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Statistical-thermodynamic description within the ring approximation. II. Ising model

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The results obtained previously [R. V. Chepulskii, Phys. Rev. B **69**, 134431 (2004)] within the ring approximation in the case of the lattice gas model are generalized to the case of the Ising model with a complex crystal lattice and arbitrary magnetic order. The nonpair spin interactions of any order and effective radii of action are taken into account. The verification of the numerical accuracy of the ring approximation in the cases that are typical at consideration of the Ising model is performed.

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I. INTRODUCTION

The spin-1/2 Ising model with two possible directions of the spin (up and down) is statistically equivalent to the two-component lattice gas model.[1,2] However, in contrast to the lattice gas model, which can be directly applied to study of alloys and even fluids and amorphous materials, the Ising model is a crude model for investigation of real magnetic systems. Nevertheless, the Ising model has been one of the basic models used for development of the statistical mechanics of phase transitions. A great number of analytical and numerical, exact and approximate, results were obtained for this model.

In the previous paper,[3] the lattice gas model was considered within the ring approximation. The aim of the present paper is to generalize the obtained results to the case of spin-1/2 Ising model considering paramagnetic, ferromagnetic, and antiferromagnetic states (Secs. II–III). In Sec. IV, we outline the approximations within the Ising model that are similar to the ring one. In Sec. V, the verification of the numerical accuracy of the ring approximation is performed in the cases that have been typical at consideration of the Ising model.

II. GENERAL CASE

Let us consider the spin-1/2 Ising model. We suppose that the unit cell of the crystal lattice consists of ν crystal lattice sites $(\nu \geqslant 1)$. It is important that the case of $\nu > 1$ can be attributed not only to the complex character of the crystal lattice itself but also to the presence of a long-range antiferromagnetic order in a spin distribution. The crystal lattice can be divided into ν Bravais sublattices according to the unit cell. Taking into account the many-body spin interactions of arbitrary orders and radii of action, the Hamiltonian H of the Ising model in question can be written in the following form [see, e.g., Eq. (8.12) in Ref. 4]:

$$H = -Nj_0 - \sum_i h_i \sum_{\mathbf{R}} \sigma_{i,\mathbf{R}} - \sum_{n=2}^{N\nu} \frac{1}{n!} \sum_{i_1,i_2,\ldots,i_n} \sum_{\mathbf{R}_1,\mathbf{R}_2,\ldots,\mathbf{R}_n} J^{(n)}_{i_1,\mathbf{R}_1;i_2,\mathbf{R}_2;\ldots;i_n,\mathbf{R}_n} \times \sigma_{i_1,\mathbf{R}_1}\sigma_{i_2,\mathbf{R}_2}\cdots\sigma_{i_n,\mathbf{R}_n}, \quad (1)$$

or writing the series explicitly

$$H = -Nj_0 - \sum_i h_i \sum_{\mathbf{R}} \sigma_{i,\mathbf{R}} - \frac{1}{2}\sum_{i_1,i_2}\sum_{\mathbf{R}_1,\mathbf{R}_2} J^{(2)}_{i_1,\mathbf{R}_1;i_2,\mathbf{R}_2}\sigma_{i_1,\mathbf{R}_1}\sigma_{i_2,\mathbf{R}_2} - \frac{1}{6}\sum_{i_1,i_2,i_3}\sum_{\mathbf{R}_1,\mathbf{R}_2,\mathbf{R}_3} J^{(3)}_{i_1,\mathbf{R}_1;i_2,\mathbf{R}_2;i_3,\mathbf{R}_3}\sigma_{i_1,\mathbf{R}_1}\sigma_{i_2,\mathbf{R}_2}\sigma_{i_3,\mathbf{R}_3} - \cdots. \quad (2)$$

In Eqs. (1) and (2), the summations on the indices i and on the site radius vectors $\mathbf{R}$ are carried over all ν sublattices and over all N unit cells of the crystal lattice, respectively, h_i is the nonuniform (for a generality) external magnetic field (measured in energy units), $\sigma_{i,\mathbf{R}}$ is the configurational variable,

$$\sigma_{i,\mathbf{R}} = \begin{cases} 1 & \text{if the spin at site } (i,\mathbf{R}) \text{ is up} \\ -1 & \text{otherwise,} \end{cases} \quad (3)$$

and $J^{(n)}_{i_1,\mathbf{R}_1;i_2,\mathbf{R}_2;\ldots;i_n,\mathbf{R}_n}$ is the spin interaction potential of nth order $(n=2,3,\ldots,N\nu)$. Note that in the configurational description of the Ising model we follow the same line of reasoning as in Ref. 3 (see Sec. 2 there).

The general expression for the free energy of the lattice gas obtained within the ring approximation in Ref. 3 [see Eq. (38) there] can be transformed to the case of the Ising model as follows:

$$f_{\text{ring}} = f_{\text{MF}} - \frac{1}{2}\sum_{i=1}^{\nu} \mu_i (1 - s_i^2) + \frac{k_B T}{2N}\sum_{\mathbf{k}} \ln\det A_{\mathbf{k}}, \quad (4)$$

where T is the absolute temperature, k_B is the Boltzmann constant, s_i is the (unitless) statistical average magnetization of the sites at ith sublattice $(i=1,2,\ldots,\nu)$,

$$s_i = \langle \sigma_{i,\mathbf{R}} \rangle, \quad (5)$$

$$f_{\text{MF}} = \varepsilon_{\text{MF}} - Ts_{\text{MF}}, \quad (6)$$

$$\varepsilon_{\text{MF}} = -\tilde{\Phi}^{(0)}, \quad (7)$$

$$s_{\mathrm{MF}} = -k_{\mathrm{B}} \sum_{i=1}^{\nu} \left[\frac{1+s_i}{2} \ln \frac{1+s_i}{2} + \frac{1-s_i}{2} \ln \frac{1-s_i}{2} \right]. \tag{8}$$

The quantities μ_i are to be determined from the equations ($i=1,2,\ldots,\nu$)

$$N^{-1} \sum_{\mathbf{k}} \|A_{\mathbf{k}}^{-1}\|_{ii} = 1, \tag{9}$$

f_{MF}, $\varepsilon_{\mathrm{MF}}$, and s_{MF} are, respectively, the free energy, energy, and entropy corresponding to the mean-field approximation. The designations $\det A_{\mathbf{k}}$ and $\|A_{\mathbf{k}}^{-1}\|_{ii}$ mean, respectively, the determinant of the matrix $A_{\mathbf{k}}$ and the ith diagonal element of the matrix $A_{\mathbf{k}}^{-1}$ inverse to $A_{\mathbf{k}}$, which has the following elements:

$$A_{\mathbf{k}}^{i_1,i_2} = \delta_{i_1,i_2} - \frac{\sqrt{1-s_{i_1}^2}\,[\tilde{\Phi}^{(2)}_{i_1,\mathbf{k};i_2} - \mu_{i_1}\delta_{i_1,i_2}]\sqrt{1-s_{i_2}^2}}{k_{\mathrm{B}}T}. \tag{10}$$

The functions $\tilde{\Phi}^{(n)}_{i_1,\mathbf{k}_1;i_2,\mathbf{k}_2;\ldots;i_{n-1},\mathbf{k}_{n-1};i_n}$ ($n=1,2,\ldots,N\nu$) are defined as (for $n=0,1,\ldots,4$ see the Appendix)

$$\begin{aligned}\tilde{\Phi}^{(n)}_{i_1,\mathbf{k}_1;i_2,\mathbf{k}_2;\ldots;i_{n-1},\mathbf{k}_{n-1};i_n} &= \sum_{t=0}^{N\nu-n} \frac{1}{t!} \sum_{i'_1,i'_2,\ldots,i'_t} s_{i'_1} s_{i'_2} \cdots s_{i'_t} \\ &\quad \times \tilde{J}^{(t+n)}_{i'_1,\mathbf{0};i'_2,\mathbf{0};\ldots;i'_t,\mathbf{0};i_1,\mathbf{k}_1;i_2,\mathbf{k}_2;\ldots;i_{n-1},\mathbf{k}_{n-1};i_n},\end{aligned} \tag{11}$$

where $\tilde{J}^{(n)}_{i_1,\mathbf{k}_1;i_2,\mathbf{k}_2;\ldots;i_{n-1},\mathbf{k}_{n-1};i_n}$ ($n=2,3,\ldots,N\nu$) are the Fourier transforms of the interaction potentials:

$$\tilde{J}^{(0)} = j_0, \quad \tilde{J}^{(1)}_i = J^{(1)}_i = h_i,$$

$$\begin{aligned}\tilde{J}^{(n)}_{i_1,\mathbf{k}_1;i_2,\mathbf{k}_2;\ldots;i_{n-1},\mathbf{k}_{n-1};i_n} &= \sum_{\mathbf{R}_1,\mathbf{R}_2,\ldots,\mathbf{R}_{n-1}} J^{(n)}_{i_1,\mathbf{R}_1;i_2,\mathbf{R}_2;\ldots;i_{n-1},\mathbf{R}_{n-1};i_n,\mathbf{0}} \\ &\quad \times \exp\left[-i\sum_{i=1}^{n-1} \mathbf{k}_i \mathbf{R}_i\right],\end{aligned}$$

$$\begin{aligned}J^{(n)}_{i_1,\mathbf{R}_1;i_2,\mathbf{R}_2;\ldots;i_{n-1},\mathbf{R}_{n-1};i_n,\mathbf{R}_n} &= N^{-(n-1)} \sum_{\mathbf{k}_1,\mathbf{k}_2,\ldots,\mathbf{k}_{n-1}} \tilde{J}^{(n)}_{i_1,\mathbf{k}_1;i_2,\mathbf{k}_2;\ldots;i_{n-1},\mathbf{k}_{n-1};i_n} \\ &\quad \times \exp\left[i\sum_{i=1}^{n-1} \mathbf{k}_i(\mathbf{R}_i - \mathbf{R}_n)\right].\end{aligned} \tag{12}$$

In Eqs. (4), (9), and (12) and below in this paper, the summations on **k** are carried over all the points specified by the cyclic boundary conditions in the corresponding first Brillouin zone. From Eq. (4) one can obtain the following expressions for the energy $\varepsilon_{\mathrm{ring}}$ and entropy s_{ring} within the ring approximation:

$$\varepsilon_{\mathrm{ring}} = \varepsilon_{\mathrm{MF}} - \frac{1}{2}\sum_{i=1}^{\nu} \mu_i(1-s_i^2), \tag{13}$$

$$s_{\mathrm{ring}} = s_{\mathrm{MF}} - \frac{k_{\mathrm{B}}}{2N}\sum_{\mathbf{k}} \ln\det A_{\mathbf{k}}. \tag{14}$$

Note that moving from the lattice gas model to the Ising model we used the following relationships:

$$C_{i,\mathbf{R}} = \frac{1+\sigma_{i,\mathbf{R}}}{2}, \quad P_i = \frac{1+s_i}{2}, \tag{15}$$

where $C_{i,\mathbf{R}}$ is the configurational variable and P_i is atom distribution probability within the lattice gas model [see Eqs. (3) and (15) in Ref. 3]. For a convenience, the above defined

$$\mu_i \equiv \mu_i^{\mathrm{Ising}}$$

and

$$\tilde{\Phi}^{(n)}_{i_1,\mathbf{k}_1;i_2,\mathbf{k}_2;\ldots;i_{n-1},\mathbf{k}_{n-1};i_n} \equiv \tilde{\Phi}^{(n)\mathrm{Ising}}_{i_1,\mathbf{k}_1;i_2,\mathbf{k}_2;\ldots;i_{n-1},\mathbf{k}_{n-1};i_n}$$

are different from those defined in Ref. 3 [with sign LG (lattice gas) below] by the factors (-2^{-n}) and 4, respectively:

$$\mu_i^{\mathrm{Ising}} \equiv 4\mu_i^{\mathrm{LG}}, \tag{16}$$

$$\begin{aligned}\tilde{\Phi}^{(n)\mathrm{Ising}}_{i_1,\mathbf{k}_1;i_2,\mathbf{k}_2;\ldots;i_{n-1},\mathbf{k}_{n-1};i_n} &\equiv -2^{-n}\tilde{\Phi}^{(n)\mathrm{LG}}_{i_1,\mathbf{k}_1;i_2,\mathbf{k}_2;\ldots;i_{n-1},\mathbf{k}_{n-1};i_n}.\end{aligned} \tag{17}$$

The values of the quantities s_i corresponding to the thermodynamically stable or metastable states are to be found from the condition of the absolute or local, respectively, minima of the free energy, according to the variational property of the free energy (see, e.g., Sec. 4.2.2 in Ref. 2). The corresponding equations of state for determination of such s_i within the ring approximation in the case of the Ising model can be obtained from Eq. (66) in Ref. 3 as ($i=1,2,\ldots,\nu$)

$$\frac{k_{\mathrm{B}}T}{2} \ln\frac{1+s_i}{1-s_i} = G_i \tag{18}$$

or, equivalently,

$$s_i = \tanh[G_i/(k_{\mathrm{B}}T)], \tag{19}$$

where

$$\begin{aligned}G_i &= \tilde{\Phi}^{(1)}_i - \mu_i s_i \\ &\quad + \frac{1}{2N}\sum_{\mathbf{q}}\sum_{j,l} \sqrt{(1-s_j^2)(1-s_l^2)}\,\tilde{\Phi}^{(3)}_{i,\mathbf{0};j,\mathbf{q};l} \|A_{\mathbf{q}}^{-1}\|_{lj}.\end{aligned} \tag{20}$$

In the derivation of Eqs. (18) and (19) we took into account that, in contrast to the lattice gas model, within the Ising model there is no such constraint as the total concentration of *A*-type atoms. Note that within the mean-field approximation, the equations of state are the same as Eqs. (18) and (19) but with $G_i = \tilde{\Phi}_i^{(1)}$.

The critical temperature of the absolute instability of any structure is determined by the equation [see Eq. (97) in Ref. 3]

$$\det \beta_{\mathbf{k}} = 0, \tag{21}$$

where the elements of the matrix $\beta_{\mathbf{k}}$ are defined as

$$\begin{aligned}\beta_{\mathbf{k}}^{ij} = {} & A_{\mathbf{k}}^{ij} + \frac{2s_i[\|I_{\mathbf{k}}^{-1}\|_{ij} - \delta_{ij}]s_j}{\sqrt{(1-s_i^2)(1-s_j^2)}} + \sum_{l,s} T_{\mathbf{k}}^{il}\|I_{\mathbf{k}}^{-1}\|_{ls} \\ & \times\left[\frac{1}{2}T_{-\mathbf{k}}^{js} + \frac{2s_j}{\sqrt{(1-s_j^2)}}\delta_{sj}\right] \\ & - \frac{1}{2N}\sum_{i_1,i_2}\sum_{\mathbf{q}} \tilde{f}^{(4)}_{i,\mathbf{k};j,-\mathbf{k};i_1,\mathbf{q};i_2}\|A_{\mathbf{q}}^{-1}\|_{i_2,i_1} \\ & - \frac{1}{2N}\sum_{i_1,i_2,i_3,i_4}\sum_{\mathbf{q}} \tilde{f}^{(3)}_{i_1,\mathbf{q}-\mathbf{k};i_2,-\mathbf{q};i}\|A_{\mathbf{q}}^{-1}\|_{i_2,i_3} \\ & \times \tilde{f}^{(3)}_{i_3,\mathbf{q};i_4,\mathbf{k}-\mathbf{q};j}\|A_{\mathbf{q}-\mathbf{k}}^{-1}\|_{i_4,i_1},\end{aligned} \tag{22}$$

$$\begin{aligned}& \tilde{f}^{(n)}_{i_1,\mathbf{k}_1;i_2,\mathbf{k}_2;\ldots;i_{n-1},\mathbf{k}_{n-1};i_n} \\ & \quad = \frac{\prod_{m=1}^{n}\sqrt{1-s_{i_m}^2}}{k_{\mathrm{B}}T}\tilde{\Phi}^{(n)}_{i_1,\mathbf{k}_1;i_2,\mathbf{k}_2;\ldots;i_{n-1},\mathbf{k}_{n-1};i_n},\end{aligned} \tag{23}$$

$I_{\mathbf{k}}^{-1}$ is the matrix inverse to $I_{\mathbf{k}}$ with the elements

$$I_{\mathbf{k}}^{ij} = N^{-1}\sum_{\mathbf{q}} \|A_{\mathbf{k}-\mathbf{q}}^{-1}\|_{ij}\|A_{\mathbf{q}}^{-1}\|_{ij}, \tag{24}$$

$$T_{\mathbf{k}}^{ij} = N^{-1}\sum_{i_1,i_2}\sum_{\mathbf{q}} \|A_{\mathbf{q}}^{-1}\|_{ji_1}\tilde{f}^{(3)}_{i_1,\mathbf{q};i_2,-(\mathbf{k}+\mathbf{q});i}\|A_{\mathbf{k}+\mathbf{q}}^{-1}\|_{i_2j}. \tag{25}$$

Let us define the short-range order (SRO) parameters $\alpha_{\mathbf{R}}^{ij}$ and there Fourier transform $\alpha_{\mathbf{k}}^{ij}$ as

$$\alpha_{\mathbf{R}_1-\mathbf{R}_2}^{ij} = \frac{\langle(\sigma_{\mathbf{R}_1}^i - s_i)(\sigma_{\mathbf{R}_2}^j - s_j)\rangle}{\sqrt{(1-s_i^2)(1-s_j^2)}}, \tag{26}$$

$$\alpha_{\mathbf{k}}^{ij} = \sum_{\mathbf{R}} \alpha_{\mathbf{R}}^{ij}\exp(-i\mathbf{k}\mathbf{R}), \quad \alpha_{\mathbf{R}}^{ij} = N^{-1}\sum_{\mathbf{k}} \alpha_{\mathbf{k}}^{ij}\exp(i\mathbf{k}\mathbf{R}). \tag{27}$$

Within the ring approximation for the SRO, we obtain (see Sec. IX in Ref. 3)

$$\alpha_{\mathbf{k}}^{ij} = \|\beta_{\mathbf{k}}^{-1}\|_{ij}, \tag{28}$$

where matrix $\beta_{\mathbf{k}}^{-1}$ is inverse to $\beta_{\mathbf{k}}$ determined in Eq. (22).

By a direct differentiation of the equations of state, Eq. (18), we obtain the following for the generalized susceptibility χ_{ij}:

$$\chi_{ij} \equiv \frac{\partial s_i}{\partial h_j} = \frac{\sqrt{(1-s_i^2)(1-s_j^2)}}{k_{\mathrm{B}}T}\alpha_{\mathbf{k}=\mathbf{0}}^{ij}, \tag{29}$$

where $\alpha_{\mathbf{k}}^{ij}$ is determined in Eq. (28). The relationship (29) is the fluctuation-dissipation theorem [see, e.g., Eq. (124.5) in Ref. 5 and Sec. 4.3.5 in Ref. 2], which is therefore satisfied within the ring approximation and may be also rewritten as

$$\frac{\partial s_i}{\partial h_j} = \|\Phi^{-1}\|_{ij}, \tag{30}$$

where Φ^{-1} is the matrix inverse to Φ that has the following elements:

$$\Phi_{lm} \equiv \frac{\partial^2 f_{\mathrm{ring}}}{\partial s_l \partial s_m}. \tag{31}$$

Note that in the case of a paramagnetic state at the crystal lattice with two sublattices and only pair interactions, the expression (29) transforms into Eq. (21) of Ref. 6 derived within the Onsager cavity field approximation.

Using the above general expressions, one can calculate the complete (configurational) phase diagram of the Ising model with any complex crystal lattice according to the procedure suggested in Sec. X of Ref. 3. Any paramagnetic, ferromagnetic, and antiferromagnetic states can be taken into account. For example, in the cases of ferromagnetic and paramagnetic states, correspondingly $s_i = s$ and $s_i = 0$ for any values of the index *i*, which may still be necessary due to the complex character of the crystal lattice itself.

III. CASE OF A FERROMAGNETIC STATE WITHIN A BRAVAIS CRYSTAL LATTICE

A. Nonpair spin interactions

In such a particular case it is not necessary to introduce the sublattices. Correspondingly, instead of Eqs. (1) and (3) we have

$$\begin{aligned}H = {} & -Nj_0 - h\sum_{\mathbf{R}} \sigma_{\mathbf{R}} \\ & - \sum_{n=2}^{N\nu}\frac{1}{n!}\sum_{\mathbf{R}_1,\mathbf{R}_2,\ldots,\mathbf{R}_n} J^{(n)}_{\mathbf{R}_1,\mathbf{R}_2,\ldots,\mathbf{R}_n}\sigma_{\mathbf{R}_1}\sigma_{\mathbf{R}_2}\cdots\sigma_{\mathbf{R}_n},\end{aligned} \tag{32}$$

$$\sigma_{\mathbf{R}} = \begin{cases} 1 & \text{if the spin at site } \mathbf{R} \text{ is up} \\ -1 & \text{otherwise.}\end{cases} \tag{33}$$

The corresponding expressions for the free energy, energy, entropy, and equation of state can be easily obtained within the ring approximation by deleting both indices of sublattices and summations on them in all the above presented, in Sec. II, expressions. Thus, we obtain

$$f_{\mathrm{ring}}=f_{\mathrm{MF}}-\frac{1}{2}\mu(1-s^2)+\frac{k_{\mathrm{B}}T}{2N}\sum_{\mathbf{k}}\ln\det A_{\mathbf{k}}, \tag{34}$$

where $s=\langle\sigma_{\mathbf{R}}\rangle$ is the total magnetization,

$$f_{\mathrm{MF}}=\varepsilon_{\mathrm{MF}}-Ts_{\mathrm{MF}}, \tag{35}$$

$$\varepsilon_{\mathrm{MF}}=-\tilde{\Phi}^{(0)}, \tag{36}$$

$$s_{\mathrm{MF}}=-k_{\mathrm{B}}\left[\frac{1+s}{2}\ln\frac{1+s}{2}+\frac{1-s}{2}\ln\frac{1-s}{2}\right], \tag{37}$$

$$A_{\mathbf{k}}=1-\frac{1-s^2}{k_{\mathrm{B}}T}[\tilde{\Phi}^{(2)}_{\mathbf{k}}-\mu]. \tag{38}$$

The quantity μ is to be determined from the equation

$$N^{-1}\sum_{\mathbf{k}}A_{\mathbf{k}}^{-1}=1. \tag{39}$$

It is easy to find that the expression (34) satisfies the relationship $s=-\partial f/\partial h$. The equation of state can be written as (from $\partial f/\partial s=0$)

$$\frac{k_{\mathrm{B}}T}{2}\ln\frac{1+s}{1-s}=G \tag{40}$$

or, equivalently,

$$s=\tanh[G/(k_{\mathrm{B}}T)], \tag{41}$$

where

$$G=\tilde{\Phi}^{(1)}-\mu s+\frac{1-s^2}{2N}\sum_{\mathbf{q}}\frac{\tilde{\Phi}^{(3)}_{\mathbf{0},\mathbf{q}}}{A_{\mathbf{q}}}. \tag{42}$$

The corresponding expressions for the energy and entropy are the following:

$$\varepsilon_{\mathrm{ring}}=\varepsilon_{\mathrm{MF}}-\tfrac{1}{2}\mu(1-s^2), \tag{43}$$

$$s_{\mathrm{ring}}=s_{\mathrm{MF}}-\frac{k_{\mathrm{B}}}{2N}\sum_{\mathbf{k}}\ln\det A_{\mathbf{k}}. \tag{44}$$

The functions $\tilde{\Phi}^{(n)}_{\mathbf{k}_1,\mathbf{k}_2,\ldots,\mathbf{k}_{n-1}}$ $(n=0,1,\ldots,3)$ entering the above expressions one can obtain from the Appendix by deleting both indices of sublattices and summations on them. Note that within the mean-field approximation, the equations of state are the same but with $G=\tilde{\Phi}^{(1)}$.

From Eq. (106) of Ref. 3, the critical temperature of the absolute instability of the paramagnetic state is determined by the equation

$$\beta_{\mathbf{0}}|_{s=0}=0, \tag{45}$$

where

$$\beta_{\mathbf{k}}=A_{\mathbf{k}}+\frac{2s^2}{1-s^2}\left[\frac{1}{I_{\mathbf{k}}}-1\right]-\frac{(1-s^2)^2}{2k_{\mathrm{B}}T}Q_{\mathbf{k}}+\frac{2(1-s^2)}{k_{\mathrm{B}}T}T^{(1)}_{\mathbf{k}}\left\{\frac{(1-s^2)^2}{4k_{\mathrm{B}}T}\left[\frac{T^{(1)}_{\mathbf{k}}}{I_{\mathbf{k}}}-\frac{T^{(2)}_{\mathbf{k}}}{T^{(1)}_{\mathbf{k}}}\right]+\frac{s}{I_{\mathbf{k}}}\right\}, \tag{46}$$

$$I_{\mathbf{k}}=\frac{1}{N}\sum_{\mathbf{q}}\frac{1}{A_{\mathbf{q}}A_{\mathbf{k}+\mathbf{q}}},\quad Q_{\mathbf{k}}=\frac{1}{N}\sum_{\mathbf{q}}\frac{\tilde{\Phi}^{(4)}_{\mathbf{k},-\mathbf{k},\mathbf{q}}}{A_{\mathbf{q}}}, \tag{47}$$

$$T^{(1)}_{\mathbf{k}}=\frac{1}{N}\sum_{\mathbf{q}}\frac{\tilde{\Phi}^{(3)}_{\mathbf{q},-(\mathbf{k}+\mathbf{q})}}{A_{\mathbf{q}}A_{\mathbf{k}+\mathbf{q}}},\quad T^{(2)}_{\mathbf{k}}=\frac{1}{N}\sum_{\mathbf{q}}\frac{[\tilde{\Phi}^{(3)}_{\mathbf{q},-(\mathbf{k}+\mathbf{q})}]^2}{A_{\mathbf{q}}A_{\mathbf{k}+\mathbf{q}}}. \tag{48}$$

Note that within the mean-field approximation, such a critical temperature T_{c} is determined as $k_{\mathrm{B}}T_{\mathrm{c}}=\tilde{\Phi}^{(2)}_{\mathbf{0}}$.

In the considered case the SRO parameters $\alpha_{\mathbf{R}}$ and there Fourier transform $\alpha_{\mathbf{k}}$ should be defined as

$$\alpha_{\mathbf{R}_1-\mathbf{R}_2}=\frac{\langle(\sigma_{\mathbf{R}_1}-s)(\sigma_{\mathbf{R}_2}-s)\rangle}{1-s^2}, \tag{49}$$

$$\alpha_{\mathbf{k}}=\sum_{\mathbf{R}}\alpha_{\mathbf{R}}\exp(-i\mathbf{kR}),\quad \alpha_{\mathbf{R}}=N^{-1}\sum_{\mathbf{k}}\alpha_{\mathbf{k}}\exp(i\mathbf{kR}). \tag{50}$$

Within the ring approximation for the SRO, we obtain

$$\alpha_{\mathbf{k}}=\beta_{\mathbf{k}}^{-1}. \tag{51}$$

For the sucseptibility χ we have

$$\chi\equiv\frac{\partial s}{\partial h}=\frac{1-s^2}{k_{\mathrm{B}}T}\alpha_{\mathbf{k}=\mathbf{0}}, \tag{52}$$

where $\alpha_{\mathbf{k}}$ is determined in Eq. (51).

B. Pair spin interactions

Let us consider in more detail the particular case of *pair* spin interactions, which will be numerically studied below in Sec. V. In such a case, we have the following Hamiltonian:

$$H=-Nj_0-h\sum_{\mathbf{R}}\sigma_{\mathbf{R}}-1/2\sum_{\mathbf{R}_1,\mathbf{R}_2}J^{(n)}_{\mathbf{R}_1,\mathbf{R}_2}\sigma_{\mathbf{R}_1}\sigma_{\mathbf{R}_2}. \tag{53}$$

The free energy, energy, entropy, and equation of state can be easily obtained by use of the above expressions (34)–(44) where according to the Appendix

$$\tilde{\Phi}^{(0)}=j_0+hs+\tfrac{1}{2}\tilde{J}^{(2)}_{\mathbf{0}}s^2, \tag{54}$$

$$\tilde{\Phi}^{(1)}=h+s\tilde{J}^{(2)}_{\mathbf{0}},\quad \tilde{\Phi}^{(2)}_{\mathbf{k}}=\tilde{J}^{(2)}_{\mathbf{k}}, \tag{55}$$

$$\tilde{\Phi}^{(3)}_{\mathbf{k}_1,\mathbf{k}_2}=\tilde{\Phi}^{(4)}_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3}=0, \tag{56}$$

$$A_{\mathbf{k}}=1-\frac{1-s^2}{k_{\mathrm{B}}T}[\tilde{J}^{(2)}_{\mathbf{k}}-\mu]. \tag{57}$$

From Eq. (107) in Ref. 3 we have a very simple expression for the critical temperature T_c of the absolute instability of the paramagnetic state,[7]

$$\frac{1}{k_\mathrm{B}T_\mathrm{c}}=N^{-1}\sum_{\mathbf{k}}\,[\tilde{J}^{(2)}_{\mathbf{0}}-\tilde{J}^{(2)}_{\mathbf{k}}]^{-1}. \tag{58}$$

The SRO Fourier transform $\alpha_{\mathbf{k}}$ and heat capacity $c_V=\partial\varepsilon_{\mathrm{ring}}/\partial T$ are determined as

$$\alpha_{\mathbf{k}}^{-1}=A_{\mathbf{k}}+\frac{2s^2}{1-s^2}\left[\frac{1}{I_{\mathbf{k}}}-1\right], \tag{59}$$

$$c_V=\frac{1-s^2}{2T}\left\{X+\frac{2\alpha_{\mathbf{k}=\mathbf{0}}}{k_\mathrm{B}T}[h+s(\tilde{J}^{(2)}_{\mathbf{0}}-\mu)-sX]^2\right\}, \tag{60}$$

where

$$X=-\frac{k_\mathrm{B}T}{1-s^2}\left[\frac{1}{I_{\mathbf{0}}}-1\right], \tag{61}$$

$I_{\mathbf{k}}$ are determined in Eq. (47) and the quantity μ is to be determined from the Eq. (39). The expression for the sucseptibility is the same as Eq. (52) but with $\alpha_{\mathbf{k}}$ determined by Eq. (59). In the case of a *paramagnetic* state when $s=0$, we obtain

$$c_V\big|_{s=0}=\frac{k_\mathrm{B}}{2}\left[1-\frac{1}{I_{\mathbf{0}}}\bigg|_{s=0}\right]. \tag{62}$$

For comparison, within the mean-field approximation we have

$$\chi^{\mathrm{MF}}=\frac{1-s^2}{k_\mathrm{B}T}\left[1-\frac{1-s^2}{k_\mathrm{B}T}\tilde{J}^{(2)}_{\mathbf{0}}\right]^{-1}, \tag{63}$$

$$c_V=\begin{cases}\dfrac{1}{T}\chi^{\mathrm{MF}}[h+s\tilde{J}^{(2)}_{\mathbf{0}}]^2, & s\neq 0\\[1ex] 0, & s=0.\end{cases} \tag{64}$$

From Eq. (62) it follows that if $T\neq\infty$ then $c_V\neq 0$ even at $s=0$, because $I_{\mathbf{0}}\neq 1$. It is just the spin correlations that contribute to the heat capacity of the paramagnetic state within the ring approximation in contrast to the mean-field one. Note that in the case of paramagnetic state, the expressions for $\alpha_{\mathbf{k}}$ and χ transform into those obtained in Refs. 7–9.

IV. SIMILAR APPROXIMATIONS

Let us outline the approximations that are similar to the ring one in the case of the Ising model (with pair spin interactions). In the case of the lattice gas model the same was done in Sec. V of Ref. 3.

The expressions (34), (41), and (58) (with zero nonpair spin interactions) are the same as those obtained by Brout in Refs. 7–9 (see also Ref. 10). Perhaps, one may even call the ring approximation as the Brout one (correspondingly generalized to the cases of antiferromagnet, non-Bravais crystal lattice, nonpair interactions, and lattice gas model with long-range atomic order both in the present and previous[3] papers).

If the external magnetic field is zero and the temperature is higher than the critical temperature of the absolute instability of the paramagnetic state, the ring approximation for the paramagnetic state gives the same results as the spherical model (e.g., Ref. 11). This fact allowed Brout to name the ring approximation as the spherical model. Such a name seems not to be adequate enough because the ring approximation may be effectively used also at nonzero external magnetic field and/or below the critical temperature (in contrast to the spherical model).

One can find a number of similarities between the results obtained within the ring approximation and in the framework of Onsager cavity field approximation.[6,12]

In Ref. 13 (see also Refs. 10 and 14–18), Horwitz and Callen elaborated a different form of the ring approximation. By numerical calculations we found that the results of the Horwitz-Callen and ring approximations are the same qualitatively and very close to one another quantitatively. For example, in the case of face-centered-cubic crystal lattice within the Horwitz-Callen approximation we got $T_{\mathrm{c}1}=2.216$, $T_0=2.408$, and $T_{\mathrm{c}2}=2.426$, whereas within the ring approximation we have correspondingly $T_{\mathrm{c}1}=2.231$, $T_0=2.406$, and $T_{\mathrm{c}2}=2.423$. (T_0 is the temperature of the ferromagnetic phase transition of the first order, and $T_{\mathrm{c}1}$ and $T_{\mathrm{c}2}$ are the temperatures of absolute instability of the paramagnetic and ferromagnetic states, respectively, see below Sec. V.) However, Horwitz-Callen approximation is more complicated than the ring one because it contains additional integrations in the corresponding expressions. Besides, the Horwitz-Callen approximation does not satisfy the fluctuation-dissipation theorem[19] in contrast to the ring approximation [see above Eqs. (29) and (30)]. Note that in Ref. 19 (see also Chap. 9 in Ref. 7), just using the similarity between the Horwitz-Callen and ring approximations, it was *erroneously* concluded that the ring approximation does not satisfy the fluctuation-dissipation theorem as well.

The free-energy expressions similar to Eq. (34) with $\mu=0$ were derived in Ref. 20 (within the Gaussian model), in Ref. 13 [see Eq. (121) there corresponding to partial renormalization], in Ref. 21, and in Refs. 7–9 (within the random-phase approximation). All of them suffer from the same principal drawback as the ring approximation at $\mu=0$; namely, due to the presence of the logarithm, the free energy of the paramagnetic state does not exist at the temperatures lower than the critical temperature of the ferromagnetic phase transition calculated within the mean-field approximation (see also Sec. 6 in Ref. 3).

There are also similarities between Eq. (4) and the free-energy expression obtained by γ-expansion method and presented in Ref. 22 [see Eq. (17) there].

In the following section we perform the detailed numerical study of the ring approximation, which can also help us to understand the features of similar approximations.

V. NUMERICAL CALCULATIONS

This section is devoted to the verification of the adequacy and numerical accuracy of the ring approximation in the case of the spin-1/2 Ising model. Such a verification was partially performed in Refs. 7–9 and 13. However, it was not complete and some important conclusions were done erroneously (see below). We consider three classical cases of the ferromagnetic Ising model with the linear chain, simple quadratic, and face-centered-cubic (fcc) crystal lattices, and nearest-neighbor spin interactions. Such a consideration is an important addition to the numerical study of the ring approximation performed in Ref. 3. Our choice of the cases to be considered is caused by the existence of a large number of results (including the exact ones) obtained previously in such cases. We do not consider the Ising model with an antiferromagnetic order because it is equivalent to the lattice gas model with a long-range order (e.g., Sec. 2.6 in Ref. 2), which was already considered numerically in Ref. 3 to a large extent. The dependence of the numerical accuracy of the ring approximation with respect to the radius of interactions was also investigated in Ref. 3 and will not be touched here.

In Figs. 1–3, we presented the temperature dependencies of the magnetization, heat capacity, sucseptibility, free energy, energy, and entropy in zero magnetic field in the three above-mentioned cases. The temperature regions not far from the phase transition points are considered. In Figs. 4 and 5, we presented the dependencies of the magnetization with respect to the magnetic field for a number of temperatures in the cases of linear chain and fcc crystal lattices. The dependencies were obtained within the ring and mean-field approximations, by the exact calculations, series expansion, as well as by the Monte Carlo simulation. Both thermodynamically stable and metastable states were considered within the ring approximation. The values of the characteristic temperatures obtained by different methods are presented in Table I. For calculations within the ring and mean-field approximations we used the expressions listed in Sec. III of the present paper. The exact results in the case of linear chain and simple quadratic (Onsager solution) crystal lattices were taken from Refs. 23 and 24 and from the textbooks on statistical mechanics (e.g., Refs. 5, 25, and 26). The sources of the other results presented in figures one can find in their captions. Note that the low- and high-temperature series expansions can be used only for the verification of right asymptotical behavior of the ring approximation in the corresponding temperature regions.

In the present paper we do not present the verification of the spin-correlation function (or, equivalently, SRO) within the ring approximation. Actually, one can find such verification in the papers[3,27,28] devoted to the consideration of the statistically equivalent case of the lattice gas model. Besides, in all three cases considered here of nearest-neighbor spin interactions, the numerical accuracy of the nearest-neighbor spin-correlation function can be directly studied through the internal energy to which it is proportional.

From Table I and Figs. 1–5, one can conclude the following. In the cases of simple quadratic and fcc crystal lattices, the ring approximation gives the ferromagnetic phase transition temperatures T_0^{ring} that are very close to the corresponding ones obtained exactly, by series expansion, or by Monte Carlo simulation (which can be considered as a standard). In the case of the one-dimensional linear chain crystal lattice, the ring approximation gives finite phase transition temperature in contrast to zero one obtained exactly.

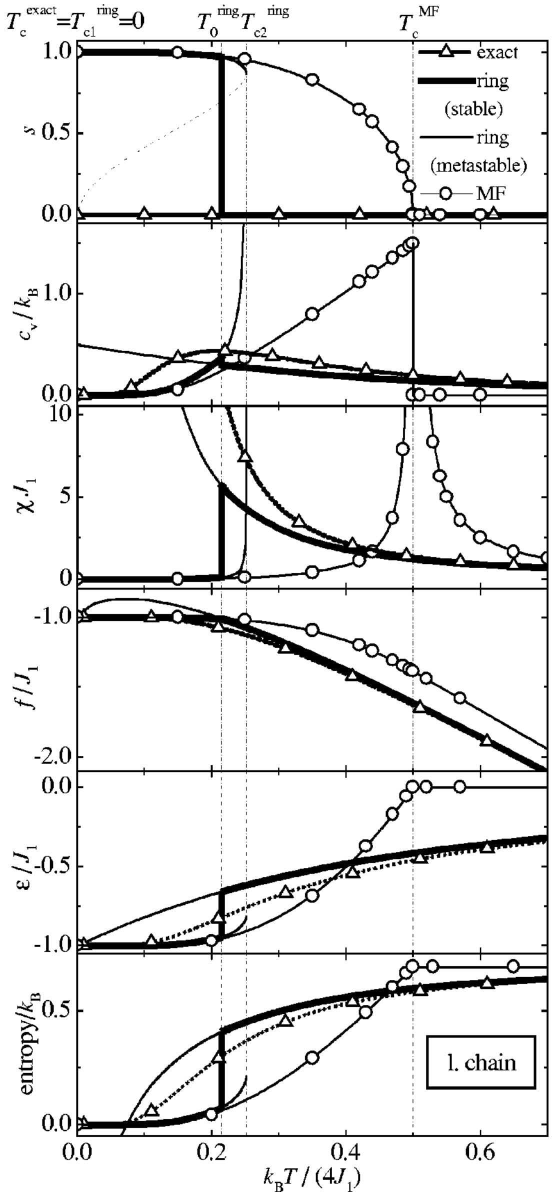

FIG. 1. The temperature dependences of the Ising model magnetization s, heat capacity c_V, sucseptibility χ, free energy f, energy ε, and entropy in zero magnetic field in the case of linear chain crystal lattice with nearest-neighbor ferromagnetic spin interactions. The dependences were obtained within the ring (thick and thin lines in case of the thermodynamically stable and metastable states, respectively) and mean-field (open circles, MF) approximations as well as by the exact calculations (open triangles, exact). The designations of curves are the same for all quantities. At the top of the figure: T_0^{ring} is the temperature of the ferromagnetic phase transition of the first order, and T_{c1}^{ring} and T_{c2}^{ring} are the temperatures of absolute instability of the paramagnetic and ferromagnetic states, respectively; all calculated within the ring approximation. T_c^{exact} and T_c^{MF} are the temperatures of the ferromagnetic phase transition of the second order calculated exactly and within the mean-field approximation, respectively.

In all the considered cases, we obtain the phase transitions

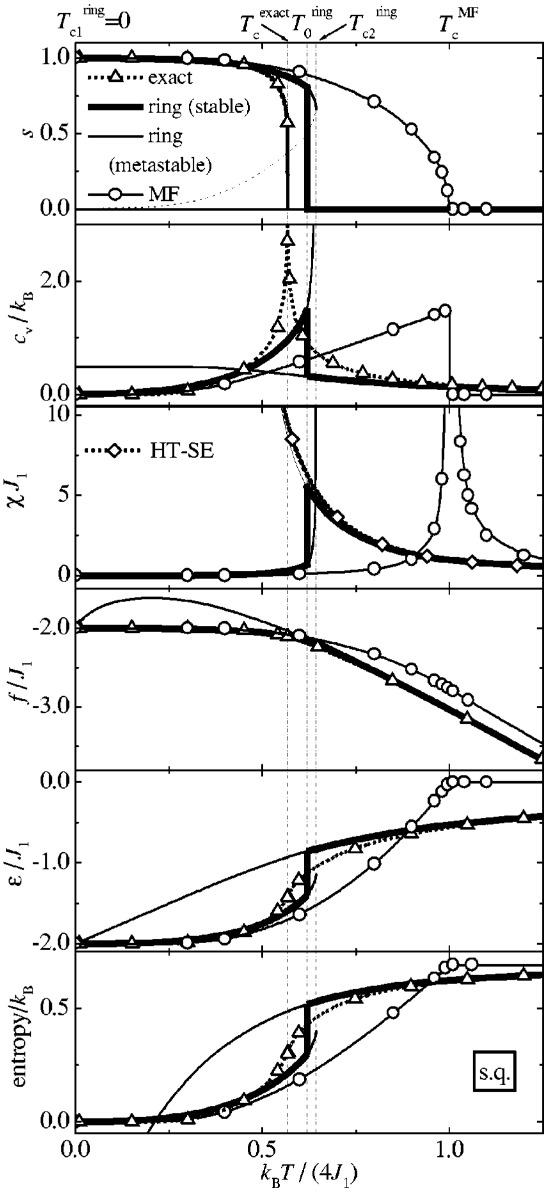

FIG. 2. The same as in Fig. 1. but in the case of simple quadratic crystal lattice. The data for sucseptibility χ corresponding to the high-temperature series expansion (open diamonds, HT-SE) were calculated using Eq. (26.2) in Ref. 29.

of the *first* order within the ring approximation in contrast to the *second* order obtained by the other standard methods. That is why within the ring approximation the temperature T_0^{ring} of the phase transition (Curie temperature) is different from the temperatures $T_{\mathrm{c1}}^{\mathrm{ring}}$ and $T_{\mathrm{c2}}^{\mathrm{ring}}$ of absolute instability of the paramagnetic and ferromagnetic states, respectively. Correspondingly, we have discontinuances in the temperature dependencies of magnetization, heat capacity, sucseptibility, energy, and entropy at the point of the phase transition. Thus, we do not study the critical quantities (e.g., indices) introduced for a description of the phase transitions of *exactly* the second order. The susceptibility takes an infinite values only for metastable paramagnetic and ferromagnetic states at $T_{\mathrm{c1}}^{\mathrm{ring}}$ and $T_{\mathrm{c2}}^{\mathrm{ring}}$, respectively. The heat capacity takes finite $k_{\mathrm{B}}/2$

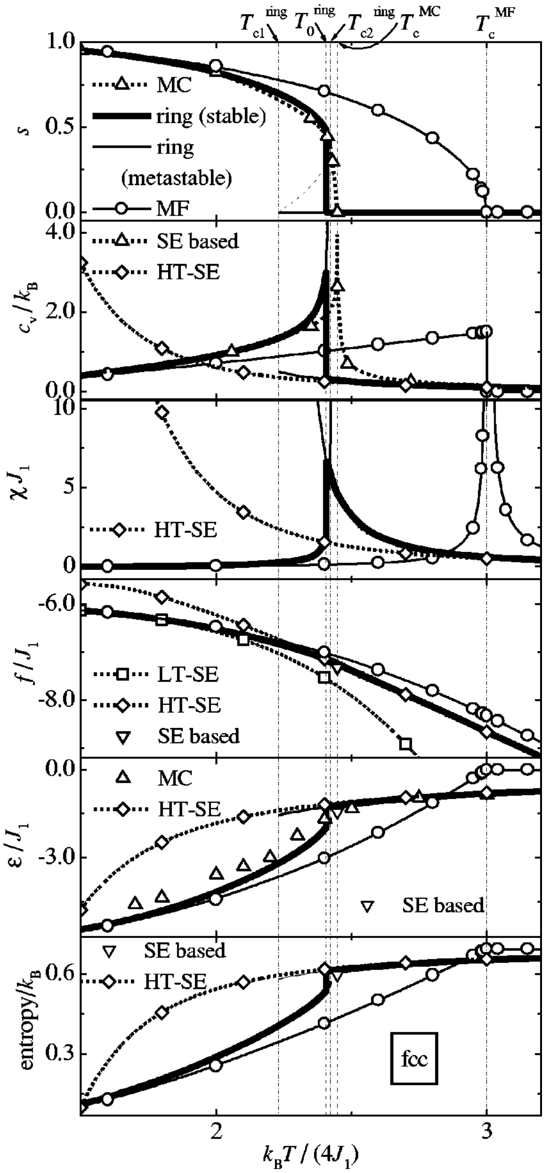

FIG. 3. The same as in Fig. 1 but in the case of fcc crystal lattice without the exact calculations which are absent. The Monte Carlo simulation data on magnetization s were calculated through the data in Fig. 1(a) in Ref. 30. The Monte Carlo data on energy ε were obtained through our own Monte Carlo simulation of the correlation function at the first coordination shell. (Unfortunately, below the phase transition temperature we failed to achieve the good convergence of our results with respect to the size of the Monte Carlo simulation sample.) $T_{\mathrm{c}}^{\mathrm{MC}}$ is the temperature of the ferromagnetic phase transition of the second order calculated by the Monte Carlo simulation (Ref. 30). The series expansion (SE) based data for heat capacity c_V were taken from Fig. 14 of Sec. 4.7.3 in Ref. 23. The data for sucseptibility χ corresponding to the high-temperature series expansion (HT-SE) were taken from Ref. 31. The data for free energy f corresponding to the low-temperature (HT) and high-temperature (LT) series expansions were calculated using, respectively, Eqs. (119) and (127) of Chap. 4 in Ref. 23. The data for energy f and entropy corresponding to the high-temperature series expansion (HT-SE) were taken Ref. 32. The series expansion (SE) based data for critical values of the free energy, energy, and entropy were taken from Table 6 of Sec. 4.7.1 in Ref. 23.

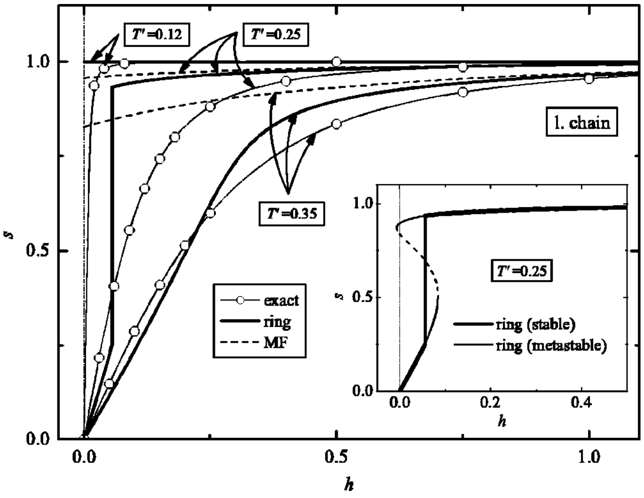

FIG. 4. The dependences of the magnetization *s* with respect to the magnetic field *h* in the case of linear chain crystal lattice for the reduced temperatures $T' = 0.12$, 0.25, and 0.35 where $T' \equiv k_B T/(4J_1)$. The dependences were obtained within the ring (thick line) and mean-field (dash line) approximations as well as by the exact calculations (open circles).

value for metastable paramagnetic state at $T_{c1}^{\rm ring}$ and infinite value for metastable ferromagnetic state at $T_{c2}^{\rm ring}$.

Note that in some cases the wrong (first) order of the phase transition within the ring or ringlike approximations was also found in Refs. 3, 16, 17, 22, and 35. In Refs. 8, 9, and 13 the second order of the phase transition was assumed *a priori* thus resulting in the wrong conclusions about the behavior of the heat capacity in the vicinity of the phase transition. In Chap. 9 of Ref. 7, assuming the second order of the phase transition and using the similarity to the spherical model, it was erroneously concluded that there is no phase transition at all within the ring approximation in one- and two-dimensional cases (at zero external magnetic field), whereas actually in these cases only the temperature $T_{c1}^{\rm ring}$ of absolute instability of the paramagnetic state vanishes rather than the temperature $T_0^{\rm ring}$ of the phase transition itself. Note that the same problem of adequate description of the order of the phase transformation was also revealed within the cluster-variation method in the two-dimensional case (see Sec. 10 in Ref. 33).

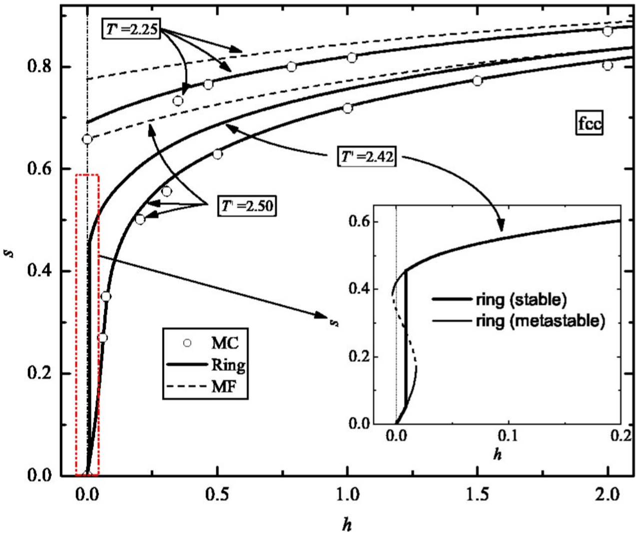

FIG. 5. The same as in Fig. 4 but in the case of fcc crystal lattice without the exact calculations which are absent. The sign MC (open circles) correspond to the Monte Carlo simulation data taken from Figs. 1(b) and 1(c) in Ref. 30.

TABLE I. The values of the characteristic temperatures obtained by different methods in the cases of linear chain (l chain), simple quadratic (sq), and face-centered-cubic (fcc) crystal lattices. $T_0^{\rm ring}$ is the temperature of the ferromagnetic phase transition of the first order, $T_{c1}^{\rm ring}$ and $T_{c2}^{\rm ring}$ are the temperatures of absolute instability of the paramagnetic and ferromagnetic states, respectively; all calculated within the ring approximation. $T_c^{\rm MC}$, $T_c^{\rm SE}$, $T_c^{\rm exact}$, $T_c^{\rm MF}$, and $T_c^{\rm CVM}$ are the temperatures of the ferromagnetic phase transition of the second order calculated by Monte Carlo simulation, by series expansion, exactly, within the mean-field approximation, and by cluster-variation method [within the square or triangle (sq) and tetrahedron-octahedron (fcc) approximations], respectively. All the temperatures are in units $k_B/(4J_1)$.

	l chain	sq	fcc
$T_{c1}^{\rm ring}$	0	0	2.231
$T_0^{\rm ring}$	0.2148	0.6186	2.406
$T_{c2}^{\rm ring}$	0.2516	0.6427	2.423
$T_c^{\rm MC}$			2.448[a]
$T_c^{\rm SE}$		0.567[b]	2.449[c]
$T_c^{\rm exact}$	0	0.5673	
$T_c^{\rm MF}$	0.5	1	3
$T_c^{\rm CVM}$		0.6057[d]	2.502[c]

[a] Reference 30.

[b] Table 5 in Sec. 4.7.1 of Ref. 23.

[c] Table III in Ref. 33.

[d] Table V in Ref. 34.

In the dependences of the magnetization with respect to the magnetic field the discontinuances take place when the magnetic field is small and the temperature is *close* to the phase-transition temperature. Such behavior was found to be inadequate (see Chap. 9 in Ref. 7 and Refs. 9 and 19) to the Lee and Yang general theorem.[1]

It is remarkable that within the mean-field approximation we obtain the right order of the phase transitions and there is not discontinuances in the dependences of the magnetization with respect to the magnetic field. But, nevertheless, the numerical accuracy of the ring approximation is much higher than that of the mean-field one in all the considered cases.

As a rule, the numerical accuracy of the ring approximation is high for all considered quantities in all temperature region except the vicinity of the phase transition. Only in the one-dimensional case, the error of magnetization and sucseptibility is substantial also at low temperatures. Remarkably high numerical accuracy of the ring approximation is obtained for the free energy in the almost all temperature region in all three cases. The error contributions of energy and entropy to the free energy seem to compensate one another.

The numerical accuracy of the ring approximation has a strong tendency of increase with increase of the dimension of the crystal lattice. In particular, the order of the phase transitions becomes closer to the second order (the temperatures T_{c1}^{ring}, T_0^{ring}, and T_{c2}^{ring} approach one another). Such a tendency is in accordance with the choice of the inverse effective number of atoms (spins) interacting with one fixed atom (spin) as a small parameter of expansion within the ring approximation.[3] According to such a tendency, one can expect also an increase of the numerical accuracy of the ring approximation with increase of the effective radius of atomic interactions. Such effect was much verified in Refs. 3,27, and 28 rather than in the present paper. Note that even in the case of the one-dimensional linear chain, the phase transition does exist in the case of sufficiently long-range spin interactions (e.g., Sec. 5.5 in Ref. 24) in accordance with the prediction of the ring approximation.

VI. CONCLUSIONS

In the present paper, we generalized the results obtained in Ref. 3 within the ring approximation to the case of the spin-1/2 Ising model with a complex crystal lattice, arbitrary magnetic order and with nonpair spin interactions of any order and effective radii of action (Secs. II–III). By the use of those results one can calculate the complete phase diagram of the Ising model as well as the correlation effects. We also performed the verification of the numerical accuracy of the ring approximation in the cases that have been typical at consideration of the Ising model (Sec. V).

In the case of the Ising model the ring approximation has the same advantages and shortcomings as in the case of the lattice gas model (for more details see conclusions in Ref. 3). The corresponding expressions are general and analytically simple. The ring approximation offers the advantages over the cluster-variation method and Monte Carlo simulation.

It should be emphasized that, actually, such mean-field-like theories as the ring approximation (as well as the cluster-variation method) are not intended to be used for a description of the critical phenomena but rather for description of phase diagrams, correlation effects, nonequilibrium processes, etc. outside the critical regions, which nevertheless is of great interest from practical point of view (e.g., Secs. 4.1 and 4.5.6 in Ref. 2, and Chap. 5 in Ref. 34). Particularly, it is impossible to require the high accurate description of the critical indices within such theories. For a description of the critical phenomena and universal characteristics of phase transitions, we have to use the special methods (e.g., series expansions and renormalization-group theory).

Nevertheless, the study performed in the present paper demonstrates that, even in the most unfavorable cases of nearest-neighbor spin interactions and phase transformations of the second order, the ring approximation gives high-accurate values for the temperatures of such phase transformations (in two- and three-dimensional cases). In such cases, within the ring approximation the order of the phase transformations is not perfectly second but close to it. There is a strong tendency of increase of the numerical accuracy of the ring approximation with increase of the effective radius of spin interactions and the dimensionality of the crystal lattice. By the use of the ring approximation one can perform the high-accuracy calculations of the magnetization, heat capacity, sucseptibility, free energy, energy, and entropy in a wide temperature region except the vicinity of the phase transition. Remarkably high numerical accuracy of the ring approximation is obtained for the free energy within the almost all temperature region. The numerical accuracy of the ring approximation is much higher than that of the mean-field one.

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APPENDIX

The general expression (11) for $\tilde{\Phi}^{(n)}_{i_1,\mathbf{k}_1;i_2,\mathbf{k}_2;\ldots;i_{n-1},\mathbf{k}_{n-1};i_n}$ takes the following forms in the particular cases of $n=0$,

$$\tilde{\Phi}^{(0)}=j_0+\sum_i h_i s_i+\frac{1}{2}\sum_{i_1,i_2}\tilde{J}^{(2)}_{i_1,\mathbf{0};i_2}s_{i_1}s_{i_2}+\frac{1}{6}\sum_{i_1,i_2,i_3}\tilde{J}^{(3)}_{i_1,\mathbf{0};i_2,\mathbf{0};i_3}s_{i_1}s_{i_2}s_{i_3}+\frac{1}{24}\sum_{i_1,i_2,i_3,i_4}\tilde{J}^{(4)}_{i_1,\mathbf{0};i_2,\mathbf{0};i_3,\mathbf{0};i_4}s_{i_1}s_{i_2}s_{i_3}s_{i_4}+\cdots; \tag{A1}$$

$n=1$,

$$\tilde{\Phi}^{(1)}_i=h_i+\sum_{i_1'} s_{i_1'}\tilde{J}^{(2)}_{i_1',\mathbf{0};i}+\sum_{i_1',i_2'}\frac{s_{i_1'}s_{i_2'}}{2}\tilde{J}^{(3)}_{i_1',\mathbf{0};i_2',\mathbf{0};i}+\sum_{i_1',i_2',i_3'}\frac{s_{i_1'}s_{i_2'}s_{i_3'}}{6}\tilde{J}^{(4)}_{i_1',\mathbf{0};i_2',\mathbf{0};i_3',\mathbf{0};i}+\cdots; \tag{A2}$$

$n=2$,

$$\tilde{\Phi}^{(2)}_{i_1,\mathbf{k};i_2}=\tilde{J}^{(2)}_{i_1,\mathbf{k};i_2}+\sum_{i_1'} s_{i_1'}\tilde{J}^{(3)}_{i_1',\mathbf{0};i_1,\mathbf{k};i_2}+\sum_{i_1',i_2'}\frac{s_{i_1'}s_{i_2'}}{2}\tilde{J}^{(4)}_{i_1',\mathbf{0};i_2',\mathbf{0};i_1,\mathbf{k};i_2}+\cdots; \tag{A3}$$

$n=3,$

$$\tilde{\Phi}^{(3)}_{i_1,\mathbf{k}_1;i_2,\mathbf{k}_2;i_3}=\tilde{J}^{(3)}_{i_1,\mathbf{k}_1;i_2,\mathbf{k}_2;i_3}+\sum_{i'_1} s_{i'_1}\tilde{J}^{(4)}_{i'_1,\mathbf{0};i_1,\mathbf{k}_1;i_2,\mathbf{k}_2;i_3}+\cdots; \tag{A4}$$

$n=4,$

$$\tilde{\Phi}^{(4)}_{i_1,\mathbf{k}_1;i_2,\mathbf{k}_2;i_3,\mathbf{k}_3;i_4}=\tilde{J}^{(4)}_{i_1,\mathbf{k}_1;i_2,\mathbf{k}_2;i_3,\mathbf{k}_3;i_4}+\cdots. \tag{A5}$$

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[1] T.D. Lee and C.N. Yang, Phys. Rev. **87**, 410 (1952).

[2] F. Ducastelle, *Order and Phase Stability in Alloys* (Elsevier, New York, 1991).

[3] R.V. Chepulskii, Phys. Rev. B **69**, 134431 (2004).

[4] R.V. Chepulskii, J. Phys.: Condens. Matter **11**, 8645 (1999).

[5] L.D. Landau and E.M. Lifshitz, *Course of Theoretical Physics* (Pergamon, Oxford, 1980), Vol. 5.

[6] G.M. Wysin, Phys. Rev. B **62**, 3251 (2000).

[7] R. Brout, *Phase Transitions* (Benjamin, New York, 1965).

[8] R. Brout, Phys. Rev. **118**, 1009 (1960); **122**, 469 (1961).

[9] R. Brout, in *Magnetism*, edited by G.T. Rado and H. Suhl (Academic Press, New York, 1965), Vol. IIA, p. 43.

[10] B. Mühlschlegel and H. Zittartz, Z. Phys. **175**, 553 (1963).

[11] G.S. Joyce, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M.S. Green (Academic Press, London, 1972), Vol. 2, p. 375.

[12] R. Brout and H. Thomas, Physics **3**, 317 (1967).

[13] G. Horwitz and H.B. Callen, Phys. Rev. **124**, 1757 (1961).

[14] Yu.A. Izyumov and F.A. Kassan-Ogly, Fiz. Met. Metalloved. **30**, 449 (1970); Yu.A. Izyumov, F.A. Kassan-Ogly, and Yu.N. Skryabin, J. Phys. (Paris) **325**, C1 (1971); Yu.A. Izyumov and Yu.N. Skryabin, *Statistical Mechanics of Magnetically Ordered Systems* (Consultants Bureau, New York, 1988), Chap. 1.

[15] M. Wortis, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M.S. Green (Academic Press, London, 1974), Vol. 3.

[16] Z. Onyszkiewicz, Phys. Lett. A **76**, 411 (1980).

[17] D.A. Garanin and V.S. Lutovinov, Teor. Mat. Fiz. **62**, 263 (1985) [Theor. Math. Phys. **62**, 177 (1985)].

[18] E. Halvorsen and M. Bartkowiak, Phys. Rev. B **63**, 014403 (2001).

[19] F. Englert, Phys. Rev. **129**, 567 (1963).

[20] T.H. Berlin and M. Kac, Phys. Rev. **86**, 821 (1952).

[21] V.G. Vaks, A.I. Larkin, and S.A. Pikin, Zh. Éksp. Teor. Fiz. **51**, 361 (1966) [Sov. Phys. JETP **24**, 240 (1966)]; see also A. Katsnelson and A. Olemskoi, *Microscopic Theory of Nonhomogeneous Structures* (Mir, Moscow, 1990), Sec. 16.3.

[22] V.I. Tokar, Comput. Mater. Sci. **8**, 8 (1997).

[23] C. Domb, Adv. Phys. **9**, 150 (1960).

[24] J.M. Ziman, *Models of Disorder* (University Press, Cambridge, 1979).

[25] T.L. Hill, *Statistical Mechanics* (McGraw-Hill, New York, 1956).

[26] K. Huang, *Statistical Mechanics* (Wiley, New York, 1963).

[27] R.V. Chepulskii and V.N. Bugaev, J. Phys.: Condens. Matter **10**, 7327 (1998); R.V. Chepulskii, J. Phys. Chem. Solids **59**, 1473 (1998).

[28] R.V. Chepulskii, J. Phys.: Condens. Matter **11**, 8661 (1999); Phys. Rev. B **61**, 8606 (2000).

[29] M.E. Fisher, *The Nature of Critical Points* (University of Colorado Press, Boulder, 1965).

[30] R. Kutner, K. Binder, and K.W. Kehr, Phys. Rev. B **26**, 2967 (1982).

[31] W.J. Camp and J.P. Van Dyke, Phys. Rev. B **11**, 2579 (1975).

[32] C. Domb and M.F. Sykes, Phys. Rev. **128**, 168 (1962).

[33] D. de Fontaine, Solid State Phys. **47**, 33 (1994).

[34] D. de Fontaine, Solid State Phys. **34**, 73 (1979).

[35] S. Shallcross and B.L. Györffy, in *Properties of Complex Inorganic Solids*, edited by A. Meike, A. Gonis, P.E.A. Turchi, and K. Rajan (Kluwer Academic, Dordrecht, 2000), Vol. II, p. 89.