A CALCULATION OF THE PARTITION FUNCTION FOR A PLANE DIPOLE LATTICE

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The partition function for the two-dimensional Ising model is calculated. The method of calculation is close to that of Kac and Ward,[3] but has a number of advantages.

We consider a plane square lattice, in which for each lattice point k, l (k, l are the coordinates of the lattice point) there is a variable σ_{kl} which can take the two values ± 1. Let the energy of interaction of two lattice points be $E\sigma_{kl}\sigma_{k'l'}$. If the interaction is confined to nearest neighbors (the Ising model), the partition function is

$$Z = \sum_{\{\sigma\}} \exp\left\{-\frac{E}{kT}\sum_{k,\,l}(\sigma_{kl}\sigma_{kl+1} + \sigma_{kl}\sigma_{k+1l})\right\}. \qquad (1)$$

This function was calculated by Onsager.[1] The algebraic method of Onsager was perfected in a paper by Kaufman.[2] Kac and Ward[3] suggested a different approach, of a combinatorial nature, and there is a closely similar method by Hurst and Green,[4,5] which is based on the use of the language of second quantization. The structure of the solution of Kac and Ward has been explained (without rigorous proof) in unpublished lectures by Feynman (cf.[6,7]). The Feynman hypothesis has been proved by Sherman[6] and by Burgoyne.[7]

Still another explanation of the Onsager solution, based on a development of the method of Kac and Ward, is proposed in the present paper. The calculation is of the nature of a direct summation and avoids as far as possible the use of concepts not contained in the formulation of the problem. In particular, no artificial "one-dimensional" denumeration of the lattice points is required (such a denumeration is absent only in the Feynman method). The calculation shows the way in which the summation over loops of a special type which occurs in partition-function sums reduces in this case to a summation over all possible loops.

After elementary manipulations (see, for example, [5]), Z can be put in the form

$$Z = 2^N(1-x^2)^{-N}S, \quad S = \sum_{r=1}^{N} x^r g_r, \qquad (2)$$

where $x = \tanh(E/kT)$, r runs through all integer values, and g_r is the total number of closed polygons (the sum over loops, see Fig. 1) constructed from r nonrepeated bonds. The further calculation consists of three stages: a) the sum over polygons is reduced to a sum over closed loops without intersections; b) the sum over closed loops without intersections is transformed into a sum over all loops; c) the sum over all loops is reduced to a random-walk problem and is calculated easily.

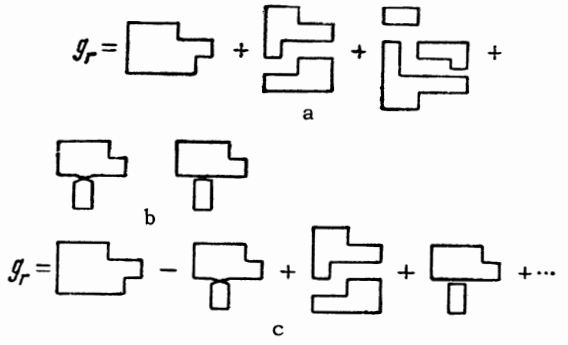

FIG. 1. The sum over loops

For what follows it is convenient to represent g_r in the form of a sum over loops without intersections and common parts. The partial sums that thus arise are: the sum of single loops, the sum of double loops—product of two single ones—the sum of triple loops, and so on. This is represented symbolically in Fig. 1, a. Such a separation is ambiguous, however, as regards figures with self-intersections, since the same figure can consist of different numbers of single loops, depending on the manner of its construction. In particular, each angle can be obtained in three different ways, as shown in Fig. 2, a. By choosing one of the last two ways—for example, the third—(the first gives loops with intersections), we obtain a sum over nonintersecting loops in which, first, all of the loops have neither repeated bonds nor intersections, and second, each polygon of the g_r is made up of only one set of loops.

To go over to a summation over all loops, we use the following simple approach. Consider the

sum over all loops that have one bond transversed twice. This bond can be traversed in two ways (see Figs. 1, b and 2, b). If we take the first way (with an intersection) with the negative sign and the second (without intersection) with the positive sign (see Fig. 1, c), then the addition of terms of this kind does not change the value of the sum, since the new terms cancel each other.

This approach can be generalized. Let us take a loop which has any number of repeated bonds. In the construction of the loop each common part enters twice: with and without an intersection (Fig. 2, b). Therefore if we consider the sum over all loops (with and without repeated bonds), with each loop taken with the sign $(-1)^n$ (n being the number of intersections), then all loops that have common parts contribute nothing to the sum, since each such loop occurs twice with opposite signs. Thus the summation can be extended to loops having common parts, if we stipulate that each loop appears with a sign which depends on the number of intersections.

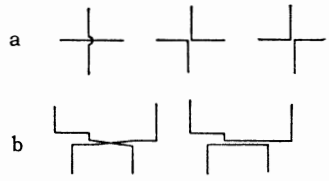

FIG. 2. Ways in which loops intersect

But then we still are not getting all possible loops, since loops corresponding to figures with self-intersections with other kinds of behavior at the corners have not been taken into account at all. Therefore we must add the sum over loops with angles of the first two types shown in Fig. 2, a, taking corners of the first type with the negative sign and those of the second type with the positive sign.

The sum over loops without intersections has been reduced to a sum over all loops, in which each loop occurs with the weight $(-1)^n$. We can connect this with a well known geometrical fact[8]: the total angle through which the tangent vector turns in going around a plane closed loop is $2\pi(l+1)$, where the parity of l is the same as that of the number of intersections n. Therefore, if to each lattice point with turning angle φ we assign the factor $e^{i\varphi/2}$, then after going around the entire loop the product of these factors will be $(-1)^{l+1}$ or $(-1)^{n+1}$, where n is the number of intersections. Thus we need not concern ourselves with the number of intersections if we take each angle with the weight $e^{i\varphi/2}$. It is easy to see, however, that for a figure made up of s closed loops the factors $e^{i\varphi/2}$ will give a factor $(-1)^{n+s}$ (where now n is the number of intersections in all of the loops). Therefore each such product is still to be multiplied by $(-1)^s$ (so as to obtain the required sign).

In order to count up the angle it is convenient to deal with directed loops. If we denote the sum over all single undirected loops consisting of r bonds by f_r (with the factors $e^{i\varphi/2}$ and x^r included), then the sum over all double loops of l bonds will be given by

$$\tfrac{1}{2}\sum_{r_1+r_2=l} f_{r_1}f_{r_2}$$

and so on, and

$$S=\sum_{s=1}^{\infty}(-1)^s\frac{1}{s!}\sum_{r_1+r_2+\cdots r_s=1}^{\infty} f_{r_1}f_{r_2}\cdots f_{r_s}.$$

The total of possible permutations of the f_{r_i} in the sum with fixed r_i gives the same combination of single loops multiplied by s! This is the reason for the factor 1/s!

In the summation over directed loops each f_r is encountered twice, and therefore if we introduce the symbol v_r for the sum over all single directed loops composed of r bonds we have

$$S=\sum_{s=1}^{\infty}(-1)^s\frac{1}{s!\,2^s}\sum_{r_1+r_2+\ldots+rs=1}^{\infty} v_{r_1}v_{r_2}\cdots v_{r_s}. \qquad (3)$$

To obtain the directed loops it is convenient to associate four possible directions with each lattice point. We denote these directions by the indices:

direction: $kl\rightarrow$ $kl\uparrow$ $kl\leftarrow$ $kl\downarrow$
index ν: $kl1$ $kl2$ $kl3$ $kl4$

and introduce the quantity $W_r(kl\nu\,|\,k'l'\nu')$ —the sum over all of the transitions from $k'l'\nu'$ to $kl\nu$ which occur in the r bonds; each bond occurs with the factor $e^{i\varphi/2}x$, where φ is the change of direction in going over to the next bond.

From the definition of W_r we have the following recurrence relations:

$$\begin{aligned}
W_{r+1}(kl1\,|\,k'l'\nu') &= xW_r(k-1,l,1\,|\,k'l'\nu')\\
&\quad + xe^{-i\pi/4}W_r(k,l-1,2\,|\,k'l'\nu')\\
&\quad + xe^{i\pi/4}W_r(k,l+1,4\,|\,k'l'\nu'),\\
W_{r+1}(kl2\,|\,k'l'\nu') &= xe^{i\pi/4}W_r(k-1,l,1\,|\,k'l'\nu') + xW_r\\
&\quad \times(k,l-1,2\,|\,k'l'\nu') + xe^{-i\pi/4}W_r(k+1,l,3\,|\,k'l'\nu'),\\
W_{r+1}(kl3\,|\,k'l'\nu') &= xe^{i\pi/4}W_r(k,l-1.2\,|\,k'l'\nu')\\
&\quad + xW_r(k+1,l,3\,|\,k'l'\nu') + xe^{-i\pi/4}W_r(k,l+1.4\,|\,k'l'\nu'),\\
W_{r+1}(kl4\,|\,k'l'\nu') &= xe^{-i\pi/4}W_r(k-1,l,1\,|\,k'l'\nu')\\
&\quad + xe^{i\pi/4}W_r(k+1,l,3\,|\,k'l'\nu') + xW_r(k,l+1.4\,|\,k'l'\nu').
\end{aligned} \qquad (4)$$

Knowing the $W_r(k l\nu \mid k' l'\nu')$, we can easily calculate the sum over all single directed loops with r bonds. Let us introduce the notation $\sum_{kl\nu} W_r(k l\nu \mid k l\nu) = b_r$. Then

$$v_r = b_r / r. \tag{5}$$

The factor $1/r$ appears because the same loop can be obtained in r different ways, depending on the choice of starting point.

Substituting (5) in (3), we get

$$S = \sum_{s=1}^{\infty} (-1)^s \frac{1}{s!\, 2^s} \sum_{r_1+\ldots+r_s=1}^{\infty} \prod_{i=1}^{s} \frac{b_{r_i}}{r_i}. \tag{6}$$

In the last sum we can take the r_i to run independently through all values from 1 to ∞. (Loops with a number of lattice points larger than N will not contribute, since they contain repeated bonds). Therefore

$$S = \sum_{s=1}^{\infty} (-1)^s \frac{1}{s!\, 2^s} \left(\sum_{r=0}^{\infty} \frac{b_r}{r} \right)^s = \exp\left(-\frac{1}{2} \sum_{r=0}^{\infty} \frac{b_r}{r} \right). \tag{7}$$

Let us denote the matrix of the system (4) by A. As can be seen by writing this matrix graphically (Fig. 3), each of its elements is the "probability" W_1 of a transition between adjacent lattice points.

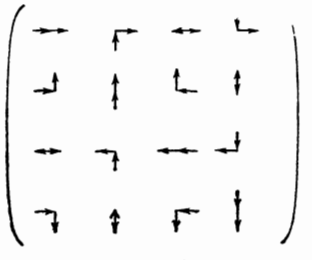

FIG. 3

The "probabilities" W_r of traversing paths with r bonds will be given by the matrix A^r, and the "probability" of return to the same point after traversing r bonds is $\mathrm{Sp}\, A^r$. Accordingly,

$$b_r = \mathrm{Sp}\, A^r = \sum_i \lambda_i^r,$$

where the λ_i are the eigenvalues of the matrix A. Let us substitute this value of b_r in (7):

$$S = \exp\left\{ -\frac{1}{2} \sum_{r=0}^{\infty} \frac{1}{r} \sum_i \lambda_i^r \right\}.$$

Changing the order of the summations, we get

$$S = \exp\left\{ -\frac{1}{2} \sum_i \sum_{r=0}^{\infty} \frac{\lambda_i^r}{r} \right\}$$

$$= \exp\left\{ \frac{1}{2} \sum_i \ln(1-\lambda_i) \right\} = \prod_i \sqrt{1-\lambda_i}. \tag{8}$$

The matrix A is easily diagonalized with respect to the indices k and l by means of a finite-dimensional Fourier transformation. In (4) we go over to a new representation:

$$W_r(p, q) = \sum_{k=0}^{n} \sum_{l=0}^{m} \exp\left\{ -2\pi i \left(\frac{pk}{n} + \frac{ql}{m} \right) \right\} W_r(k, l).$$

In this representation

$$A(p, q) = \begin{pmatrix} x\bar{\alpha}_p & x\varepsilon\bar{\beta}_q & 0 & x\varepsilon\beta_q \\ x\varepsilon\bar{\alpha}_p & x\bar{\beta}_q & x\bar{\varepsilon}\alpha_p & 0 \\ 0 & x\varepsilon\bar{\beta}_q & x\alpha_p & x\bar{\varepsilon}\beta_q \\ x\bar{\varepsilon}\bar{\alpha}_p & 0 & x\varepsilon\alpha_p & x\beta_q \end{pmatrix},$$

where to shorten the writing we have introduced the notations: $\epsilon = e^{i\pi/4}$, $\alpha_p = e^{2\pi i p/n}$, $\beta_q = e^{2\pi i q/m}$.

For a fixed p and q we get

$$\prod_{i=1}^{4} [1 - \lambda_i(p, q)] = \mathrm{Det}\, [E - A(p, q)]$$

$$= (1+x^2)^2 - 2x(1-x^2)\left(\cos\frac{2\pi p}{n} + \cos\frac{2\pi q}{m} \right).$$

It follows that

$$Z = 2^N (1-x^2)^{-N}$$

$$\times \prod_{p=0}^{n} \prod_{q=0}^{m} \left[(1+x^2)^2 - 2x(1-x^2)\left(\cos\frac{2\pi p}{n} + \cos\frac{2\pi q}{m} \right) \right]^{1/2}$$

—the usual expression for the partition function for a plane dipole lattice (see, e.g., [5]).

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