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Statistical Mechanics of "2x2x2" Ising Model

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Abstract

The partition function of 2×2×2 Ising lattice with external magnetic field was calculated by elementary enumeration of complexions. The zeros of the partition function in the complex temperature and in the complex magnetic field plane were obtained. The internal energy, specific heat, magnetic susceptibility in the absence of magnetic field, and the magnetization with external magnetic field were also calculated. The estimated critical temperatures from the zeros near the positive real axis and from the maximum of specific heat curve are compared with that obtained from the Pade' approximation for the infinite lattice system. It is shown that the zeros of partition function of ferromagnet lie on the unit circle, and those of antiferromagnet distribute on the negative real axis in the complex fugacity plane.

I. Introduction

Onsager,[1] Kaufman,[2] and Nambu[3] obtained a rigorous form of the partition function of the infinite two dimensional square Ising lattice in the absence of external magnetic field. In general case under arbitrary magnetic field the partition function has not yet been obtained. It seems impossible to obtain the exact solution for the threedimensional cubic lattice. Many approximation methods[4-6] for obtaining the partition function have been proposed and the approximate values of the critical temperature of the threedimensional Ising lattice have been estimated. Among them the Pade' approximation seems to be the best for estimating critical temperature. Another approach to this problem was attempted by Katsuras[7].

We consider the "2×2×2" cubic Ising lattice. The partition function of such system was obtained in a closed form as a function of temperatures and the external magnetic field. By using the calculated partition function the critical temperatures from the complex temperature plane and from the maxima of the specific curve were estimated. These results were compared with those of one of auther's previous work for finite system[8] and with that of Pade' approximation for infinite system. The Lee-Yang theorem[9] which states that all the zeros of the partition function of the Ising ferromagnets lie on the unit circle in the complex magnetic field plane holds for the 2×2×2 ferromagnet. It is shown that the zeros of antiferromagnet distribute on the negative real axis. This situation resembles that of antiferromagnetic finite Heisenberg systems. The internal energy, magnetization and the magnetic susceptibility were calculated as functions of temperature. The magnetization-field plot for ferromagnetic case indicates that the plot is always a convex function[10].

II. The Partition Function

Let us consider the "2×2×2" Ising lattice with usual periodic boundary conditions as shown in Fig.1. On the i-th lattice point, there is a spin which is represented by S_i. Each spin is capable of having only two orientations as $S_i=+\frac{1}{2}$ and $S_i=-\frac{1}{2}$. The energy on each spin depends on the orientation of its immediate neighbors and on the external magnetic field H. For a particular spin configuration the hamiltonian can be written as

$$\mathcal{H}_c = -2J \sum_{\langle i,j \rangle} S_i S_j - g\mu_B H \sum_i S_i \qquad (1)$$

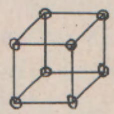
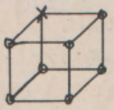
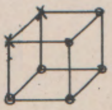
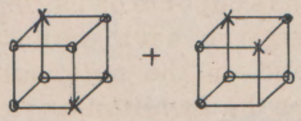
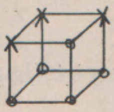
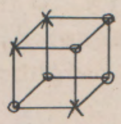
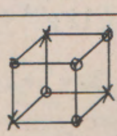
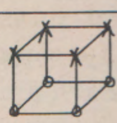
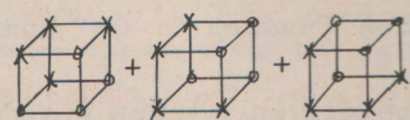
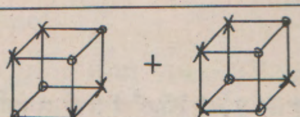
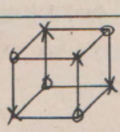
Where $\langle i,j \rangle$ sum over all nearest neighbors pairs, $\sum_i$ the sum over all spins which have total number N, μ_B is Bohr magneton, g the g factor, J the exchange integral, n the number of nearest neighbors.
The energy for this configuration is

$$E_c = -\left[\frac{1}{2}\left(\frac{2J}{4} Nn\right) - 2\left(\frac{2J}{4} P\right)\right] - \frac{1}{2}(N-2r) g\mu_B H \qquad (2)$$

Let $g(p,r)$ be the number of the configurations of which the total numbers of the anti-parallel pairs of spin and reversed spins are represented by p and r, respectively. Then the partition function can be written as

$$Z = \sum_{p,r} g(p,r) e^{-E_c/kT} \qquad (3)$$

In the ground state all spins are oriented paralled to each other with their magnetic moments point in the direction of the external magnetic field. The energy is $-\frac{3}{2}NJ-\frac{1}{2}N\mu_B gH$. The first higher state is given by the reversal of a single spin and the energy for this state is $-(\frac{3}{2}N-6)J-\frac{1}{2}(N-2)g\mu_B H$. As it does not matter which spin is reversed, the number of configurations is N. The second higher state corresponds to the reversal of two neighboring spins, with energy $-(\frac{3}{2}N-8)J-\frac{1}{2}(N-4)g\mu_B H$ and $g(p,r)=N$, and so forth. Thus we obtain:

Configurations of spins (up spin: 0 down spin: x)	E_C	g(p, r)
	$-12J-4g\mu_BH$	1
	$-6J-3g\mu_BH$	8
	$-4J-2g\mu_BH$	12
	$-2g\mu_BH$	4+12=16
	$-2J-g\mu_BH$	24
	$2J-g\mu_BH$	24
	$6J-g\mu_BH$	8
	$-4J$	6
	0	8+12+12=32
	$4J$	6+24=30
	$12J$	2

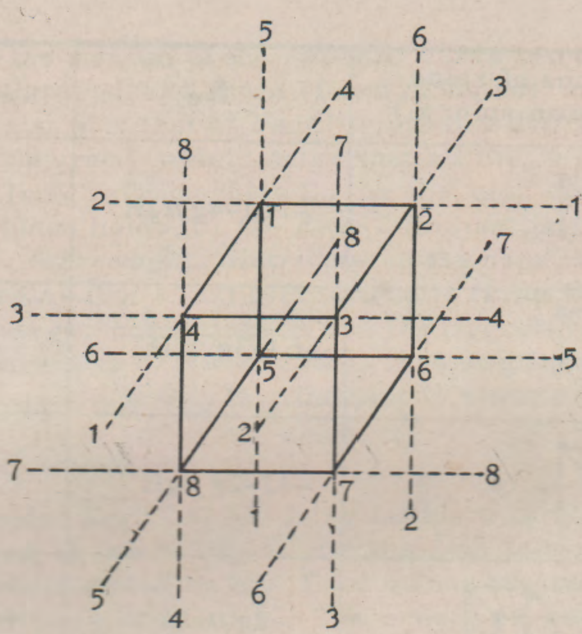


Fig. 1. $2\times2\times2$ cubic lattice with cyclic boundary condition.

In the calculation for $g(p,r)$ above we note that reversing of all spins leaves $g(p,r)$ unchanged, thus

$$g(p,r)=g(p,N-r) \tag{4}$$

The partition function now can be written as

$$Z_{2\times2\times2}(y,z)=y^{-12}(z^4+z^{-4})+8y^{-6}(z^3+z^{-3})+(12y^{-4}+16)(z^2+z^{-2})$$
$$+(24y^{-2}+24y^2+8y^6)(z+z^{-1})+6y^{-4}+32+30y^4+2y^{12} \tag{5}$$

where

$$y=e^{-J/kT}$$
$$z=e^{-g\mu_B H/kT} \tag{6}$$

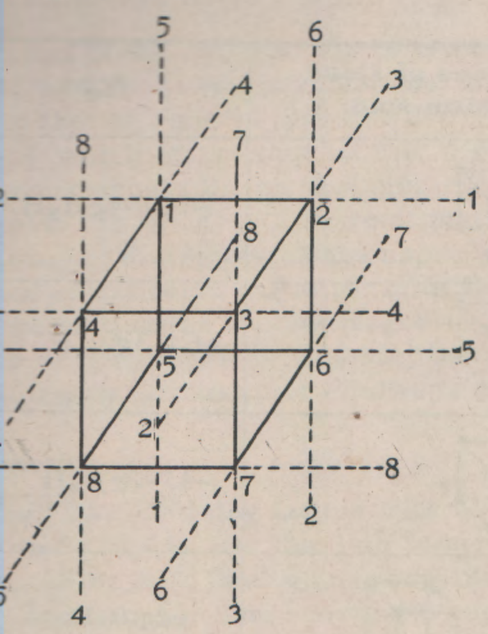
III. Distribution of Zeros of the Partition Function in the Complex Temperature Plane

In the absence of the magnetic field the partition function is reduced to

$$z(y,1)=2(y^{-12}+8y^{-6}+15y^{-4}+24y^{-2}+32+24y^2+15y^4+8y^6+y^{12}) \tag{7}$$

The distribution of zeros of the equation

$$Z(y,1)=0 \tag{8}$$



. 2×2×2 cubic lattice with
cyclic boundary condition.

r g(p,r) above we note that reversing of all spins
ged, thus

$$g(p,r)=g(p,N-r) \quad (4)$$

n now can be written as

$$=y^{-12}(z^4+z^{-4})+8y^{-6}(z^3+z^{-3})+(12y^{-4}+16)(z^2+z^{-2})$$

$$24y^2+8y^6)(z+z^{-1})+6y^{-4}+32+30y^4+2y^{12} \quad (5)$$

$$y=e^{-J/kT}$$

$$z=e^{-g\mu_B H/kT} \quad (6)$$

Zeros of the Partition Function in the Complex
lane

the magnetic field the partition function is reduced

$$8y^{-6}+15y^{-4}+24y^{-2}+32+24y^2+15y^4+8y^6+y^{12}) \quad (7)$$

of zeros of the equation

$$Z(y,1)=0 \quad (8)$$

in the complex $y=e^{-J/kT}$ plane determines the thermodynamical behaviour of the system. Since all the coefficients are positive this equation gives no zeros on the positive real axis of the complex plane. The number of zeros will increase as the size of the lattice increase. In the limit of the infinite lattice the distribution of these zeros will become a continous curve which will intersect with the positive real axis at the value $y=e^{-J/kT}$ corresponding to the critical temperature T_c. The zeros are plotted on the complex y plane as shown in Fig. 2.

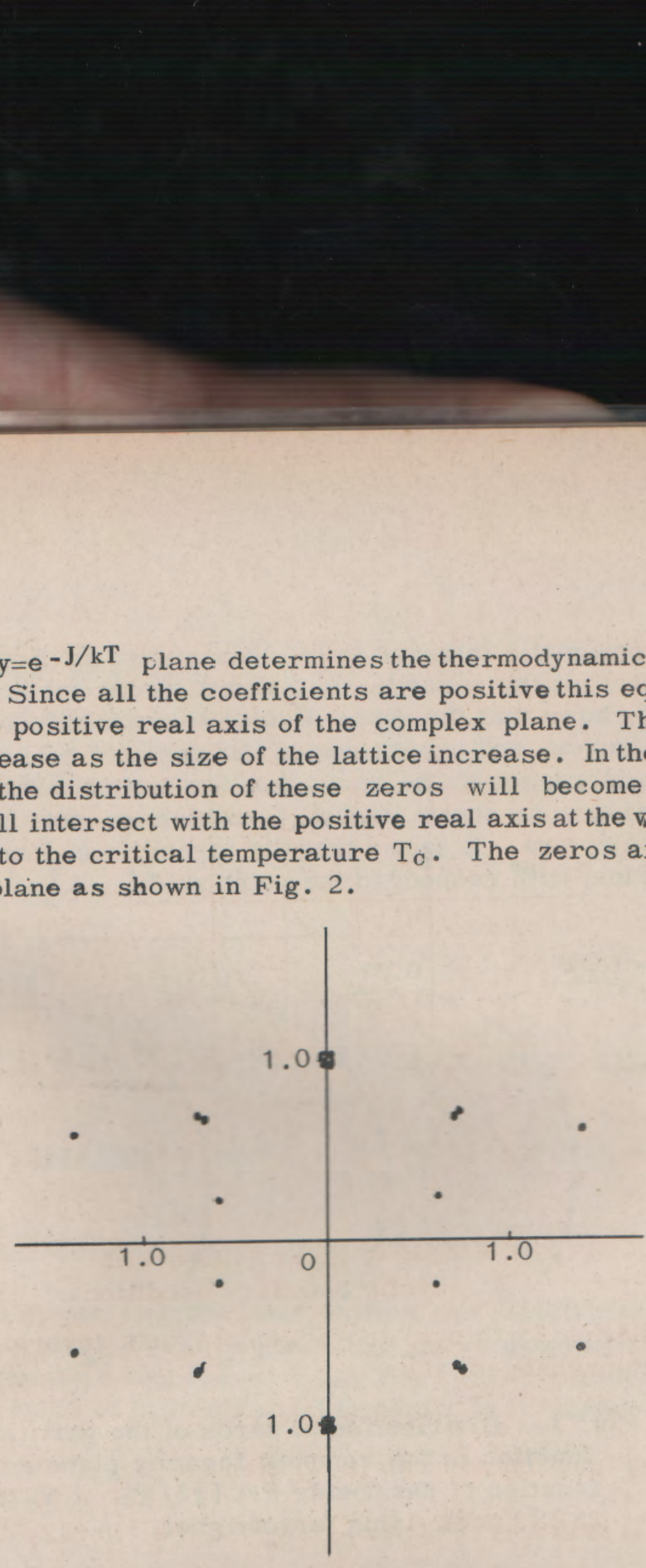


Fig. 2. Distribution of zeros in the $e^{-|J|/kT}$ plane for the "2×2×2" cubic Ising lattice.

The value of y corresponding to the critical temperature of which the value is estimated from zeros near the positive real axis is $y_c=0.595$ which is smaller than the critical value $y_c=0.642$ obtained from the Pade' approximation[11]. It is shown that the value of y_c seems to approach to y_c as the system of the lattice increase[8,12].

IV. Distribution of Zeros of the Partition Function in the Fugacity Plane

Lee-Yang and Asano[13] indicate that the zeros of the partition function lie on the unit circle in the fugacity plane and this concept is very useful for the purpose of investigating critical behaviours in magnetic system.[14-26] The distribution of zeros of the partition function, given by

$$Z(y,z)=0 \quad (9)$$

for the ferromagnetic interaction ($J>0$) is shown in Fig. 3, from which it is found that all the zeros lie on the unit circle in the complex fugacity plane. It is shown that the zeros distribute uniformly on the circle for high temperatures, and crowd toward the negative real half plane as the temperature increases. The zeros for the antiferromagnet lie on the negative real axis as shown in Fig. 4, which is not inconsistent with Suzukis' conjecture. It seems that the logarithmic locations of zeros are symmetrical with respect to the point $z=-1$.

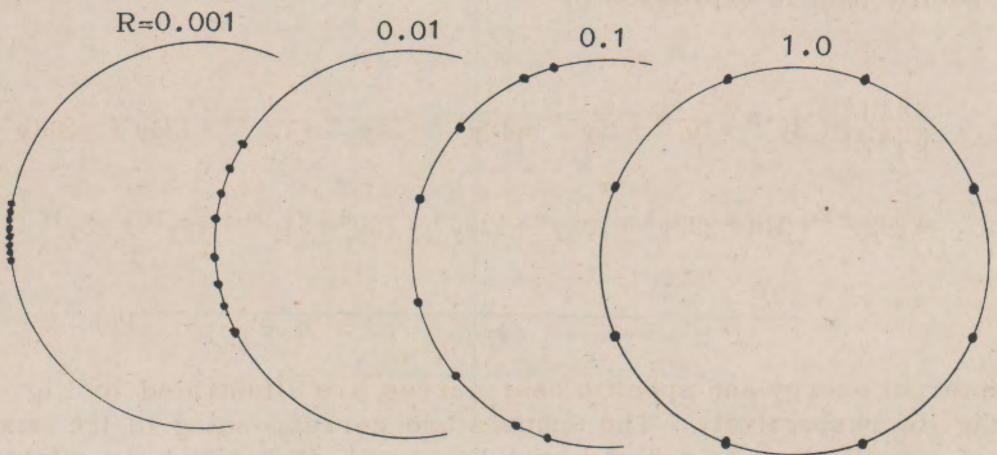


Fig. 3. Distribution of zeros of the partition function in the complex fugacity plane as a function of parameter $R \equiv |J|/kT$ for the $2\times2\times2$ cubic Ising ferromagnet.

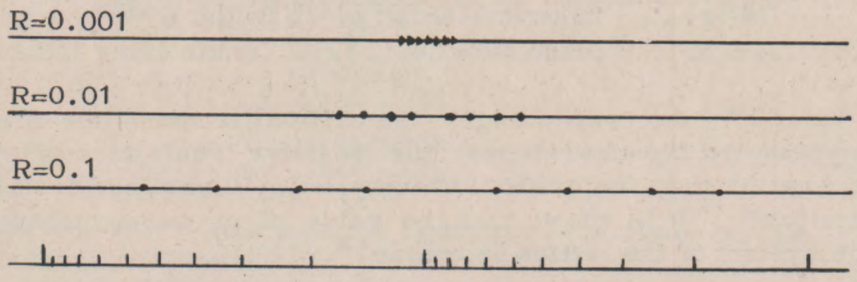


Fig. 4. Distribution of zeros of the partition function in the complex fugacity plane for the $2\times2\times2$ cubic Ising antiferromagnet $R \equiv J/kT$.

V. Thermodynamic properties

Owing to the symmetry in the coefficients of the zero--field (z=1) partition function, all the thermodynamic properties are identical for both ferro--and antiferro--interactions. The internal energy is given by

$$E = \frac{24J}{Z} \left(-y^{-12} - 4y^{-6} - 5y^{-4} - 4y^{-2} + 4y^{2} + 5y^{4} + 4y^{6} + y^{12} \right) \qquad (10)$$

The specific heat is expressed by

$$C = \frac{384\,J^2}{KT^2Z^2} (3y^{-18} + 10^{-16} + 25y^{-14} + 48y^{-12} + 54y^{-10} + 72y^{-8} + 138y^{-6} + 208y^{-4}$$

$$+ 292y^{-2} + 348 + 292y^{2} + 208y^{4} + 138y^{6} + 72y^{8} + 54y^{10} + 48y^{12} + 25y^{14}$$

$$+ 1\ y^{16} + 3y^{18}) \qquad (11)$$

The internal energy and specific heat curves are illustrated in Fig. 5 and Fig. 6, respectively. The temperature corresponding to the maximum of specific heat as denoted by KT_m / J is 1.81 , which is slightly smaller than the value of 2.26 obtained from the Pade' approximation.

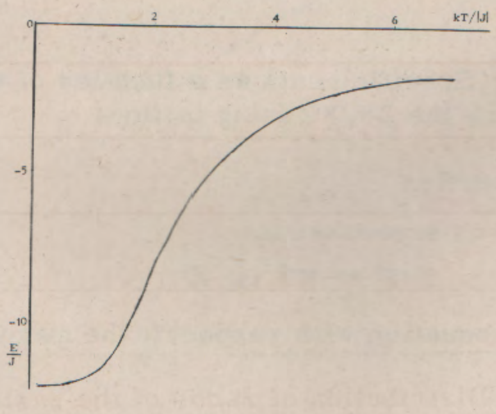


Fig. 5. Internal energy as a function of the temperature kT/J for simple cubic 2×2×2 Ising lattice.

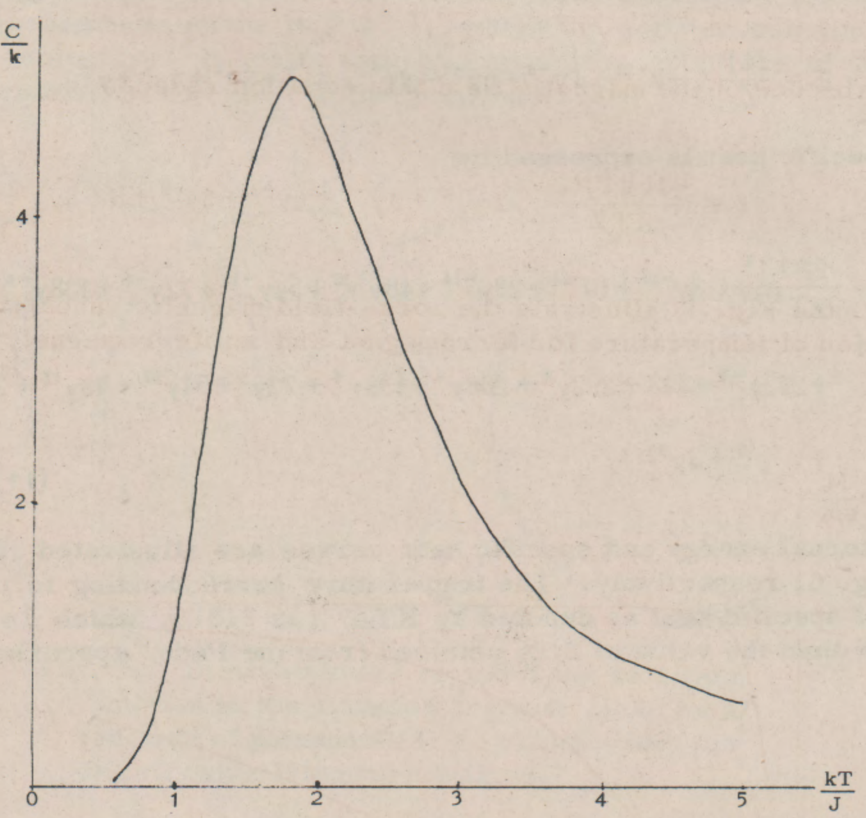


Fig. 6. Specific heats as a function of temperature kT/J for the 2×2×2 Ising lattice.

VI. Magnetic Properties

The free energy is expressed as

$$F = -KT \log Z \tag{12}$$

Differentiating this equation with respect to the magnetic field, we obtain the magnetization

$$M = \frac{g\mu_B}{Z}\left[4y^{-12}(z^4 - z^{-4}) + 24y^{-6}(z^3 - z^{-3}) + (24y^{-4} + 32)(z^2 - z^{-2}) + (24y^{-2} + 24y^2 + 8y^6)(z - z^{-1})\right]$$

This indicated that the spontaneous magnetization can not be observed for the finite system of lattice. The variation of the magnetization as a function of the magnetic field and of the temperature are given through Fig. 7 to Eig. 9 respectively. The magnetic susceptibility is calculated by differentiating the magnetization with respect to H as

$$\chi = -\frac{g^2 \mu_B^2}{KYZ^2} \left[Z\frac{\partial Z}{\partial z} + zZ\frac{\partial^2 Z}{\partial z^2} - z\left(\frac{\partial Z}{\partial z}\right)^2 \right] \tag{14}$$

In the absence of the magnetic field this equation reduces to

$$\chi = \frac{-16 g^2 \mu_B^2}{KTZ} \left(2y^{-12} + 9y^{-6} + 6y^{-4} + 3y^{-2} + 8 + 3y^2 + y^6 \right) \tag{15}$$

Fig. 10 and Fig. 11 illustrate the zero--field magnetic susceptibility as a function of temperature for ferromagnet and antiferromagnet, respectively.

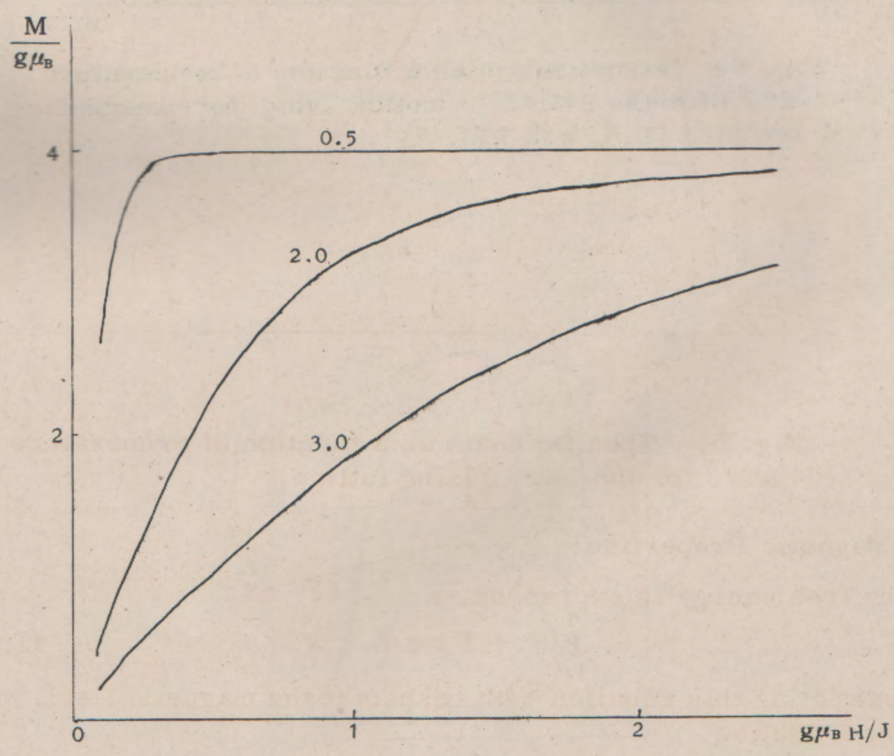


Fig. 7. Variation of magnetization as a function of magnetic field $g\mu_B H/J$ for the $2\times2\times2$ cubic Ising ferromagnet; kT/J=3.0, 2.0 and 0.5.

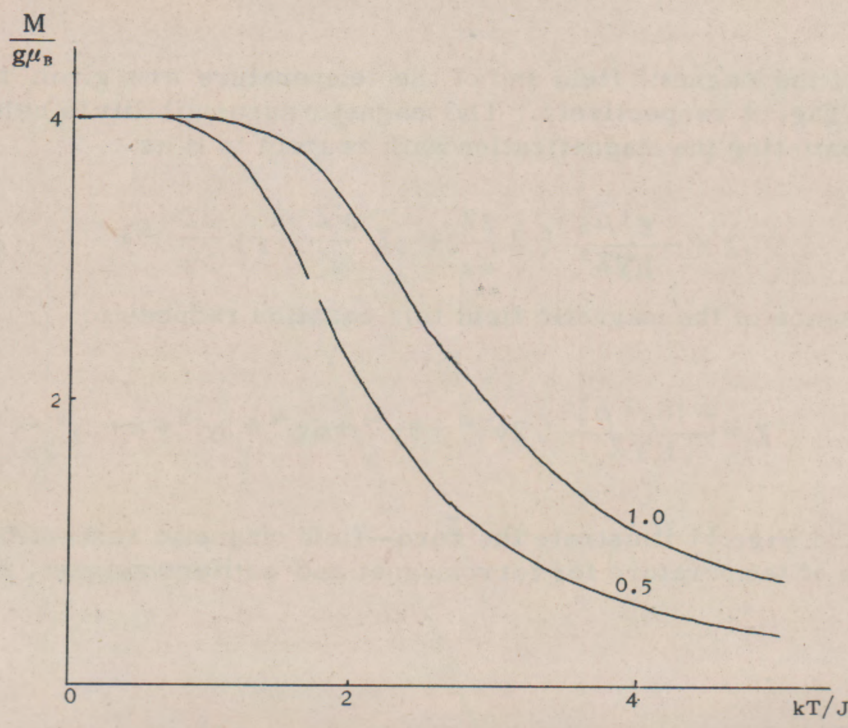


Fig. 8. Magnetization as a function of temperature kT/J for the 2×2×2 cubic Ising ferromagnet; $g\mu_B H/J = 0.5$, and 1.0.

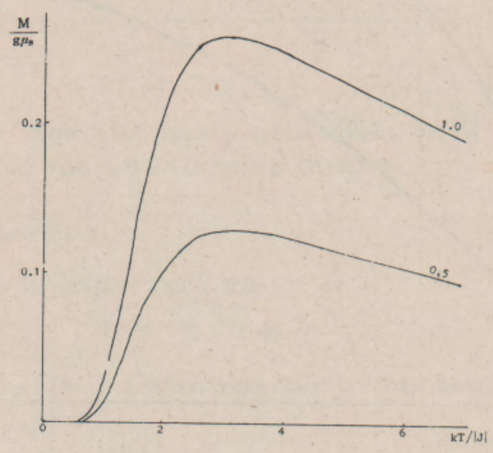


Fig. 9. Magnetization as a function of temperature kT/J for the 2×2×2 cubic Ising antiferromagnet; $g\mu_B H/J = 0.5$ and 1.0.

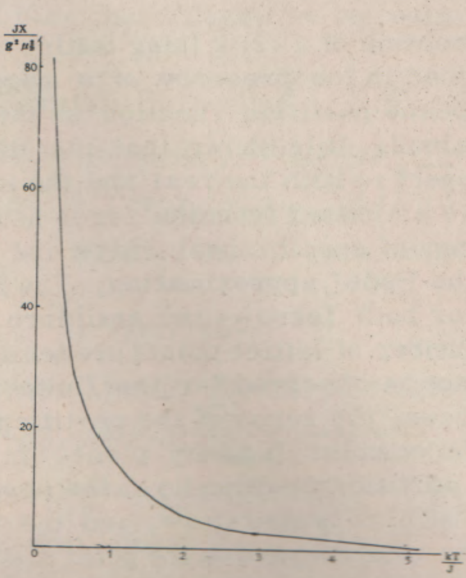


Fig. 10 Zero-field susceptibility as a function of temperature kT/J for the 2×2×2 cubic Ising ferromagnet.

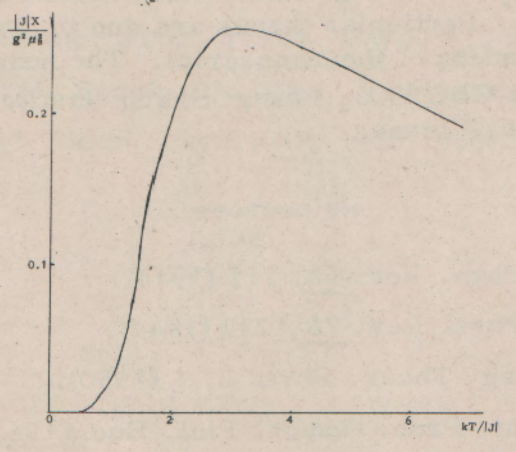


Fig. 11 Zero-field susceptibility as a function of temperature kT/|J| for the 2×2×2 Ising antiferromagnet.

VII. Summery

The partition function of $2\times2\times2$ Ising lattice with periodic boundary condition was obtained in the presence of a magnetic field. The distribution of zeros of the partition function in the complex temperature plane has been obtained. It is shown that the distribution of zeros is symmetric with respect to both the real and the imaginary axes, and the critical temperature estimated from the zeros near the positive real axis and from the maximum of specific heat curve are smaller than the Curie temperature from the Pade' approximation. The thermodynamic properties are identical for both ferro -- and antiferro -- interactions for the system with even number of lattice points in each side. The spontaneous magnetization can not be observed for the finite size of the lattice. In the ferromagnetic case, the zeros of the partition function distribute on the unit circle in the complex fugacity plane. In the antiferromagnetic case, the zeros of partition function lie on the negative real axis of complex fugacity plane at high temperature, and the logalithmic location of zeros are symmetric with respect to the point $z=-1$. Since it is expected that there should be a phase transition for the infinite lattice in antiferromagnetic interaction, where the zeros of the partition function should accumulate near the positive real axis, thus the fact that the zeros of partition function of antiferromagnetic case lie on the negative real axis of the complex fugacity plane must be due to the small size of the lattice or due to not sufficiently low temperature.

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