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ISING MODEL IN THE MAGNETIC FIELD *iπkT*/2

K.Y. LIN and F.Y. WU†

Physics Department, National Tsing Hua University, Hsinchu, Taiwan 30043, China

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It is shown that the free energy and the magnetization of an Ising model in the magnetic field $H = i\pi kT/2$ can be obtained directly from corresponding expressions of these quantities in zero field, provided that the latter are known for sufficiently anisotropic interactions. Using this approach we derive explicit expressions of the free energy and the magnetization at $H = i\pi kT/2$ for a number of two-dimensional lattices.

It is now a widely-known knowledge that the free energy and the magnetization of two-dimensional Ising models can be exactly evaluated when there is no magnetic field. A lesser known fact, first noted by Lee and Yang,[1] is that both of these quantities can also be evaluated at the special value of the magnetic field $H = i\pi kT/2$. Discussions in the past, however, have focussed on considerations of the different and alternate ways which the square lattice results can be rederived,[2-6] and on some extensions to specific checkerboard lattices.[7-9] There have been very little generality discussions on possible extensions to other lattices.[2]

In this paper we present a general, yet simple, formulation of the Ising model in the magnetic field $H = i\pi kT/2$, which is valid for any lattice in any dimension. This formulation, which generalizes an earlier treatment by Merlini[5] for a square lattice, permits a direct evaluation of the free-energy and magnetization at $H = i\pi kT/2$ from the corresponding zero-field expressions, provided that the latter are known for sufficiently anisotropic interactions. Using this approach and related considerations, we derive explicit expressions of the free energy and magnetization at $H = i\pi kT/2$ for several two-dimensional lattices.

Consider an Ising model on a lattice of N sites with pair interactions and in an external magnetic field H. For definiteness we assume periodic boundary conditions and N to be integral multiples of 2. The partition function is given by the expression

$$Z_N(L) = \sum_{\sigma_i} \exp\left(\sum_{\langle ij \rangle} K_{ij}\sigma_i\sigma_j + L \sum_i \sigma_i \right), \tag{1}$$

†Permanent address: Department of Physics, Northeastern University, Boston, MA 02115, USA.

where $\sigma_i = \pm 1$ denotes the spin located at the ith site, $L = H/kT$, and $J_{ij} = kTK_{ij}$ is the interaction between spins σ_i and σ_j. In the most general case, J_{ij} are arbitrary and can all be distinct. The quantities of interest are the per-site "free energy"

$$f(L) = \lim_{N\to\infty} \frac{1}{N} \ln Z_N(L)\,, \tag{2}$$

and the per-site magnetization

$$I(L) = \lim_{N\to\infty} M_N(L)\,, \tag{3}$$

with

$$M_N(L) = \left[\sum_{\sigma_i} \sigma_1 \exp\left(\sum_{\langle ij\rangle} K_{ij}\sigma_i\sigma_j + L\sum_i \sigma_i\right)\right] / Z_N(L)\,, \tag{4}$$

where σ_1 is a spin located in the interior of the lattice. We shall assume that $Z_N(0)$, $M_N(0)$, $f(0)$ and $I(0)$ are known for interactions sufficiently anisotropic in a manner we shall describe, and show that $Z_N\left(i\frac{\pi}{2}\right)$, $M_N\left(i\frac{\pi}{2}\right)$, $f\left(i\frac{\pi}{2}\right)$, and $I\left(i\frac{\pi}{2}\right)$ can be derived from these known expressions by effecting a simple transformation.

Consider first the evaluation of $Z_N\left(i\frac{\pi}{2}\right)$, assuming that $Z_N(0)$, defined by (1) with $L = 0$, is known. Using the identity

$$\exp(i\pi\,\sigma/2) = i\sigma\,, \qquad \sigma = \pm 1\,, \tag{5}$$

we obtain from (1)

$$Z_N\left(i\frac{\pi}{2}\right) = i^N \sum_{\sigma_i=\pm 1} \left(\prod_{i=1}^{N} \sigma_i\right) \prod_{\langle ij\rangle} \exp(K_{ij}\sigma_i\sigma_j)\,. \tag{6}$$

The factor i^N in (6) contributes to $f\left(i\frac{\pi}{2}\right)$ an additive term $i\frac{\pi}{2}$ which we shall keep explicitly in our expressions of $f\left(i\frac{\pi}{2}\right)$.

Following Merlini[5], we split the product $\prod_{i=1}^{N} \sigma_i$ in (6) into a product of $N/2$ factors $\sigma_i\sigma_j$ associated with a set of $N/2$ interactions $\{K'_{ij}\}$ covering all N lattice sites. This splitting permits us to combine the two products in (6) into one. Furthermore, upon associating a factor i to each of the $N/2$ factors $\sigma_i\sigma_j$, we rewrite (6) as

$$Z_N\left(i\frac{\pi}{2}\right) = i^{N/2} \sum_{\sigma_i} \prod_{\langle ij \rangle} B_{ij}(\sigma_i\sigma_j), \tag{7}$$

where

$$\begin{aligned} B_{ij}(\sigma_i\sigma_j) &= i\sigma_i\sigma_j \exp(K'_{ij}\sigma_i\sigma_j), \quad K_{ij} = K'_{ij}, \\ &= \exp(K_{ij}\sigma_i\sigma_j), \quad \text{otherwise.} \end{aligned} \tag{8}$$

Using (5) once more to write

$$i\sigma_i\sigma_j \exp(K'_{ij}\sigma_i\sigma_j) = \exp\left[\left(K'_{ij} + i\frac{\pi}{2}\right)\sigma_i\sigma_j\right], \tag{9}$$

we see that, aside from the extra factor $i^{N/2}$, $Z_N\left(i\frac{\pi}{2}\right)$ is precisely $Z_N(0)$, provided that we make the following replacement for *each* of the $N/2$ interactions in the set $\{K'_{ij}\}$:

$$K'_{ij} \rightarrow K'_{ij} + i\frac{\pi}{2}. \tag{10}$$

Thus we obtain the identity,

$$Z_N\left(i\frac{\pi}{2}\right) = i^{N/2} Z^*(0), \tag{11}$$

where the asterisk in (11) indicates the replacement (10). Taking the thermodynamic limit of (11), we obtain

$$f\left(i\frac{\pi}{2}\right) = i\frac{\pi}{4} + f^*(0). \tag{12}$$

In a similar fashion we obtain for the magnetization

$$M_N\left(i\frac{\pi}{2}\right) = M_N^*(0)\,, \tag{13}$$

and

$$I\left(i\frac{\pi}{2}\right) = I^*(0)\,. \tag{14}$$

Relations (11)–(14) are exact expressions valid for any lattice in any dimension with periodic boundary conditions. It should be noted here that Merlini[5] has previously obtained similar relations for the square lattice by assuming an open boundary condition and the introduction of a boundary field; he also introduced the dual for the square lattice, which is not needed in our consideration.

It is clear that the usefulness of (11)–(14) for computing quantities of interest at $H = i\pi kT/2$ rests on the prior knowledge of the corresponding zero-field expressions for a lattice whose $\{K'_{ij}\}$ are distinct from all other interactions. This is an important and crucial aspect of this approach. It is also clear that the choice of the set $\{K'_{ij}\}$ is not unique and, in the simplest case, all $N/2$ interactions K'_{ij} can be made equal by setting $K'_{ij} = K'$.

It is convenient to regard each K'_{ij} as being covered by a dimer placed along the lattice edge connecting sites i and j. Consequently, each choice of the set $\{K'\}$ corresponds to a close-pact dimer covering of the lattice. While any dimer covering will suffice our purposes, it is most natural to choose one which is commensurate with the underlying lattice structure and for which the zero-field quantities can be computed. This implies that the Ising interactions must be appropriately anisotropic for the purpose of distinguishing the interactions K'. The example of a suitable dimer covering for the square lattice is shown in Fig. 1.

It is quite simple to effect the transformation (10) in practice by using the equivalent replacements:

$$\begin{aligned} &\sinh K' \to i\cosh K', \qquad \cosh K' \to i\sinh K'\,. \\ &\exp(2K') \to -\exp(2K')\,, \\ &\sinh K' \to i\cosh K', \qquad \cosh K' \to i\sinh K'\,. \end{aligned} \tag{15}$$

In the following, we present results of the computation of $f\left(i\frac{\pi}{2}\right)$ and $I\left(i\frac{\pi}{2}\right)$ for

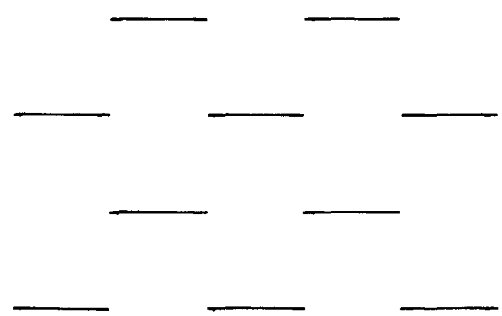

Fig. 1. A dimer covering of the square lattice. Each interaction covered by a dimer is K' and is distinct from all other interactions.

some two-dimensional lattices. These results can be summarized by the expressions

$$f\left(i\frac{\pi}{2}\right) = i\frac{\pi}{2} + \frac{1}{16\pi^2}\iint_0^{2\pi} d\theta\, d\phi \ln F(\theta, \phi)\,, \tag{16}$$

and

$$I\left(i\frac{\pi}{2}\right) = (1 - N/D)^{1/8}\,, \tag{17}$$

where the factors $F(\theta, \phi)(\geqslant 0)$, N and D differ from lattice to lattice. In order to explicitly display the additive term $i\frac{\pi}{2}$ occurring in $f\left(i\frac{\pi}{2}\right)$ as mentioned in discussions after (6), we have used the following identity in rewriting (12):

$$i\frac{\pi}{4} = i\frac{\pi}{2} - \frac{1}{16\pi^2}\iint_0^{2\pi} d\theta\, d\phi \ln(-1)\,, \tag{18}$$

and combined the second term in (18) with $f^*(0)$.

1. Checkerboard Lattice

The checkerboard lattice is a square lattice with four distinct coupling constants K_1, K_2, K_3, K_4 arranged as shown in Fig. 2. The free energy $f(0)$ of this lattice has been computed by Utiyama[10] and the magnetization $I(0)$ by Baxter[11] confirming an earlier conjecture by Syozi and Naya.[12] Using the dimer covering shown in Fig. 1, which corresponds to using the replacement $K_1 \rightarrow K_1 + i\frac{\pi}{2}$ in

$f(0)$ and $I(0)$, we obtain $f\left(i\frac{\pi}{2}\right)$ and $I\left(i\frac{\pi}{2}\right)$ as given by (16) and (17) respectively, with

$$F(\theta, \phi) = 8[\Pi C_i + \Pi S_i - 1 + S_2 S_4 \cos(\theta + \phi) - S_1 S_3 \cos(\theta - \phi) - (S_1 S_2 - S_3 S_4) \cos\theta - (S_1 S_4 - S_2 S_3) \cos\phi], \quad (19)$$

where $C_i = \cosh 2K_i$, $S_i = \sinh 2K_i$, and

$$N = 2(1 - \Pi C_i - \Pi S_i) + \Sigma S_i^2,$$

$$D = (2 + \Sigma S_i^{-2}) \Pi S_i^2 + 2(\Pi C_i - 1) \Pi S_i. \quad (20)$$

2. Honeycomb Lattice

The honeycomb lattice with anisotropic interactions K_1, K_2 and K_3 is derived from the checkerboard lattice with $K_4 = 0$. This leads to, after setting $K_4 = 0$ in (19) and (20), the following expressions:

$$F(\theta, \phi) = 8[C_1 C_2 C_3 - 1 - S_1 S_3 \cos(\theta - \phi) - S_1 S_2 \cos\theta + S_2 S_3 \cos\phi],$$

$$N = 2(1 - C_1 C_2 C_3) + S_1^2 + S_2^2 + S_3^2 \quad (21)$$

$$D = S_1^2 S_2^2 S_3^2.$$

The same results can also be derived by setting directly $K_3 \to K_3 + i\frac{\pi}{2}$ in expres-

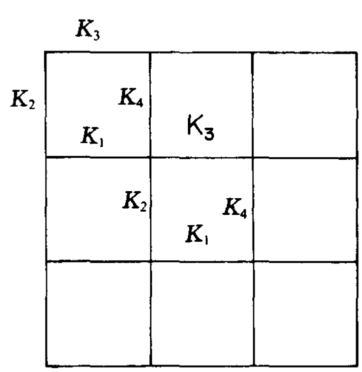

Fig. 2. The checkerboard lattice.

sions of $f(0)$ and $I(0)$ for the honeycomb lattice given in Ref. 13. G. Baxter[2] has also computed $f(0)$ using a graphical approach.

3. Triangular Lattice

The triangular lattice with anisotropic interactions K_1, K_2 and K_3 can be covered by dimers placed along, say, every other K_1. This situation can be visualized by arranging the lattice in a rectangular pattern in which interactions K_1 are in the horizontal direction, interactions K_2 in the vertical direction, and interactions K_3 in, say, the NW-SE diagonal direction. Then the dimer covering in Fig. 1 covers every other horizontal interaction which we denote by K_1'. To compute $f(0)$ as a function of K_1, K_2, K_3, K_1', we regard the Ising model as an eight-vertex model with staggered weights.[14] The desired expression for $f\left(i\frac{\pi}{2}\right)$ is then obtained by setting $K_1' \to K_1' + i\frac{\pi}{2}$ in $f(0)$. Using Eq. (19) of Ref. 14 for $f(0)$ and omitting detailed steps we obtain $f\left(i\frac{\pi}{2}\right)$ as given by (16) with

$$\begin{aligned} F(\theta, \phi) &= 2[G - D\cos(\theta - \phi) - E\cos(\theta + \phi) + \Delta\cos 2\phi], \\ G &= 2[-1 + e^{4(K_1+K_2+K_3)} + e^{4(K_1-K_2-K_3)} + e^{4(-K_1+K_2-K_3)} + e^{4(-K_1-K_2+K_3)}], \\ D &= -4\sinh^2 2K_1, \\ E &= -4\sinh^2 2K_2, \\ \Delta &= 4\sinh^2 2K_3. \end{aligned} \tag{22}$$

Here, for comparison purposes, D, E, and Δ are the same as those defined in Ref. 14 and $G = \Delta - A$ with A defined in Ref. 14. Unfortunately, the expression $I(0)$ needed for evaluating $I\left(i\frac{\pi}{2}\right)$ has not yet being computed. Note that the resulting expression for $f\left(i\frac{\pi}{2}\right)$ is symmetric in K_1, K_2, K_3, and reduces to that of a square lattice by setting, e.g., $K_3 = 0$. The expression (22) agrees with that obtained by G. Baxter and Dyson who derived it by evaluating a 36×36 determinant.[2]

4. Union Jack Lattice

Consider the Union Jack lattice shown in Fig. 3. The dimer covering of Fig. 1 with dimers placed along interactions K_1 again suffices our purposes. Using (12) and the expression for $f(0)$ obtained recently by us,[15] we obtained $f\left(i\frac{\pi}{2}\right)$ in the

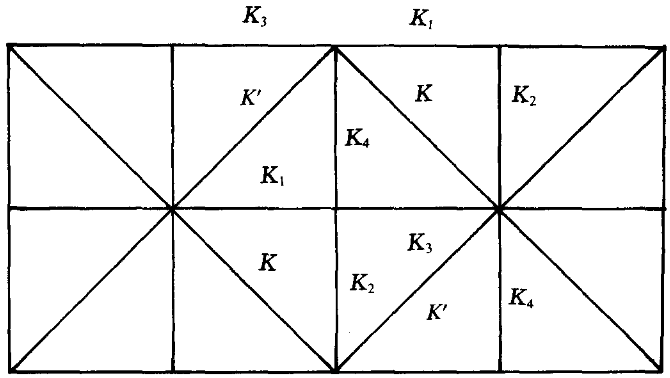

Fig. 3. The Untion Jack lattice.

form of (16) with

$$
\begin{aligned}
F(\theta, \phi) &= 2[a + b\cos\theta + c\cos\phi + d\cos(\theta - \phi) \\
&\quad + e\cos(\theta + \phi)], \qquad (23) \\
2a &= \omega_1^2 + \omega_2^2 + \omega_3^2 + \omega_4^2 \\
b &= \omega_1\omega_3 - \omega_2\omega_4\,, \qquad c = \omega_1\omega_4 - \omega_2\omega_3\,, \\
d &= \omega_3\omega_4 - \omega_7\omega_8\,, \qquad e = \omega_3\omega_4 - \omega_5\omega_6\,, \\
\omega_1 &= 2e^{K+K'}\sinh(K_1 + K_2 + K_3 + K_4)\,, \\
\omega_2 &= 2e^{-K-K'}\sinh(K_1 - K_2 + K_3 - K_4)\,, \\
\omega_3 &= 2e^{-K+K'}\sinh(K_1 - K_2 - K_3 + K_4)\,, \\
\omega_4 &= 2e^{K-K'}\sinh(K_1 + K_2 - K_3 - K_4)\,, \\
\omega_5 &= 2\sinh(K_1 - K_2 + K_3 + K_4)\,, \\
\omega_6 &= 2\sinh(K_1 + K_2 + K_3 - K_4)\,, \\
\omega_7 &= 2\sinh(K_1 + K_2 - K_3 + K_4)\,, \\
\omega_8 &= 2\sinh(-K_1 + K_2 + K_3 + K_4)\,.
\end{aligned}
$$

It can be verified that (23) reduces to (19) for the checkerboard lattice upon taking $K = K' = 0$.

The zero-field magnetization $I(0)$ for this general Union Jack lattice is not yet known and, consequently, $I\left(i\frac{\pi}{2}\right)$ has not been computed.

5. Other Two-dimensional Lattices

Both $f\left(i\frac{\pi}{2}\right)$ and $I\left(i\frac{\pi}{2}\right)$ can also be evaluated for a number of other two-dimensional lattices. Since these derivations are straightforward and the results lengthy, we include here only the relevant references from which interested readers can derive the results. For the 4–8 (bathroom tile) lattice shown in Fig. 4 the free energy $f(0)$ has been computed by Utiyama[10] and the magnetization $I(0)$ by Baxter and Choy.[16] By choosing a dimer covering with dimers placed along, say, K_1' and K_2', we can use (12) and (14) to compute $f\left(i\frac{\pi}{2}\right)$ and $I\left(\frac{\pi}{2}\right)$. For the

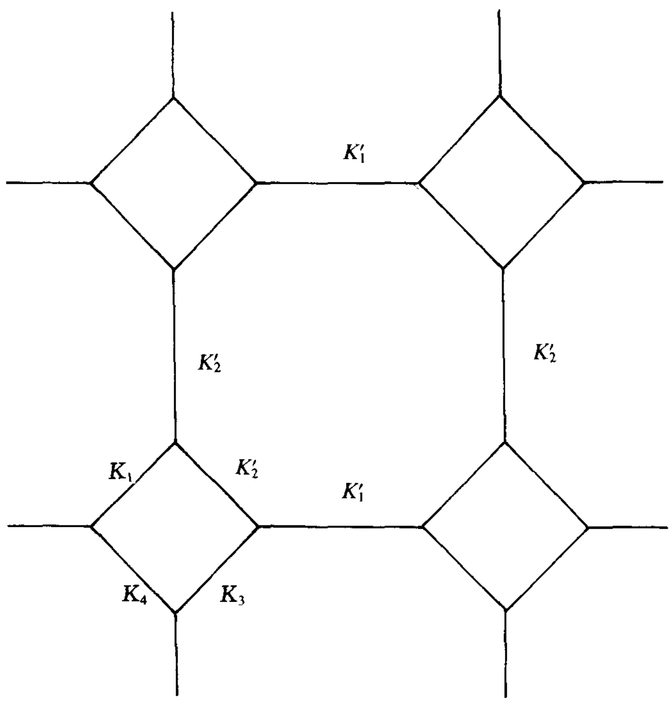

Fig. 4. The 4–8 (bathroom tile) lattice.

general 3–12 lattice shown in Fig. 5 both $f(0)$ and $I(0)$ have been obtained by Lin and Chen.[17] Using a dimer covering with dimers placed along interactions K_1'', K_2'', K_3'', we can compute $f\left(i\frac{\pi}{2}\right)$ and $I\left(i\frac{\pi}{2}\right)$ from (12) and (14). Finally, for the layered square lattice shown in Fig. 6, Lin and Ma[18] have obtained $f(0)$ and pro-

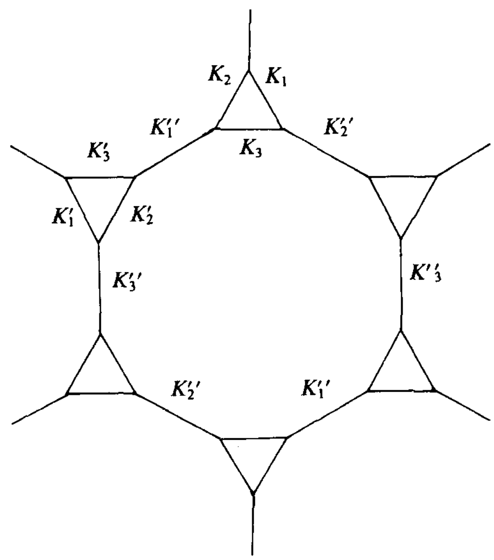

Fig. 5. The 3–12 lattice.

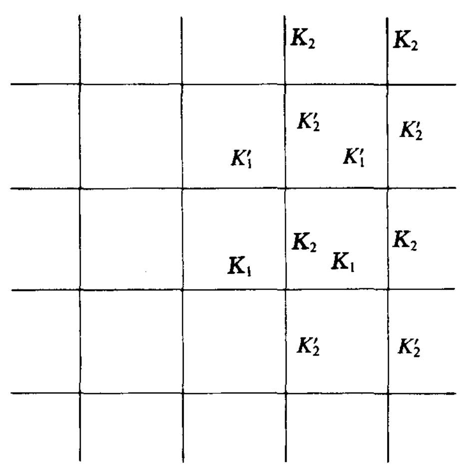

Fig. 6. The layered square lattice.

posed a conjectured formula for $I(0)$. We can then compute $f\left(i\frac{\pi}{2}\right)$ and $I\left(i\frac{\pi}{2}\right)$ by making in these expressions the replacement of, say, $K_2' \to K_2' + i\frac{\pi}{2}$. It should be pointed out that in these applications the form of $I(0)$, and hence $I\left(i\frac{\pi}{2}\right)$, is modified with the appearance of a factor G in the RHS of (17).

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References

1. T. D. Lee and C. N. Yang, *Phys. Rev.* **87** (1952) 410.
2. G. Baxter, *J. Math. Phys.* **6** (1965) 1015.
3. B. M. McCoy and T. T. Wu, *Phys. Rev.* **155** (1967) 438.
4. T. W. Marshall, *Mol. Phys.* **21** (1971) 847.
5. D. Merlini, *Lett. Nuovo Cimento* **9** (1974) 100.
6. A. Gaaff, *Phys. Lett.* **A49** (1974) 103.
7. F. Y. Wu, *J. Stat. Phys.* **44** (1986) 455.
8. K. Y. Lin, *J. Phys.* **A21** (1988) 1055.
9. K. Y. Lin and F. Y. Wu, *J. Stat. Phys.* (1988), to be published.
10. T. Utiyama, *Prog. Theor. Phys.* **6** (1951) 907.
11. R. J. Baxter, *Proc. Roy. Soc. Lond* **A404** (1986) 1.
12. I. Syozi and S. Naya, *Prog. Theor. Phys.* **23** (1960) 374; **24** (1960) 829.
13. S. Naya, *Prog. Theor. Phys.* **6** (1951) 907.
14. C. S. Hsue, K. Y. Lin and F. Y. Wu, *Phys. Rev.* **B12** (1975) 429.
15. F. Y. Wu and K. Y. Lin, *J. Phys.* **A20** (1987) 5737.
16. R. J. Baxter and T. C. Choy, *J. Phys.* **A** (1988), to be published.
17. K. Y. Lin and J. L. Chen, *J. Phys.* **A20** (1987) 5695.
18. K. Y. Lin and S. K. Ma, *J. Stat. Phys.* **51** (1988) 491.