# THERMODYNAMICS OF A PLANE ISING-ONSAGER DIPOLE LATTICE

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THE thermodynamics of a dipole lattice is of considerable interest since this is the only model of a system experiencing a second-order phase transition which admits an exact solution. Onsager[1] and Kaufman[2] gave a solution of this problem. The method developed by them does as a matter of principle not admit a generalization to the case of a three-dimensional lattice.

One of the present authors (Yu. B. R.) gave in 1954 a survey of the above-mentioned papers.[3]

Recently a paper by Hurst and Green[4] appeared in which there was made considerable progress and essentially new ideas in the approach to the problem. The new method gives a solution which is simpler than the one given in references 1 and 2 and which above all does not exclude the possibility of generalizing it to a three-dimensional lattice. We therefore thought it expedient to give an exposition of the new method in the form of a survey, which may be considered to be a continuation of the survey in reference 3.

## 1. THE PARTITION FUNCTION

Let there be given a square lattice consisting of m columns and n rows, containing N = nm lattice sites. We renumber the lattice sites in lexicological order, i.e., we assign to each site a number

$$k=(k_2-1)m+k_1, \quad 1\leqslant k_1\leqslant m, \quad 1\leqslant k_2\leqslant n, \tag{1}$$

where $k_1$ and $k_2$ are the numbers of the column and the row in which a given site is situated.

To get rid of edge effects we impose upon the lattice a periodic boundary condition, closing it in both directions, i.e., we identify the (m+1)-st column with the first column, and the (n+1)-st row with the first row.

In each lattice site we place a dipole with axes along the direction normal to the plane of the lattice. Each dipole can have one of two possible opposite directions. It is clear that the general number of possible configurations of dipoles in the lattice is equal to $2^N$.

To describe the different configurations we proceed in the following way. We ascribe to each dipole a discrete variable $\sigma$ which can take on only two values: $\sigma = +1$, if the dipole is oriented toward the right, and $\sigma = -1$, if the dipole is oriented to the left.

If we restrict ourselves to taking only nearest-neighbor interactions into account and neglect interactions between farther neighbors, the configurational energy $E(\sigma_1, \ldots \sigma_N)$ can be written in the form

$$E(\sigma_1, \ldots, \sigma_N)=\sum_{k=1}^{N}(I_1\sigma_k\sigma_{k+1}+I_2\sigma_k\sigma_{k+m}). \tag{2}$$

Here, $\pm I_1$ is the energy of the interaction between two neighbor dipoles on the same row with parallel and antiparallel orientations of the dipoles, respectively. Similarly we denote by $\pm I_2$ the energy of the interaction between two neighbor dipoles on the same column. For the partition function we have the expression

$$\begin{aligned} Z(T)&=\sum_{\sigma_1\ldots\sigma_N}\exp\left[\frac{-E(\sigma_1, \ldots, \sigma_N)}{T}\right]\\ &=\sum_{(\sigma)}\exp\left\{-\sum_{k=1}^{N}(\theta_1\sigma_k\sigma_{k+1}+\theta_2\sigma_k\sigma_{k+m})\right\}\\ &=\sum_{(\sigma)}\prod_{k=1}^{N}\exp(-\theta_1\sigma_k\sigma_{k+1})\exp(-\theta_2\sigma_k\sigma_{k+m}), \end{aligned} \tag{3}$$

where $\Sigma_{(\sigma)}$ indicates a sum over all $2^N$ possible dipole configurations and where we have introduced the notation

$$\theta_1=\frac{I_1}{T}, \quad \theta_2=\frac{I_2}{T}. \tag{4}$$

Taking into consideration that $\sigma_1^2 = 1$, we get the formula*

$$\exp\alpha\sigma_i\sigma_k=\operatorname{ch}\alpha+\sigma_i\sigma_k\operatorname{sh}\alpha=\frac{1-\sigma_i\sigma_k\operatorname{th}\alpha}{(1-\operatorname{th}^2\alpha)^{1/2}}. \tag{5}$$

Using this formula and introducing the notation

$$x=\operatorname{th}\theta_1, \quad y=\operatorname{th}\theta_2,$$

we can rewrite Z(T) in the form

$$Z(x, y)=[(1-x^2)(1-y^2)]^{-\frac{N}{2}}\sum_{(\sigma)}\prod_{k=1}^{N}(1-x\sigma_k\sigma_{k+1})(1-y\sigma_k\sigma_{k+m}). \tag{6}$$

## 2. DIAGRAM TECHNIQUE

The product

$$G(x, y, \sigma_1, \ldots, \sigma_N)=\prod_{k=1}^{N}(1-x\sigma_k\sigma_{k+1})(1-y\sigma_k\sigma_{k+m}), \tag{7}$$

occurring in (6) is a polynomial in the variables x, y, $\sigma_1, \ldots, \sigma_N$. Since G occurs in (6) under the summation sign over all configurations, not all terms in the polynomial will give a non-vanishing contribution to the partition function. We show that only those terms give a non-vanishing contribution which contain all variables $\sigma_1, \ldots, \sigma_N$ to the zeroth, second, or fourth

*ch = cosh, sh = sinh, th = tanh.

power. It is clear that it is sufficient to prove this statement for just one arbitrarily chosen separate variable $\sigma_i$.

We split off from G all factors containing $\sigma_i$.

It is clear that there are four such factors, and we can write (6) in the form

$$Z(x, y) = [(1-x^2)(1-y^2)]^{-\frac{N}{2}} \times \sum_{\sigma_1, \ldots, \sigma_{i-1}, \sigma_{i+1}, \ldots, \sigma_N} G^{(i)}(x, y, \sigma_1, \ldots, \sigma_{i-1}, \sigma_{i+1}, \ldots, \sigma_N) \times \sum_{\sigma_i} (1 - x\sigma_i\sigma_{i-1})(1 - x\sigma_i\sigma_{i+1})(1 - y\sigma_i\sigma_{i-m})(1 - y\sigma_i\sigma_{i+m}), \quad (8)$$

where $G^{(i)}$ denotes the product of all those factors which do not contain the variable $\sigma_i$. Performing in (8) the last summation over $\sigma_i$ we see that nonvanishing contributions to $Z(x, y)$ are only made by those terms in G which contain $\sigma_i$ to the zeroth, the second, and the fourth power. The discussion given here is, clearly, valid for all variables $\sigma_i$.

Since $\sigma_i^2 = 1$, each term of the polynomial which contains all variables $\sigma_1, \ldots, \sigma_N$ in even powers will after summation over all configurations give a contribution proportional to the total number of configurations $2^N$.

We go over to a diagram technique, noting that to each term in the polynomial $G(x, y, \sigma_1, \ldots, \sigma_N)$ we can uniquely assign an aggregate of lines joining several pairs of neighboring lattice sites.

The diagrams given, for instance, in Figs. 1 a—c correspond to the following terms in the polynomial

a) $\sigma_k\sigma_{k+1}^2\sigma_{k+m+1}$,

b) $\sigma_k^2\sigma_{k+1}^2\sigma_{k+m-1}^2\sigma_{k+m}^4\sigma_{k+m+1}^2\sigma_{k+2m-1}^2\sigma_{k+2m}^2$,

c) $\sigma_k^2\sigma_{k+1}^2\sigma_{k+m-2}^2\sigma_{k+m-1}^2\sigma_{k+m}^2\sigma_{k+m+1}^2\sigma_{k+2m-2}^2\sigma_{k+2m-1}^2 \times \sigma_{k+3m-2}^2\sigma_{k+3m-1}^2$.

Equation (7) shows that each horizontal line corresponds to a factor x and each vertical line to y.

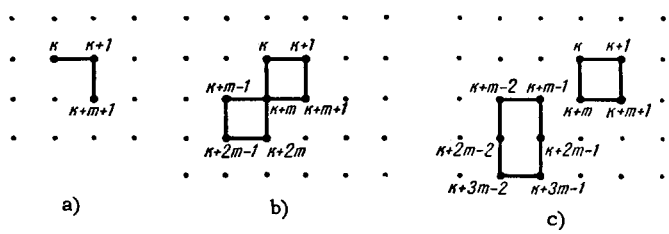


FIG. 1

We have shown above that only those terms in G, which contain the variables $\sigma_1, \ldots, \sigma_N$ to the zeroth, second, and fourth power, give a nonvanishing contribution to the partition function.

This means geometrically that, out of all possible diagrams, only those for which zero, two, or four lines meet in each lattice site give a nonvanishing contribution to the partition function. The simplest examples of such diagrams are given in Figs. 1 b and c. All diagrams making a nonvanishing contribution must thus be closed, and in some lattice sites there is the possibility of multiple intersections (the site k+m in Fig. 1b).

The partition function can thus be written in the following form

$$Z(x, y) = 2^N [(1-x^2)(1-y^2)]^{-\frac{N}{2}} S(x, y), \quad (9)$$

$$S(x, y) = \sum_{\alpha, \beta} g_{\alpha\beta} x^\alpha y^\beta, \quad (10)$$

where $g_{\alpha\beta}$ is the number of closed diagrams consisting of $\alpha$ horizontal and $\beta$ vertical lines, with any multiply connected diagram counted as one in the calculation (for instance, the diagram of Fig. 1c).

## 3. INTRODUCTION OF FERMI OPERATORS

To evaluate the sum $S(x, y)$ by Eq. (10) we introduce for each lattice site two pairs of Fermi-operators ($a_k^+$, $a_k$ and $b_k^+$, $b_k$) which satisfy the relations

$$a_k^+ a_i + a_i a_k^+ = \delta_{ik}, \qquad b_k^+ b_i + b_i^+ b_k = \delta_{ik}. \quad (11)$$

(All other anticommutators are equal to zero.)

Let us calculate the expression

$$S^*(x, y) = \mathrm{Sp} \prod_k (1 + 4xy a_{k+1} b_{k+m} a_k^+ b_k^+ + 4xy a_k^+ b_k^+ + a_{k+1} b_{k+m} + 2x a_k^+ b_{k+m} + 2y b_k^+ a_{k+1} + 2x a_{k+1} a_k^+ + 2y b_{k+m} b_k^+) \quad (12)$$

and show that $S^*(x, y) = S(x, y)$.

We note that for convenience we denote henceforth by Sp C the quantity Sp C/Sp E, where E is the unit matrix of the same dimensions as C. With this notation the dimensions of the matrices under the Sp sign will not affect the results.

We expand the product under the Sp sign and gather together terms with the same powers of 2x and 2y. We get

$$S^*(x, y) = \sum_{\alpha, \beta} (2x)^\alpha (2y)^\beta \mathrm{Sp} \sum_\lambda f_{\alpha\beta}^{(\lambda)}, \quad (13)$$

where we have under the Sp sign sums of different products of the Fermi operators $a_k^+$, $a_{k'}$ and $b_j^+$, $b_{j'}$.

To visualize the structure of these products it is convenient to use again a diagram technique.

To do this we introduce the eight elementary diagrams depicted in Fig. 2, corresponding to each of the eight terms from which the factors in the product (12) are constructed.

We agree to draw the lines going up or to the left from a lattice site as solid lines and we assign creation operators to them, while lines going down or to the right from a lattice site are dotted and correspond to annihilation operators. Moreover, we write down for each creation operator $a_k^+$ a factor 2x and for each creation operator $b_k^+$ a factor 2y.

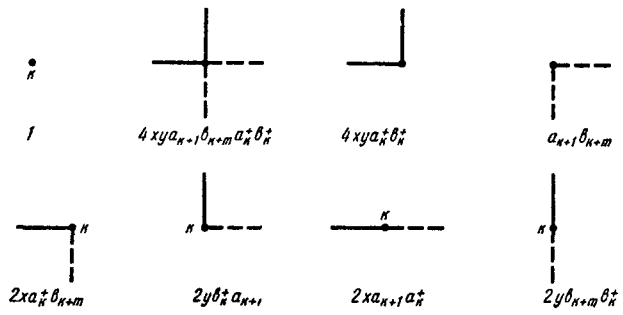


FIG. 2

We place arbitrarily on each lattice site one of the eight elementary diagrams drawn in Fig. 2.

We call a diagram a "duplicated" one, if in it any two neighboring sites are either not joined at all or are joined by one solid and one dotted line. We note that diagrams in which some of the duplicated lines turn out to be both solid or both dotted cannot be encountered at all, since it can be shown from Fig. 2 that in the elementary diagrams all solid lines are directed opposite the corresponding dotted line.

We show that all duplicated diagrams are closed. Indeed, one can see from Fig. 2 that an even number of single lines depart from each site. These lines are duplicated only by lines starting from neighboring sites. In the duplicated diagrams an even number of duplicated lines pass through each site, i.e., such a diagram is a closed one.

It is clear that to each duplicated diagram there corresponds some set of paired creation and annihilation operators. A duplicated horizontal line, for instance, joining the $(k-1)$-st and the k-th site can be constructed if we place on the $(k-1)$-st site one of the diagrams of Fig. 3a, and on the k-th site one of the diagrams of Fig. 3b.

The part of the resultant diagram of interest to us is shown in Fig. 4a.

Similarly, a vertical duplicated line can be constructed if we place on the $(k-m)$-th site one of the diagrams of Fig. 5a, and on the k-th site one of the diagrams of Fig. 5b. The diagram obtained then is conventionally shown in Fig. 4b.

It is clear that the system of "duplicated" diagrams constructed here is completely equivalent to the system of diagrams of the preceding section and leads to

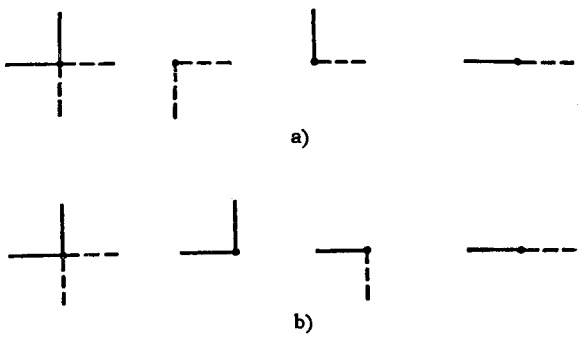


FIG. 3

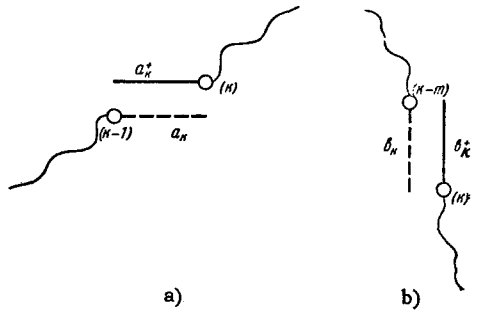


FIG. 4

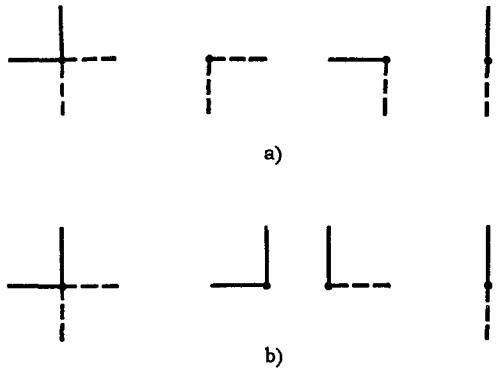


FIG. 5

it if we replace each duplicated line by a single one.

Apart from the duplicated diagrams considered up to now, we will encounter also diagrams in which some of two neighboring lattices are joined by a single (solid or dotted) line.

It is clear that such diagrams will correspond to products of Fermi operators containing unpaired (creation or annihilation) operators.

However, if we substitute such products under the Sp sign in Eq. (13), they give a vanishing contribution to the sum. They need therefore not be considered and the only products remaining in the sum correspond to duplicated closed diagrams.

For $S(x,y)$ and $S^*(x,y)$ we have the expressions

$$S(x, y)=\sum_{\alpha,\beta} g_{\alpha\beta}x^\alpha y^\beta \qquad (10)$$

where $g_{\alpha\beta}$ is the number of closed diagrams composed of $\alpha$ horizontal and $\beta$ vertical lines, and

$$S^*(x, y)=\sum_{\alpha,\beta}(2x)^\alpha(2y)^\beta\sum \mathrm{Sp}\,(a_\lambda^+ \ldots a_{\lambda'} \ldots b_\mu^+ \ldots b_{\mu'}), \qquad (14)$$

where paired products of $\alpha$ Fermi operators $a_\lambda^+$, $a_\lambda$ and $\beta$ Fermi operators $b_\lambda^+$, $b_\lambda$ are under the Sp sign.

In view of the proved equivalence of single and duplicated diagrams, the number of terms in the second sum will be exactly equal to $g_{\alpha\beta}$.

Bearing in mind that when we evaluate the trace of a product of Fermi operators

$$\mathrm{Sp}\,a_\lambda^+a_\lambda=\mathrm{Sp}\,a_\lambda a_\lambda^+=\frac{1}{2},$$

we get from Eq. (14)

$$S^*(x, y)=\sum_{\alpha,\beta} x^{\alpha}y^{\beta}(\pm 1\pm 1\pm 1\pm \ \dots\ \pm 1), \quad (15)$$

where the brackets contain $g_{\alpha\beta}$ terms, each equal to $\pm 1$.

The sign of the corresponding term is determined by the parity of the permutation that must be made in order that the original arrangement of Fermi operators determined by Eq. (12) go over into the "paired" arrangement, wherein creation operators stand next to the corresponding annihilation operators.

We shall show in Appendix I that it turns out that when the operators are paired off, the sign is conserved and that one must thus everywhere take the plus-sign. It is thereby shown that

$$S(x, y)=S^*(x, y).$$

## 4. CALCULATION OF THE FUNCTION S(x,y)

To evaluate the function S(x,y) using Eq. (12) we must evaluate the trace of the product of N factors, each of which is a sum of eight terms: unity, a single product of four Fermi operators, and six products of two Fermi operators.

We derive in Appendix II an equation which enables us to evaluate conveniently the trace of products of factors containing Fermi operators, i.e., a product of the type

$$\prod_{i=1}^{N}\Big[\sum_{k}(a_{ik}c_k^{+}+b_{ik}c_k)\Big]. \quad (16)$$

We could use this equation were we able to write each of the factors in (12) as a product of factors linear in the Fermi-operators contained in them.

To carry out this program of "linearizing" the product in (12) we calculate the product

$$(A_k^{(1)}+2xa_k^{+})(A_k^{(2)}+2yb_k^{+})(A_k^{(3)}+a_{k+1})(A_k^{(4)}+b_{k+m}), \quad (17)$$

where the $A_k^{(\lambda)}$ are four operators that anticommute with the operators $a_k^{+}$, $a_{k+1}$, $b_k^{+}$, $b_{k+m}$. We get then

$$\begin{aligned}&A_k^{(1)}A_k^{(2)}A_k^{(3)}A_k^{(4)}+4xya_k^{+}b_k^{+}a_{k+1}b_{k+m}+A_k^{(1)}A_k^{(2)}a_{k+1}b_{k+m}\\&\quad+A_k^{(1)}A_k^{(3)}2yb_{k+m}b_k^{+}+A_k^{(1)}A_k^{(4)}2yb_k^{+}a_{k+1}+A_k^{(2)}A_k^{(3)}2xa_k^{+}b_{k+m}\\&\quad+A_k^{(2)}A_k^{(4)}2xa_{k+1}a_k^{+}+A_k^{(3)}A_k^{(4)}4xya_k^{+}b_k^{+}. \quad (18)\end{aligned}$$

If we impose upon the four operators $A_k^{(\lambda)}$ the conditions

$$\mathrm{Sp}(A_1A_2A_3A_4)=1, \quad \mathrm{Sp}\,A_k^{(\lambda)}A_k^{(\mu)}=\delta_{\lambda\mu} \quad (\lambda,\mu=1,2,3,4), \quad (19)$$

we can write S(x,y) as the product of 4N factors

$$S(x, y)=\mathrm{Sp}\prod_{k=1}^{N}(A_k^{(1)}+2xa_k^{+})(A_k^{(2)}+2yb_k^{+})(A_k^{(3)}+a_{k+1})(A_k^{(4)}+b_{k+m}). \quad (20)$$

One can easily verify that one can satisfy condition (19) by introducing six extra pairs of Fermi operators $c_k^{+(\lambda)}$, $c_k^{(\lambda)}$, ($\lambda$ = 1, 2, 3, 4, 5, and 6), and put

$$\left.\begin{aligned}A_k^{(1)}&=\sqrt{2}(c_k^{(1)}+c_k^{(2)}+c_k^{(3)}),\\A_k^{(2)}&=\sqrt{2}(c_k^{+(1)}+c_k^{+(4)}+c_k^{(5)}),\\A_k^{(3)}&=\sqrt{2}(c_k^{+(2)}+c_k^{+(4)}+c_k^{(6)}),\\A_k^{(4)}&=\sqrt{2}(c_k^{+(3)}+c_k^{+(5)}+c_k^{+(6)}).\end{aligned}\right\} \quad (21)$$

Equations (20) and (21) enable us to write the trace of the product (13) as the trace of the product of 4N factors linear in the operators

$$a_k^{+},\ a_k,\ b_k^{+},\ b_k,\ c_k^{+(\lambda)},\ c_k^{(\lambda)}.$$

By Eq. (12) of Appendix II we can write the square of this trace in the form of the determinant of a 4N by 4N antisymmetric matrix D, the elements of which are numbered by two indices $(k,\lambda)$, where k = 1, 2, ..., N, $\lambda$ = 1,2,3,4. The elements of D are

$$\left.\begin{aligned}(k,\lambda\,|\,D\,|\,k,\lambda)&=1,\\(k,3\,|\,D\,|\,k+1,1)&=x,\\(k,4\,|\,D\,|\,k+m,2)&=y.\end{aligned}\right\} \quad (22)$$

The other matrix elements are equal to zero. We see that the matrix D can be represented as a hypermatrix consisting of 4 by 4 blocks

$$D=\begin{pmatrix}U & X & 0 & \dots & Y0 & \dots\\ -X^T & U & X & \dots & 0Y & \dots\\ 0 & -X^T & UX & \dots & 0Y & \dots\\ \dots & \dots & \dots & \dots & \dots & \dots\end{pmatrix}, \quad (23)$$

where according to Eq. (22)

$$U=\begin{pmatrix}0&1&1&1\\-1&0&1&1\\-1&-1&0&1\\-1&-1&-1&0\end{pmatrix},\quad X=\begin{pmatrix}0&0&x&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix},\quad Y=\begin{pmatrix}0&0&0&0\\0&0&0&y\\0&0&0&0\\0&0&0&0\end{pmatrix}. \quad (24)$$

The structure of the matrix D shows that it can be written as a sum of direct products of N by N matrices E, $E_1$, and $E_m$ by four by four matrices U, X, and Y, respectively:

$$D=E\times U+E_1\times X+E_m\times Y-E_1^T\times X^T-E_m^T\times Y^T, \quad (25)$$

where

$$(i\,|\,E\,|\,k)=\delta_{ik},\quad (i\,|\,E_1\,|\,k+1)=\delta_{ik},\quad (i\,|\,E_m\,|\,k+m)=\delta_{ik}.$$

We have according to (12) of Appendix II

$$S(x, y)^2=\det|D|. \quad (26)$$

When evaluating the determinant of the matrix D we can perform a similarity transformation upon it, using the equations of Appendix III:

$$\begin{aligned}D'=(S\times E)\,D\,(S^{-1}\times E)&=E\times U+E_1'\times X+E_m'\\&\quad\times Y-E_1'^T\times X^T-E_m'^T\times Y^T, \quad (27)\end{aligned}$$

and choose the matrix S such that $E_1'$ and $E_m'$ turn out to be diagonal.

Since N = mn is a large number, we can impose the periodicity condition upon the elements of the matrix D

$$(N+k, \lambda \mid D \mid N+k', \lambda') = (k, \lambda \mid D \mid k', \lambda'). \tag{28}$$

In that case

$$E_m = E_1^m,\ E = (E_1)^N,\ E_1^{N-1} = E_1^{-1} = E_1^T,\ E_1^{N-m} = E_1^{-m} = E_m^T, \tag{29}$$

from which it follows that the eigenvalues of the matrices $E_1$ and $E_m$ will be the N-th roots of unity:

$$(p \mid E_1' \mid p) = \exp\frac{2\pi i}{N} p \equiv \alpha_p, \quad (p \mid E_m' \mid p) = \exp\left(\frac{2\pi i}{N} mp\right) \equiv \beta_p. \tag{30}$$

The matrix D′ can be written in the form of a block matrix:

$$D' = \begin{pmatrix} U_1 & & & \\ & U_2 & & \\ & & \ddots & \\ & & & U_p \end{pmatrix}, \tag{31}$$

where according to (27) and (30)

$$U_p' = U + \alpha_p X + \beta_p Y - \alpha_p X^T - \beta_p Y^T, \tag{32}$$

or, using Eq. (24)

$$U_p = \begin{pmatrix} 0 & 1 & 1+\alpha_p x & 1 \\ -1 & 0 & 1 & 1+\beta_p y \\ -1-\alpha_p^* x & -1 & 0 & 1 \\ -1 & -1-\beta_p^* y & -1 & 0 \end{pmatrix}. \tag{33}$$

Evaluating the determinant, we get

$$\det \mid U_p \mid = (1+x^2)(1+y^2) - 2y(1-x^2)\cos\frac{2\pi}{N} p - 2x(1-y^2)\cos\frac{2\pi}{N} mp.$$

We use the notation $p = p_2 n + p_1$, $1 \le p_1 \le n$, $0 \le p_2 \le m-1$,

$$\cos\frac{2\pi}{N} p = \cos\frac{2\pi}{m}\left(p_2 + \frac{p_1}{n}\right), \quad \cos\frac{2\pi}{N} mp = \cos\frac{2\pi}{n} p_1 \tag{34}$$

and we write the final expression for $S^2(x, y)$ as a double product:

$$S^2(x, y) = \prod_{p_1=1}^{n} \prod_{p_2=0}^{m} \left[(1+x^2)(1+y^2) - 2x(1-y^2)\cos\frac{2\pi}{n} p_1 - 2y(1-x^2)\cos\frac{2\pi}{m}\left(p_2 + \frac{p_1}{n}\right)\right], \tag{35}$$

and taking the logarithm we get from this

$$\ln S(x, y) = \frac{1}{2}\sum_{p_1=1}^{n}\sum_{p_2=0}^{m-1} \ln\left[(1+x^2)(1+y^2) - 2x(1-y^2)\cos\frac{2\pi}{n} p_1 - 2y(1-x^2)\cos\frac{2\pi}{m}\left(p_2 + \frac{p_1}{n}\right)\right]. \tag{36}$$

For large n and m this sum goes over into an integral

$$\ln S(x, y) = \frac{N}{2(2\pi)^2}\int_0^{2\pi}\int \ln\left[(1+x^2)(1+y^2) - 2x(1-y^2)\cos\omega_1 - 2y(1-x^2)\cos\omega_2\right] d\omega_1\, d\omega_2. \tag{37}$$

## 5. FREE ENERGY, PHASE TRANSITION

Since we have an expression for ln S(x, y) we can use Eq. (9) to write down an expression for the free energy F(x, y) in the form

$$-\frac{F(x, y)}{TN} = \frac{1}{N}\ln Z(x, y) = \ln 2 - \frac{1}{2}\ln(1-x^2)(1-y^2) + \frac{1}{2}\frac{1}{(2\pi)^2}\int_0^{2\pi}\int \ln\left[(1+x^2)(1+y^2) - 2x(1-y^2)\cos\omega_1 - 2y(1-x^2)\cos\omega_2\right] d\omega_1\, d\omega_2. \tag{38}$$

Substituting $x = \tanh\theta_1$ and $y = \tanh\theta_2$, we get

$$-\frac{F(x, y)}{TN} = \ln 2 + \frac{1}{2}\frac{1}{(2\pi)^2} \times \int_0^{2\pi}\int \ln\left[\operatorname{ch} 2\theta_1 \operatorname{ch} 2\theta_2 - \operatorname{sh} 2\theta_1 \cos\omega_1 - \operatorname{sh} 2\theta_2 \cos\omega_2\right] d\omega_1\, d\omega_2. \tag{39}$$

This expression was obtained in Onsager's original paper.[1]

We show that the expression occurring under the logarithm sign in (38) is non-negative. We have

$$[(1-x^2)(1-y^2) - 4xy]^2 = (1-x^2)^2(1-y^2)^2 + 16x^2y^2 - 8xy(1-x^2)(1-y^2) \geqslant 0, \tag{40}$$

or

$$(1+x^4-2x^2)(1+y^4-2y^2) \geqslant 8xy(1-x^2)(1-y^2) - 16x^2y^2.$$

Adding to both sides of the inequality the positive expression

$$4x^2(1+y^4) + 4y^2(1+x^4) = 4x^2(1-y^2)^2 + 4y^2(1-x^2)^2 + 16x^2y^2,$$

we get

$$(1+x^4+2x^2)(1+y^4+2y^2) \geqslant [2x(1-y^2) + 2y(1-x^2)]^2,$$

from which it follows that

$$A(x, y) = (1+x^2)(1+y^2) - 2x(1-y^2) - 2y(1-x^2) \geqslant 0, \tag{41}$$

where the equality sign occurs for the values $x = x_c$ and $y = y_c$ for which

$$(1-x_c^2)(1-y_c^2) - 4x_c y_c = 0. \tag{42}$$

Using (41) we can write the free energy in the form

$$-\frac{F(x, y)}{TN} = R(x, y) + \frac{1}{2}\frac{1}{(2\pi)^2}\int_0^{2\pi}\int \ln\left[A(x, y) + 2x(1-y^2)(1-\cos\omega_1) + 2y(1-x^2)(1-\cos\omega_2)\right] d\omega_1\, d\omega_2 \tag{43}$$

where R(x, y) is a function which is regular at $x = x_c$, $y = y_c$.

We see that the singularity of the free energy is connected with the fact that the expression under the logarithm sign vanishes for $\omega_1 = \omega_2 = 0$ and a temperature $T_c$ determined by the equation

$$\text{th}\,\frac{I_1}{T_c} = x_c, \qquad \text{th}\,\frac{I_2}{T_c} = y_c, \tag{44}$$

where $x_c$ and $y_c$ satisfy Eq. (42).

Since the equation

$$A(x, y) + 2x(1-y^2)(1-\cos\omega_1) + 2y(1-x^2)(1-\cos\omega_2)$$

has a minimum at the values $\omega_1 = 0$, $\omega_2 = 0$, $x = x_c$, $y = y_c$ and vanishes there, we can expand it in a power series and we get

$$\frac{1}{2}\left[2\left(\frac{\partial^2 A}{\partial x\,\partial y}\right)\Delta x\,\Delta y + \left(\frac{\partial^2 A}{\partial x^2}\right)_c \Delta x^2 + \frac{\partial^2 A}{\partial y^2}\Delta y^2\right]$$
$$+ x_c(1-y_c^2)\omega_1^2 + y_c(1-x_c^2)\omega_2^2. \tag{45}$$

Since by virtue of (44)

$$\Delta x = -(1-x_c^2)\frac{y_1}{T_c^2}\Delta T, \qquad \Delta y = -(1-y_c^2)\frac{y_2}{T_c^2}\Delta T,$$

we have for the free energy in the vicinity of the singularity

$$-\frac{F(T)}{TN} = R(x_c, y_c) + \frac{1}{2}\frac{1}{(2\pi)^2}\int_0^{2\pi}\int \ln\left[C(T_c)(T-T_c)^2\right.$$
$$\left. + x_c(1-y_c^2)\omega_1^2 + y_c(1-x_c^2)\omega_2^2\right] d\omega_1 d\omega_2, \tag{46}$$

where

$$C(T_c) = \frac{1}{2T_c^2}\left[I_1^2\left(\frac{\partial^2 A}{\partial x^2}\right)_c (1-x_c^2) + 2I_1 I_2\left(\frac{\partial^2 A}{\partial x\,\partial y}\right)_c^2 (1-x_c^2)(1-y_c^2)\right.$$
$$\left. + I_2^2\left(\frac{\partial^2 A}{\partial y^2}\right)_c (1-y_c^2)^2\right]. \tag{47}$$

Integrating (46) we get for the free energy the expression

$$-\frac{F}{TN} = R_1(T_c) + C_1(T_c)(T-T_c)^2\ln(T-T_c)^2. \tag{48}$$

The internal energy U is found from the formula

$$\frac{U}{N} = -\frac{d}{dT}\left(\frac{F}{NT}\right) = R_2(T_c) + 2C_1(T_c)(T-T_c)\ln(T-T_c)^2. \tag{49}$$

We note that it is continuous in the point $T = T_c$. The specific heat, however, has a logarithmic discontinuity:

$$\frac{c}{N} = \frac{d}{dT}\left(\frac{U}{N}\right) = R_3(T_c) + 2C_1(T_c)\ln(T-T_c)^2. \tag{50}$$

## CONCLUSION

We note in conclusion that the method expounded here cannot immediately be generalized to the case of a three-dimensional lattice. We shall number the corresponding equations for the three-dimensional lattice by the same numbers as for the two-dimensional one, but with an asterisk. We assign to each lattice site a number

$$k = (k_3-1)mn + (k_2-1)m + k_1, \quad N = mnp,$$
$$1 \leqslant k_1 \leqslant m, \quad 1 \leqslant k_2 \leqslant n, \quad 1 \leqslant k_3 \leqslant p. \tag{1*}$$

We readily arrive at the equations

$$Z(x, y, z) = 2^N\left[(1-x^2)(1-y^2)(1-z^2)\right]^{-\frac{N}{2}} S(x, y, z), \tag{9*}$$
$$S(x, y, z) = \sum_{\alpha,\beta,\gamma} g_{\alpha\beta\gamma} x^\alpha y^\beta z^\gamma. \tag{10*}$$

Here $g_{\alpha\beta\gamma}$ is the number of closed spatial diagrams with $\alpha$, $\beta$, and $\gamma$ lines in three mutually perpendicular directions.

Moreover, we can introduce, as in (12), Fermi operators corresponding to the three mutually perpendicular directions in the lattice, namely $a_k^+$, $a_k$, $b_k^+$, $b_k$, $c_k^+$, $c_k$. The elementary diagrams similar to the ones depicted in Fig. 2 can also be easily constructed. One verifies easily that there are thirty-two of them in the three-dimensional case. One can develop a diagram technique for the quantity S*, and one obtains easily the equation

$$S^*(x, y, z) = \sum_{\alpha,\beta,\gamma} x^\alpha y^\beta z^\gamma (\pm 1 \pm 1 \pm 1 \pm \ldots \pm 1), \tag{15*}$$

where there are $g_{\alpha\beta\gamma}$ terms within the brackets. However, in contradistinction to the plane case, it is impossible to prove here that all terms in (15*) have a plus sign. Furthermore, there is a simple example showing that this is not the case. The diagram of Fig. 6 serves as such an example:

$$a_2 c_5 c_6 a_2^+ a_4 c_7 c_8 a_4^+ b_7 c_5^+ b_8 c_6^+ b_7^+ c_7^+ b_8^+ c_8^+. \tag{*}$$

Performing the pairing as shown in (*) we get the result that the diagram of Fig. 6 gives a negative contribution to the partition function. This fact is independent of the order of the operators at the vertices since a vertex of each type occurs twice in the diagram considered.

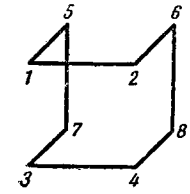


FIG. 6

## APPENDIX I

We show that for the given order of the operators in (12) all diagrams make a non-negative contribution to the partition function.

In order to go over from an arbitrary term of the sum in (14) to the diagrams, it is necessary to write down the Fermi operators in such a way that one can go from the lexicological order which we took in (12)

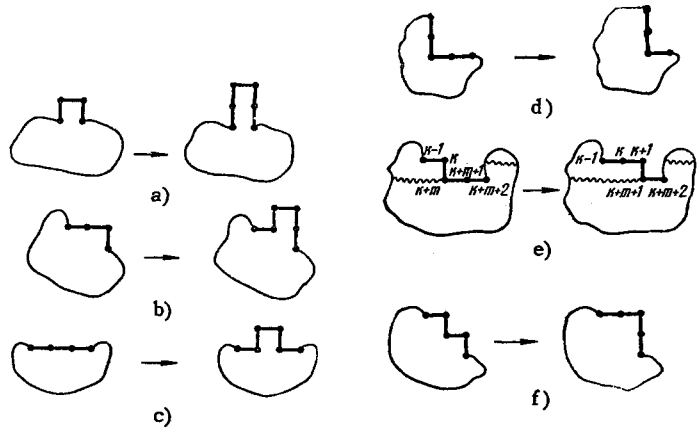


FIG. 7

to an order where each creation operator stands next to the corresponding annihilation operator. We note that the order in which the corresponding creation and annihilation operators are situated with respect to one another is immaterial, by virtue of the validity of the relation

$$\mathrm{Sp}\, a_k^+ a_k = \mathrm{Sp}\, a_k a_k^+.$$

It is sufficient to prove this for connected diagrams, since an unconnected diagram is equal to the product of the connected parts occurring in it. We prove this by induction. To do this we verify that the simplest diagram Fig. 1c has a plus sign. This diagram corresponds to the operators

$$a_{k+1} b_{k+m} b_{k+m+1} a_{k+1}^+ a_{k+m+1} b_{k+m}^+ a_{k+m+1}^+ b_{k+m+1}^+.$$

Performing the permutations in the usual way, we satisfy ourselves that the diagram has a plus sign.

We consider first an arbitrary connected diagram without intersections. It is clear that any such diagram can be constructed from an elementary one by successive applications of one of the operations shown in Fig. 7.

It is sufficient for us to show that any one of those operations leaves the sign of the diagram unchanged. Since the elementary diagram gives a positive contribution to (15), we show thereby that a positive contribution is made by all diagrams that contain no intersections. The proof proceeds in the same way for all operations in Fig. 7; we can here thus consider any one as an example, say, Fig. 7e.

We write down the operators corresponding to the diagram on the left of Fig. 7e:

$$\alpha \underbrace{a_k^+ b_{k+m}} \beta \underbrace{b_{k+m}^+ a_{k+m+1}} a_{k+m+2} \underbrace{a_{k+m+1}^+} \gamma. \qquad (1)$$

Here $\alpha$ denotes the totality of all Fermi operators pertaining to sites preceding the k-th site, $\beta$ to the sites included between the k-th and the (k+m)-th sites (in Fig. 7e the corresponding part of the diagram is shown by a wavy line), and $\gamma$ to the sites following the (k+m+1)-st site.

After adding the elementary square, the left diagram of Fig. 7e, goes over into the one on the right. We write out the operators corresponding to it:

$$\alpha \underbrace{a_{k+1} a_k^+} \underbrace{a_{k+1}^+ b_{k+m+1}} \beta b_{k+m+1}^+ a_{k+m+2} \gamma. \qquad (2)$$

Pairing in (1) the operators $b_{k+m}$ and $b_{k+m}^+$, and also $a_{k+m+1}$ and $a_{k+m+1}^+$ we get

$$\mathrm{sgn}\,(1) = -\mathrm{sgn}\,\alpha a_k^+ \beta a_{k+m+1}^+ \gamma.$$

In the same way we verify that

$$\mathrm{sgn}\,(2) = -\mathrm{sgn}\,\alpha a_k^+ \beta a_{k+m+1}^+ \gamma.$$

We have thus

$$\mathrm{sgn}\,(1) = \mathrm{sgn}\,(2),$$

and the diagrams in Fig. 7e have the same sign.

The proof in all the other cases is performed in the same way.

To perform the proof for diagrams with intersections it is necessary to include operations of the kind depicted in Fig. 8 among the extension operations.

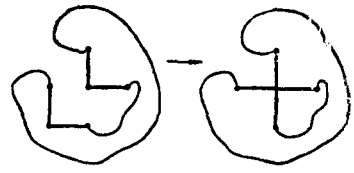

FIG. 8

The proof is then given in an exactly similar way as in the preceding case.

## APPENDIX II

Let there be given $2\tau$ expressions linear in the Fermi operators $c_k^+$ and $c_k$:

$$L_i = \sum_{k=1} (a_{ik} c_k^+ + b_{ik} c_k). \qquad (3)$$

We introduce an equation with which to calculate the trace of the product of such linear expressions

$$S_{2\tau} = \mathrm{Sp}\,(L_1 L_2 \ldots L_{2\tau}). \qquad (4)$$

$$[L_jL_i]_+ = L_jL_i + L_iL_j = \sum_{k,k'} (a_{jk}b_{ik'}[c_k^+c_{k'}] + b_{jk}a_{ik'}[c_kc_{k'}]) = \sum_k (a_{jk}b_{ik} + a_{ik}b_{jk}),$$

$$\mathrm{Sp}\, L_jL_i = \frac{1}{2}\sum_k (a_{jk}b_{ik} + a_{ik}b_{jk}) = \frac{1}{2}[L_jL_i]_+. \tag{5}$$

We draw up a sequence of $2\tau - 1$ identities:

$$\left.\begin{aligned} &\mathrm{Sp}\,(L_1L_2L_3 \ldots L_{2\tau}) + \mathrm{Sp}\,(L_2L_1L_3 \ldots L_{2\tau}) = [L_1L_2]\,\mathrm{Sp}\,(L_3L_4 \ldots L_{2\tau}),\\ &-\mathrm{Sp}\,(L_2L_1L_3 \ldots L_{2\tau}) - \mathrm{Sp}\,(L_2L_3L_1 \ldots L_{2\tau}) = -[L_1L_3]\,\mathrm{Sp}\,(L_2L_4 \ldots L_{2\tau}),\\ &\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\\ &\mathrm{Sp}\,(L_2L_3 \ldots L_1L_{2\tau}) + \mathrm{Sp}\,(L_2L_3 \ldots L_{2\tau}L_1) = [L_1L_{2\tau}]\,\mathrm{Sp}\,(L_2L_3 \ldots L_{2\tau-1}). \end{aligned}\right\} \tag{6}$$

Since the trace of a product is invariant under cyclic permutation of the factors, we get, adding (6),

$$\left.\begin{aligned} 2\mathrm{Sp}\,(L_1L_2 \ldots L_{2\tau}) &= \sum_{i=1}^{2\tau} (-1)^i [L_1L_i]\,\mathrm{Sp}\,(L_2 \ldots L_{i-1}L_{i+1} \ldots L_{2\tau}),\\ S_{2\tau} &= \sum_{i=2}^{2\tau} (-1)^i\,\mathrm{Sp}\,(L_1L_i)\,\mathrm{Sp}\,(L_2L_3 \ldots L_{i-1}L_{i+1} \ldots L_{2\tau}), \end{aligned}\right\} \tag{7}$$

a recurrence formula to evaluate the trace in which we are interested. Applying Eq. (7) consecutively, we get

$$S_{2\tau} = \sum{}' (-1)^p\,\mathrm{Sp}\,(L_{k_1}L_{k_2})\,\mathrm{Sp}\,(L_{k_3}L_{k_4}) \ldots \mathrm{Sp}\,(L_{2\tau-1}L_{2\tau}), \tag{8}$$

where the $\Sigma'$ sign indicates that the summation is taken over all permutations

$$\begin{pmatrix} k_1k_2 \ldots k_{2\tau-1}\,k_{2\tau} \\ 1\ 2 \ldots 2\tau-1\ 2\tau \end{pmatrix}, \tag{9}$$

satisfying the conditions

$$\begin{aligned} &k_1 < k_2,\ k_3 < k_4, \ldots, k_{2n-1} < k_{2n},\\ &k_1 < k_3 < k_5 < \ldots < k_{2\tau-1}, \end{aligned} \tag{10}$$

while p is the parity of the permutation (9).

An expression of the kind (8) is called the Pfaffian of the triangular table of quantities[5]

$$S_{2\tau} = \begin{pmatrix} \mathrm{Sp}\,(L_1L_2)\,\mathrm{Sp}\,(L_1L_3) \ldots \mathrm{Sp}\,(L_1L_{2\tau}) \\ \mathrm{Sp}\,(L_2L_3) \ldots \mathrm{Sp}\,(L_2L_{2\tau}) \\ \ldots\ldots\ldots\ldots\ldots \\ \mathrm{Sp}\,(L_{2\tau-1}L_{2\tau}) \end{pmatrix}. \tag{11}$$

The minor of the Pfaffian corresponding to the element $\mathrm{Sp}\,(L_iL_j)$, $j > i$, is defined as the Pfaffian obtained from the Pfaffian of (7) by striking out two rows (the i-th and k-th) and two columns (the j-th and the k-th).

Equation (7) is the expansion of the Pfaffian (11) in terms of the elements of the first row.

A fundamental theorem in the theory of Pfaffians, which we give without proof, establishes a connection between the square of the Pfaffian and the determinant of the corresponding antisymmetric matrix:

$$S_{2\tau}^2 = \begin{pmatrix} 0 & \mathrm{Sp}\,(L_1L_2) & \mathrm{Sp}\,(L_1L_3) \ldots \mathrm{Sp}\,(L_1L_{2\tau}) \\ -\mathrm{Sp}\,(L_1L_2) & 0 & \mathrm{Sp}\,(L_2L_3) \ldots \mathrm{Sp}\,(L_2L_{2\tau}) \\ -\mathrm{Sp}\,(L_1L_3) & -\mathrm{Sp}\,(L_2L_3) & 0 \ \ldots \mathrm{Sp}\,(L_3L_{2\tau}) \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ -\mathrm{Sp}\,(L_1L_{2\tau}) & \ldots\ldots\ldots\ldots\ldots & 0 \end{pmatrix}. \tag{12}$$

The calculation of the trace through Eq. (4) is thus reduced through Eqs. (5) and (12) to an evaluation of a determinant.

## APPENDIX III

We call the nm by nm block matrix

$$A \times B = \begin{pmatrix} A_{11}B & A_{12}B \ldots A_{1m}B \\ A_{21}B & A_{22}B \ldots A_{2m}B \\ \ldots\ldots\ldots\ldots \\ A_{n1}B & A_{n2}B \ldots A_{nn}B \end{pmatrix} \tag{13}$$

the direct product of an n by n matrix A and an m by m matrix B. It is clear that $A \times B \neq B \times A$.

From the definition the following formulae for products follow

$$\begin{aligned} &(A\times B)\,(C\times D) = AC\times BD,\\ &(A\times B)\,(C\times D)\,(F\times G) = ACF\times BDG. \end{aligned} \tag{14}$$

One can perform a similarity transformation to a direct product

$$(S_1\times S_2)\,(A\times B)\,(S_1^{-1}\times S_2^{-1}) = S_1AS_1^{-1}\times S_2BS_2^{-1}. \tag{15}$$

In the particular case $S_1 = E$ we get the formula

$$(E\times S_2)\,(A\times B)\,(E\times S_2^{-1}) = A\times S_2BS_2^{-1}, \tag{16}$$

given in the text.

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