Journal of Statistical Physics, Vol. 98, Nos. 5/6, 2000

Distribution of Energies for the Two-Dimensional Ising Model

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Received August 26, 1999

We calculate the number of polygons with fixed total length drawn on a square lattice with periodic boundary conditions. In addition, we study the statistics of polygons with the number of horizontal and vertical links fixed separately. The analysis is performed via a mapping to the Ising model with isotropic and anisotropic interactions. We deal with the case of finite lattice sizes as well as the thermodynamic limit.

KEY WORDS: Polygon statistics; Ising model; exact solution.

1. INTRODUCTION

The exact solution of the 2d Ising model has been found more than half a century ago, and recently some new interesting aspects of this solution have been raised. In particular, the calculation of the *distribution of energies* for finite lattices attracted considerable attention.(1) This function is very important. Among many possible applications, it can serve as a reference point in testing the correctness of Monte Carlo methods.

In ref. 1 it has been shown how to calculate the distribution of energies for the isotropic model (i.e., the model with same coupling constants for the two perpendicular directions) using the exact solution given by Kaufman(3) for finite $M \times N$ lattices. This distribution is given by the set of coefficients for the partition function:

$$Z_{M,N} = e^{2MN\beta J} \sum_{k=0}^{MN} g_k x^{2k} \tag{1}$$

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where N is the number of columns, M the number of rows of the lattice, J is the coupling constant, k_B is Boltzmann's constant, $\beta = k_B J$, $x = e^{-2\beta J}$ is the low-temperature expansion variable, and the coefficient g_k is the number of configurations with energy $4kJ$ above (one of the two) ground states. (It turns out that g_k is also the number of closed polygons of total length $2k$ on the lattice).

The coefficients g_k have been calculated by Beale using the exact solution given by Kaufman. The result is exact, but is effectively calculable only for relatively small sizes of the lattice due to the computational complexity of the problem. This complexity grows exponentially with N. In ref. 1 the result for lattice size 32×32 has been given. Our own computations for the 40×40 lattice (by a method different from Beale's method, see below) took about 1 day on a standard workstation. In contrast to these systems, the lattice sizes of MC simulations can be of the order of a thousand, see for instance[5] where simulations of square lattices up to size 1000×1000 have been performed. For lattices of this size the possibility to obtain an exact distribution of energies seems to be hopeless. Still it is very desirable to have some reference point also for large lattices.

It turns out that it is relatively simple to calculate some asymptotic quantity, namely $(\log g_k)/MN$ which is finite for all M, N, and takes a finite thermodynamic limit.

The interpretation of this quantity is obvious: g_k is the *number of states* with energy $4kJ$ over the two (degenerate) ground states. So the quantity $(\log g_k)/MN$ is simply an *entropy per spin* in the microcanonical ensemble. In other words, it is the entropy expressed as a function of the internal energy. Besides the simplicity of this result, we like to mention that this relation was not pointed out in the literature. This is the reason why we explore this quantity a little further.

An expression for the quantity $(\log g_k)/MN$ can also be obtained from the product form of the partition function (see formulas (10)–(14) below for the anisotropic case), using for example the steepest descent path method for calculating the coefficients of the polynomial. In this way one obtains the same expression as for the entropy in the microcanonical ensemble. However, an immediate interpretation of $(\log g_k)/MN$ as the entropy in the microcanonical ensemble is conceptually simpler and more esthetic.

The outline of the paper is as follows. In Section 2, we derive the formula for the entropy in the isotropic case expressed as a function of the internal energy. Some properties of this function are also discussed. In Section 3 the anisotropic case is considered (i.e., coupling constants are different in vertical and horizontal directions). An expression for the number of states with given energies in the horizontal and vertical directions is

derived and illustrated for some lattice sizes. In Section 4 we calculate analogous quantities in the TD limit. In Section 5 we summarize our results and discuss prospects for future work.

2. ISOTROPIC CASE: THERMODYNAMIC LIMIT

All quantities necessary for expressing the entropy as a function of internal energy have been calculated in Onsager's seminal paper.[2] In the isotropic case (in the rest of this part we consider a square lattice $M = N$) we have for the internal energy

$$u = -J \frac{1+x^2}{2x} \left(1 + \frac{2}{\pi} k' K(k) \right) \tag{2}$$

where $x = \tanh \beta J$ is the "high-temperature" variable, $k = 2 \sinh 2\beta J / \cosh^2 2\beta J = 4x(1-x^2)/(1+x^2)^2$ and $k' = \pm\sqrt{1-k^2} = 2 \tanh^2 2\beta J - 1$ are elliptic moduli, and $K(k)$ is an elliptic integral of the second kind. The relation between internal energy u and (scaled) length of polygons $\kappa = k/N^2$ is obvious:

$$\kappa = \frac{1}{2J} u + 1 \tag{3}$$

The formula for entropy s does not appear in Onsager's paper, but it can be calculated in straightforward manner from $f = u - Ts$:

$$s = -\frac{1}{2} \log \left(\frac{1+x}{1-x} \right) \frac{1+x^2}{2x} \left(1 + \frac{2}{\pi} k' K(k) \right) + \log \frac{2(1+x^2)}{1-x^2} + \frac{1}{2\pi} F(k) \tag{4}$$

where

$$F(k) = \int_0^{\pi} \log[\tfrac{1}{2}(1 + \sqrt{1 - k^2 \sin^2 \phi})] \, d\phi$$

It is easy to check that both functions s and u are monotonic functions of the argument x for $x \in (0, 1)$, so that $s(u)$ is well defined by the expressions (2) and (4) above.

A plot of $s(\kappa)$ is presented in Fig. 1. We denote $s(\kappa) \equiv s(u(\kappa))$, where u and κ are related by (3). We do not present plots for finite N, because these are practically indistinguishable for $N = 40$ and $N = \infty$. For instance, for the largest coefficient g_{800}, the quotient $\ln g_{800}/1600$ is equal to 0.6904, whereas the corresponding value of entropy is $\ln 2 = 0.6932$. In general, the values for $N = 40$ and the limiting values deviate by less than 1%.

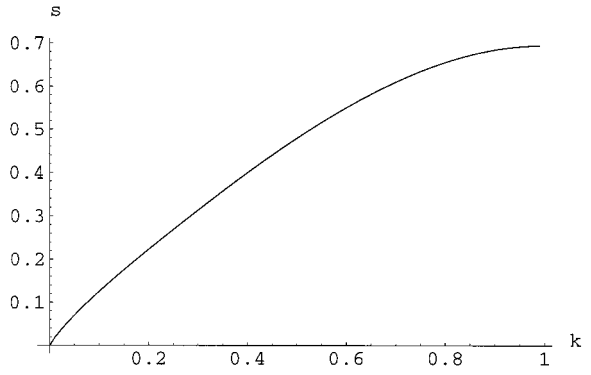

Fig. 1. Entropy s as a function of (scaled) polygon length κ for isotropic Ising model in thermodynamic limit.

An interesting property of the $s(\kappa)$ function is its convexity. The $s(\kappa)$ function is convex (i.e., its second derivative is negative) almost everywhere. An exception is the critical value of κ ($\kappa_{cr} = 1 - 1/\sqrt{2}$). The second derivative of $s(\kappa)$ is zero at this point, but the third derivative diverges (logarithmically). This corresponds to a phase transition at this value of κ.

3. ANISOTROPIC CASE: FINITE LATTICES

The main achievement of Beale's paper for the isotropic case can be extended to the more general situation of an *anisotropic* model having coupling constants different in the two directions (say, J in horizontal direction and J' in vertical direction). Using results of ref. 3 one can obtain expressions for the distribution of energies for the anisotropic model. In order to do so, let us start with the "polygonal" form of the partition function given by van der Waerden,[6] see also:[7]

$$Z_{M,N} = e^{MN\beta(J+J')} \sum_{k=0}^{MN} \sum_{l=0}^{MN} g_{kl} u^k v^l \tag{5}$$

where $u = \exp(-2\beta J)$, $v = \exp(-2\beta J')$. The coefficient g_{kl} is the number of configurations with energy $2kJ + 2lJ'$ above the two (degenerate) ground states. (It turns out that g_{kl} is also the number of closed polygons with k horizontal bonds and l vertical bonds on the lattice). It is clear that the coefficients g_{kl} determine the distribution of energies.

To obtain the coefficients g_{kl}, we must rewrite formula (39) of ref. 3 giving the partition function for finite M, N. It is possible to do it in

such a manner that the polynomial structure of the resulting expression will be transparent. It can be done by a method borrowed from ref. 4.

According to formula (39) in ref. 3 the partition function is

$$Z=\frac{1}{2}(2\sinh 2H)^{MN/2}\cdot\left\{\prod_{r=1}^{N}\left(2\cosh\frac{M\gamma_{2r}}{2}\right)+\prod_{r=1}^{N}\left(2\sinh\frac{M\gamma_{2r}}{2}\right)+\prod_{r=1}^{N}\left(2\cosh\frac{M\gamma_{2r-1}}{2}\right)+\prod_{r=1}^{N}\left(2\sinh\frac{M\gamma_{2r-1}}{2}\right)\right\} \tag{6}$$

where γ_j is determined by

$$\cosh\gamma_j=\cosh 2H^*\cosh 2H'-\sinh 2H^*\sinh 2H'\cos(\pi j/N) \tag{7}$$

where $H=\beta J$, $H'=\beta J'$ and H^* is determined from $e^{-2H}=\tanh H^*$.

Using an elementary identity:[4]

$$\cosh l\theta=2^{l-1}\prod_{s=0}^{l-1}\left(\cosh\theta-\cos\frac{(2s+1)\,\pi}{2l}\right) \tag{8}$$

and a twin identity

$$\sinh l\theta=2^{l-1}\sinh\theta\prod_{k=1}^{l-1}\left(\cosh\theta-\cos\frac{k\pi}{l}\right) \tag{9}$$

we obtain the following expression for the partition function:

$$Z_{M\times N}=(\cosh\beta J\cosh\beta J')^{MN}(I+II+III+IV) \tag{10}$$

where:

$$I=\prod_{r=1}^{N}\prod_{s=0}^{M/2-1}\left[(1+x^2)(1+y^2)-2y(1-x^2)\cos\frac{2\pi r}{N}-2x(1-y^2)\cos\frac{(2s+1)\,\pi}{M}\right] \tag{11}$$

$$III=\prod_{r=1}^{N}\prod_{s=0}^{M/2-1}\left[(1+x^2)(1+y^2)-2y(1-x^2)\cos\frac{(2r-1)\,\pi}{N}-2x(1-y^2)\cos\frac{(2s+1)\,\pi}{M}\right] \tag{12}$$

$$IV = \prod_{r=1}^{N/2} \left[\left(1 + x^2)(1 + y^2) - 2y(1 - x^2) \cos \frac{(2r-1)\,\pi}{N} \right)^2 - (2x(1 - y^2))^2 \right]$$
$$\times \prod_{r=1}^{N} \prod_{s=1}^{M/2-1} \left[(1 + x^2)(1 + y^2) - 2y(1 - x^2) \cos \frac{(2r-1)\,\pi}{N} \right.$$
$$\left. - 2x(1 - y^2) \cos \frac{2s\pi}{M} \right] \tag{13}$$

$$II = (1 + x + y - xy)(1 - x + y + xy)(1 + x - y + xy)(1 - x - y - xy)$$
$$\times \prod_{r=1}^{N/2-1} \left[\left((1 + x^2)(1 + y^2) - 2y(1 - x^2) \cos \frac{2r\pi}{N} \right)^2 - (2x(1 - y^2))^2 \right]$$
$$\times \prod_{r=1}^{N} \prod_{s=1}^{M/2-1} \left[(1 + x^2)(1 + y^2) \right.$$
$$\left. - 2y(1 - x^2) \cos \frac{2r\pi}{N} - 2x(1 - y^2) \cos \frac{2s\pi}{M} \right] \tag{14}$$

and $x = \tanh \beta J$, $y = \tanh \beta J'$.

In expression (10) above, the partition function is expressed as a polynomial in the "high-temperature" variables $x = \tanh \beta J$, $y = \tanh \beta J'$, whereas in (5) we need an expression in the "low-temperature" variables $u = \exp(-2\beta J)$, $v = \exp(-2\beta J')$. However, from duality and cyclic boundary conditions, it follows that the *coefficients g_{kl} in both expressions (5) and (10) must be identical.*

Let us denote the sum of expressions (11)–(14) by $P(x, y)$:

$$P(x, y) \equiv I + II + III + IV = \sum_{k=0}^{MN} \sum_{l=0}^{MN} g_{kl} x^k y^l \tag{15}$$

The interpretation of this expression is that the coefficient g_{kl} is the number of polygons with k *horizontal* and l *vertical* bonds.

The correctness of the expression for $P(x, y)$ has been checked in several ways. First of all, for the isotropic case (i.e., $x = y$), the known expression is reproduced. In other words, we have checked that an equality $\sum_{l=0}^{k} g_{k-l,\,l} = g_k$ holds. The second test consists of an examination of certain properties of the polynomial. It turns out that the only nonzero coefficients are the even-even ones, and all these coefficients are positive. Indeed, our polynomial satisfies these conditions. Specializing from this moment to $M = N$, the P_{kl} polynomial turns out to be symmetric with respect to the change of indices $k \to N^2 - k$, as it should be. The third test

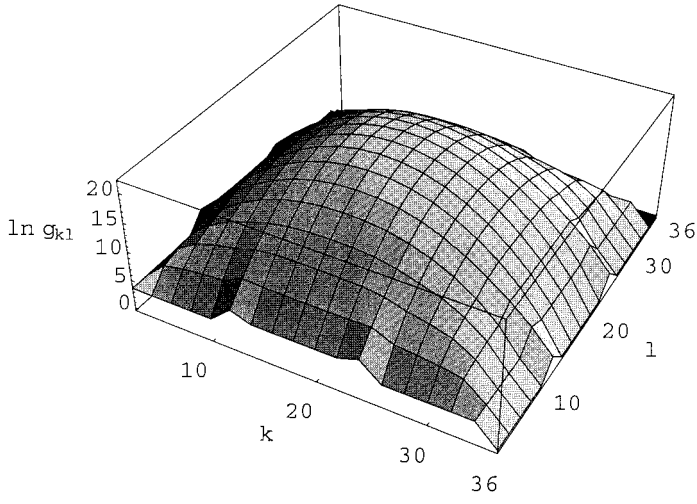

Fig. 2. Anisotropic lattice 6×6. Logarithm of number of states as a function of (scaled) polygon lengths: horizontal k and vertical l.

was a direct calculation of some coefficients g_{kl} for small k and l (for example, $g_{0,2N} = g_{2N,0} = N(N-1)/2$; $g_{2,2} = g_{2,4} = g_{4,2} = N^2$; $g_{4,4} = N^2(N^2+5)/2$) and a check that they are the same as appearing in the $P(x, y)$ polynomial, for all N considered, up to $N = 10$.

The plots of $\log g_{kl}$ as functions of k and l are presented on Figs. 2 and 3 for $N = 6$ and $N = 10$.

4. FORMULA FOR $\ln g_{kl}/MN$ IN THE TD LIMIT

Let us begin with an interpretation of the (scaled) lengths of polygons in horizontal and vertical directions. It is obvious that these lengths correspond to *average energies of interactions* in horizontal and vertical directions. Denote these by u_h and u_v, respectively. Of course we have $u = u_v + u_h$, where u is the total internal energy. Furthermore

$$u_h = J \frac{\partial(\beta f)}{\partial H}, \qquad u_v = J' \frac{\partial(\beta f)}{\partial H'} \tag{16}$$

Relations between u_v, u_h and $\kappa \equiv k/N^2$, $\lambda \equiv l/N^2$ are:

$$\kappa = \frac{1}{2J} u_v + \frac{1}{2}, \qquad \lambda = \frac{1}{2J'} u_h + \frac{1}{2} \tag{17}$$

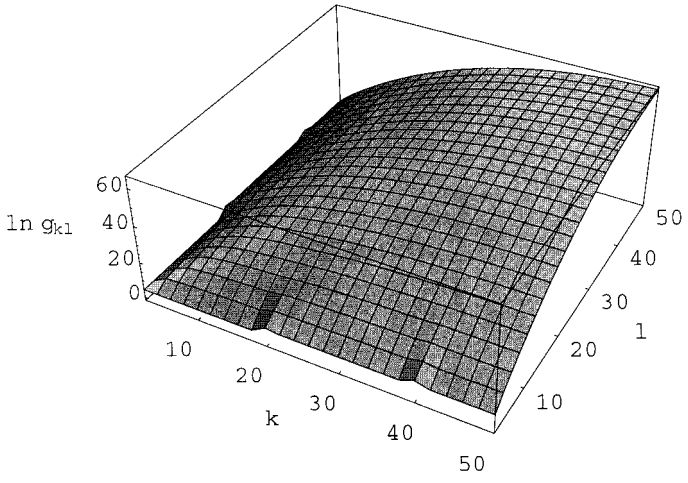

Fig. 3. Anisotropic lattice 10×10. Logarithm of number of states as a function of polygon lengths: horizontal k and vertical l. *Remark*. Only half of the range of k and l is taken because of symmetry.

We see that the problem of calculation of $\ln g_{kl}/N^2$ as functions of κ and λ is equivalent to expressing the entropy as a function of u_v, u_h. The technicalities are the following. From given values of (u_v, u_h) we calculate the corresponding values of (x, y). It is not possible by some explicit formulas, but from the inverse function theorem we conclude that there exists a unique mapping $x = x(u_v, u_h)$, $y = y(u_v, u_h)$. From x, y calculated in this manner, we calculate in turn the entropy.

Explicit formulas for all necessary quantities are as follows. The free energy (ref. 7) is given by

$$-\beta f = \frac{1}{2\pi} \int_0^{\pi} \ln \left\{ 2 \left[\cosh 2H \cosh 2H' + \frac{1}{k} \sqrt{1 + k^2 - 2k \cos 2\theta} \right] \right\} \mathrm{d}\theta \quad (18)$$

where $k = (\sinh 2H \sinh 2H')^{-1}$. "Vertical" and "horizontal" contributions to the internal energy are:[2]

$$-\frac{u_h}{J'} = \coth 2H'(2y + (2K/\pi)\, Z[2yK', k']) \quad (19)$$

$$-\frac{u_v}{J} = \coth 2H(1 - 2y + (2K/\pi)\, Z[(1 - 2y)\, K', k']) \quad (20)$$

where these expressions are valid below the critical temperature, and above the critical temperature we have

$$-\frac{u_h}{J'} = \coth 2H'(2y - (2K/\pi)\, Z[(1-2y)\, K', k']) \tag{21}$$

$$-\frac{u_v}{J} = \coth 2H(1 - 2y - (2K/\pi)\, Z[2yK', k']) \tag{22}$$

In the formulas for u_v, u_h the notation is: $k = (\sinh 2H \sinh 2H')^{-1}$ $(T < T_c)$; $k' = \sqrt{1-k^2}$; $k \equiv K(k)$ is a complete elliptic integral of first kind; $K' = K(k')$; $g' = \mathrm{gd}\, 2H'$, $g = \mathrm{gd}\, 2H$ (where gd is the gudermannian angle, defined as $\mathrm{gd}\, u = 2\, \mathrm{arctg}(\tanh \frac{1}{2} u)$), and $y = F(k', g')/2K'$ where $F(k, \phi)$ denotes the elliptic integral of the first kind: $F(k, \phi) = \int_0^\phi (1 - k^2 \sin^2 \theta)^{-1/2}\, \mathrm{d}\theta$. $Z[u, k]$ is the Jacobi elliptic function. For $T > T_c$ one must take $k = (\sinh 2H \sinh 2H')$.

Other important thermodynamic functions (i.e., total internal energy u and entropy s) can be calculated from the relations $f = u - Ts$, $u = u_v + u_h$. The plot of the entropy as function of vertical and horizontal scaled polygon lengths is presented on Fig. 4.

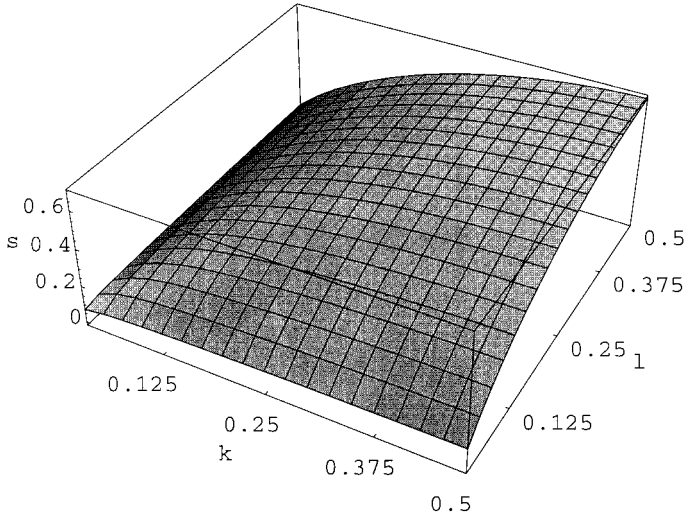

Fig. 4. Anisotropic lattice. Entropy s as a function of (scaled) polygon lengths: horizontal κ and vertical λ in thermodynamic limit. Again, due to symmetry, only half of range of variables κ, λ is taken.

5. OUTLOOK

We have calculated the number of polygons for fixed total length as well as the number of polygons for separately fixed horizontal and vertical lengths. By use of the exact expression of the Ising model free energy on the square lattice with periodic boundary conditions we have numerically obtained the distribution functions (entropies) for system sizes up to $N \leqslant 40$ (for isotropic lattices) and $N \leqslant 10$ (for anisotropic ones).

It is seen that for increasing N, the corresponding entropies s_N converge to the entropy calculated in the thermodynamic limit. It would be interesting (although technically involved) to calculate the asymptotics of the entropy for large N via correction terms in the saddle point approximation.

We believe that our results concerning the distribution of energies provide useful checks for Monte Carlo calculations.

The two-dimensional Ising model is a unique nontrivial statistical-mechanical model (with finite range interactions) for which it is possible to calculate the partition function in closed form not only in TD limit, but also for finite lattices. The corrections to finite size scaling, i.e., higher order terms in asymptotic expansions for large N, are of great importance in determining properties of large but finite systems. However, the structure of such correction-to-scaling terms is clear only in the leading terms for which renormalization-group results or exact solutions have been obtained. The structure of next-to-leading FSS terms remains unclear even for the Ising model. The main reason of this situation is the fact that FSS corrections are difficult to determine both theoretically as well as numerically. The sources of these difficulties have been discussed recently in ref. 8. By an extension of the method presented here (a generalization of the exact expression for the partition function to other thermodynamic quantities) it should be possible to determine higher-order FSS corrections. The realization of this programme is in progress.

ACKNOWLEDGMENTS

A substantial part of the calculations have been performed during the stay of one of us (J.W.) at the Institut für Theoretische Physik, Universität zu Köln. J.W. would like to express his gratitude towards DAAD for financial support and for the ITP for kind hospitality. A.K. acknowledges financial support by the *Deutsche Forschungsgemeinschaft* under grant No. Kl 645/3-1 and support by the research program of the Sonderforschungsbereich 341, Köln-Aachen-Jülich.

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