THERMODYNAMICS OF A SIMPLE CUBIC ISING LATTICE

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It is shown that the logarithm of the partition function for a simple cubic lattice cannot be represented in the form (4) where F(x,y,z, cos p, cos q, cos r) is a polynomial, symmetric in all its arguments, such that for z = 0 (or x = 0, or y = 0) the partition function reduces to the corresponding Onsager formula for the two-dimensional Ising lattice. In contrast to the work of other authors[1-9] the series for the partition function are calculated for the case of a nonsymmetric lattice ($I_x \neq I_y \neq I_z$) both in the "high temperature" and in the "low temperature" approximations.

IN this paper we use two systems of variables*

$$x_i = \operatorname{th}(I_i / kT), \qquad \xi_i = \exp(-2I_i / kT),$$

interrelated by the expressions

$$x_i = \frac{1-\xi_i}{1+\xi_i}, \qquad \xi_i = \frac{1-x_i}{1+x_i} \quad (i = 1, 2, 3), \tag{1}$$

where I_1, I_2, and I_3 are the energies of interaction between two neighboring dipoles having respectively the same x-coordinate, the same y-coordinate, and the same z-coordinate; k is the Boltzmann constant, and T is the temperature. The logarithm of the partition function for a plane square lattice can be represented[8-16] in terms of the variables x_i in the form

$$\ln Z^{(2)} = \ln 2 - {}^1/_2 \ln(1-x^2)(1-y^2) + \frac{1}{2\pi^2}\int_0^\pi\int_0^\pi \ln(1 - 2x\cos p - 2y\cos q + x^2 + y^2 + 2x^2 y\cos q + 2xy^2\cos p + x^2y^2)\,dp\,dq, \tag{2}$$

and in terms of the variables ξ_i in the form

$$\ln Z^{(2)} = -{}^1/_2 \ln(\xi\eta) + \frac{1}{2\pi^2}\int_0^\pi\int_0^\pi \ln(1 - 2\xi\cos q - 2\eta\cos p + \xi^2 + \eta^2 + 2\xi^2\eta\cos p + 2\xi\eta^2\cos q + \xi^2\eta^2)\,dp\,dq. \tag{3}$$

Formulas (2) and (3) go over into one another under the transformations (1).

An exact solution has not yet been found for the logarithm of the partition function for a cubic lattice and, therefore, methods have been developed which enable us to obtain the expansion of the partition function in a series in two limiting cases: for $T \to 0$[1-4] and for $T \to \infty$[3,5-9]. It is shown below that for $T \to \infty$ the logarithm of the partition function can be expanded into the series (8). If the last term in (2) is expanded into a series in the neighborhood of the point x = y = 0, then we obtain a series which goes over into (8) for z = 0 (i.e., $I_3 = 0$). For $T \to 0$ the logarithm of the partition function can be expanded into the series (9). If the last term of formula (3) is expanded into a power series in the neighborhood of the point $\xi = \eta = 0$, then we obtain a series into which (9) goes over for $\zeta = 1$ (i.e., $I_3 = 0$).

Comparing formulas (2), (3), (8), (9), with one another it is sensible to assume that the formula for the partition function of a simple cubic lattice in terms of the variable x_i can be represented in the form[17]

$$\ln Z^{(3)} = \ln 2 - {}^1/_2 \ln[(1-x^2)(1-y^2)(1-z^2)] + \frac{1}{2\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \ln F_1(x, y, z, p, q, r)\,dp\,dq\,dr, \tag{4}$$

and in terms of the variables ξ_i in the form

$$\ln Z^{(3)} = -{}^1/_2 \ln(\xi\eta\zeta) + \frac{1}{2\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \ln F_2(\xi, \eta, \zeta, p, q, r)\,dp\,dq\,dr. \tag{5}$$

In the above: a) the functions F_1 and F_2 are symmetric in all their arguments; b) formula (4) goes over into (2) for z = 0; c) formula (5) goes over into (3) for $\zeta = 1$; d) formulas (4) and (5) go over

*th = tanh.

into each other under the transformations (1); e) formula (4) goes over into (8) if the last term of (4) is expanded in a power series about the point $x = y = z = 0$; f) formula (5) goes over into (9) if the last term of (5) is expanded into a series about the point $\zeta = \eta = \xi = 0$. It can be easily shown that in order for conditions a), b), e) to be satisfied the function F_1 must have the following form:

$$F_1 = 1 - x\,2\cos p - y\,2\cos q - z\,2\cos r + x^2 + y^2 + z^2 + xy^2\,2\cos p + x^2y\,2\cos q + xz^2\,2\cos p + x^2z\,2\cos r + yz^2\,2\cos q + y^2z\,2\cos r + x^2y^2 + x^2z^2 + y^2z^2 + xyz\mathcal{P}(x, y, z, p, q, r). \qquad (6)$$

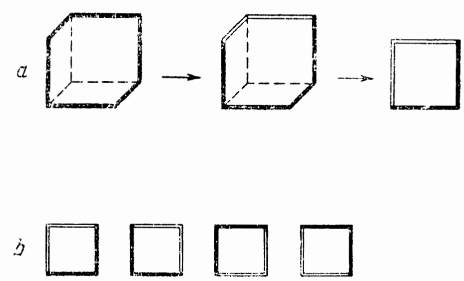
Indeed, we substitute (6) into (4) and, assuming $z = 0$, we obtain (2), while expanding the last term of (4) into a series we obtain the coefficients of all the terms of formula (8) in the form $a(2k, 2l, 0)$.

The function $\mathcal{P}(x, y, z, p, q, r)$ can either be a finite polynomial in the variables x, y, z, or can be expanded into an infinite power series about the point $x = y = z = 0$. In the former case substituting (6) into (4), expanding (4) into a series and comparing the series so obtained with (8), we can write a finite system of equations for the determination of all the terms of the polynomial $\mathcal{P}$. In the latter case, following the procedure described above we shall obtain a finite system of equations (due to the fact that we know a finite number of terms of formula (8) for an infinite number of unknowns). One can hope to be successful in this latter case only when one is able to derive a formula for the general term of the series (8). Therefore, in this paper we consider only the first possibility, viz., that the function $\mathcal{P}$, and, therefore, also F_1 are finite polynomials in the arguments x, y, z. The variables p, q, r can appear in the function $\mathcal{P}$ only in the form of arguments of trigonometric functions, since in the opposite case some of the coefficients in the expansion (8) will contain powers of π. It is shown below that the coefficients referred to above are rational. Since the coefficient of the term $(a_1a_2a_3)$ is equal to zero if any one of the a_i is odd, the function can depend only on cos p, cos q, cos r and on their linear combinations and in each term the total power of x and cos p, y and cos q, z and cos r must be even.

In view of the above discussion the function $\mathcal{P}$ can be represented in the form

$$\mathcal{P} = A\cos p\cos q\cos r\,(111) + \left\{\begin{array}{l} B\cos q\cos r\,(211) + C\cos r\,(221) \\ B\cos p\cos r\,(121) + C\cos q\,(212) + D\,(222) \\ B\cos p\cos q\,(112) + C\cos p\,(122) \end{array}\right\} + \text{terms of higher order.} \qquad (7)$$

We substitute (7) into (6) and (6) into (4), carry out the replacement of variables (1), bring in (4) the expression in the argument of the logarithm to a common denominator, remove this denominator from the logarithm and from the integral, combine similar terms and comparing the resultant expression with (5) we find that all terms of higher order not written out in (7) must be equal to zero. Then by expanding (4) in series and comparing the resultant expression with (8) we obtain a system of equations for obtaining the coefficients A, B, C, D. The system of equations obtained above for the unknowns A, B, C, D is incompatible. Therefore, the logarithm of the partition function of the simple cubic Ising lattice cannot be represented in the form (4) where F_1 is a finite polynomial in terms of the variables x, y, and z.



The red lines are replaced by thin double lines, and the black ones by thick lines. The number of graphs of type a is four. All of them are shown in Fig. b.

The method of evaluating the "high temperature" expansion of the partition function for a cubic nonsymmetric Ising lattice is a simple generalization of the method utilized in a number of papers[1,2,7,8] for the case of a symmetric lattice. It can be shown that the partition function evaluated for a single lattice point is equal to

$$Z^{(3)} = 2(1-x^2)^{-1/2}(1-y^2)^{-1/2}(1-z^2)^{-1/2}\Lambda(x, y, z),$$

$$\Lambda(xyz) = \lim_{N\to\infty}\left\{1 + \sum_{k+l+m\geqslant 2} P(2k, 2l, 2m)\,x^{2k}y^{2l}z^{2m}\right\}^{1/N},$$

where N is the number of lattice points in the lattice, while $P(2k, 2l, 2m)$ is the number of noncoincident spatial graphs constructed from 2k, 2l, 2m segments parallel respectively to the X, Y, Z axes. Moreover, 1) either 0, 2, 4, or 6 and no more segments can meet at each lattice point; 2) the segments must be parallel to the coordinate axes; 3) a segment may connect only the two nearest neighboring lattice points; 4) no two neighboring points can be connected by more than one segment; 5) a graph may be multiply connected.

Since the three coordinate axes have equal status we have:

$$P(2k, 2l, 2m) = P(2k, 2m, 2l) = P(2m, 2k, 2l) = \text{etc.}$$

The plane graphs can be evaluated in the usual manner[1]. A spatial graph of the form (2k, 2l, 2m) can be replaced by a plane multicoloured polygon of the form (2k, 2l). The number of different colors needed to color the sides of this polygon does not exceed m + 1. We illustrate this method on a simple example. Let us consider some spatial graph of the form (2, 2, 2). We shall color the lines lying in the upper plane "red." We shall then plot the projection of this spatial graph on the XY plane retaining the color of the lines, and we shall obtain a plane polygon but a two-colored one. It is evident that two identical spatial graphs shall have identical projections, while different graphs shall be characterized by different projections. It is not difficult to establish a one-to-one correspondence between a colored projection and a spatial graph.

As a result of the calculations carried out above the formula for the logarithm of the partition function for a simple cubic nonsymmetric lattice assumes the form

$$\ln Z^{(3)} = \ln 2 - {}^1\!/_2 \ln\left[(1-x^2)(1-y^2)(1-z^2)\right] + \ln\Lambda(x, y, z); \tag{8}$$

for x = y = z = u

$$\ln\Lambda(u) = 3u^4 + 22u^6 + {}^{375}\!/_2 u^8 + 1980u^{10} + 24044u^{12} + \ldots,$$

where

$$3u^4 = (220) + (202) + (022),$$

$$22u^6 = (420) + (204) + (042) + (240) + (402) + (024) + 16(222),$$

$${}^{375}\!/_2\, u^8 = (620) + (206) + (062) + (260) + (602) + (026) + {}^5\!/_2(440) + {}^5\!/_2(404) + {}^5\!/_2(044) + 58(422) + 58(242) + 58(224),$$

$$1980\, u^{10} = (820) + (208) + (082) + (280) + (802) + (028) + 5(640) + 5(406) + 5(064) + 5(460) + 5(604) + 5(046) + 128(622) + 128(226) + 128(262) + 520(442) + 520(424) + 520(244),$$

$$24044\, u^{12} = (10,2,0) + (2,0,10) + (0,10,2) + (2,10,0) + (10,0,2) + (0,2,10) + {}^{17}\!/_2(840) + {}^{17}\!/_2(408) + {}^{17}\!/_2(084) + {}^{17}\!/_2(480) + {}^{17}\!/_2(804) + {}^{17}\!/_2(048) + {}^{55}\!/_3(660) + {}^{55}\!/_3(606) + {}^{55}\!/_3(066) + 226(822) + 226(228) + 226(282) + 2262(642) + 2262(426) + 2262(264) + 2262(462) + 2262(624) + 2262(246) + 9682(444).$$

The symbol (ik$l$) denotes $x^i y^k z^l$.

Since the coefficient of the term (ik$l$) in the formula for the expansion of the partition function in a series is the number of graphs of a definite kind, it is clear that this coefficient must be an integer, and the corresponding coefficient in formula (8) in the logarithm of the partition function can not be irrational.

The method of evaluating the "low temperature" expansion of the partition function is a simple generalization to the case of a nonsymmetric lattice of the method utilized by many authors[1,3,4,7]. In the case when there is no external magnetic field present the formula for the partition function of a simple cubic lattice assumes the following form:

$$Z^{(3)} = (\xi\eta\zeta)^{-1/2}\Lambda(\xi, \eta, \zeta),$$

$$\Lambda(\xi, \eta, \zeta) = \lim_{N\to\infty}\left\{1 + \sum_{n;\,k,l,m} G(n; k, l, m)\, \xi^{2(n-k)}\, \eta^{2(n-l)}\, \zeta^{2(n-m)}\right\}^{1/N},$$

where G(n; k, l, m) is the number of graphs of the most general form containing n lattice points, k connections joining these lattice points, parallel to the X axis, l connections parallel to the Y axis, and m connections parallel to the Z axis.

Utilizing the technique described above of replacing the spatial graphs by plane colored polygons, we obtain the series expansion of the partition function,

$$\ln Z^{(3)} = -{}^1\!/_2 \ln(\xi\eta\zeta) + \ln\Lambda(\xi, \eta, \zeta); \tag{9}$$

for $\xi = \eta = \zeta = t$ we obtain

$$\ln\Lambda(t) = t^6 + 3t^{10} - {}^7\!/_2 t^{12} + 15t^{14} - 33t^{16} + {}^{313}\!/_3 t^{18} - {}^{561}\!/_2 t^{20} + 849t^{22} - {}^{9847}\!/_4 t^{24} + \ldots,$$

where

$$t^6 = (222),$$

$$3t^{10} = (442) + (424) + (244),$$

$$-{}^7\!/_2 t^{12} = -{}^7\!/_2(444),$$

$$15\, t^{14} = (266) + (626) + (662) + 4(446) + 4(464) + 4(644),$$

$$-33\, t^{16} = (448) + (484) + (844) - 12(466) - 12(646) - 12(664),$$

$${}^{313}\!/_3\, t^{18} = (288) + (828) + (882) + 8(468) + 8(846) + 8(684) + 8(648) + 8(486) + 8(864) + {}^{160}\!/_3(666),$$

$$-{}^{561}\!/_2\, t^{20} = 4(4,6,10) + 4(6,10,4) + 4(10,4,6) + 4(6,4,10) + 4(4,10,6) + 4(10,6,4) - {}^{51}\!/_2(488) - {}^{51}\!/_2(848) - {}^{51}\!/_2(884) - 76(668) - 76(686) - 76(866),$$

$$849\, t^{22} = (2,10,10) + (10,2,10) + (10,10,2) + 12(4,8,10) + 12(8,10,4) + 12(10,4,8) + 12(8,4,10)$$

$$+12(4,10,8)+12(10,8,4)+9(6,6,10)+9(6,10,6)$$
$$+9(10,6,6)+247(688)+247(868)+247(886)$$
$$+(4,6,12)+(6,12,4)+(12,4,6)+(6,4,12)$$
$$+(4,12,6)+(12,6,4),$$

$$-{}^{9847}/_{4}t^{24}=8(4,8,12)+8(8,12,4)+8(12,4,8)$$
$$+8(8,4,12)+8(4,12,8)+8(12,8,4)+24(6,6,12)$$
$$+24(6,12,6)+24(12,6,6)-44(4,10,10)$$
$$-44(10,4,10)-44(10,10,4)-240(6,8,10)$$
$$-240(8,10,6)-240(10,6,8)-240(8,6,10)$$
$$-240(6,10,8)-240(10,8,6)-{}^{4039}/_{4}(888).$$

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