International Journal of Theoretical Physics, Vol. 39, No. 2, 2000

One-, Two-, and Three-Dimensional Ising Model in the Static Fluctuation Approximation

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Received March 16, 1999

Viewed as a prototype for strongly interacting many-body systems, the spin-1/2 n-dimensional Ising model ($n = 1, 2, 3$) is studied within the so-called *static fluctuation approximation* (SFA). The underlying physical picture is that the local field *operator* σ_f^z with *quadratic* fluctuations is replaced with its mean value $[(\sigma_f^z)^2 \cong \langle(\sigma_f^z)^2\rangle]$. This means that the true quantum mechanical spectrum of the operator σ_f^z is replaced with a distribution; along with the calculation of its mean value, we take into account *self-consistently* the moments of this distribution. It is shown that this sole approximation is sufficient for deducing the equilibrium correlation functions and the main thermodynamic characteristics of the system. Special new features of this study include an analysis of the two-dimensional model *without* periodic boundary conditions, and the demonstration that the phase-transition scenario is quite sensitive to the boundary conditions in the two- and three-dimensional cases. In passing, new boundary problems in mathematical physics are emphasized.

1. INTRODUCTION

The spin-1/2, or two-state, Ising model was introduced in 1925 (Brush, 1967). Since then it has been one of the most thoroughly studied models in statistical mechanics and many-body theory. This is not surprising in view of its relative simplicity, which has led to rigorous solutions for both one-dimensional and certain two-dimensional lattices, as well as its broad range of applicability to real physical systems (Honmura and Kaneyoshi, 1979; Taggart and Fittipaldi, 1982). In addition, it has been treated as a "laboratory" for testing a variety of theories and techniques. Recently (Bune *et al.*, 1998) it has even been invoked for modeling ferroelectricity in two-dimensional polymer films.

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0020-7748/00/0200-0405$18.00/0

It is its appeal as a prototype for strongly interacting many-body systems that has motivated the present paper. The main objective is to develop a new general approach for many-body systems which is simple, transparent, and avoids the complications and shakey approximations of conventional many-body theories, especially of the perturbative variety—diagrammatic techniques, Green's functions, the heavy reliance on an expansion parameter that is not really small, and so forth (Abrikosov *et al.*, 1965; Fetter and Walecka, 1971). The spin-l/2 Ising model in an arbitrary integral dimension will be regarded as a mere application of this approach; other applications for Fermi and Bose systems with strong interparticle correlations and arbitrary interaction will follow in subsequent papers. [A preliminary study of electronic correlations within this approach has, in fact, already been carried out (Loskutov *et al.,* 1996)].

Earlier versions of our approach, which has been called the static fluctuation approximation (SFA) for reasons that will become apparent shortly, have already been presented in a series of papers (Nigmatullin and Toboev, 1986, 1988, 1989). The key physical idea lies in the optimal, and (from our point of view) physically obvious, modification of the mean-field approximation in that the operator of *quadratic fluctuations*, which can have either a scalar or a vector nature, is replaced with its mean value. It turns out that this sole approximation is sufficient for calculating the equilibrium correlation functions as well as all principal characteristics of the system. To this end it is necessary to obtain the linearized, self-consistent (difference) long-range equation ([D]LRE) [an exact [D]LRE was obtained for the first time for the one-dimensional Ising model by Jelifonov (1971) for the corresponding Hamiltonian], the qualifier 'difference' being applicable to lattice systems.

Among the highlights of the present study of the spin-1/2 Ising model within the framework of the SFA are (i) an analysis of the two-dimensional model *without periodic boundary conditions*, (ii) the identification of SFA solutions with new boundary problems in mathematical physics, and (iii) the demonstration that the phase-transition scenario is quite sensitive to the boundary conditions in the two- and three-dimensional cases. This fact was first discovered and discussed by Jelifonov (1971).

It should be emphasized right at the outset that the present approach is *not* just one version of a mean-field theory; the SFA goes beyond the mean-field approximation (MFA) and its known modifications. In particular, in the MFA, it is impossible to calculate the equilibrium correlation functions of the system with an *arbitrary* interaction and in an *arbitrary* geometrical configuration. In the SFA, however, knowing the DLRE, it will be shown *how* to obtain these functions to *any* order for any integral dimension and for boundary conditions *other than periodic conditions* which are commonplace in statistical mechanics.

The synopsis of the rest of the paper is as follows: In Section 2 the linearized DLREs for the spin-1/2 Ising model of an arbitrary integral dimension are derived. This is followed, in Section 3, by an analysis of the one-dimensional model; comparison with exact solutions (Jelifonov, 1971) is meticulously made. Next, in Section 4, the two-dimensional model is studied; the thermodynamic properties of an infinite plane are determined. Section 5 is devoted to the three-dimensional model, complete with the effects of boundary conditions. The paper closes, in Section 6, with general conclusions.

2. THE LINEARIZED DIFFERENCE LONG-RANGE EQUATIONS FOR THE ISING MODEL ($S = 1/2$)

We start with a system of spins localized at the nodes of a lattice and related to each other by an overall attractive potential, $U(f - f') < 0$. The Hamiltonian of the system is in the form

$$H = -\omega_0 \sum_f S_f^z - \frac{1}{2} \sum_{f,f'} U(f - f') S_f^z S_{f'}^z = -\sum_f S_f^z \sigma_f^z \tag{1}$$

Here $U(f - f') \equiv U_{ff'} = U\Phi(|\mathbf{r}_f - \mathbf{r}_{f'}|/a)$ is positive-definite (the minus sign being explicitly shown in the Hamiltonian), a is the lattice constant, and

$$\sigma_f \equiv \omega_0 + \sum_{f'} U_{ff'} S_{f'}^z \tag{2}$$

is the operator of the total local field acting on the spin localized in the node f. We write down the Heisenberg equations of motion ($\hbar \equiv 1$):

$$\frac{dS_f^x}{dt} = i[H, S_f^x] = \sigma_f^z S_f^y \tag{3a}$$

$$\frac{dS_f^y}{dt} = i[H, S_f^y] = -\sigma_f^z S_f^x \tag{3b}$$

The principal approximation on which our whole approach is based is that the square of the operator of the total local field, defined by expression (2), is replaced with its average value:

$$(\sigma_f^z)^2 \cong \langle(\sigma_f^z)^2\rangle \tag{4}$$

The *physical meaning* of this approximation is the following. The true quantum mechanical spectrum of the operator σ_f^z is replaced with a distribution; along with the calculation of its mean value (MFA), we take into account the moments of this distribution (SFA). As a first step we shall calculate here *self-consistently* the *quadratic fluctuations* of σ_f^z which lead to the approximate but *linearized* DLRE, which, in turn, can be solved by well-known mathematical methods.

Based on the definition of the Euclidean norm of an operator,

$$\|A\| = [\mathrm{Tr}(AA^+)]^{1/2} \tag{5}$$

together with the Cauchy–Schwarz inequality, one can show that the Euclidean norm of the difference,

$$\|(\sigma_f^z)^2 - \langle(\sigma_f^z)^2\rangle\| \leq \sum_{f',f''} U_{ff'} U_{ff''} \left| \frac{S(S+1)}{3} - \langle S_{f'}^z S_{f''}^z \rangle \right| \tag{6}$$

is bounded at all temperatures and can be estimated for any given S and $U_{ff'}$.

The substitution of the operator of the total local field by its average value allows us to extend the range of validity of the SFA and obtain the DLREs for a wide class of Hamiltonians. This supersedes the approximation used in previous papers (Nigmatullin and Toboev, 1986, 1988, 1989), where, from the operator of the total local field, its mean value was subtracted and then the *remaining* operator of relative quadratic fluctuations was substituted by its average value:

$$(\Delta\sigma_f^z)^2 \cong \langle(\Delta\sigma_f^z)^2\rangle \tag{7}$$

Here $\Delta\sigma_f^z \equiv \Sigma_{f'} U_{ff'} \Delta S_{f'}^z$, and $\Delta S_f^z \equiv S_f^z - \langle S_f^z \rangle$ is the operator of relative spin deviations of the node f.

With approximation (4), the equations of motion (3) assume a closed form. The solutions can be written down at once:

$$S_f^x(t) = \cos(\Omega_f t)\, S_f^x(0) + \frac{\sin(\Omega_f t)}{\Omega_f} \sigma_f^z S_f^y(0) \tag{8a}$$

$$S_f^y(t) = \cos(\Omega_f t)\, S_f^y(0) - \frac{\sin(\Omega_f t)}{\Omega_f} \sigma_f^z S_f^x(0) \tag{8b}$$

Here $\Omega_f \equiv \sqrt{\langle(\sigma_f^z)^2\rangle}$ is the frequency of the total field, together with its quadratic fluctuations. The required mean values are found in accordance with the formula

$$\langle B(-i\beta)C \rangle = \langle CB \rangle \tag{9}$$

The notation $\langle \cdots \rangle \equiv \mathrm{Tr}[\exp(-\beta H) \ldots]/Q$ denotes the averaging procedure over the canonical ensemble: Q is the partition function, $\beta \equiv 1/T$ is the inverse temperature (Boltzmann's constant k_B being set to unity), and B and C are arbitrary operators. Putting $B \equiv S_f^x$ and $C \equiv S_f^x A$, with A being a set of spin operators except for the node f, we obtain the equation (or equations for other cases) relating the spin of the node f with all other spins via $U(f - f')$.

For the one-dimensional Ising model such equations have been called the *difference long-range equations* (DLREs) (Jelifonov, 1971); the exact solution for this model has been obtained for various boundary conditions. In this paper we shall retain this abbreviation. Simple manipulations lead to the following linearized DLRE in the SFA:

$$\langle S_f^z A\rangle = \eta_f \langle \sigma_f^z A\rangle \tag{10a}$$

where

$$\eta_f \equiv \frac{1}{2\Omega_f}\tanh\left(\frac{\beta\Omega_f}{2}\right) \tag{10b}$$

The DLRE allows one to obtain closed equations for all microscopic values and to calculate completely the thermodynamics of the system considered.

We show here how to close the system of equations for the ferromagnetic Ising lattice of an arbitrary integral dimension.

If the lattice is regular and has translational symmetry, then Ω_f does not depend on the index of the node f. Putting $A = 1$ in DLRE (10a), we have

$$\langle S_f^z\rangle = \eta\langle \sigma_f^z\rangle = \eta\left(\omega_0 + \sum_{f'} U_{ff'}\langle S_{f'}^z\rangle\right) \tag{11}$$

We are interested in the homogeneous solutions of this equation. With the notation

$$\langle S_f^z\rangle \equiv \mu/2; \qquad p \equiv \eta\sum_{f'} U_{ff'} = \eta U(0) = \eta U\Phi(0) \tag{12}$$

$U(0)$ being the zero Fourier component of the interaction, we can write (11) in the form

$$\mu(1 - p) = 2p\omega_0/U(0) \tag{13}$$

Using the operators of spin deviations $\Delta S_f^z \equiv S_f^z - \langle S_f^z\rangle$ and subtracting Eq. (11) from (10a), we can rewrite the DLRE in the form

$$\langle \Delta S_f^z A\rangle = \eta\langle \Delta\sigma_f^z A\rangle \tag{14}$$

where $\Delta\sigma_f^z \equiv \Sigma_{f'} U_{ff'}\Delta S_{f'}^z$. From (14) we obtain the equations for the pair correlation function. For this purpose, we put $A \equiv \Delta S_{f'}^z$ in (14):

$$\begin{aligned}\langle \Delta S_f^z\, \Delta S_{f'}^z\rangle_c &= \eta\sum_{f''} U(f - f'')\langle \Delta S_f^z\, \Delta S_{f'}^z\rangle \\ &= \eta U(f - f')\langle(\Delta S_{f'}^z)^2\rangle + \eta\sum_{f''} U(f - f'')\langle \Delta S_f^z\, \Delta S_{f''}^z\rangle_c \end{aligned} \tag{15}$$

The index c in the correlation function means that all pair correlations are taken into account except the case when $f = f'$. To find the pair correlation function from (15), we assume the validity of cyclic boundary conditions. In this case we use the Fourier transforms in accordance with

$$\langle \Delta S_f^z \, \Delta S_{f'}^z \rangle_c = \frac{1}{N} \sum_{\mathbf{k}} K(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{r}_{ff'}) \tag{16a}$$

$$U(f - f') = \frac{1}{N} \sum_{\mathbf{k}} U(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{r}_{ff'}) \tag{16b}$$

Invoking orthogonality,

$$\sum_{\mathbf{q}} \exp(i\mathbf{q} \cdot \mathbf{r}_{ff'}) = N\delta_{ff'}; \qquad \sum_{f} \exp[i\mathbf{r}_f(\mathbf{k} - \mathbf{k}')] = N\Delta(\mathbf{k} - \mathbf{k}') \tag{17}$$

we obtain

$$K(\mathbf{k}) = \langle (\Delta S^z)^2 \rangle \frac{\eta U(\mathbf{k})}{1 - \eta U(\mathbf{k})} = \langle (\Delta S^z)^2 \rangle \left(\frac{1}{1 - \eta U(\mathbf{k})} - 1 \right) \tag{18a}$$

The pair correlation function is found from (16a) and (18a):

$$\begin{aligned} \langle \Delta S_f^z \, \Delta S_{f'}^z \rangle_c &= \frac{\langle (\Delta S^z)^2 \rangle}{N} \sum_{\mathbf{k}} [(1 - \eta U(\mathbf{k}))^{-1} - 1] \exp(i\mathbf{k} \cdot \mathbf{r}_{ff'}) \\ &= \frac{\langle (\Delta S^z)^2 \rangle}{N} \sum_{\mathbf{k}} \frac{\exp(i\mathbf{k} \cdot \mathbf{r}_{ff'})}{1 - pU(\mathbf{k})/U(0)} \end{aligned} \tag{18b}$$

We now show how to close the set of equations and obtain the self-consistent equation for an unknown value η as well as the necessary formulas for investigating the Ising model of an arbitrary integral dimension.

From Eq. (13) it follows that, at $\omega_0 \to 0$, $p = 1$ is a singular point. At $p = 1$, $\mu \neq 0$; then this relation defines the equation for spontaneous magnetization. If $\omega_0 \neq 0$, the equation for the magnetization μ, which follows from (13), has the form

$$\mu = \frac{2p}{1 - p} \left(\frac{\omega_0}{U(0)} \right) \tag{19}$$

This observation shows that one can choose the variable p as an independent parameter determined by (12). Its values lie in the interval $0 \leq p \leq p_{\mathrm{up}}$, where p_{up} (≤ 1) is determined, in turn, from the condition $\mu = 1$ and is given by $p_{\mathrm{up}} = 1/[1 + 2\omega_0/U(0)]$. The value $p = 1$ defines a possible phase transition for the spontaneous magnetization.

In order to obtain the self-consistent equation for magnetization, we transform the expression for $\Omega_f \equiv \sqrt{\langle (\sigma_f^z)^2 \rangle} \equiv \Omega$:

$$\Omega = \sqrt{\langle\sigma_f^z\rangle^2 + \langle(\Delta\sigma_f^z)^2\rangle} \tag{20}$$

The values $\langle\sigma_f^z\rangle$ and $\Delta\sigma_f^z$ are defined according to (11) and (14). Let us rewrite the expression for the square fluctuations of the mean field $\langle(\Delta\sigma_f^z)^2\rangle$ in the **k**-representation:

$$\langle(\Delta\sigma_f^z)^2\rangle = \sum_{f',f''} U(f-f')U(f-f'')[\langle\Delta S_{f'}^z\,\Delta S_{f''}^z\rangle_c + \langle(\Delta S^z)^2\rangle\delta_{f'f''}] \tag{21}$$

Incorporating the expressions (16) and (18), we get

$$\begin{aligned}\langle(\Delta\sigma_f^z)^2\rangle &= \frac{\langle(\Delta S^z)^2\rangle}{N}\sum_k \frac{U(\mathbf{k})U(-\mathbf{k})}{1-pU(\mathbf{k})/U(0)}\\ &= \langle(\Delta S^z)^2\rangle\,\frac{U^2(0)}{p^2}\,[G(p)-1]\end{aligned} \tag{22}$$

In expression (22)

$$G(p) \equiv \frac{1}{N}\sum_k \frac{1}{1-pU(\mathbf{k})/U(0)} \tag{23}$$

is the lattice Green function, which depends on both the dimension of the system and the form of the interaction. Taking into account the definition of potential $U_{ff'} \equiv U\Phi(|\mathbf{r}_f - \mathbf{r}_{f'}|/a)$, one can define the dimensionless dispersion relation of the local field from

$$\langle(\Delta\sigma_f^z)^2\rangle = U^2B^2(p) \tag{24}$$

where

$$B(p) \equiv \frac{\Phi(0)}{2p}\,(1-\mu^2)^{1/2}[G(p)-1]^{1/2} \tag{25}$$

For systems with a short-range interaction, the zero-Fourier component is $\Phi(0) = z$, where z is the number of the nearest spins involved in the interaction.

Taking into account (24) and (25), we see that the expression for the energy Ω has the form

$$\Omega(p) = \left[\left(\omega_0 + \frac{U\Phi(0)\mu}{2}\right)^2 + U^2B^2(p)\right]^{1/2} \tag{26}$$

Equation (10b) represents the self-consistent equation and defines the so-called temperature function $T(p)$. It can also be presented in the form

$$\frac{p}{U(0)} = \frac{1}{2\Omega(p)}\tanh\left(\frac{\Omega(p)}{2T}\right) \tag{27a}$$

or

$$T(p) = \frac{1}{2}\frac{\Omega(p)}{\tanh^{-1}(2p\Omega(p)/U(0))} \tag{27b}$$

For completeness, we derive the expressions for the mean energy and the partition function. From (1) it follows that

$$\langle H \rangle = -\sum_f \langle S_f^z \sigma_f^z \rangle = -N\langle S_f^z \sigma_f^z \rangle \tag{28a}$$

Putting $A = \sigma_f^z$ in the DLRE (10a) and using the approximation (4) and the self-consistent equation (27a), we finally get

$$-\frac{\langle H \rangle}{N} = \frac{\Omega}{2}\tanh\left(\frac{\Omega}{2T}\right) = \frac{p}{U(0)}\,\Omega^2(p) \tag{28b}$$

which is the expression for the mean energy as a function of the parameter p.

The expression for the partition function is obtained, within the framework of approximation (7), from

$$\cosh(a\sigma_f^z) = \cosh(a\Omega) \tag{29}$$

Thus, we have

$$Q = \prod_f \sum_{s=\pm 1/2} \exp(\beta S_f^z \sigma_f^z) = \prod_f \left[2\cosh\left(\frac{\sigma_f^z}{2T}\right)\right] = \left[2\cosh\left(\frac{\Omega}{2T}\right)\right]^N \tag{30}$$

From this it is easy to obtain the expressions for the free and the mean energy, respectively: $F = -T \ln Q$, $\langle H \rangle = -\partial \ln Q/\partial\beta$. The last expression for the mean energy reproduces (28b), obtained above from the DLRE.

We also give the explicit expression for the spontaneous magnetization by putting $p = 1$ in (27a):

$$\frac{1}{U\Phi(0)} = \frac{1}{2\Omega(1)}\tanh\left[\frac{\Omega(1)}{2T}\right] \tag{31}$$

Here

$$\Omega(1) \equiv \frac{U\Phi(0)}{2}\,[\mu^2 + (G(1) - 1)(1 - \mu^2)]^{1/2} \tag{32}$$

If one puts $\mu = 0$ in (32), one will obtain the expression for the critical temperature T_c:

$$\frac{4T_c}{U\Phi(0)} = \frac{[G(1) - 1]^{1/2}}{\tanh^{-1}[G(1) - 1]^{1/2}} \tag{33}$$

In short, then, Eqs. (19), (20), (24), and (26)–(33) form a closed system of equations and define completely the thermodynamics of the spin-1/2 Ising model for a regular lattice of an arbitrary integral dimension; these equations are related to each other through an arbitrary interaction. If in (26) we neglect the quadratic fluctuations, $\langle(\Delta\sigma_f^z)^2\rangle = 0$, we recover the mean-field approximation. If, on the other hand, we put $U_{ff'} = 0$, the problem reduces to the trivial statistical problem of noninteracting spins.

It is necessary to stress the fact that approximation (4) embraces the molecular field fluctuations of higher orders. The nth-order fluctuations are given by

$$\begin{aligned}(\sigma_f^z)^{2n} &= \langle(\sigma_f^z)^2\rangle^n \\ (\sigma_f^z)^{2n+1} &= \sigma_f^z \, \langle(\sigma_f^z)^2\rangle^n\end{aligned} \tag{34}$$

The main difference of the SFA from exact solutions is that, in the SFA, the exact value of the mean field is determined by finite or (in general) infinite numbers of fluctuations leading finally to the nonlinear DLRE. Since the analytical methods of solving nonlinear difference equations are not yet fully known, the DLREs are approximately linearized and the problem of nonlinearity is carried over to the self-consistent equations [in the present case, Eq. (10b) for the value of η or p].

It is worth remarking here that the rather involved method of temporal Green functions has been deliberately avoided (Zubarev, 1960); in any case, the direct, simple computations of the correlation functions in the Heisenberg representation, together with (9), give the same result.

Before giving our results for complex cases, it is useful to compare the approximate and exact results for one and two dimensions.

3. THE ONE-DIMENSIONAL ISING MODEL IN THE SFA: COMPARISON WITH EXACT SOLUTIONS

For the one-dimensional Ising model with short-range interaction, the lattice Green function (23) can easily be calculated:

$$G(p) = \frac{1}{N}\sum_k \frac{1}{1 - pU(k)/U(0)} = \frac{1}{2\pi}\int_{-\pi}^{+\pi} \frac{d\varphi}{1 - p\cos\varphi} = \frac{1}{\sqrt{1 - p^2}} \tag{35}$$

Clearly, $G(p)$ goes to infinity at $p = 1$. On the other hand, thanks to the boundedness of the function $\Omega(p)$ at any p, there should exist a limiting value $p_L < 1$ for which Eqs. (18b), (27a) make sense. It is easy to see that p_L is determined from the condition ($\omega_0 = 0$, $\mu = 0$, $z = 2$)

$$\frac{2p_L\Omega(p_L)}{U(0)} = 1 \qquad \text{or} \qquad G(p_L) = 2 \tag{36}$$

We have $p_L = \sqrt{3}/2 = 0.866025\ldots$

We can therefore conclude that in the one-dimensional Ising model a phase transition for periodic boundary conditions does not exist. This conclusion is in agreement with the exact solutions (Jelifonov, 1971). It is interesting to unmask the reasons for the appearance of the singularity in the lattice Green function at $p = 1$. We shall presently show that this singularity is intimately related to the use of cyclic boundary conditions (the Born–von Karman periodic boundary conditions); we have already shown that, thanks to these cyclic conditions, we get the closed solution for the pair correlation function in the form (18b).

Let us find the solution of (15) without using Fourier transforms. We introduce the notation

$$\langle \Delta S_f^z \, \Delta S_{f'}^z \rangle_c \equiv K(j) \tag{37}$$

where $f - f' \equiv j$. Then, for the short-range potential ($z = 2$), Eq. (15) can be written in the form of the difference equation

$$\frac{p}{2}\,[K(j+1) + K(j-1)] - K(j) = 0 \tag{38}$$

where $p \equiv 2\eta U$. The solution of (38) reads

$$K(j) = C_1 \lambda_+^j + C_2 \lambda_-^j \tag{39a}$$

Here

$$\lambda_\pm \equiv \frac{1 \pm \sqrt{1 - p^2}}{p} \tag{39b}$$

are the roots of the characteristic equation

$$\lambda^2 - \frac{2}{p}\lambda + 1 = 0 \tag{40}$$

For the infinite chain the pair correlations should decrease with the growth of j; the solution for the infinite chain can then be written as

$$K(j) = \langle (\Delta S^z)^2 \rangle \, \lambda_-^j \tag{41}$$

Expression (41) correctly describes the correlations near the critical "point"; these attain their maximum value $\langle (\Delta S^z)^2$ at $p = 1$ and remain constant. Based on this result, we can readily calculate $\Omega^2(p)$ at $\omega_0 = 0$, $\mu = 0$:

$$\begin{aligned}\Omega^2(p) &= \langle (\Delta \sigma_f^z)^2 \rangle = U^2 \langle (\Delta S_{f+1}^z + \Delta S_{f-1}^z)^2 \rangle = 2U^2(K(0) + K(2)) \\ &= \frac{U^2}{2}(1 + \lambda_-^2) = \frac{U^2}{1 + \sqrt{1 - p^2}}\end{aligned} \tag{42}$$

The value $2p\Omega(p)/2U$ at the critical point $p = 1$ is finite and, by virtue of (42), equals unity. As follows from (27a), this value corresponds to the critical temperature $T_c = 0$.

Thus, one can conclude that the appearance of the singularity is associated with cyclic boundary conditions, but no phase transition occurs in the one-dimensional infinite chain. All these conclusions equally apply for the exact solution with short-range interactions. It is easy to show that the exact DLRE (Jelifonov, 1971) for the one-dimensional model can be given in a form rather similar to (10a):

$$\langle S_f^z A\rangle = \eta_{ex} U \langle (S_{f+1}^z + S_{f-1}^z) A\rangle \tag{43}$$

where

$$\eta_{ex} U = \frac{\tanh(\beta U/2)}{2[\cosh^2(\beta\omega_0/2) + \sinh^2(\beta\omega_0/2)\tanh(\beta U/2)]} \tag{44}$$

Further investigation of the approximate DLRE (10a) for $d_E = 1$ can be realized in complete analogy with the exact DLRE of the type (43). We omit here the details. We only remark that excellent agreement is obtained with the exact solutions. Figure 1a gives a plot of the two functions $\eta U = p$ [Eq. (38)] and $\eta_{ex} U = p_{ex}$ [Eq. (44)] versus the 'reduced' temperature T/U. As was shown by Jelifonov (1971), these functions play a dominant role in calculating the main thermodynamic characteristics of the Ising model with $d_E = 1$. It is clear from Fig. 1b that the relative error is $\delta \equiv (|p - p_{ex}|/p_{ex}) \cdot 100\% \leq 9.3\%$, which inspires confidence in the SFA. The dependence of the local field fluctuations B on T/U is shown in Fig. 2.

4. THE TWO-DIMENSIONAL ISING MODEL IN THE SFA: THERMODYNAMIC PROPERTIES OF AN INFINITE PLANE

For the two-dimensional Ising model with a short-range (nearest neighbor interaction) the exact expression for the Green function has the form (Morita and Horiguchi, 1971; Oitmaa, 1971)

$$\begin{aligned} G(p) &= \frac{1}{N}\sum_k \frac{1}{1 - pU(\mathbf{k})/U(0)} \\ &= \frac{1}{(2\pi)^2}\int_{-\pi}^{+\pi}\int_{-\pi}^{+\pi} \frac{d\varphi_1 d\varphi_2}{1 - p(\cos\varphi_1 + \cos\varphi_2)/2} \equiv \frac{2}{\pi} K(p) \end{aligned} \tag{45}$$

Here $\mathbf{K}(p)$ is a complete elliptic integral of the first type:

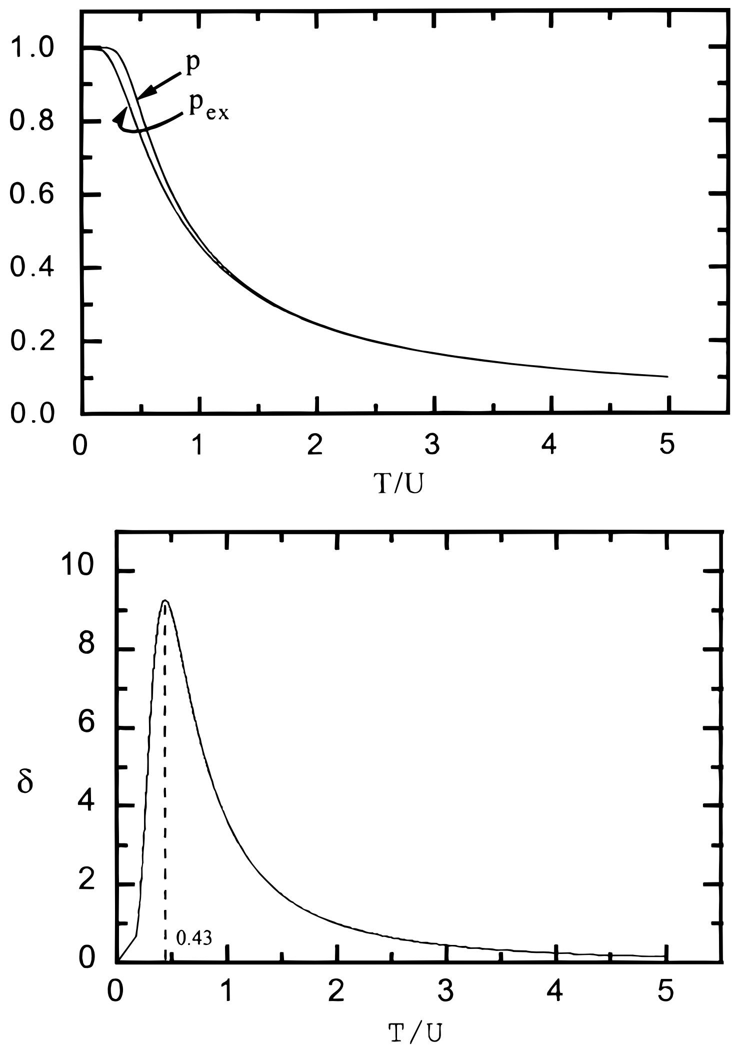

Fig. 1. (a) Direct comparison of the parameters $p = 2\eta U$ (upper curve) [entering into the approximate DLRE (38)] and $p_{ex} = 2\eta_{ex}U$ [Eq. (44)] at $\omega_0 = 0$ (lower curve) versus the reduced temperature T/U. Visually these curves are almost fused with each other. (b) To see the difference we calculated the value of the relative error $\delta \equiv (|p - p_{ex}|/p_{ex}) \cdot 100\%$ as a function of the temperature ($\omega_0 = 0$). The value of this error is $\leq 9.3\%$.

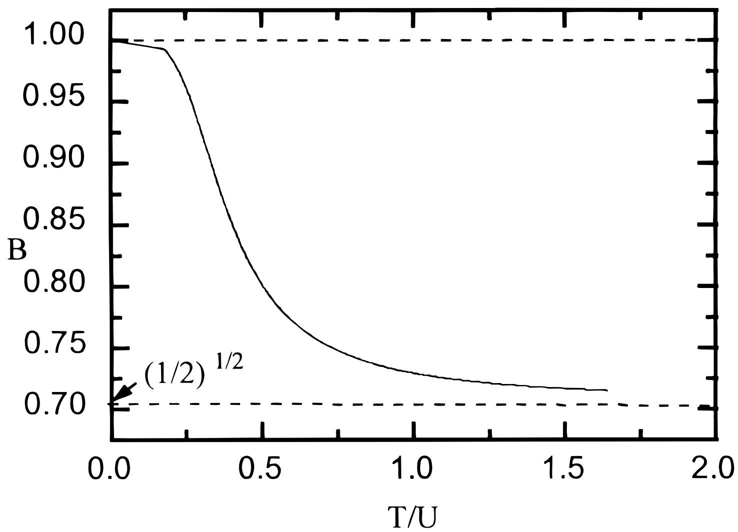

Fig. 2. The dependence of the local field fluctuations B versus T/U for the one-dimensional Ising model. The maximum value $B(T) = 1$ occurs at zero temperature. The limiting value at infinite temperature is $B(\infty) = 1/\sqrt{2} = 0.707$.

$$K(p) \equiv \int_0^{\pi/2} (1 - p^2 \sin^2\theta)^{-1/2}\, d\theta \tag{46}$$

From (46) it follows that, as $p \to 1$, the function $K(p)$ has a logarithmic divergence $\sim \ln[1/(1 - p)]$. However, from a condition analogous to (36), it follows that the lattice Green function should be finite. In fact, the limiting value for $d_E = 2$ is also found from (36):

$$G(p_L) = 2 \qquad \text{or} \qquad K(p_L) = \pi \tag{47}$$

The solution of the last transcendental equation gives the value $p_L = 0.9844606\ldots$, which *slightly* differs from unity. If for the critical region we require the fulfilment of the stringent constraint $p = 1$, we should conclude that within the framework of the SFA the incorporation of only *quadratic fluctuations* for cyclic boundary conditions is not sufficient to yield the phase transition for the spontaneous magnetization. Preliminary investigations of the influence of higher order fluctuations on the phase transition for the two-dimensional case with periodic boundary conditions clearly show that the consideration of third-order fluctuations of the local field *is* sufficient for restoring the phase transition in this case. The results obtained are very close to Onsager's results. The complete investigation of the influence of the higher order fluctuations of the local field on the phase-transition phenomenon will be the subject of a subsequent publication.

In fact, the exact DLRE for the two-dimensional Ising model reads

$$\langle S_f^z A\rangle = \tau_0\langle A\rangle + \tau_1\langle \Sigma_f A\rangle + \tau_2\langle \Sigma_f^2 A\rangle + \tau_3\langle \Sigma_f^3 A\rangle + \tau_4\langle \Sigma_f^4 A\rangle \qquad (48)$$

where

$$\Sigma_f \equiv S_{m+1,n}^z + S_{m-1,n}^z + S_{m,n+1}^z + S_{m,n-1}^z \qquad (49)$$

Σ_f is the sum of spins interacting with spin $S_f^z \equiv S_{m,n}^z$. The parameters τ_i in (48) are given by

$$\tau_0 = \frac{1}{2}\, t_0 \qquad (50a)$$

$$\tau_1 = \frac{1}{3}\,(t_+ - t_-) - \frac{1}{24}\,(t_{+2} - t_{-2}) \qquad (50b)$$

$$\tau_2 = \frac{1}{3}\,(t_+ + t_-) - \frac{1}{48}\,(t_{+2} + t_{-2}) - \frac{5}{8}\, t_0 \qquad (50c)$$

$$\tau_3 = -\frac{1}{12}\,(t_+ - t_-) + \frac{1}{24}\,(t_{+2} - t_{-2}) \qquad (50d)$$

$$\tau_4 = -\frac{1}{12}\,(t_+ + t_-) + \frac{1}{48}\,(t_{+2} + t_{-2}) + \frac{1}{8}\, t_0 \qquad (50e)$$

where

$$t_0 \equiv \tanh\left(\frac{\beta\omega_0}{2}\right); \qquad t_\pm \equiv \tanh\left[\frac{\beta}{2}\,(\omega_0 \pm U)\right];$$

$$t_{\pm 2} \equiv \tanh\left[\frac{\beta}{2}\,(\omega_0 \pm 2U)\right]$$

For the two-dimensional case the exact DLREs are nonlinear; all attempts to obtain exact solutions based on (48) have so far been ineffective. The SFA, it should be emphasized, has arisen, as a new method of solution in the many-body problem and statistical mechanics, from the idea of the replacement of the nonlinear, exact DLRE of type (48) with the linearized, approximate, and self-consistent DLRE of type (14). This linearized DLRE allows one to also consider boundary conditions other than cyclic.

To this end, let us examine the DLRE for an infinite plane.

We have already seen that, for cyclic boundary conditions, the consideration of only the quadratic fluctuations of the molecular field *is not sufficient* for the realization of phase-transition conditions in the Ising system.

In view of this, it is interesting to pose the following problem: *Are there any boundary conditions, other than cyclic, where quadratic fluctuations of* *the molecular field are sufficient for the realization of the phase-transition phenomenon*?

To answer this question, we should find the solution of the DLRE of type (15) without using the Fourier transform in the **k**-representation. We assume that the set of spins is located in an infinite plane and that they interact only with nearest neighbors. For this case, introducing the translationally invariant correlation function

$$\langle \Delta S_f^z \, \Delta S_{f'}^z \rangle = K(m, n) \tag{51}$$

where $(x - x')/a \equiv m$ and $(y - y')/a \equiv n$, with a being the lattice constant, we can write down the DLRE (15) in the form

$$\begin{aligned} K(m, n) = \eta U[&K(m+1, n) + K(m-1, n) + K(m, n+1) \\ &+ K(m, n-1)] \end{aligned} \tag{52}$$

For an infinite plane, taking into account the rotational symmetry as well, we look for a particular solution of $K(m, n)$ in the form

$$K(m, n) = K(0, 0)\lambda^{|m|+|n|}, \qquad |\lambda| \le 1 \tag{53}$$

Usually this form of solution for two-dimensional difference equations is ineffective because the conditions for finding the value λ are unknown. In our case, however, these additional conditions *do* exist and an equation for λ is found for the nearest neighbor correlation functions. Let us write the DLRE for $K(0, 1)$:

$$K(0, 1) = \frac{p}{4}[K(1, 1) + K(-1, 1) + K(0, 2) + K(0, 0)] \tag{54}$$

Here, as before, the parameter p is determined from the condition $\eta U(0) = 4\eta U = p$. Substituting the particular solution (53) into (54), we get the desired equation for λ:

$$\lambda = \frac{p}{4}(3\lambda^2 + 1) \tag{55}$$

or

$$\lambda_{\pm}(p) = \frac{2}{3p} \pm \frac{\sqrt{4 - 3p^2}}{3p} \tag{56}$$

Since $|p| \le 1$, the root $\lambda_+(p)$ should be rejected $[|\lambda_+(p)| > 1]$ except for the critical point, where $\lambda_+(1) = 1$. Thus, the solution for the pair correlation function can be written in the form

$$K(m, n) = \begin{cases} K(0, 0)[\lambda_-(p)]^{|m|+|n|} \\ C_1 + C_2\left(\dfrac{1}{3}\right)^{|m|+|n|}; \qquad C_1 + C_2 = K(0, 0) \end{cases} \tag{57}$$

On the other hand, at the critical point $p = 1$, the correlation function should be a decreasing and a single-valued function. It follows that $C_1 = 0$, and the pair correlation function for all p is determined by the expression

$$K(m, n) = K(0, 0)(\lambda_-(p))^{|m|+|n|} \tag{58}$$

Based on (58), one can derive the full thermodynamics of this system.

Consider first the case ($T \geq T_c$, $\omega_0 = 0$, $\mu = 0$): The critical dispersion $B(1)$ and the temperature T_c are found from the conditions

$$\begin{aligned} B(1) &= \langle (S^z_{1,0} + S^z_{-1,0} + S^z_{0,1} + S^z_{0,-1})^2 \rangle^{1/2} \\ &= [4K(0, 0) + 2K(2, 0) + 2K(0, 2) + 8K(1, 1)]^{1/2} \\ &= \tfrac{2}{3}\sqrt{3} = 1.1547\ldots \end{aligned} \tag{59a}$$

$$4X_c \equiv \frac{4T_c}{U} = \frac{2B(1)}{\tanh^{-1}[B(1)/2]} = 3.507175\ldots \tag{59b}$$

The normalized temperature $\tau(p)$ is defined by

$$\tau(p) \equiv \frac{X(p)}{X_c} - 1 \tag{60}$$

where

$$X(p) \equiv \frac{B(p)}{2\tanh^{-1}[pB(p)/2]}; \qquad B(p) \equiv \sqrt{3[\lambda_-(p)]^2 + 1}$$

$\lambda_-(p)$ is given by (56).

Let us find the decomposition of $\tau(p)$ near the critical point $p = 1$. In terms of $\varepsilon \equiv (1 - p)^{1/2}$,

$$\tau(\varepsilon) = \theta_1^{>}\varepsilon^2 + \theta_2^{>}\varepsilon^4 + O(\varepsilon^6) \tag{61}$$

$\theta_1^{>} = 1.4728$, $\theta_2^{>} = 0.33492$. Inverting this, we find the inverse decomposition:

$$\varepsilon(\tau) = \delta_1^{>}\tau^{1/2} - \delta_2^{>}\tau^{3/2} + O(\tau^2) \tag{62}$$

$\delta_1^{>} = 0.824002$, $\delta_2^{>} = 0.0636138$. To find the behavior of the specific heat to the right of the critical point, we first find the decomposition for the average energy:

$$\frac{\langle H\rangle}{N} = -\frac{pB^2(p)}{4}U = U[-g_0^2 + e_1^> \varepsilon^2 - e_2^> \varepsilon^4 + O(\varepsilon^6)] \tag{63}$$

$g_0^2 = 1/3$, $e_1^> = 2/3$, $e_2^> = 4/3$. Using (62), we finally get the decomposition for the mean energy as a function of τ:

$$\frac{\langle H\rangle}{N} = U[-g_0^2 + k_1^> \tau - k_2^> \tau^2 + O(\tau^3)] \tag{64}$$

$k_1^> = 0.4526$, $k_2^> = 0.6846$. From the last expression, by differentiation, we find the specific heat decomposition to the right of T_c:

$$\frac{1}{U}\frac{C_H}{N} = \frac{1}{UN}\left(\frac{d\langle H\rangle}{dT}\right) = \frac{1}{UX_c}\frac{d}{d\tau}\left(\frac{\langle H\rangle}{N}\right) = \Delta^> - D^>\tau \tag{65}$$

$\Delta^> = 0.516256$, $D^> = 1.51653$. From this result it follows that the critical exponent for the specific heat is $\alpha' = 0$.

Let us now find the behavior of the specific heat to the left of the critical point ($T \leq T_c$, $\mu \neq 0$). We define the reduced temperature for this region as

$$\tau \equiv 1 - \frac{X(\mu)}{X_c} = 1 - \frac{Z(\mu)}{X_c \tanh^{-1}[Z(\mu)]} \tag{66}$$

where

$$Z(\mu) \equiv \Omega(\mu)/(2U) = \{\mu^2 + (1 - \mu^2)[B(1)/2]^2\}^{1/2}$$

It is then convenient to determine the inverse relation $\mu \equiv \mu(Z)$ and define a new variable ξ by the relation

$$\mu(Z) = \left[\frac{Z^2 - [B(1)/2]^2}{1 - [B(1)/2]^2}\right]^{1/2} = \frac{\xi^{1/2}}{\{1 - [B(1)/2]^2\}^{1/2}} \tag{67}$$

From this last expression the decomposition of $\tau(\xi)$ follows:

$$\tau = 1 - \frac{\sqrt{\xi + [B(1)/2]^2}}{X_c \tanh^{-1}\sqrt{\xi + [B(1)/2]^2\}}} = \theta_1^< \xi + \theta_2^< \xi^2 + O(\xi^3) \tag{68}$$

$\theta_1^< = 0.472786$, $\theta_2^< = 0.192294$. Inverting (68), we find the decomposition for $\xi(\tau)$:

$$\xi = \varphi_1^< \tau - \varphi_2^< \tau^2 + \varphi_3^< \tau^3 + O(\tau^4) \tag{69}$$

$\varphi_1^< = 2.11512$, $\varphi_2^< = 1.81958$, $\varphi_3^< = 0.0779139$. Putting (69) into (67), we find the desired decomposition for the magnetization as a function of τ:

$$\mu(\tau) = m_1\tau^{1/2} - m_2\tau^{3/2} - m_3\tau^{5/2} + O(\tau^{7/2}) \tag{70}$$

$m_1 = 1.7812$, $m_2 = 0.76616$, $m_3 = 0.13197$. Having obtained decompositions

(69) and (70), one can find the corresponding decompositions for the mean energy:

$$\frac{\langle H \rangle}{N} = U[-g_0^2 - k_1^< \tau + k_2^< \tau^2 + O(\tau^3)] \tag{71}$$

$k_1^< = 2.11512$, $k_2^< = 1.01950$. By differentiation, we finally obtain the decomposition for the specific heat to the left of the critical point:

$$\frac{1}{U}\frac{C_H}{N} = \frac{1}{UN}\left(\frac{d\langle H \rangle}{dT}\right) = \frac{1}{UX_c}\frac{d}{d\tau}\left(\frac{\langle H \rangle}{N}\right) = \Delta^< - D^< \tau \tag{72}$$

$\Delta^< = 2.41231$, $D^< = 4.15054$.

It follows that the specific heat has a finite jump $\Delta \equiv \Delta^< - \Delta^>$ that gives the critical exponent $\alpha = 0$. It is crucial to note that this finite jump is intimately related to the breakdown of the nearest order correlation function at the critical point. This relation will be delineated in detail for the three-dimensional case.

From the solution of the transcendental equation

$$\frac{1}{2U} = \frac{1}{\Omega(\mu, \omega_0)} \tanh\left[\frac{\Omega(\mu,\omega_0)}{2T_c}\right] \tag{73}$$

where $\Omega(\mu, \omega_0) \equiv [(\omega_0 + 2U\mu)^2 + (2U)^2 (1 - \mu^2)B^2(1)]^{1/2}$, one can find $\mu = \mu(h)$ $[h \equiv \omega_0/2U]$ at the critical point $T = T_c$. The critical exponent $\delta = 3$ can be determined from the Griffith relation (Stanley, 1971) $\alpha' + \beta(1 + \delta) = 2$. Plots illustrating the thermodynamics of the Ising infinite plane are given in Figs. 3–7.

5. THE THREE-DIMENSIONAL ISING MODEL: THE EFFECTS OF BOUNDARY CONDITIONS

In contrast to the one- and two-dimensional cases, no exact solution exists for the three-dimensional case, as is well known. With various approximate methods, however, it is possible to obtain some important and reliable results. The main techniques of solving for the Ising model in three dimensions are the low- and high-temperature decompositions of thermodynamic values, the Padé-approximant method, and various modifications of the mean-field theory.

In all these methods the effects of boundary conditions have not been considered; the problem has been approximately solved only with periodic boundary conditions. In the framework of the SFA method, however, it is possible to consider other boundary conditions.

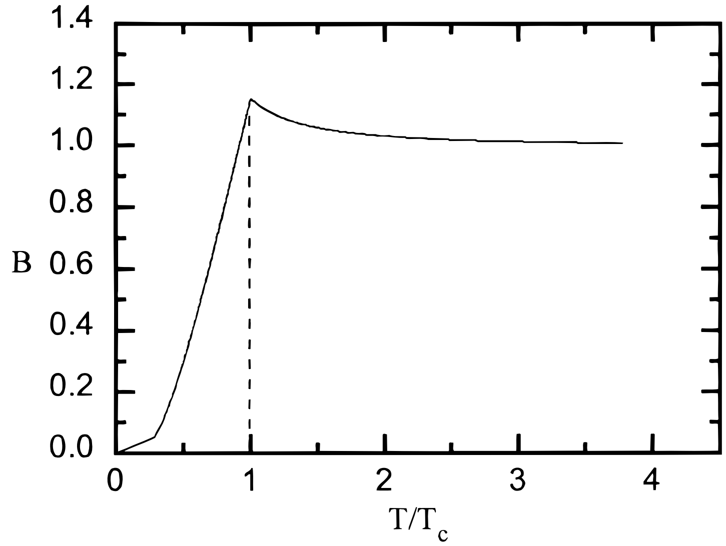

Fig. 3. The dimensionless local field dispersion $B(T)$ versus the normalized temperature T/T_c for an infinite plane. At the critical point, $B(T) = 2/\sqrt{3}$. The limiting value at high temperatures equals unity: $B(\infty) = 1$.

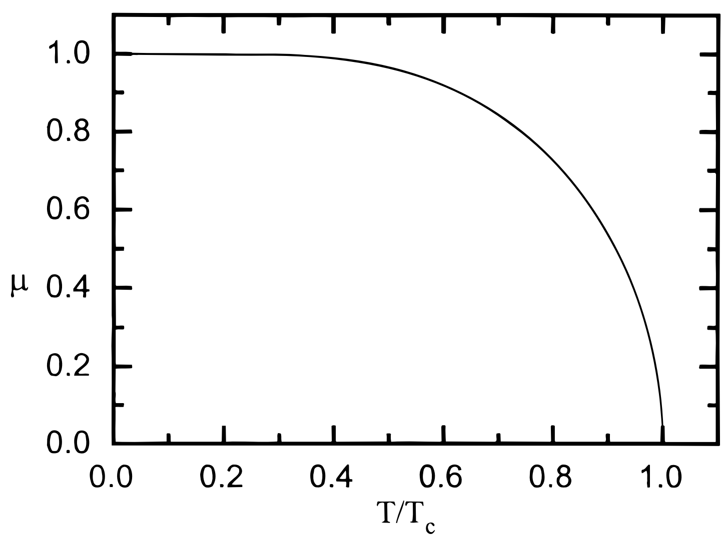

Fig. 4. The spontaneous magnetization versus the normalized temperature T/T_c. The critical exponent to the left of the critical point is $\beta = 1/2$, which agrees with the prediction of mean-field theory.

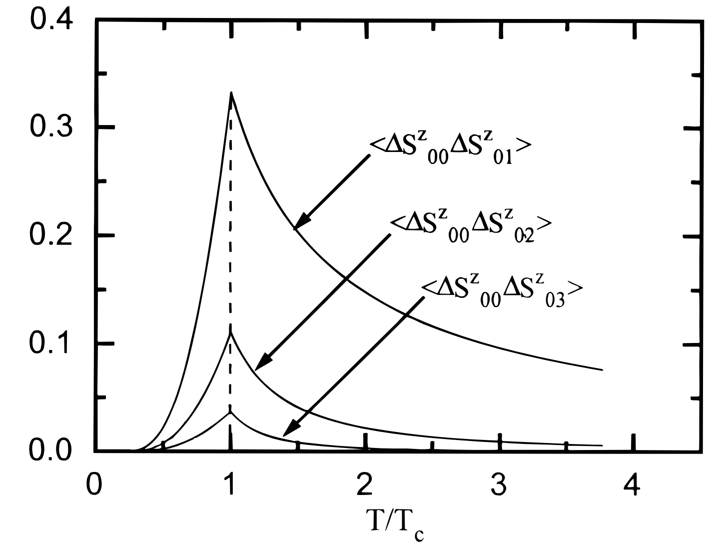

Fig. 5. The behavior of the nearest order correlation functions as a function of the normalized temperature T/T_c.

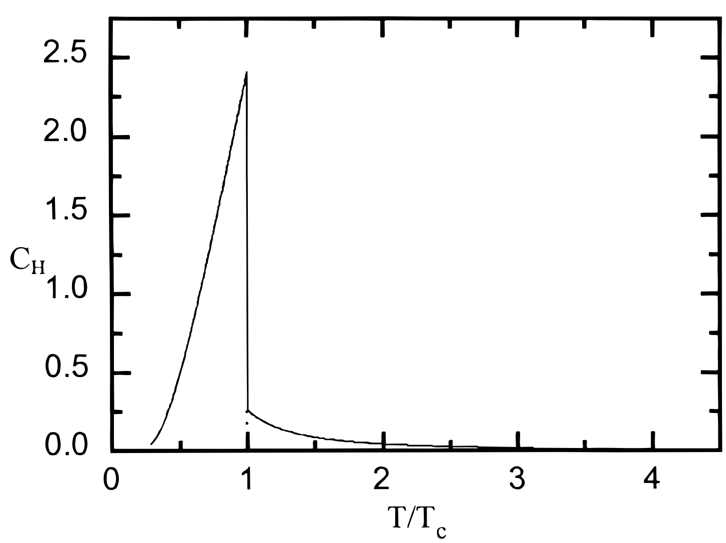

Fig. 6. The specific heat for an infinite plane as a function of the normalized temperature T/T_c. Note the finite jump at the critical point.

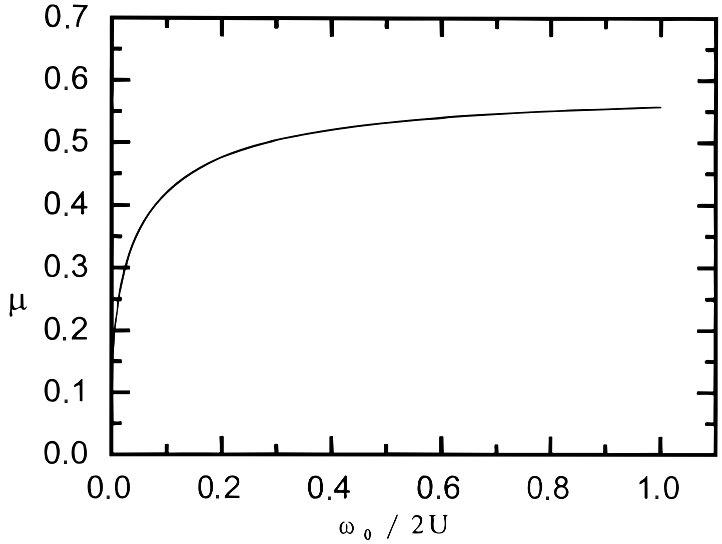

Fig. 7. The magnetization versus the magnetic field $h \equiv \omega_0/2U$ at the critical point $T = T_c$. The critical exponent can be determined from the Griffith relation (Stanley, 1971) and is $\delta = 3$.

As for the one-dimensional (Jelifonov, 1971) and two-dimensional cases considered above, the change of boundary conditions can lead to a considerable modification of the phase-transition scenario in the three-dimensional case. To avoid misunderstanding concerning this point, we emphasize that the term 'boundary conditions' is used here in a strict mathematical sense; the present work can be regarded as a generalization of the previous one-dimensional study (Jelifonov, 1971), where it was stressed that the change of boundary conditions affects the critical behavior of the system.

Before considering this problem, we give the complete thermodynamics of the three-dimensional model in the SFA method with periodic boundary conditions and compare the results to the data obtained by conventional methods.

5.1. The Cyclic Boundary Conditions

We consider the system of spins to be localized at the nodes of a Bravais lattice. These spins interact with each other via an attractive short-range potential. The lattice Green function in this case can be written in the form

$$\begin{aligned} G_L(p) &= \frac{1}{N}\sum_{\mathbf{k}} \{1 - p[U_L(\mathbf{k})/U_L(0)]\}^{-1} \\ &= \frac{1}{(2\pi)^3}\int_{-\pi}^{\pi} d\varphi_1 \int_{-\pi}^{\pi} d\varphi_2 \int_{-\pi}^{\pi} d\varphi_3 \, \{1 - p[U_L(\varphi_1, \varphi_2, \varphi_3)/U_L(0)]\}^{-1} \end{aligned} \tag{74}$$

where the Fourier components of the potential depend on the type of cubic lattice. The explicit expressions are given by

$$\begin{aligned} &U_L(\varphi_1, \varphi_2, \varphi_3)/U_L(0) \\ &\quad = (\cos\varphi_1 + \cos\varphi_2 + \cos\varphi_3)/3, \quad L \equiv \mathrm{SC} \\ &U_L(\varphi_1, \varphi_2, \varphi_3)/U_L(0) \\ &\quad = (\cos\varphi_1 \cos\varphi_2 + \cos\varphi_1 \cos\varphi_3 + \cos\varphi_2 \cos\varphi_3)/3, \quad L \equiv \mathrm{FCC} \\ &U_L(\varphi_1, \varphi_2, \varphi_3)/U_L(0) \\ &\quad = \cos\varphi_1 \cos\varphi_2 \cos\varphi_3, \quad L \equiv \mathrm{BCC} \end{aligned} \tag{75}$$

For the three-dimensional case the lattice Green function does not have singularities at the critical point (Morita and Horiguchi, 1971; Oitmaa, 1971). Based on these results, we can directly use Eqs. (18)–(33) for cyclic boundary conditions.

We find the critical temperature T_c from (27b) at $p = 1$, where the lattice Green functions have a branching point (Morita and Horiguchi, 1971). It conforms with the usual definition of T_c because, at $p = 1$, the magnetization becomes zero. From (27b), we obtain the following expression for the dimensionless ratio T_c/U:

$$X_c \equiv \frac{4T_c}{U} = \frac{z[G_L(1) - 1]}{\tanh^{-1}[G_L(1) - 1]} \tag{76}$$

Here $G_L(1)$ is the Watson integral. The values of T_c/U calculated from (76), together with the corresponding results obtained from other methods, are given in Table I. The values of $G_L(1)$ for the principal types of cubic lattices are also given in this table.

The dependence of the dimensionless local field dispersion $B(p)$ on the reduced temperature in the whole temperature region can be obtained from the following system of equations:

For $T > T_c$:

$$B(p) = \frac{z}{2p}[G_L(p) - 1]^{1/2} \tag{77a}$$

$$X(p) = \frac{4T}{U} = \frac{2B(p)}{\tanh^{-1}[2pB(p)/z]} \tag{77b}$$

Table I. The Critical Temperature T_c/U for the Three-Dimensional Ising Model, Obtained by Various Methods[a]

Method	SC lattice ($z = 6$)	BCC lattice ($z = 8$)	FCC lattice ($z = 12$)
Weiss mean field (Smart, 1966)	6.0	8.0	12.0
Oguchi's method (Smart, 1966)	5.7194	7.7819	11.8487
P. R. Weiss (Honmura and Kaneyoshi, 1979)	5.5866	7.5692	11.5495
Green functions (Smart, 1966)	5.3	7.36	?
Effective field ($n = 0$; $n = z$) (Honmura and Kaneyoshi, 1979)	5.0733	7.0633	11.0446
	4.9326	6.9521	10.9696
Zhang and Min (1981)	4.890	6.914	10.651
Taggart and Fittipaldi (1982)	4.632	6.560	10.284
Frank and Mitran (1977)	4.530	6.392	9.828
RPA (Smart, 1966)	3.96	5.74	?
High-temperature decomposition (Smart, 1966)	3.7760	5.2865	8.3073
Constant-bond approximation (Kasteleijn and Van Kranendonk, 1956)	3.6410	5.7708	9.8652
SFA (this work)	4.7655	6.8107	10.4649
$G_L(1)$	1.51638	1.393204	1.34466
$B_L(1)$	2.1558	2.5082	3.5225
$B_L(\infty)$	1.2247	1.4142	1.73205

[a] The values of $G_L(1)$ and of the dimensionless local field dispersion at the critical point $B(1)$ and at high temperatures $B(\infty)$ are also given.

For $T < T_c$:

$$B(\mu) = \frac{z}{2}(1 - \mu^2)^{1/2}[G_L(1) - 1]^{1/2} \tag{77c}$$

$$X(\mu) = \frac{4T}{U} = \frac{2\Omega(\mu)}{U \tanh^{-1}[2\Omega(\mu)/Uz]} \tag{77d}$$

$$\Omega(\mu) = \frac{zU}{2}\{\mu^2 + (1 - \mu^2)[G_L(1) - 1]\}^{1/2} \tag{77e}$$

Analytical expressions of Green functions defined by (74) are given by Morita and Horiguchi (1971) and by Oitmaa (1971). The corresponding plots of $B(T/T_c)$ are given in Fig. 8.

To find the temperature dependence of the nearest order correlation functions, $4\langle S_f^z S_{f+\delta}^z\rangle$, we put $A = \sigma_f^z$ in DLRE (10a). With (28), we find

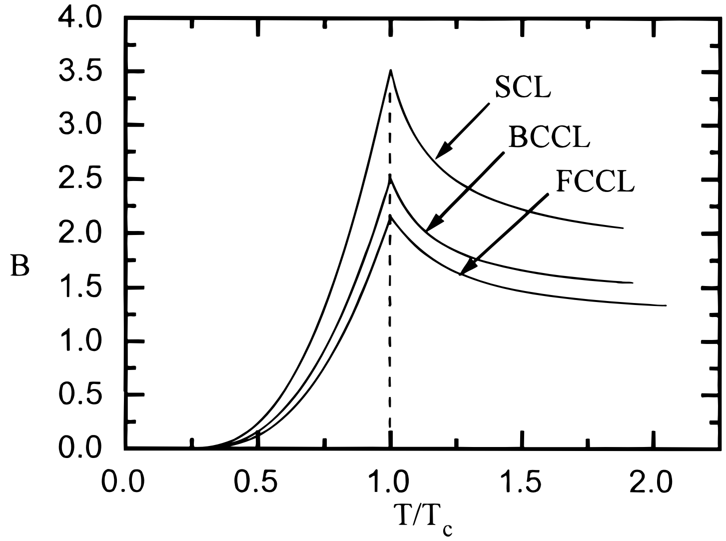

Fig. 8. The dependence of the dimensionless local field dispersion on the normalized temperature T/T_c. The numerical values of $B_L(T/T_c)$ and $B_L(\infty)$ are given in Table I.

$$zU\langle S_f^z S_{f+\delta}^z\rangle = \frac{p\Omega^2(p)}{U(0)} \tag{78a}$$

More explicitly, we have the following results.

For $T > T_c$:

$$4\langle S_f^z S_{f+\delta}^z\rangle = 4\,\frac{pB^2(p)}{z^2} \tag{78b}$$

For $T < T_c$:

$$4\langle S_f^z S_{f+\delta}^z\rangle = \left(\frac{2\Omega(\mu)}{zU}\right)^2 \tag{78c}$$

Equations (78), together with (77), define the temperature dependence of the nearest order correlators on the normalized temperature T/T_c. The corresponding plots for the three principal types of cubic lattices are given in Fig. 9. From this figure it is shown that the nearest order correlator has a monotonic behavior near the critical point. It means that the specific heat does not have a jump at the transition point; the SFA with periodic boundary conditions predicts a phase transition of the *first kind*. This conclusion differs from the Weiss theory and its modifications, which predict a phase transition of the second kind; the correlation function of the nearest order has a kink

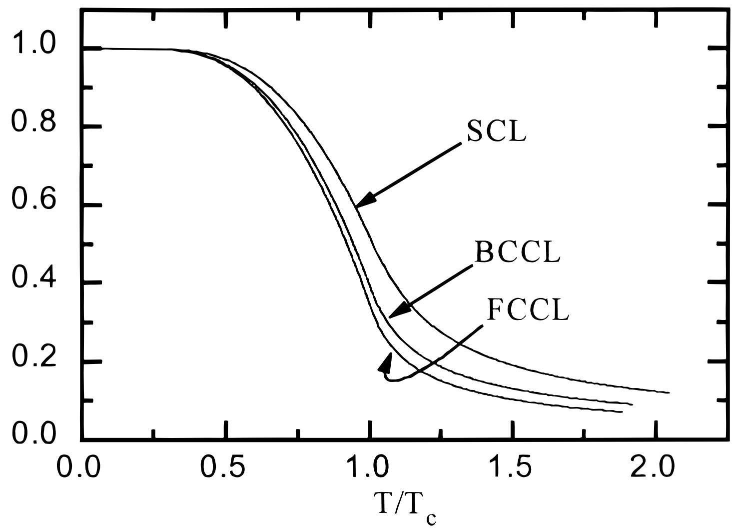

Fig. 9. The correlators of the nearest order $4\langle S_j^z S_{j+\delta}^z \rangle$ as functions of the normalized temperature T/T_c.

at the critical point that leads, in turn, to the jump of the specific heat at T_c. The comparative plots of the nearest order correlators obtained by various methods for a simple cubic lattice (SC) are given in Fig. 10. The values of the correlators at T_c for $z = 6$ are listed in Table II.

It is convenient to define the pair correlation function of any order for an arbitrary potential $U_{ff'} \equiv U\Phi(|r_f - r_{f'}|/a)$ in the SFA by the expression

$$K(f - f') = 4\langle \Delta S_f^z \, \Delta S_{f'}^z \rangle = 4 \frac{\langle (\Delta S^z)^2 \rangle}{N} \sum_{\mathbf{k}} \frac{\exp(i\mathbf{k}\mathbf{r}_{ff'})}{1 - pU(\mathbf{k})/U(0)} \qquad (79)$$

Here $U(\mathbf{k})$ is the Fourier transform of the potential. It follows that the pair correlation function contains the Fourier transform of the Green function. It is impossible to obtain an analytical expression of this transform for an arbitrary potential; in general, therefore, it is estimated numerically (Morita and Horiguchi, 1971; Oitmaa, 1971). As an example, we give in Fig. 11 the plots of the correlation functions $4\langle \Delta S_{000}^z \, \Delta S_{100}^z \rangle$, $4\langle \Delta S_{000}^z \, \Delta S_{110}^z \rangle$, and $4\langle \Delta S_{000}^z \, \Delta S_{200}^z \rangle$ for the SC lattice.

Equations (77c)–(77e) allow one to find the temperature dependence of the spontaneous magnetization. This quantity can be expressed in the following parametric form:

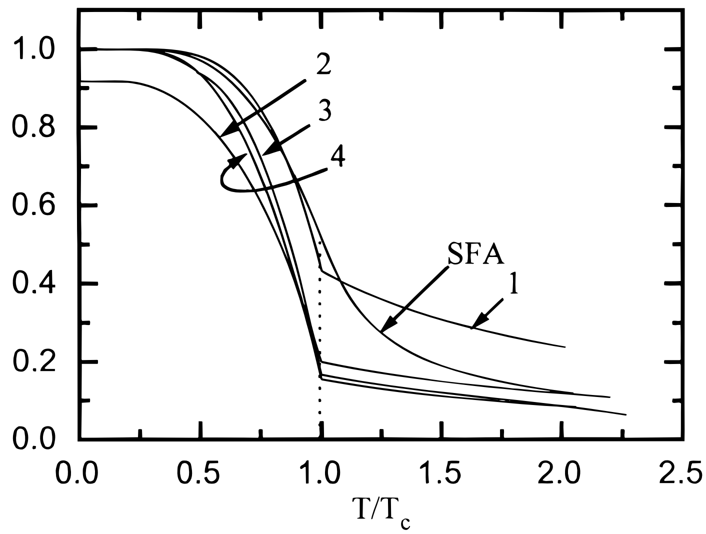

Fig. 10. The correlation functions of the nearest order $4\langle S_j^z S_{j+\delta}^z\rangle$ as functions of the normalized temperature T/T_c, calculated by various methods. (1) Oguchi's method (Honmura and Kaneyoshi, 1979; Smart, 1966), (2) the constant-bond method (Kasteleijn and Van Kranendonk, 1956); (3) P. R. Weiss approximation (Honmura and Kaneyoshi, 1979; Smart, 1966); (4) effective-field approximation (Honmura and Kaneyoshi, 1979; Smart, 1966) at $n = 0$.

$$\mu(Z) = \left(\frac{Z^2 - [G_L(1) - 1]}{1 - [G_L(1) - 1]}\right)^{1/2} \tag{80a}$$

$$X(\mu) = \frac{zy}{4\tanh^{-1}[Z(\mu)]} \tag{80b}$$

where $Z(\mu) = 2\Omega(\mu)/zU$, $0 \le Z^2(\mu) \le G_L(1) - 1$. The plot of the spontaneous magnetization versus temperature for the FCC lattice is shown in Fig. 12.

Table II. Values of the Nearest Order Correlators at the Critical Point, Obtained by Various Methods ($z = 6$)

SFA	Oguchi's method (Smart, 1966)	Constant-bond approximation (Kasteleijn and Van Kranendonk, 1956)	Effective-field method ($n = 0$) (Honmura and Kaneyoshi, 1979; Smart, 1966)	P. R. Weiss approximation (Honmura and Kaneyoshi, 1979; Smart, 1966)	Mean-field theory (Honmura and Kaneyoshi, 1979; Smart, 1966)
0.5164	0.4316	0.2000	0.1667	0.1552	0.0

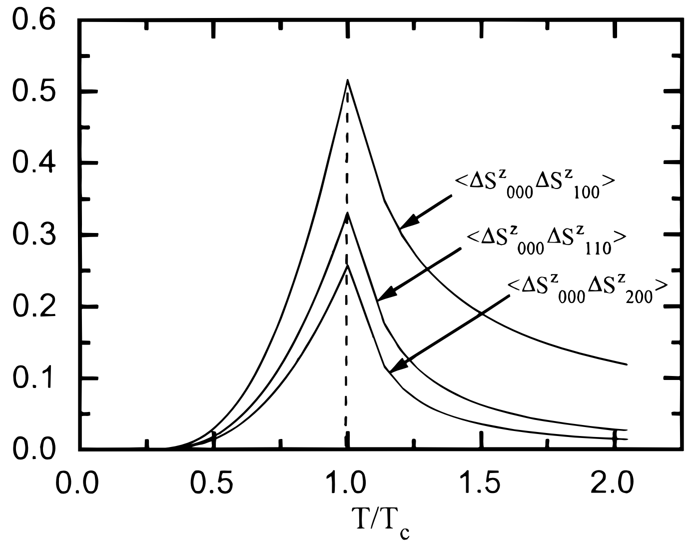

Fig. 11. The dependence of the pair correlation functions for an SC lattice ($z = 6$) on the normalized temperature T/T_c. The values of these correlators at the critical point are, respectively, $4\langle \Delta S^z_{000}\ \Delta S^z_{100}\rangle_c = 0.516$, $4\langle \Delta S^z_{000}\ \Delta S^z_{110}\rangle_c = 0.331$, and $4\langle \Delta S^z_{000}\ \Delta S^z_{200}\rangle_c = 0.257$.

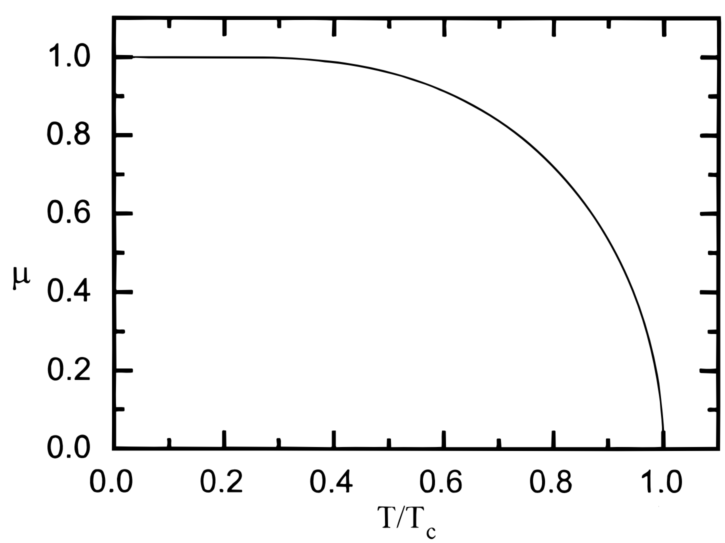

Fig. 12. The dependence of the spontaneous magnetization for an FCC lattice on the normalized temperature T/T_c.

For SC and BCC lattices the plots look almost the same, so they are not given here.

In the framework of the SFA [see (13)], it is possible to find the dependence of the magnetization on the external magnetic field:

$$\mu = \frac{2p\omega_0}{(1 - p)zU} \tag{81}$$

the parameter p being itself a function of ω_0. The functional dependence of $p(\omega_0)$ can be recovered from the following system of equations:

$$\Omega(p) = \left\{\left(\omega_0 + \frac{Uz\mu}{2}\right)^2 + [UB(p)]^2\right\}^{1/2} \tag{82a}$$

$$B(p) = \frac{z}{2p}(1 - \mu^2)[G_L(p) - 1]^{1/2} \tag{82b}$$

$$p = \frac{Uz}{2\Omega(p)}\tanh\left(\frac{\Omega(p)}{2T}\right) \tag{82c}$$

This, in turn, reduces to the following self-consistent equation:

$$p\left[\left(\mu(p, \omega_0) + \frac{2\omega_0}{Uz}\right)^2 + \frac{1 - \mu^2(p, \omega_0)}{p^2}[G_L(p - 1]\right]^{1/2} \\ = \tanh\frac{z[[\mu(p, \omega_0) + 2\omega_0/Uz]^2 + \{[1 - \mu^2(p, \omega_0)]/p^2\}[G_L(p) - 1]]^{1/2}}{X} \tag{83}$$

where $\mu(p, \omega_0)$ is defined by (81), and $X = 4T/U$. A plot of $\mu(2\omega_0/Uz)$ for an FCC lattice is given in Fig. 13.

The specific heat is found from the defining expression

$$G_H = \frac{1}{N}\frac{\partial\langle H\rangle}{\partial T} \tag{84}$$

the mean energy being

$$\frac{1}{N}\langle H\rangle = -\langle S_f^z\sigma_f^z\rangle = -zU\langle S_f^z S_{f+\delta}^z\rangle = -\frac{p\Omega^2(p)}{zU} \tag{85}$$

The plot of the specific heat versus the normalized temperature T/T_c for $z = 8$ (a BCC lattice) is shown in Fig. 14. In Fig. 15 we also give, for comparison, the set of plots of specific heats for $z = 6$ (SC) obtained by other methods.

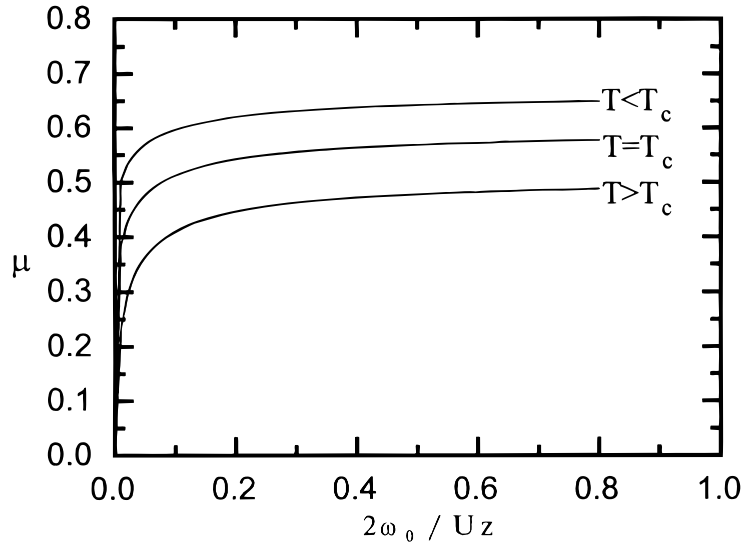

Fig. 13. The dependence of the magnetization for an FCC lattice ($z = 12$) on the reduced external magnetic field $h \equiv 2\omega_0/Uz$.

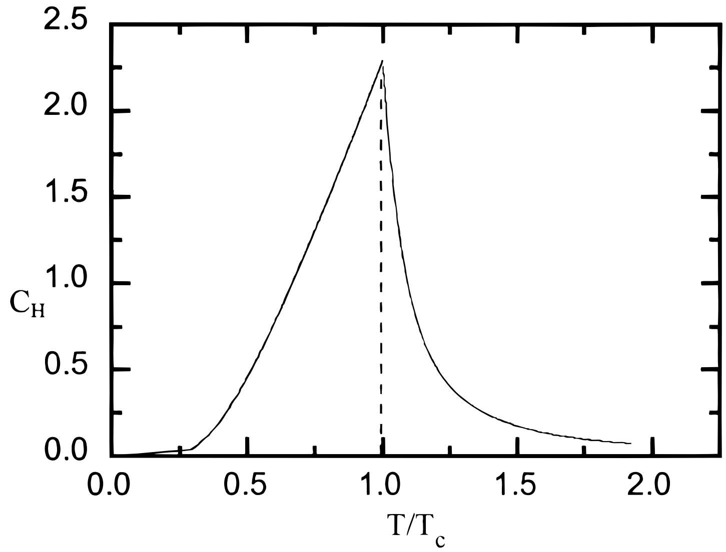

Fig. 14. The specific heat dependence on the dimensionless temperature for a BCC lattice ($z = 8$) with periodic boundary conditions.

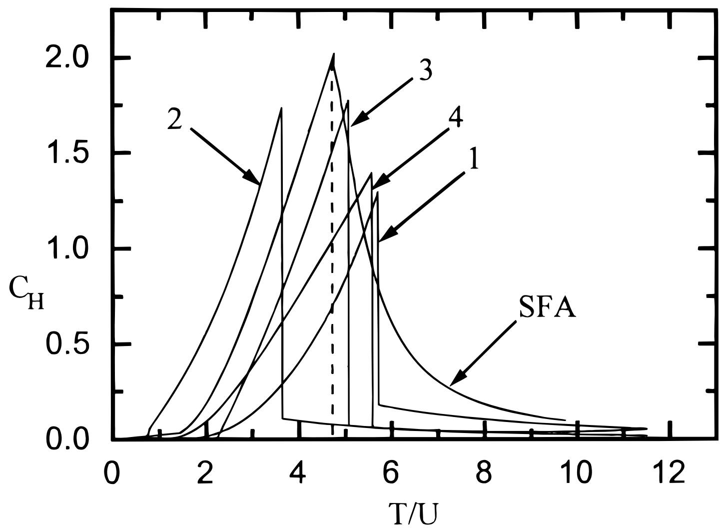

Fig. 15. The dependence of $C_H(T/T_c)$ on the normalized temperature T/T_c for $z = 6$ (periodic boundary conditions): (1) Oguchi's method (Honmura and Kaneyoshi, 1979; Smart, 1966); (2) the constant-bond method (Kasteleijn and Van Kranendonk, 1956); (3) P. R. Weiss approximation (Honmura and Kaneyoshi, 1979; Smart, 1966); (4) effective-field approximation (Honmura and Kaneyoshi, 1979; Smart, 1966) at $n = 0$.

It should be noted that the experimental data for $C_H(T)$ cannot give a categorical answer to the question: Does the jump shown imply a critical point; or does C_H simply decrease rapidly for $T > T_c$?

For simple cubic lattices the behavior of the lattice Green functions has been investigated in the vicinity of the branching point $p = 1$ for $d_E = 3$ (Mannari and Kogeyama, 1968; Morita and Horiguchi, 1971); it has the form

$$G_L(p) = G_L(1) - g_{1L}\varepsilon - g_{2L}\varepsilon^2 + g_{3L}\varepsilon^3 + \ldots \tag{86}$$

The constants g_{iL} depend on the lattice ($L \equiv$ SC, BCC, FCC) and are given by Mannari and Kogeyama (1968); $\varepsilon \equiv (1 - p)^{1/2}$. The decomposition (86) allows one to clarify the behavior of the main thermodynamic values in the vicinity of the critical point and to find the critical exponents α, α' for the specific heat as well as β for the magnetization:

A. Case $T > T_c$ ($\mu = 0$): Defining the parameter $\tau(p) \equiv X(p)/X_c - 1$, where $X(p)$, X_c are defined by (76), (77a), respectively, one can show that the decomposition $\tau(p)$ near X_c has the form

$$\tau \cong \vartheta_{1L}^{>}\,\varepsilon + \vartheta_{2L}^{>}\,\varepsilon^2 + \vartheta_{3L}^{>}\,\varepsilon^3 + O(\varepsilon^4) \tag{87}$$

The positive constants $\vartheta_{iL}^{>}$ ($i = 1, 2, 3$) have been calculated for all three main cubic lattices and are shown in Table III. In the same manner one can find the decomposition coefficients g_{0L}^2 and e_{iL} ($i = 1, 2, 3$) for the mean energy (Table III):

$$\frac{1}{N}\langle H\rangle \cong \frac{Uz}{4}\,[-g_{0L}^2 + e_{1L}^{>}\,\varepsilon - e_{2L}^{>}\,\varepsilon^2 + e_{3L}^{>}\,\varepsilon^3 + O(\varepsilon^4)] \qquad (88)$$

Inverting decomposition (87), we obtain

Table III. Decomposition Coefficients of Thermodynamic Values for the Three-Dimensional Ising Model (Periodic Boundary Conditions)

Decomposition coefficients	SC lattice	BCC lattice	FCC lattice
g_{1L}	1.1695	0.9003	0.8270
g_{2L}	1.0705	0.8421	0.7995
g_{3L}	0.8772	0.6763	0.6206
$\theta_{1L}^{>}$	0.7274	0.4614	0.3968
$\theta_{2L}^{>}$	0.1549	0.3820	0.4805
$\theta_{3L}^{>}$	2.7899	1.3033	1.0480
g_{0L}^2	0.5164	0.3932	0.3447
$e_{1L}^{>}$	1.1695	0.9003	0.8270
$e_{2L}^{>}$	1.5949	1.2353	1.1442
$e_{3L}^{>}$	2.0467	1.5767	1.4476
$\delta_{1L}^{>}$	1.3747	2.1674	2.5203
$\delta_{2L}^{>}$	0.4025	−3.0097	−7.6928
$\delta_{3L}^{>}$	−9.7293	−14.7906	4.6806
$k_{1L}^{>}$	1.6078	1.9513	2.0843
$k_{2L}^{>}$	2.5434	9.3049	13.6295
$k_{3L}^{>}$	7.8260	23.5582	71.4122
$\Delta_{L}^{>}$	2.0243	2.2921	2.3900
$D_{1L}^{>}$	6.4046	21.8595	31.2576
$\theta_{1L}^{<}$	0.6220	0.5125	0.4798
$\theta_{2L}^{<}$	0.3539	0.2300	0.1987
$\theta_{3L}^{<}$	0.3901	0.2009	0.1604
1_{1L}	1.6078	1.9513	2.0843
1_{2L}	1.4711	1.7087	1.7988
1_{3L}	0.0852	0.0801	0.0783
a_{1L}	1.8233	1.7933	1.7834
a_{2L}	0.8342	0.7851	0.7696
a_{3L}	0.1424	0.1351	0.1325
$k_{1L}^{<}$	1.6078	1.9513	2.0843
$k_{2L}^{<}$	1.4711	1.7087	1.7988
$k_{3L}^{<}$	0.0852	0.0801	0.0783
$\Delta_{L}^{<}$	2.0243	2.2921	2.3901
$D_{1L}^{<}$	3.7044	4.0141	4.1253

$$\varepsilon \cong \delta_{1L}\,\tau + \delta_{2L}\,\tau^2 + \delta_{3L}\,\tau^3 + O(\tau^4) \tag{89}$$

where the positive parameters δ_{iL} are listed in Table III. Putting this into (88), we find the decomposition of the mean energy and the nearest order correlators as functions of the parameter τ:

$$\frac{1}{N}\langle H\rangle \cong \frac{Uz}{4}\,(-g_{0L}^2 + k_{1L}^{>}\tau - k_{2L}^{>}\tau^2 - k_{3L}^{>}\tau^3 + \ldots) \tag{90}$$

where the decomposition coefficients $k_{iL}^{>}$ are again given in Table III. From the last decomposition it is easy to find the specific heat behavior at small τ:

$$C_v \cong \Delta_L^{>} - D_{1L}^{>}\tau \tag{91}$$

Numerical values of $\Delta_L^{>}$, $K_{1L}^{>}$ are given for all three types of cubic lattices in Table III. From (91) it follows that, in the SFA framework, the critical exponent α to the right of the critical point equals zero exactly. The high-temperature decomposition leads to the value $\alpha = 0.125 \pm 0.015$; see, for example, Potashinsky and Pokrovsky (1975).

B. Case $T \leq T_c$: For this temperature region we define in a similar manner the parameter $\tau \equiv 1 - X(\mu)/X_c$, $X(\mu)$ being given by expression (77d). From (80) one can see that, near the critical point, the value

$$\xi \equiv Z(\mu)^2 - [G_L(1) - 1] \tag{92}$$

is a small parameter; therefore it is possible to find the decomposition $\tau(\xi)$:

$$\tau \cong \vartheta_{1L}^{<}\xi + \vartheta_{2L}^{<}\xi^2 + \vartheta_{3L}^{<}\xi^3 + O(\xi^4) \tag{93}$$

The coefficients $\vartheta_{iL}^{<}$ ($I = 1, 2, 3$) are shown in Table III. Inverting (93), we find

$$\xi \cong 1_{1L}\tau - 1_{2L}\tau^2 + 1_{3L}\tau^3 + O(\tau^4) \tag{94}$$

where the calculated values 1_{iL} are again listed in Table III. Putting (94) into the expression for μ^2 [see (80)],

$$\mu^2 = \frac{\xi}{2 - G_L(1)} \tag{95}$$

we obtain the decomposition for the spontaneous magnetization:

$$\mu_L \cong a_{1L}\tau^{1/2} - a_{2L}\tau^{3/2} - a_{3L}\tau^{5/2} + O(\tau^{7/2}) \tag{96}$$

Here we have explicitly denoted the magnetization by μ_L to stress the dependence of the constants a_{iL} on the lattice type for the three-dimensional case. It follows from (96) that the SFA is not capable of improving the “classical” values of the critical exponents; it gives $\beta = 1/2$, which coincides with the result of the mean-field theory and its modifications (see, for example, Smart, 1966; Honmura and Kaneyoshi, 1979; Zhang and Min, 1981; Taggart and Fittipaldi, 1982).

To find the behavior of the specific heat to the left of the critical point, it is necessary to find the mean energy as a function of λ. Based on the decompositions given above, it is possible to realize this; we get

$$\frac{1}{N}\langle H\rangle = -\frac{zU}{4}\{\lambda + [G_L(1) - 1]\} \tag{97}$$

which gives the desired decomposition:

$$\frac{1}{N}\langle H\rangle \cong \frac{zU}{4}(-g_{0L}^2 - k_{1L}^{<}\tau + k_{2L}^{<}\tau^2 - k_{3L}^{<}\tau^3 + \ldots) \tag{98}$$

The coefficients $K_{iL}^{<}$ for the cubic lattices are also given in Table III.

It should be noted that the expressions in parentheses in (90) and (98) themselves represent the decompositions of the nearest order correlators from the right and the left, respectively. Comparison of the coefficients $k_{1L}^{>}$, $k_{1L}^{<}$ shows that the correlation functions are monotonic at the critical point; this, in turn, gives only the kink of the specific heat at the critical point. This conclusion follows from the comparison of the expressions for the specific heat at $T > T_c$ and $T < T_c$:

$$C_v \cong \Delta_L^{<} - K_{1L}^{<}\tau \tag{99}$$

The coincidence of $\Delta_L^{>}$ and $\Delta_L^{<}$ leads to the kink of the specific heat and predicts a phase transition of the first kind for this type of boundary conditions. The critical exponent coincides with $\alpha' = 0$ [see (91)].

From the relations for the critical exponents given in, for example, Frank and Mitran (1977), if the exponents α, α', β are known, it is easy to calculate the remaining exponents: $\gamma = \gamma' = 1$, $\delta = 3$, $\nu = \nu' = 2/3$, $\eta = 1/2$ [numerical calculation taken from Potashinsky and Pokrovsky (1975) give the following results: $\gamma \cong 1.25 \pm 0.03$; $\delta = 5.0 \pm 0.2$; $\nu = 0.642 \pm 0.03$].

5.2. The Infinite Lattice

As remarked above, in the present framework, the possibility exists for considering boundary conditions other than the conventional periodic boundary conditions. In particular, we shall now consider infinite cubic lattices and show that the change of boundary conditions can modify the scenario of the phase transition.

To this end it is necessary to get the analytical solution of the corresponding DLRE; but analytical solutions of multidimensional difference equations are not known and have not yet been considered in mathematical physics. It is possible, however, to suggest a method based on the concrete form of three-dimensional difference equations. In Section 5.2.1 we shall first consider the solution of a model based, in its turn, on the solution of multidimensional difference equations. Next, in Section 5.2.2 we shall give for comparison purposes the continuous approach, based on the solution of the Helmholtz equation for the pair correlation function. Insofar as the form of the difference equation is dictated by the geometry of the lattice, for complex lattices (BCC, FCC) the solutions will differ by purely mathematical complications of the corresponding expressions. For demonstration purposes, we shall limit ourselves here to the SC lattice.

5.2.1. *Discrete Approach*

The equation for the pair correlation function can be given in the form of a three-dimensional difference equation of the second order. For nearest neighbor interactions ($z = 6$), it reads

$$K(m, n, l) = \frac{p}{6}[K(m+1, n, l) + K(m-1, n, l) + K(m, n+1, l) + K(m, n-1, l) + K(m, n, l+1) + K(m, n, l-1)] \quad (100)$$

$K(m, n, l) \equiv 4\langle \Delta S_f^z \, \Delta S_{f'}^z \rangle$; $f - f' \equiv j(m, n, l)$. The solution of this equation can readily be obtained by the method of separation of variables. By analogy with the one-dimensional case, we find as for $d_E = 2$ [see expression (53)]

$$K(m, n, l) = Cx^{|m|}y^{|n|}z^{|l|} \quad (101)$$

where x, y, z are unknown functions of p, and C is a constant.

We impose the following limitations on x, y, z:

1. $|x|, |y|, |z| \leq 1$ (the correlation function at infinity should go to zero).
2. $K(m, n, l)$ for the SC lattice should be a symmetric function of the parameters m, n, l.

To determine the unknown functions x, y, and z, (100) is written down for the correlators of the nearest order, using the fact *that the value of the correlator* $K(0, 0, 0)$ *is known*:

$$K(1, 0, 0) = \frac{p}{6}[K(2, 0, 0) + K(0, 0, 0) + K(1, 1, 0) + K(1, -1, 0) + K(1, 0, 1) + K(1, 0, -1)]$$

$$K(0, 1, 0) = \frac{p}{6}[K(1, 1, 0) + K(-1, 1, 0) + K(0, 1, 0) \quad (102)$$

$$+ K(0, 0, 0) + K(0, 1, 1) + K(0, 1, -1)]$$

$$K(0, 0, 1) = \frac{p}{6}[K(1, 0, 1) + K(-1, 0, 1) + K(0, 1, 1)$$

$$+ K(0, -1, 1) + K(0, 0, 1) + K(0, 0, 0)]$$

Substituting (101) into (102) gives the following system of equations for x, y, z:

$$\begin{aligned} x &= \frac{p}{6}(x^2 + 1 + 2xy + 2xz) \\ y &= \frac{p}{6}(2xy + y + 1 + 2yz) \\ z &= \frac{p}{6}(2xz + 2yz + z + 1) \end{aligned} \tag{103}$$

From (103) we obtain only *one* solution satisfying the two limitations imposed above:

$$x = y = z = \lambda = \frac{3 - \sqrt{9 - 5p^2}}{5p} \tag{104}$$

Thus the desired solution of (100) assumes the form

$$K(m, n, l) = K(0, 0, 0)\lambda^{|m|+|n|+|l|} \tag{105}$$

This allows one to regain easily the dimensionless dispersion of the local field as a function of the parameter p ($T > T_c$):

$$B(p) = [6K(0, 0, 0) + 6K(2, 0, 0) + 24K(1, 1, 0)]^{1/2} = \left(\frac{3}{2} + \frac{15}{2}\lambda^2\right)^{1/2} \tag{106}$$

The critical temperature is readily found from the dimensionless ratio $X = 4T/U$, (77a), by putting $p = 1$; for the infinite SC lattice $T_c/U = 5.5761$. This is greater than $T_c/U = 4.7655$ (SC) for periodic boundary conditions. The critical temperature serves as a measure of interaction and has a tendency to increase with an increasing number of total spins. We therefore conclude that the boundary conditions affect the value of the critical temperature.

The plot of the dimensionless local field dispersion for an infinite SC lattice as a function of the normalized temperature is given in Fig. 16. In Fig. 17 we also show the nearest order correlation function (the nearest order parameter) as a function of the normalized temperature T/T_c.

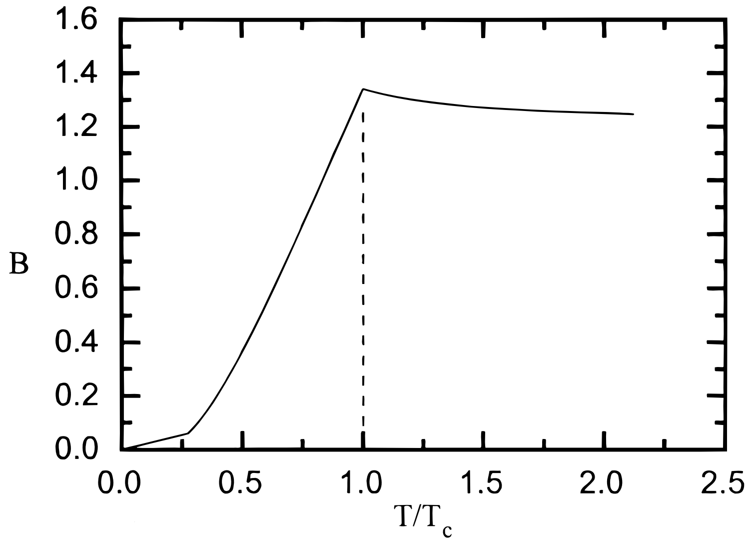

Fig. 16. The dependence of $B(T/T_c)$ on the normalized temperature T/T_c for an infinite SC lattice. $B(1) = 1.3416$; $B(\infty) = 1.2247$.

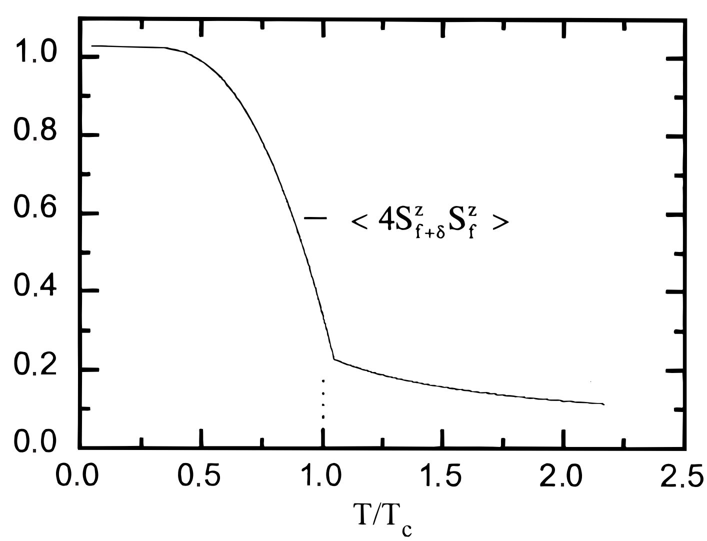

Fig. 17. The dependence of the nearest order correlation function on the normalized temperature T/T_c for an infinite SC lattice.

As is clear from this figure, modification of the boundary conditions leads to the kink of the nearest order parameter at the critical point, which, in turn, can lead to a finite jump of the specific heat (see Fig. 18). Using (106), we can easily find the dependence of the spontaneous magnetization for an infinite SC lattice on the normalized temperature T/T_c. The corresponding plot is given in Fig. 19. In Fig. 20 we give some plots of the nearest order correlation functions versus the dimensionless temperature. In Fig. 21 we show the calculated function $\mu(h)$. Based on expression (106), we are able to investigate the region near the critical point. The procedure is the same as before; we only point out some peculiarities of the present case:

A. $T \geq T_c$ ($\mu = 0$):

$$\tau \cong \vartheta_{1\infty}^{>}\varepsilon^2 + \vartheta_{2\infty}^{>}\varepsilon^4 + O(\varepsilon^5) \tag{107}$$

$$\frac{1}{N}\langle H\rangle \cong \frac{Uz}{4}\left(-g_{0\infty}^2 + e_{1\infty}^{>}\varepsilon^2 - e_{2\infty}^{>}\varepsilon^4 + \cdots\right) \tag{108}$$

$$\tau \cong \delta_{1\infty}^{>}\tau^{1/2} - \delta_{2\infty}^{>}\tau^{3/2} + O(\tau^{5/2}) \tag{109}$$

$$\frac{1}{N}\langle H\rangle \cong \frac{Uz}{4}\left(-g_{0\infty}^{2>} + k_{1\infty}^{>}\tau - k_{2\infty}^{>}\tau^2 + k_{3\infty}^{>}\tau^3 + \cdots\right) \tag{110}$$

$$C_H \cong \Delta_\infty^{>} - D_{1\infty}^{>}\tau \tag{111}$$

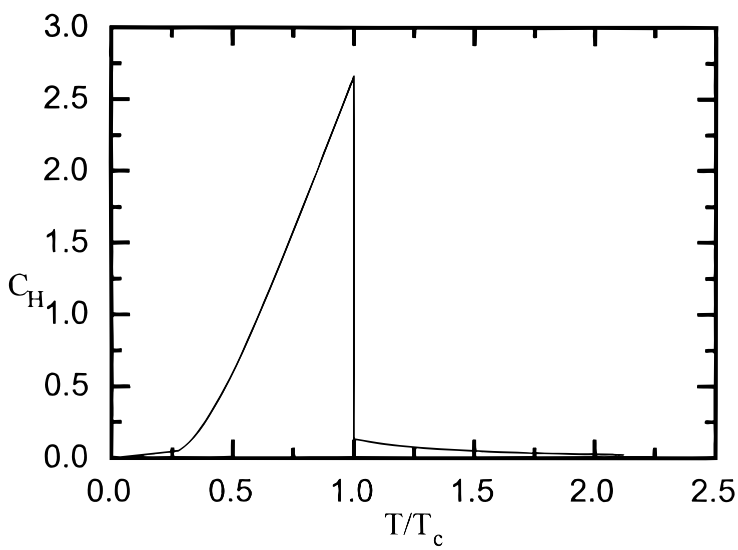

Fig. 18. The dependence of $C_v(T/T_c)$ on the normalized temperature T/T_c for an infinite SC lattice. At the critical point we see the finite jump that is associated with a phase transition of the second kind.

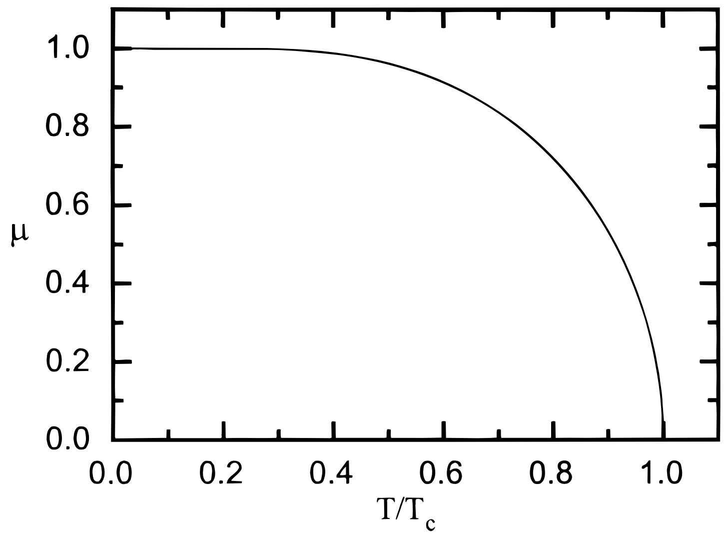

Fig. 19. The dependence of the spontaneous magnetization $\mu(T/T_c)$ on the normalized temperature T/T_c for an infinite SC lattice.

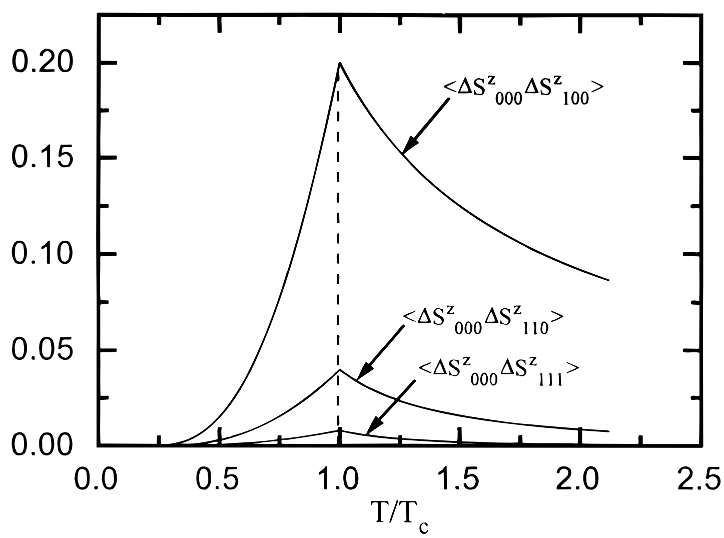

Fig. 20. The dependence of the nearest order correlation functions $4\langle \Delta S^z_{000} \Delta S^z_{100} \rangle$, $4\langle \Delta S^z_{000}\, \Delta S^z_{110} \rangle$, and $4\langle \Delta S^z_{000}\, \Delta S^z_{111} \rangle$ on the normalized temperature T/T_c for an infinite SC lattice ($z = 6$). The corresponding values of these correlation functions at the critical point are 0.2, 0.04, and 0.008.

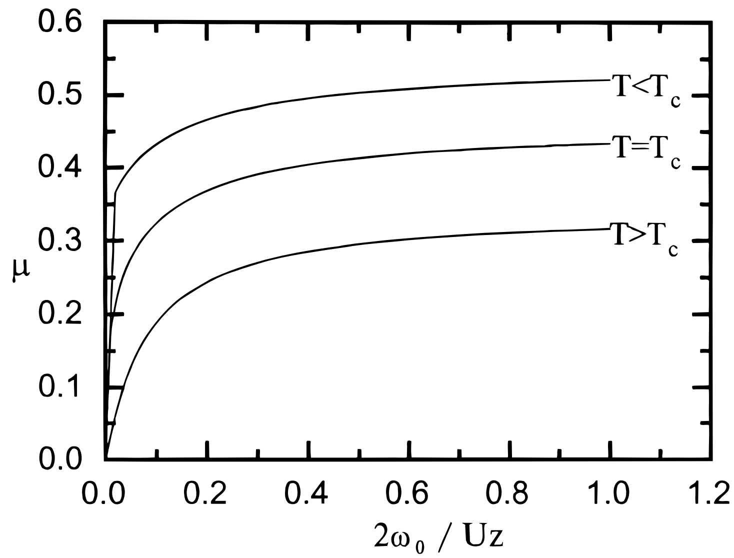

Fig. 21. The dependence of $\mu(h)$ on the magnetic field h at temperatures close to the critical value for an infinite SC lattice ($z = 6$). $h \equiv 2\omega_0 U/z$.

Clearly, from (111) we note that the change of boundary conditions does not change the value of the critical exponent α.

B. $T \leq T_c$:

$$\tau \cong \vartheta_{1\infty}^{<}\xi + \vartheta_{2\infty}^{<}\xi^2 + \vartheta_{3\infty}^{<}\xi^3 + O(\xi^4) \tag{112}$$

$$\lambda \cong 1_{1\infty}\tau - 1_{2\infty}\tau^2 + 1_{3\infty}\tau^3 + O(\tau^4) \tag{113}$$

$$\mu \cong a_{1\infty}\tau^{1/2} - a_{2\infty}\tau^{3/2} - a_{3\infty}\tau^{5/2} + O(\tau^3) \tag{114}$$

$$\frac{1}{N}\langle H\rangle \cong \frac{Uz}{4}\left(-g_{0\infty}^2 + k_{1\infty}^{<}\tau - k_{2\infty}^{<}\tau^2 + k_{3\infty}^{<}\tau^3 + \cdots\right) \tag{115}$$

$$C_H \cong \Delta_{\infty}^{<} - D_{1\infty}^{<}\tau \tag{116}$$

The coefficients of these decompositions are listed in Table IV.

Thus, the change of boundary conditions does not change the values of critical exponents; but the specific heat C_H has a finite jump at the critical point (for $z = 6$, $\Delta C_H = \Delta_{\infty}^{<} - \Delta_{\infty}^{>} = 2.3967$). For an infinite model, as remarked above, we have a phase transition of the second kind—in agreement with other methods.

5.2.2. Continuous Approach

In this subsection we demonstrate the alternative approach of investigating phase transitions in an infinite lattice. We transform the corresponding

Table IV. Decomposition Coefficients of Thermodynamic Values for an Infinite SC Lattice

$\theta_{1\infty}^{>}$	$\theta_{2\infty}^{>}$	$\delta_{1\infty}^{>}$	$\delta_{2\infty}^{>}$	$g_{0\infty}^{2}$	$e_{1\infty}^{>}$	$e_{2\infty}^{>}$	$k_{1\infty}^{>}$	$k_{2\infty}^{>}$
1.2021	0.9407	0.9121	0.2969	0.2000	0.3000	0.2625	0.2496	0.3441
$k_{3\infty}^{>}$	$\Delta_{\infty}^{>}$	$D_{1\infty}^{>}$	$\theta_{1\infty}^{<}$	$\theta_{2\infty}^{<}$	$\theta_{3\infty}^{<}$	$1_{1\infty}$	$1_{2\infty}$	$1_{3\infty}$
0.5131	0.2685	0.7406	0.4042	0.1359	0.0896	2.4739	2.0583	0.0737
$a_{1\infty}$	$a_{2\infty}$	$a_{3\infty}$	$k_{1\infty}^{<}$	$k_{2\infty}^{<}$	$k_{3\infty}^{<}$	$\Delta_{\infty}^{<}$	$D_{1\infty}^{<}$	
1.7585	0.7315	0.1260	2.4739	2.0583	0.0737	2.6620	4.4296	

difference equation (100) to its continuous equivalent. Since this procedure is conventional and is described in any text of mathematical physics, we omit the routine calculations and write down only the final result:

$$\Delta K(u, v, t) - \chi^2 K(u, v, t) = -\frac{K(0, 0, 0)}{\mathrm{z}} \sum_{\varepsilon=1}^{Z} \delta(|R - R_\varepsilon|) \qquad (117)$$

Here $K(u, v, t)$ is the pair correlation function of continuous variables u, v, t; Δ is the three-dimensional Laplacian; δ is the delta function; $\chi = [z(1 - p)/p]^{1/2}$, and $z = 6$.

Equation (117) is the Helmholtz equation; its solution is well known and reads

$$K(u, v, t) = \frac{K(0, 0, 0)}{z} \sum_{\varepsilon=1}^{z} \frac{\exp(-\chi|\mathbf{R} - \mathbf{R}_\varepsilon|)}{|\mathbf{R} - \mathbf{R}_\varepsilon|} \qquad (118)$$

This expression correctly describes the interspin correlations when the separation between the chosen spin and others is increased. Based on this solution, it is easy to derive the expression for the dimensionless dispersion of the local field for $z = 6$:

$$B(p) = \left(\frac{3}{2} + \frac{9}{4} e^{-\chi} + \frac{1}{12} e^{-3\chi} + \frac{3}{5^{1/2}} e^{-5^{1/2}\chi} + \frac{2}{3^{1/2}} e^{-3^{1/2}\chi}\right)^{1/2} \qquad (119)$$

Having obtained this expression, one can find the value of $T_c/U = 4.1362$. The substantial difference from the foregoing value of $T_c/U = 5.5761$ can be attributed to the transformation to continuous variables. The remaining thermodynamic values can be calculated in complete analogy with the procedures described above for an infinite SC lattice.

6. CONCLUSIONS

In this paper we have developed a remarkably powerful approach to strongly interacting many-body systems based on an exceedingly simple mean-field picture, albeit modified in that the operator of quadratic fluctuations is replaced with its mean value [Eq. (4)]. We have applied this approach to the spin-1/2 n-dimensional Ising model ($n = 1, 2, 3$), undertaking in the process a novel analysis of the two-dimensional model *without periodic boundary conditions*, and demonstrating the sensitivity of the phase-transition scenario in the two- and three-dimensional cases to the boundary conditions.

The present work also goes well beyond the previous work (Nigmatullin and Toboev, 1986, 1988, 1989). Specifically, in those papers the treatment of the mean-field operator σ_f^z was *inconsistent*. Approximation (7) did not allow one to derive in detail the full thermodynamics of the Ising model for any integral dimension. In contrast, approximation (4) for σ_f^z, on which our present approach is based, has allowed us to work out in meticulous detail all the fundamental properties of the system and to obtain the DLREs for related systems: The Ising model of antiferromagnets, the lattice gas systems, the Ising model in the transverse field with dipole–dipole interaction, the X–Y model, the Hubbard model, and so forth. The detailed investigation of these systems will be the subject of subsequent publications. The next natural step would be to generalize our treatment to the Ising model with an arbitrary spin, type of lattice, interaction, and geometry. Other applications being envisaged include strongly interacting Bose and Fermi systems.

It should be admitted, however, that the SFA is not capable of describing the phase transition in the two-dimensional model with periodic boundary conditions, thereby precluding a comparison with Onsager's exact solution. In addition, the SFA is clearly unable to improve the values of the critical exponents for the magnetization and the specific heat in the limit of nearest neighbor interaction, these values coinciding with the predictions of the mean-field theory and its modified versions. This implies that a full description of the phase transition presumably requires higher orders of fluctuations of the local field operator (2). In principle, one can incorporate these orders into the present picture by solving a nonlinear DLRE of the type (48). Unfortunately, this is a mathematically complicated problem; analytical methods for solving nonlinear DLREs have hardly been developed. The intricate problems involved here surely constitute a major challenge for physicists and mathematicians alike.

ACKNOWLEDGMENTS

Two of us (H.B.G. and R.R.N.) gratefully acknowledge partial financial support from the Deanship of Scientific Research, University of Jordan.

REFERENCES

Abrikosov, A. A., Gor'kov, L. P., and Dzyaloshinskii, I. Ye. (1965). *Quantum Field Theoretical Methods in Statistical Physics*, 2nd ed., Pergamon Press, Oxford.
Brush, S. G. (1967). *Reviews of Modern Physics*, **39**, 883.
Bune, A. V., Fridkin, Y. M., Ducharme, S., Blinov, L. M., Palto, S. P., Sorokin, A. V., Yudin, S. G., and Zlatkin, A. (1998). *Nature*, **391**, 874.
Fetter, A. L., and Walecka, J. D. (1971). *Quantum Theory of Many-Particle Systems*, McGraw-Hill, New York.
Frank, B., and Mitran, O. (1977). *Journal of Physics C: Solid State Physics*, **10**, 2641.
Honmura, R, and Kaneyoshi, T. (1979). *Journal of Physics C: Solid State Physics*, **12**, 3979.
Jelifonov, M. P. (1971). *Teoreticheskaiya i Matematicheskaiya Fizika*, **8**, 401 [in Russian].
Kasteleijn, P. W., and Van Kranendonk, J. (1956). *Physica*, **22**, 317.
Loskutov, V. V., Mironov, G. I., and Nigmatullin, R. R. (1996). *Low Temperature Physics*, **22**, 220.
Mannari, T., and Kogeyama, A. (1968). *Progress of Theoretical Physics (Supplement)*, 269.
Morita, T., and Horiguchi, T. (1971). *Journal of Mathematical Physics*, **12**, 981, 986.
Nigmatullin, R. R., and Toboev, V. A. (1986). *Teoreticheskaiya i Matematicheskaiya Fizika*, **68**, 88 [in Russian].
Nigmatullin, R. R., and Toboev, V. A.(1988). *Teoreticheskaiya i Matematicheskaiya Fizika*, **74**, 11 [in Russian].
Nigmatullin, R. R., and Toboev, V. A. (1989). *Teoreticheskaiya i Matematicheskaiya Fizika*, **80**, 94 [in Russian].
Oitmaa, J. (1971). *Solid State Communications*, **9**, 745.
Potashinsky, A. Z., and Pokrovsky, V. L. (1975). *The Fluctuation Theory of Phase Transitions*, Nauka, Moscow [in Russian].
Smart, S. (1966). *Effective Field in the Theory of Magnetism*, IBM Watson Research Center, Yorktown Heights, and Saunders, Philadelphia.
Stanley, H. E. (1971). *Introduction to Phase Transitions and Critical Phenomena*, Clarendon Press, Oxford.
Taggart, G. B., and Fittipaldi, J. P. (1982). *Physical Review B*, **25**, 7026.
Zhang, H., and Min, B. (1981). *Journal of Physics C: Solid State Physics*, **14**, 1769.
Zubarev, D. N. (1960). *Uspekhi Fizicheskikh Nauk*, **71**, 71 [English transl., *Soviet Physics - Uspekhi*, **3**, 320 (1960)].