of the transformation (6.17) is left as an exercise. Using (6.17), we can express the operators  $\mathbf{V}_1$ , and  $\mathbf{V}_2$  in terms of the fermion operators. The operator  $\mathbf{V}_2$  presents no difficulties and is immediately given by

$$\mathbf{V}_2 = (2 \sinh 2K)^{M/2} \exp \left\{ 2K^* \sum_{j=1}^M \left( c_j^\dagger c_j - \frac{1}{2} \right) \right\}. \quad (6.18)$$

In the case of  $\mathbf{V}_1$ , there is a slight difficulty due to the periodic boundary conditions. We first note that for  $j \neq M$  the term

$$(\sigma_j^+ + \sigma_j^-) (\sigma_{j+1}^+ + \sigma_{j+1}^-) = c_j^\dagger c_{j+1}^\dagger + c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j + c_{j+1} c_j.$$

For the specific case  $j = M$ ,

$$\begin{aligned} (\sigma_M^+ + \sigma_M^-) (\sigma_1^+ + \sigma_1^-) &= \exp \left\{ \pi i \sum_{j=1}^{M-1} c_j^\dagger c_j \right\} c_M^\dagger (c_1^\dagger + c_1) \\ &\quad + \exp \left\{ \pi i \sum_{j=1}^{M-1} c_j^\dagger c_j \right\} c_M (c_1^\dagger + c_1) \\ &= \exp \left\{ \pi i \sum_{j=1}^M c_j^\dagger c_j \right\} \left[ e^{\pi i c_M^\dagger c_M} (c_M^\dagger + c_M) (c_1^\dagger + c_1) \right] \\ &= (-1)^n (c_M - c_M^\dagger) (c_1^\dagger + c_1) \end{aligned}$$

where  $n = \sum_j c_j^\dagger c_j$  is the total fermion number operator. The operator  $n$  commutes with  $\mathbf{V}_2$  but not with  $\mathbf{V}_1$ . On the other hand,  $(-1)^n$  commutes with both  $\mathbf{V}_1$ , and  $\mathbf{V}_2$  as the various terms in  $\mathbf{V}_1$  change the total fermion

number by 0 or  $\pm 2$ . Thus if we consider separately the subspaces of even and odd total number of fermions, we may write  $\mathbf{V}_1$  in a simple universal way, that is,

$$\mathbf{V}_1 = \exp \left\{ K \sum_{j=1}^M (c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1}) \right\} \quad (6.19)$$

where

$$\begin{aligned} c_{M+1} &\equiv -c_1, \quad c_{M+1}^\dagger \equiv -c_1^\dagger && \text{for } n \text{ even} \\ c_{M+1} &\equiv c_1, \quad c_{M+1}^\dagger \equiv c_1^\dagger && \text{for } n \text{ odd} . \end{aligned} \quad (6.20)$$

With this choice of boundary condition on the fermion creation and annihilation operators, we have recovered translational invariance and now carry out the *canonical* transformation

$$\begin{aligned} a_q &= \frac{1}{\sqrt{M}} \sum_{j=1}^M c_j e^{-iqj} \\ a_q^\dagger &= \frac{1}{\sqrt{M}} \sum_{j=1}^M c_j^\dagger e^{iqj} \end{aligned} \quad (6.21)$$

with inverse

$$\begin{aligned} c_j &= \frac{1}{\sqrt{M}} \sum_q a_q e^{iqj} \\ c_j^\dagger &= \frac{1}{\sqrt{M}} \sum_q a_q^\dagger e^{-iqj} . \end{aligned} \quad (6.22)$$

To reproduce the boundary conditions (6.20), we take  $q = j\pi/M$  with

$$\begin{aligned} j &= \pm 1, \pm 3, \dots, \pm(M-1) && \text{for } n \text{ even} \\ j &= 0, \pm 2, \pm 4, \dots, \pm(M-2), M && \text{for } n \text{ odd} \end{aligned}$$

and where we have also assumed, without loss of generality, that  $M$  is even. It is easy to see that the operators  $a_q, a_q^\dagger$  obey fermion commutation relations, that is,  $[a_q, a_{q'}^\dagger]_+ = \delta_{q,q'}$  and  $[a_q, a_{q'}]_+ = [a_q^\dagger, a_{q'}^\dagger]_+ = 0$  for all  $q$  and  $q'$ . Substituting into (6.18) and (6.19), we find for  $n$  even,

$$\begin{aligned} \mathbf{V}_2 &= (2 \sinh 2K)^{M/2} \exp \left\{ 2K^* \sum_{q>0} (a_q^\dagger a_q + a_{-q}^\dagger a_{-q} - 1) \right\} \\ &= (2 \sinh 2K)^{M/2} \prod_{q>0} \mathbf{V}_{2q} \end{aligned} \quad (6.23)$$

and

$$\begin{aligned} \mathbf{V}_1 &= \exp \left\{ 2K \sum_{q>0} [\cos q (a_q^\dagger a_q + a_{-q}^\dagger a_{-q}) - i \sin q (a_q^\dagger a_{-q}^\dagger + a_q a_{-q})] \right\} \\ &= \prod_{q>0} \mathbf{V}_{1q} \end{aligned} \quad (6.24)$$

where, in (6.23) and (6.24), we have combined the terms corresponding to  $q$  and  $-q$ , and recognized in writing the resulting operators as products, that bilinear operators with different wave vectors commute. This is a great simplification since the eigenvalues of the transfer matrix can now be written as a product of eigenvalues of, as we shall see, at most  $4 \times 4$  matrices. For the case of odd  $n$  we also need the operators  $\mathbf{V}_{1q}$  and  $\mathbf{V}_{2q}$  for  $q = \pi$  and  $q = 0$ . These are given by

$$\begin{aligned} \mathbf{V}_{10} &= \exp \left\{ 2K a_0^\dagger a_0 \right\} & \mathbf{V}_{20} &= \exp \left\{ 2K^* (a_0^\dagger a_0 - \frac{1}{2}) \right\} \\ \mathbf{V}_{1\pi} &= \exp \left\{ -2K a_\pi^\dagger a_\pi \right\} & \mathbf{V}_{2\pi} &= \exp \left\{ 2K^* (a_\pi^\dagger a_\pi - \frac{1}{2}) \right\} \end{aligned} \quad (6.25)$$

which are already in diagonal form and, of course, commute with each other.

### 6.1.3 Calculation of eigenvalues

We proceed to calculate the eigenvalues of the operator

$$\mathbf{V}_q = \mathbf{V}_{2q}^{1/2} \mathbf{V}_{1q} \mathbf{V}_{2q}^{1/2}$$

for  $q \neq 0$  and  $q \neq \pi$ . Since we are dealing with fermions, we have only four possible states:  $|0\rangle, a_q^\dagger|0\rangle, a_{-q}^\dagger|0\rangle,$  and  $a_q^\dagger a_{-q}^\dagger|0\rangle$ , where  $|0\rangle$  is the zero particle state defined by  $a_q|0\rangle = a_{-q}|0\rangle = 0$ . These states are already eigenstates of  $\mathbf{V}_2$ , and since the operator  $\mathbf{V}_1$  has nonzero off-diagonal matrix elements only between states that differ by two in fermion number, the problem reduces to finding the eigenvalues of  $\mathbf{V}_q$  in the basis  $|0\rangle$  and  $|2\rangle = a_q^\dagger a_{-q}^\dagger|0\rangle$ . We note that

$$\mathbf{V}_{1q} a_{\pm q}^\dagger |0\rangle = \exp \{ 2K \cos q \} a_{\pm q}^\dagger |0\rangle \quad (6.26)$$

and

$$\begin{aligned} \mathbf{V}_{2q}^{1/2} |0\rangle &= \exp \{-K^*\} |0\rangle \\ \mathbf{V}_{2q}^{1/2} |2\rangle &= \exp \{K^*\} |2\rangle . \end{aligned} \quad (6.27)$$

To obtain the matrix elements of  $\mathbf{V}_{1q}$  in the basis  $|0\rangle, |2\rangle$ , we let

$$\mathbf{V}_{1q}|0\rangle = \alpha(K)|0\rangle + \beta(K)|2\rangle .$$

Differentiating this expression with respect to  $K$ , we obtain

$$\begin{aligned} \frac{d\alpha}{dK}|0\rangle + \frac{d\beta}{dK}|2\rangle &= 2 \left[ \cos q \left\{ a_q^\dagger a_q + a_{-q}^\dagger a_{-q} \right\} \right. \\ &\quad \left. - i \sin q \left\{ a_q^\dagger a_{-q}^\dagger + a_q a_{-q} \right\} \right] \{ \alpha |0\rangle + \beta |2\rangle \} \\ &= 2i\beta \sin q |0\rangle + [4\beta \cos q - 2i\alpha \sin q] |2\rangle \end{aligned} \quad (6.28)$$

or

$$\begin{aligned} \frac{d\alpha}{dK} &= 2i\beta(K) \sin q \\ \frac{d\beta}{dK} &= 4\beta(K) \cos q - 2i\alpha(K) \sin q. \end{aligned} \quad (6.29)$$

We solve these equations subject to the boundary conditions  $\alpha(0) = 1$ ,  $\beta(0) = 0$ . The result is

$$\begin{aligned} \langle 0 | \mathbf{V}_{1q} | 0 \rangle &= \alpha(K) = e^{2K \cos q} (\cosh 2K - \sinh 2K \cos q) \\ \langle 2 | \mathbf{V}_{1q} | 0 \rangle &= \beta(K) = -ie^{2K \cos q} \sinh 2K \sin q. \end{aligned} \quad (6.30)$$

By the same method we can find the matrix elements  $\langle 2 | \mathbf{V}_{1q} | 2 \rangle$  and  $\langle 0 | \mathbf{V}_{1q} | 2 \rangle = \langle 2 | \mathbf{V}_{1q} | 0 \rangle^*$  and obtain the matrix

$$\mathbf{V}_{1q} = e^{2K \cos q} \begin{bmatrix} \cosh 2K - \sinh 2K \cos q & i \sinh 2K \sin q \\ -i \sinh 2K \sin q & \cosh 2K + \sinh 2K \cos q \end{bmatrix} \quad (6.31)$$

and

$$\mathbf{V}_q = \begin{bmatrix} \exp \{-K^*\} & 0 \\ 0 & \exp \{K^*\} \end{bmatrix} [\mathbf{V}_{1q}] \begin{bmatrix} \exp \{-K^*\} & 0 \\ 0 & \exp \{K^*\} \end{bmatrix}. \quad (6.32)$$

The eigenvalues of this matrix are easily determined. Since we wish, eventually, to take the logarithm of the largest eigenvalue of the complete transfer matrix in order to calculate the free energy, we write the eigenvalues in the form

$$\lambda_q^\pm = \exp \{ 2K \cos q \pm \epsilon(q) \} \quad (6.33)$$

and after a bit of algebra, we obtain the equation

$$\cosh \epsilon(q) = \cosh 2K \cosh 2K^* + \cos q \sinh 2K \sinh 2K^* \quad (6.34)$$

for  $\epsilon(q)$ . By convention we choose  $\epsilon(q) \geq 0$ . We see that the minimum of the right-hand side of (6.34) occurs as  $q \rightarrow \pi$  and that, for all  $q$ ,

$$\epsilon(q) > \epsilon_{min} = \lim_{q \rightarrow \pi} \epsilon(q) = 2|K - K^*| \quad (6.35)$$

and also note that

$$\lim_{q \rightarrow 0} \epsilon(q) = 2(K + K^*). \quad (6.36)$$

We are now in a position to combine all this information. Consider first the subspace in which all states contain an even number of fermions. In this case the allowed wave vectors do not include  $q = 0$  or  $q = \pi$ , and comparing (6.33) and (6.26), we see that the largest eigenvalue of  $\mathbf{V}_q$  for each  $q$  is  $\lambda_q^+$ . Thus the largest eigenvalue in this subspace,  $\Lambda_e$ , is given by

$$\begin{aligned} \Lambda_e &= (2 \sinh 2K)^{M/2} \prod_{q>0} \lambda_q^+ \\ &= (2 \sinh 2K)^{M/2} \exp \left\{ \sum_{q>0} [2\sqrt{\cos q + \epsilon(q)}] \right\} \\ &= (2 \sinh 2K)^{M/2} \exp \left\{ \frac{1}{2} \sum_q \epsilon(q) \right\} \end{aligned} \quad (6.37)$$

where, in the last step, we have used  $\sum_q \cos q = 0$  and have also extended the summation over the entire range  $-\pi < q < \pi$ .

The other subspace must be examined more carefully. For  $q \neq 0$  and  $q \neq \pi$  the maximum possible eigenvalue is  $\lambda_q^+$ . The corresponding eigenstates are all states with  $(-1)^n = -1$ . To make the overall state have  $(-1)^n = -1$ , we occupy the  $q = 0$  state and leave the  $q = \pi$  state empty and obtain a contribution of  $(2 \sinh 2K)^{M/2} \exp \{ 2K \}$  to the eigenvalue  $\Lambda_o$ . Therefore the largest eigenvalue in the odd subspace is

$$\Lambda_o = (2 \sinh 2K)^{M/2} \exp \left\{ 2K + \frac{1}{2} \sum_{q \neq 0, \pi} \epsilon(q) \right\}. \quad (6.38)$$

Since the wave vectors in the two subspaces are not identical, a direct comparison between the two largest eigenvalues is somewhat complicated. However, we note that

$$\begin{aligned} \frac{1}{2} \lim_{q \rightarrow 0} \epsilon(q) + \frac{1}{2} \lim_{q \rightarrow \pi} \epsilon(q) &= |K - K^*| + (K + K^*) \\ &= 2K \quad \text{for } K > K^* \\ &= 2K^* \quad \text{for } K^* > K. \end{aligned}$$

Thus if  $K > K^*$ , it is quite plausible, and can be shown rigorously in the thermodynamic limit  $M \rightarrow \infty$ , that  $\Lambda_o$  and  $\Lambda_e$  are degenerate. A little reflection will convince the reader that unless such a degeneracy exists, the order

parameter  $m_0(T)$  will be strictly zero. Therefore, the critical temperature of the two-dimensional Ising model is given by the equation  $K = K^*$ , or using the identity [from (6.6)]

$$\sinh 2K \sinh 2K^* = 1 \quad (6.39)$$

by the more usual expression

$$\sinh \frac{2J}{k_B T_c} = 1 \quad (6.40)$$

or  $k_B T_c / J = 2.269185 \dots$

The degeneracy of the two largest eigenvalues of the transfer matrix contributes only an additive term of  $\ln 2$  to the dimensionless free energy and is thus negligible. Therefore, at any temperature the free energy is given by

$$\begin{aligned} \frac{\beta G(0, T)}{M^2} &= \beta g(0, T) = -\frac{1}{2} \ln(2 \sinh 2K) - \frac{1}{2M} \sum_q \epsilon(q) \\ &= -\frac{1}{2} \ln(2 \sinh 2K) - \frac{1}{4\pi} \int_{-\pi}^{\pi} dq \epsilon(q) \end{aligned} \quad (6.41)$$

where we have converted the sum over wave vectors to an integral.

### 6.1.4 Thermodynamic functions

With a bit more algebra, we can simplify the expression (6.41) for the zero-field free energy. Using (6.39) and  $\cosh 2K^* = \coth 2K$ , which follows from (6.6), we have

$$\cosh \{\epsilon(q)\} = \cosh 2K \coth 2K + \cos q. \quad (6.42)$$

Consider, now, the function

$$f(x) = \frac{1}{2\pi} \int_0^{2\pi} d\phi \ln(2 \cosh x + 2 \cos \phi). \quad (6.43)$$

Differentiating with respect to  $x$  and evaluating the resulting integral by contour integration, we find

$$\frac{df(x)}{dx} = \text{sign}(x) \quad \text{or} \quad f(x) = |x|. \quad (6.44)$$

Taking  $x = \epsilon(q)$  we obtain the integral representation:

$$\epsilon(q) = \frac{1}{\pi} \int_0^{\pi} d\phi \ln(2 \cosh 2K \coth 2K + 2 \cos q + 2 \cos \phi). \quad (6.45)$$

We define

$$I = \frac{1}{2\pi} \int_0^{\pi} dq \epsilon(q) = \frac{1}{2\pi^2} \int_0^{\pi} dq \int_0^{\pi} d\phi \ln[2 \cosh 2K \coth 2K + 2 \cos q + 2 \cos \phi]. \quad (6.46)$$

Using the trigonometric identity

$$\cos q + \cos \phi = 2 \cos \frac{q+\phi}{2} \cos \frac{q-\phi}{2}$$

and changing variables of integration to

$$\omega_1 = \frac{q-\phi}{2} \quad \omega_2 = \frac{q+\phi}{2}$$

we have

$$I = \frac{1}{\pi^2} \int_0^{\pi} d\omega_2 \int_0^{\pi/2} d\omega_1 \ln[2 \cosh 2K \coth 2K + 4 \cos \omega_1 \cos \omega_2]. \quad (6.47)$$

The integration over  $\omega_2$  is almost in the form (6.43) and we can put it into this form by writing

$$\begin{aligned} I &= \frac{1}{\pi^2} \int_0^{\pi} d\omega_2 \int_0^{\pi/2} d\omega_1 \ln(2 \cos \omega_1) \\ &\quad + \frac{1}{\pi^2} \int_0^{\pi/2} d\omega_1 \int_0^{\pi} d\omega_2 \ln \left( \frac{\cosh 2K \coth 2K}{\cos \omega_1} + 2 \cos \omega_2 \right) \\ &= \frac{1}{\pi} \int_0^{\pi/2} d\omega_1 \ln(2 \cos \omega_1) \\ &\quad + \frac{1}{\pi} \int_0^{\pi/2} d\omega_1 \cosh^{-1} \frac{\cosh 2K \coth 2K}{2 \cos \omega_1}. \end{aligned} \quad (6.48)$$

But  $\cosh^{-1} x = \ln[x + \sqrt{x^2 - 1}]$  and hence

$$I = \frac{1}{2} \ln(2 \cosh 2K \coth 2K) + \frac{1}{\pi} \int_0^{\pi} d\theta \ln \frac{1 + \sqrt{1 - q^2(K) \sin^2 \theta}}{2} \quad (6.49)$$

where

$$q(K) = \frac{2 \sinh 2K}{\cosh^2 2K}. \quad (6.50)$$

Substituting in (6.41), we finally arrive at the form

$$\beta g(0, T) = -\ln(2 \cosh 2K) - \frac{1}{\pi} \int_0^{\pi/2} d\theta \ln \frac{1 + \sqrt{1 - q^2 \sin^2 \theta}}{2} \quad (6.51)$$

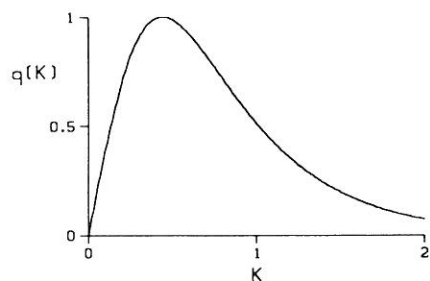


Figure 6.2: The function  $q(K)$  defined in (6.50).

for the free energy per spin.

The function  $q(K)$ , defined in (6.50), has the form shown in Figure 6.2. It takes on a maximum value,  $q = 1$ , at  $\sinh 2K = 1$ , and it is clear that the integral on the right-hand side of equation (6.51) can only be nonanalytic at that point since the term inside the square root cannot vanish for  $q < 1$ . The internal energy per spin of the system is given by

$$u(T) = \frac{d}{d\beta} [\beta g(T)] = -J \coth 2K \left[ 1 + \frac{2}{\pi} (2 \tanh^2 2K - 1) K_1(q) \right] \quad (6.52)$$

where

$$K_1(q) = \int_0^{\pi/2} \frac{d\phi}{\sqrt{1 - q^2 \sin^2 \phi}}$$

is the complete elliptic integral of the first kind. As  $q \rightarrow 1$ , the term  $(2 \tanh^2 2K - 1) \rightarrow 0$ , and the internal energy is continuous at the transition. The specific heat per spin  $c(T)$  can be obtained by differentiating once more with respect to temperature. Some analysis (Problem 6.2) shows that

$$\frac{1}{k_B} c(T) = \frac{4}{\pi} (K \coth 2K)^2 \left\{ K_1(q) - E_1(q) - (1 - \tanh^2 2K) \left[ \frac{\pi}{2} + (2 \tanh^2 2K - 1) K_1(q) \right] \right\} \quad (6.53)$$

where

$$E_1(q) = \int_0^{\pi/2} d\phi \sqrt{1 - q^2 \sin^2 \phi}$$

is the complete elliptic integral of the second kind. Near  $T_c$  the specific heat (6.53) is given, approximately, by

$$\frac{1}{k_B} c(T) \approx -\frac{2}{\pi} \left( \frac{2J}{k_B T_c} \right)^2 \ln \left| 1 - \frac{T}{T_c} \right| + \text{const.} \quad (6.54)$$

The internal energy and specific heat are shown in Figure 6.3.

The difference between the exact specific heat and that obtained in Chapter 3 from mean field and Landau theories is striking. Instead of a discontinuity in  $c(T)$ , we find a logarithmic divergence. In modern theories of critical phenomena, the form assumed for the specific heat is

$$c(T) \sim \left| 1 - \frac{T}{T_c} \right|^{-\alpha} \quad (6.55)$$

Onsager's result is a special case of this power law behavior. The limiting form of the function

$$\lim_{\alpha \rightarrow 0} \frac{1}{\alpha} (X^{-\alpha} - 1) = -\ln X.$$

The formula (6.54) is thus seen to be a special case of the power law singularity with  $\alpha = 0$ .

The calculation of the spontaneous magnetization is a nontrivial extension of the present derivation and may be found in Schultz *et al.* [270]. The result is

$$m_0(T) = -\lim_{h \rightarrow 0} \frac{\partial}{\partial h} g(h, T) = \begin{cases} \left[ 1 - \frac{(1 - \tanh^2 K)^4}{16 \tanh^4 K} \right]^{1/8} & T < T_c \\ 0 & T > T_c \end{cases} \quad (6.56)$$

$$= 0 \quad T > T_c. \quad (6.57)$$

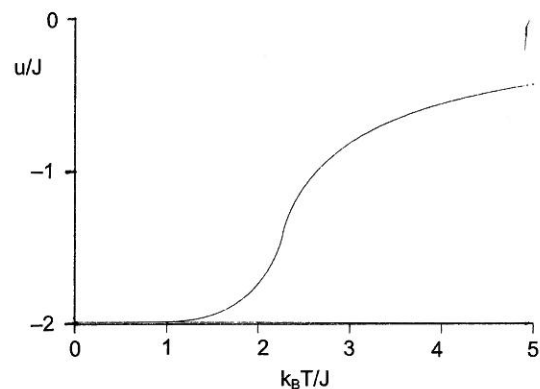
As  $T \rightarrow T_c$  from below, the limiting form of the spontaneous magnetization is given by

$$m_0(T) \approx (T_c - T)^{1/8} \equiv (T_c - T)^\beta.$$

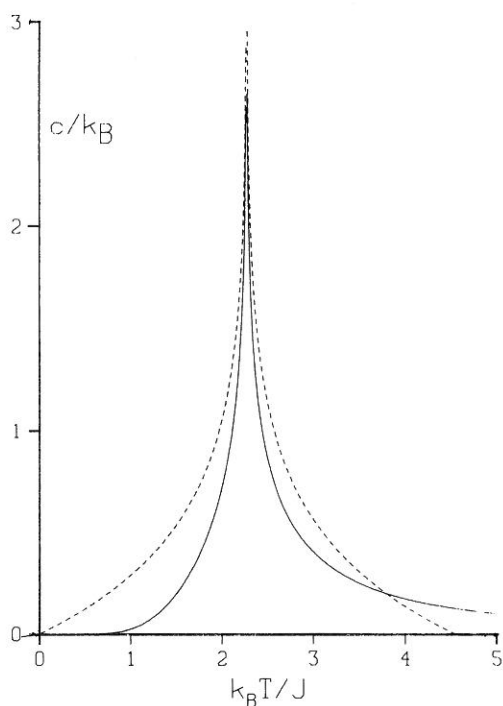
As in mean field theories, the order parameter has a power law singularity at the critical point but the exponent  $\beta = \frac{1}{8}$ , not  $\frac{1}{2}$  as obtained from mean field and Landau theories. The derivation of (6.56) was first published by Yang [331], but Onsager had previously announced the result at a conference. The asymptotic form as  $T \rightarrow T_c$  of the zero-field susceptibility is also known [198]:

$$\chi(0, T) = \lim_{h \rightarrow 0} \frac{\partial m(h, T)}{\partial h} \sim |T - T_c|^{-7/4} = |T - T_c|^{-\gamma}. \quad (6.58)$$

The exponent  $\gamma = \frac{7}{4}$  in (6.58) again is to be compared with the classical value  $\gamma = 1$ . It is clear from the exact results described above that the form of the free energy near a critical point is quite different from that postulated in the Landau theory.



(a)



(b)

Figure 6.3: The internal energy (a) and specific heat (b) of the two-dimensional Ising model on the square lattice. The dotted curve corresponds to the approximation (6.54).

### 6.1.5 Concluding remarks

The reader who has worked through the details of the preceding subsections will appreciate the difficulty of calculating even the zero-field free energy exactly. One can easily write down the transfer matrix of the two-dimensional Ising model in a finite magnetic field and arrive at a generalization of (6.15). However, the subsequent transformation to fermion operators yields a transfer matrix which is not bilinear in fermion operators and which cannot be diagonalized, at least by presently known techniques.

Similarly, one can construct the transfer matrix of the three-dimensional Ising model. In this case the matrix  $\mathbf{V}$  is of dimension  $2^L \times 2^L$ , where  $L = M^2$  if the lattice is an  $M \times M \times M$  simple cubic lattice. The reader can verify that the difficulty here is not this increase in the dimensionality of the transfer matrix but rather that the Jordan–Wigner transformation (6.17) does not produce a bilinear form in fermion operators.

Since Onsager's solution appeared, a small number of other two-dimensional problems have been solved exactly. The reader is referred to the book by Baxter [30] for an account of this work. The exact solution for the Ising model on a fractal is presented in Section 7.3. Since exact results near the critical point were so elusive, workers in the field devised various approximate techniques to probe the critical behavior of strongly interacting systems. We first discuss the method of series expansions which initially provided the greatest amount of information on critical behavior.

## 6.2 Series Expansions

The method of series expansions was first introduced by Opechowski [225] and has proved to be, with the help of modern computers, a powerful tool for the study of critical phenomena. To motivate the approach, let us consider first a simple function  $f(z)$  and its power series expansion about  $z = 0$ :

$$f(z) = \left(1 - \frac{z}{z_c}\right)^{-\gamma} = \sum_{n=0}^{\infty} \binom{\gamma}{n} \left(\frac{z}{z_c}\right)^n \quad (6.59)$$

where

$$\binom{\gamma}{n} = \frac{\gamma(\gamma+1)(\gamma+2)\cdots(\gamma+n-1)}{n!}.$$

The power series (6.59) converges for  $|z| < |z_c|$ . Now suppose that we have available a certain number of terms in the power series of an unknown function.