

Thermodynamic characteristics of the classical n -vector magnetic model in three dimensions

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A method of calculating the free energy and thermodynamic characteristics of the classical n -vector three-dimensional magnetic model at the microscopic level without any adjustable parameters is proposed. Mathematical description is performed with the collective variables method used within the framework of the ρ^4 model approximation. The exponentially decreasing function of the distance between the particles situated at the N sites of a simple cubic lattice is used as the interaction potential. Explicit analytical expressions for entropy, internal energy and specific heat near the phase-transition point as functions of the temperature are obtained. The dependence of the amplitudes of the thermodynamic characteristics of the system for $T > T_c$ and $T < T_c$ on the microscopic parameters of the system are studied for the cases $n = 1, 2, 3$. The obtained results provide the basis for accurate analysis of the critical behavior in three dimensions including the nonuniversal characteristics of the system.

I. INTRODUCTION

Investigating the behavior of the real three-dimensional systems near the phase-transition (PT) point is one of the most important problems of condensed-matter physics. In the present paper we propose a theoretical description scheme of the critical behavior of the classical n -vector magnetic model in three dimensions on the microscopic level without any adjustable parameters. The description is based on the original method of calculating the thermodynamic and structural characteristics of three-dimensional (3D) model systems near the PT point, which is known as the collective variables (CV) method.^{1,2} The method of collective variables as well as Wilson's approach³ are based on Kadanoff's idea⁴ of using effective spin blocks near the phase-transition point instead of initial spins. The description of the critical behavior of the model in Wilson's works^{3,5} was based on Gaussian distributions. The recursion relations between the coefficients of successive block Hamiltonians were obtained as corresponding combinations of the moments of Gaussian distribution. It is known that in the case of 3D model different types of divergent diagrams appear in the frame of this approach. At the present time there are a number of powerful series resummation techniques (see Refs. 6–10 as an example of its application) which enable us to remove divergences appearing in calculating universal values. However, the present methods make it impossible for us to calculate the nonuniversal characteristics of the system. The investigation of the nonuniversal properties of the system near the PT point require the use of non-Gaussian measure densities of the spin-density fluctuations.¹¹

Unlike Wilson's approach,⁵ the method of collective variables,^{1,12} uses non-Gaussian basis distributions. In this case divergent terms do not appear either in the analysis of recursion relations or in the calculation of the free energy near the phase-transition point. Hence it follows that the presence of the divergent terms appearing in Wilson's approach is of purely mathematic character and is connected with limitation in calculations by Gaussian measure (and Gaussian moments) the dispersion of which strives to infinity

in the vicinity of the phase-transition point. Such basis measure does not describe the system in the critical region and must be replaced by the non-Gaussian measure, the fourfold one in particular.

We have devoted this paper to the widely studied classical n -vector magnetic model¹³ on three-dimensional simple cubic lattice, which is also known as the Heisenberg classical $O(n)$ spin model or, in field-theoretic language, as the lattice $O(n)$ nonlinear σ model. The investigation of the critical behavior of the classical n -vector model and its partial cases was conducted in the frame of different methods such as high- and low-temperature series, the field theory, semi-microscopic scaling-field theory and Monte Carlo calculations. Much attention in these works was given to investigating the universal properties of the system such as critical exponents^{14–19} and some combinations of the critical amplitudes of thermodynamic functions.^{20–33} Besides, the equation of state of Ising system was obtained to order ϵ^2 by Avdejeva and Migdal³⁴ and by Bresin, Wallace, and Wilson.³⁵ Later these results were generalized for the case of the n -vector model.³⁵

Some important results were also obtained for calculating the thermodynamic functions near the critical point. One of the first works in this sphere is a paper by Wegner (the so-called Wegner's expansion),³⁶ suggesting the expression for the free energy with "irrelevant" operators in the Wilson approach taken into account. The works by Fisher and Aharony,³⁷ Nicoll and Albright,³⁸ and Nelson³⁹ were also devoted to receiving crossover scaling functions for temperatures $T > T_c$ in zero external field near four dimensions. In 1974, Riedel and Wegner⁴⁰ developed a numerical technique, called the scaling-field method, for obtaining crossover scaling functions of the free energy and susceptibility. Crossover functions rather than power laws^{41–43} have described the nonasymptotic region between criticality and the noncritical "background." In the frame of the massive field theory by Bagnuls and Bervillier^{18,44} the nonasymptotic critical behavior for $d = 3$ in the disordered phase case was analyzed. They obtained explicit expressions for the correlation length ξ , the susceptibility χ , and the specific heat C as tem-

perature functions in the disordered phase along the critical isohore for one-, two-, and three-component models. The description of nonasymptotical (though still critical) behavior was obtained as crossover between the Wilson-Fisher (near the critical temperature T_c) and mean-field (very far from T_c) behaviors with three adjustable parameters used.

At the present time the actual task of the critical phenomena physics is elaborating the methods giving quantity description of the critical behavior of the system without using any adjustable parameters. This has been demonstrated, for example, in the works of Dohm and co-workers⁴⁵⁻⁴⁷ in which calculation of the temperature dependence of the thermodynamic characteristics of the system was performed without using ϵ expansion in the frame of the minimal subtraction scheme for the n -vector model in three dimensions on the basis of high-order perturbation theory and Borel resummation. In these papers the amplitude functions of the susceptibility, the correlation length and the specific heat above and below T_c up to two-loop order within the ϕ^4 model for the cases $n=1,2,3$ were calculated. This approach exploits simultaneously the experimental information and simple relation between the specific heat above and below T_c for defining the effective renormalized static coupling of the model in the terms of the measured specific heat. The effective renormalized static coupling determined in such a way allows to obtain expressions for other thermodynamic characteristics of the model above and below T_c without using additional adjustable parameters. These results were extended for higher approximations in Ref. 48. Besides, in the recent works by Butera and Comi⁴⁹ high- and low-temperature expansions for the free energy, the susceptibility, and the second correlation moment of the classical n -vector model on the simple cubic (sc) and the body-centered-cubic (bcc) lattices were extended to order β .²¹ This research only contains temperature dependence of the thermodynamic characteristics and does not give the possibility to describe the functional dependence of basic thermodynamic functions on the microscopic parameters of the interaction potential and characteristics of the crystal lattice. All this indicates that nonuniversal properties of the 3D systems near the phase-transition point have not been studied sufficiently yet. However, the precise role and significance of a lattice structure and interaction potential parameters for the approach to asymptotic critical behavior still seems open to question. We hope that our explicit representations may provide useful benchmarks in studying this question.

The approach to the investigation of the critical properties of the n -vector magnetic model, suggested in Ref. 50 provides the necessary conditions for our complex approach to the study of the universal and nonuniversal phase-transition characteristics. The approach suggested in this paper allows us to perform the analysis of the dependence of the thermodynamic characteristics of the n -vector 3D magnetic model in the vicinity of the phase-transition point as functions of temperature and study their dependence on the microscopic parameters of the interaction potential and characteristics of the crystal lattice without any adjustable parameters being used. These results are interesting from the point of view of comparing the theoretical investigations and experimental data.

In Sec. II of the present paper we perform the calculation

of the partition function of the n -vector model using non-Gaussian measure density. The explicit analytical expressions for partial partition functions and general recursion relations (RR) between coefficients of the ‘‘effective Hamiltonian blocks’’ which arise in that case are obtained in the ρ^4 -model approximation. We define the scope of application of these approximate solutions and show that RR as partial solution have a saddle-type fixed point for all n . We perform the calculation of the eigenvectors and eigenvalues of the RG transformation matrix and give the results of the investigation of the dependence of the PT temperature on the microscopic parameters of the interaction potential and the characteristics of the crystal lattice.

Section III is devoted to the calculation of the free energy of the n -vector magnetic model for temperatures above and below the phase-transition point. The main idea of such calculation lies in considering separately the contribution from the critical region (CR) where renormalization-group symmetry takes place and the contribution from the region of the long-wavelength fluctuations (LWF) of the spin moment density. It shown that in the case of the temperatures $T < T_c$ in the region of the LWF the fluctuations are described by non-Gaussian distribution with negative coefficient at square term. The distributions of the spin moment density fluctuations after the selection of the ordering free energy is reduced to the Gaussian distribution. The dependence of the coefficients of the complete expression of the free energy on the microscopic parameters of the initial interaction potential and characteristics of the crystal lattice is investigated for the cases $n=1,2,3$. The contributions into the expressions for entropy and specific heat from the CR and LWF region are analyzed. It has been shown that considering the contribution of the LWF region satisfies the positiveness of the specific heat of the n -vector model and system stability.

In Sec. V the explicit expressions for thermodynamic functions of the model as functions of the temperature are obtained. The dependence of the critical amplitudes of the thermodynamic functions on the microscopic parameters of the interaction potential and the characteristics of the crystal lattice is investigated for the cases $n=1,2,3$. It has been shown that in the case $n=3$ (the Heisenberg model) the specific heat at the $T=T_c$ has the finite value. The dependence of the maximum of the specific heat on the microscopic parameters of the interaction potential is examined for the case $n=3$. The ratio of the critical amplitudes of the thermodynamic functions at the temperatures $T > T_c$ and $T < T_c$ is calculated in order to compare the obtained results with the results of the other methods.

II. CALCULATION OF THE PARTITION FUNCTION AND INVESTIGATION OF THE RECURSION RELATIONS

The critical behavior of different physical systems is characterized by their belonging to a specific class of universality which is defined by the dimensionality of the system d and the symmetry of the order parameter n . The Stanley model¹³ is selected as the object of our investigation of the critical phenomena. This model describes the system of interacting n -component classical spins localized at the N sites of the d -dimensional crystal lattice. The Stanley model is a generalization of a series of different models. In the case $n=0$ it is

reduced to the task of a self-avoiding walk and is used for describing the polymerization phenomena. The cases $n = 1, 2, 3$ correspond to the Ising model, the XY , and the Heisenberg model, respectively. The boundary case $n \rightarrow \infty$ is equivalent to the Berlin-Kac spherical model⁵¹ for which the exact result is known. The Stanley model is described by the Hamiltonian

$$\hat{H} = -\frac{1}{2} \sum_{\mathbf{R}, \mathbf{R}'} J(|\mathbf{R} - \mathbf{R}'|) \hat{\mathbf{S}}_{\mathbf{R}} \hat{\mathbf{S}}_{\mathbf{R}'}, \quad (2.1)$$

where $\hat{\mathbf{S}}_{\mathbf{R}} = (\hat{S}_{\mathbf{R}}^{(1)}, \dots, \hat{S}_{\mathbf{R}}^{(n)})$ is the n -component classical spin with the length m ($\sum_{\alpha=1}^n |\hat{S}_{\mathbf{R}}^{(\alpha)}|^2 = m^2$). Spins are localized at the N sites of the d -dimensional simple cubic lattice with coordinates \mathbf{R} . The interaction has an exchange character and can be described by the exponentially decreasing function of distance between the particles

$$J(|\mathbf{R} - \mathbf{R}'|) = A_0 \exp\left(-\frac{|\mathbf{R} - \mathbf{R}'|}{b}\right), \quad (2.2)$$

where A_0 , b are the constants. In the CV $\rho_{\mathbf{k}} = (\rho_{\mathbf{k}}^{(1)}, \dots, \rho_{\mathbf{k}}^{(n)})$ representation the partition function of the model (2.1) is written as^{1,50}

$$Z = \int \exp\left[\frac{1}{2} \sum_{\mathbf{k}} \beta \Phi(k) \rho_{\mathbf{k}} \rho_{-\mathbf{k}}\right] J[\rho] (d\rho_{\mathbf{k}})^N, \quad (2.3)$$

where $\Phi(k)$ is the Fourier transform of the interaction potential (2.2), the element of the phase space is⁵²

$$(d\rho_{\mathbf{k}})^N = \prod_{a=1}^n d\rho_0^a \prod_{\mathbf{k}} d\rho_{\mathbf{k}}^{a,c} d\rho_{\mathbf{k}}^{a,s}$$

and $J[\rho]$ is the transition Jacobian from the spin variables to the CV. The expression for $J[\rho]$ is given in Appendix A. In the coordinate CV representation

$$\rho(\mathbf{R}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \rho_{\mathbf{k}} \exp(-i\mathbf{k}\mathbf{R}) \quad (2.4)$$

the expression for $J[\rho]$ is factored

$$J[\rho] = \exp(u'_0 N') J'[0] \prod_{\mathbf{R}} J[\rho(\mathbf{R})] \quad (2.5)$$

where

$$J[\rho(\mathbf{R})] = \sum_{l \geq 1} \frac{a'_{2l}}{(2l)!} |\rho(\mathbf{R})|^{2l}. \quad (2.6)$$

The expressions for a'_{2l} were obtained in Refs. 1 and 11. The partition function (2.3) contains the contributions of two different types. The first is energy contributions

$$\frac{1}{2} \sum_{\mathbf{k} \in B} \beta \Phi(k) \rho_{\mathbf{k}} \rho_{-\mathbf{k}}. \quad (2.7)$$

They are diagonal in $\rho_{\mathbf{k}}$ representation and connected with the interaction potential. The second is entropy contributions

$$\sum_{\mathbf{R}} \ln J[\rho(\mathbf{R})]. \quad (2.8)$$

They are diagonal in $\rho(\mathbf{R})$ coordinate CV representation.

There are two possible approaches to calculating Eq. (2.3). The first one is using $\rho_{\mathbf{k}}$ variables in the calculation of the partition function of the system. In such case the energy contributions are diagonal and the nondiagonality of the entropy contributions leads to an approximate method of calculation. One of such approximations is writing Eq. (2.3) in the following form:

$$Z = \int \exp\left(-\frac{1}{2} \sum_{\mathbf{k} \in B} [a'_2 - \beta \Phi(k)] \rho_{\mathbf{k}} \rho_{-\mathbf{k}}\right) \times \left[1 + \eta + \frac{1}{2} \eta^2 + \dots\right] (d\rho_{\mathbf{k}})^N, \quad (2.9)$$

where

$$\eta = \sum_{l \geq 2} \frac{a'_{2l}}{(2l)!} N^{1-l} \sum_{\mathbf{k}_i} \rho_{\mathbf{k}_1}, \dots, \rho_{\mathbf{k}_{2l}} \delta_{\mathbf{k}_1 + \dots + \mathbf{k}_{2l}}. \quad (2.10)$$

As rule, such a way of calculation assumes that for the value η it is sufficient to restrict the consideration to one term ($l = 2$) and in addition it is presupposed that¹¹

$$[a'_2 - \beta \Phi(k)]^l \gg a'_{2l}. \quad (2.11)$$

The second way of calculating the partition function (2.3) assumes the use of the $\rho(\mathbf{R})$ CV representation. In that case the entropy contributions are diagonal (2.5) and the approximation relates to the energy contribution (2.7), as it is non-diagonal in the $\rho(\mathbf{R})$ representation. The essence of such fitting leads to a certain approximation of $\Phi(k)$ (see Ref. 1) which allows to diagonalize the expressions in the exponent under the integrand for the partition function

$$Z = \prod_{\mathbf{R}} \int \exp\left(-\frac{1}{2} (a'_2 - \beta \Phi_{apr}) \rho(\mathbf{R})^2 - \sum_{l \geq 2} \frac{a'_{2l}}{(2l)!} \rho(\mathbf{R})^{2l}\right) d\rho(\mathbf{R}). \quad (2.12)$$

We use such approximation for $\Phi(k)$ where $\Phi(k)$ is a constant Φ_{apr} for every interval $k \in (B_l, B_{l-1})$ and equals the respective mean value $\Phi(k)$.

The first way corresponds to considering the moments of a certain Gaussian distribution. It allows us to calculate only certain classes of the graphs and does not solve the problem of the description of the critical behavior as such. Besides, the condition (2.11) is too strong in the vicinity of the phase-transition point. Nevertheless, such an approach has its advantages owing to considering the wave-vector dependence of $\Phi(k)$. The second way is not restricted to Gaussian moments and is based on the use of the non-Gaussian measure density.⁵³ In this case we do not need to perform the summation of various types of infinite series of perturbation theory, certain terms of which strive to infinity with $T \rightarrow T_c$. Besides, the condition (2.11) becomes optional. In our

opinion this condition is the basic barrier in the description of the critical behavior of three-dimensional systems.

The calculation of the nonuniversal characteristics of the phase transition, particularly the PT temperature T_c , is connected with the choice of the interaction potential. The Fourier transform of the interaction potential (2.2) takes the form

$$\Phi(k) = \frac{\Phi(0)}{(1+b^2k^2)^2}, \quad (2.13)$$

where $\Phi(0) = 8\pi A_0(b/c)^3$. The value of $\Phi(k)$ for the wave vectors similar to the boundary of the Brillouin half zone ($B = \pi/c$) is much smaller than $\Phi(0)$. In this region of the wave vectors a weak dependence of $\Phi(k)$ on the wave vector is observed. This allows us to accept the following approximation for $\Phi(k)$:

$$\Phi(k) = \begin{cases} \Phi(0)(1-2b^2k^2), & k < B' \\ \Phi = \text{const}, & B' \leq k < B. \end{cases} \quad (2.14)$$

The coordinate B' is obtained from the condition of the applicability of the parabolic approximation for $\Phi(k)$ and equals $B' = (b\sqrt{2})^{-1}$.

Among the set of the CV $\rho_{\mathbf{k}}$ there are those connected with the order parameter. In the case of the model with the exponentially decreasing interaction potential (2.2) it is the ρ_0 variable. The investigation of the critical behavior of this model is largely determined by considering the contribution from the ρ_0 variable in calculating the free energy. The mean value ρ_0 describes the behavior of the order parameter. Nevertheless, as seen from Eqs. (2.3) and (A1), all the CV $\rho_{\mathbf{k}}$ are interconnected, and the contribution of the variable ρ_0 alone cannot be separated in the partition function (2.3). The given task can be accomplished if we use the method suggested in Ref. 1. Its essence lies in sequentially integrating the $\rho_{\mathbf{k}}$ variables with $k \neq 0$ and investigating the functional from the ρ_0 variable. The functional representation of the partition function of the n -vector magnetic model in the ρ^4 -model approximation has the form⁵⁴

$$Z = J'[0] \exp(u'_0 N') \int \exp \left[-\frac{1}{2} \sum_{k < B'} d(k) \rho_{\mathbf{k}} \rho_{-\mathbf{k}} - \frac{a_4}{4! N'} \sum_{\mathbf{k}_1, \dots, \mathbf{k}_4, k_i < B'} \rho_{\mathbf{k}_1} \dots \rho_{\mathbf{k}_4} \delta_{\mathbf{k}_1 + \dots + \mathbf{k}_4} \right] (d\rho_{\mathbf{k}})^{N'}. \quad (2.15)$$

Part of the interaction potential is contained in the coefficient

$$d(k) = a_2 - \beta \Phi(k).$$

The expressions for the coefficients a_{2l} are shown in Appendix B. The calculation of Eq. (2.15) employs the smoothing procedure suggested by Wilson.¹⁴ However, unlike Ref. 14's approach it is based on the use of the non-Gaussian basic measure densities. It enables us to avoid the necessity of renormalizing a whole class of diverging diagrams. It should be mentioned that divergences of the kind are of mathematical nature and are not directly connected with the physics of the problem. The basic idea of the calculation (2.15) lies in a sequential exclusion from the consideration of the short-wavelength variables $\rho_{\mathbf{k}}$. After each of such step-by-step

exclusions the size of effective spin blocks is increased by the factor s ($s \geq 1$). The set of the CV $\rho_{\mathbf{k}}$ is divided into subsets. Each of these subsets contains the variables $\rho_{\mathbf{k}}$ with certain values of the wave vectors \mathbf{k} . For the l subset we have $k \in (B_{l+1}, B_l)$, where $B_{l+1} = B_l/s$, and $B_0 = B'$. In each of the layers of the CV phase space the value $\Phi(k)$ is replaced by the corresponding mean value.¹¹ After the layer integration the partition function (2.15) can be represented as a product of the partial partition functions Q_l of separate layers,

$$Z = C'_l Q_0 Q_1 \dots Q_l \int (d\rho_{\mathbf{k}})^{N_{l+1}} \omega_{l+1}(\rho), \quad (2.16)$$

where

$$\omega_{l+1}(\rho) = \exp \left[-\frac{1}{2} \sum_{k < B_{l+1}} d^{(n,l+1)}(k) \rho_{\mathbf{k}} \rho_{-\mathbf{k}} - \frac{a_4^{(n,l+1)}}{4! N_{l+1}} \sum_{\mathbf{k}_1, \dots, \mathbf{k}_4, k_i < B_{l+1}} \rho_{\mathbf{k}_1} \dots \rho_{\mathbf{k}_4} \delta_{\mathbf{k}_1 + \dots + \mathbf{k}_4} \right], \quad (2.17)$$

$$C'_l = \sqrt{2}^{(N_l - N_{l-1})n}, \quad Q_0 = [Q(u)Q(d_0)]^{N'},$$

$$Q_l = [Q(d_l)Q(P_{l-1})]^{N_l}, \quad N_l = N' s^{-dl}. \quad (2.18)$$

The value $\ln \omega_{l+1}(\rho)$ corresponds to the l -block Hamiltonian which depends on the N_l variables $\rho_{\mathbf{k}}$ connected with the fluctuation of the spin moment density in the blocks. The values which are part of the expressions for the partial partition functions Q_l are written in the form

$$Q(d_l) = (2\pi)^{n/2} \left(\frac{3}{a_4^{(n,l)}} \right)^{n/4} U \left(\frac{n-1}{2}, x_l \right) \exp \left(\frac{x_l^2}{4} \right),$$

$$Q(P_{l-1}) = (2\pi)^{-n/2} \left(\frac{n+2}{3} s^d \frac{a_4^{(n,l-1)}}{\varphi_n x_{l-1}} \right)^{n/4} \times U \left(\frac{n-1}{2}, y_{l-1} \right) \exp \left(\frac{y_{l-1}^2}{4} \right), \quad (2.19)$$

$$Q^{N'}(u) = J'[0] \exp(u'_0 N'). \quad (2.20)$$

For coefficients $a_2^{(n,l)}$ and $a_4^{(n,l)}$ the recursion relations (RR) are valid:

$$a_2^{(n,l+1)} = a_2^{(n,l)} + d^n (B_{l+1}, B_l) M_n(x_l),$$

$$a_4^{(n,l+1)} = a_4^{(n,l)} s^{-d} E_n(x_l), \quad (2.21)$$

where $d^n (B_{l+1}, B_l)$ corresponds to the mean value in the l layer. Special functions introduced here have the following form:

$$E_n(x_l) = s^{2d} \frac{\varphi_n(y_l)}{\varphi_n(x_l)}, \quad M_n(x_l) = N_n(x_l) - 1,$$

$$N_n(x_l) = \frac{y_l U_n(y_l)}{x_l U_n(x_l)}, \quad (2.22)$$

where the functions $\varphi_n(t), U_n(t)$ are combinations of the parabolic cylinder functions $U(a, t)$,

$$\varphi_n(t) = (n+2)U_n^2(t) + 2tU_n(t) - 2,$$

$$U_n(t) = \frac{U((n+1)/2, t)}{U((n-1)/2, t)}.$$

The variables

$$x_l = \sqrt{\frac{3}{a_4^{(n,l)}}} d^n(B_{l+1}, B_l),$$

$$y_l = s^{d/2} U_n(x_l) \left(\frac{n+2}{\varphi_n(x_l)} \right)^{1/2} \quad (2.23)$$

serve as arguments. The obtained expression (2.16) for the partition function enables us to calculate the free energy of the system,

$$F = -kT \sum_{l \geq 1} \ln Q_l, \quad (2.24)$$

when the explicit analytical expressions for the partial partition functions Q_l (2.18) and (2.19) are familiar to us. But, the calculation of Eq. (2.24) can only be done if the explicit solutions of the RR (2.21) are obtained as functions of the phase layer number l .⁵⁵ In this work we briefly present the results of the investigation of the RR (2.21),⁵⁴ which allows us to perform the calculation of the nonuniversal system characteristics. The RR (2.21) can be represented in the following form:

$$r_{l+1}^{(n)} = s^2 [-q + (r_l^{(n)} + q)N_n(x_l)],$$

$$u_{l+1}^{(n)} = s^{4-d} u_l^{(n)} E_n(x_l). \quad (2.25)$$

We introduce the following substitutes:

$$r_l^{(n)} = s^{2l} d^n(0), \quad u_l^{(n)} = s^{4l} a_4^{(n,l)}, \quad (2.26)$$

with

$$r_l^{(n)} + q = d^n(B_{l+1}, B_l) s^{2l}, \quad (2.27)$$

where

$$q = \beta \Phi(0) \bar{q}, \quad \bar{q} = \frac{d}{(d+2)} \frac{(1-s^{-(d+2)})}{(1-s^{-d})}, \quad (2.28)$$

\bar{q} is the geometric mean value of k^2 in the interval $(1/s, 1)$. Equations (2.25) as a partial solution have a fixed point

$$r_n^* = -f_n \beta \Phi(0), \quad u_n^* = \varphi_n(\beta \Phi(0))^2, \quad (2.29)$$

where

$$f_n = \frac{s^2(N_n(x^*) - 1)}{s^2 N_n(x^*) - 1} \bar{q},$$

$$\varphi_n = \frac{3}{(x^*)^2} \bar{q}^2 \left\{ \frac{1-s^{-2}}{N_n(x^*) - s^{-2}} \right\}^2. \quad (2.30)$$

TABLE I. The dependence of the fixed-point coordinates and the eigenvalues of the transition matrix on the s parameter of dividing the phase space into the layers and the n component number of the model.

s	n	x^*	E_1	E_2	f_n	φ_n
1.1	1	10.9487	1.2077	0.9092	0.0181	0.0201
	2	11.9534	1.2074	0.9089	0.0202	0.0168
	3	12.8801	1.2072	0.9086	0.0217	0.0144
1.5	1	3.3645	2.1521	0.6753	0.0998	0.1088
	2	3.5927	2.1379	0.6710	0.1134	0.0914
	3	3.8088	2.1273	0.6676	0.1234	0.0787
2.0	1	1.5562	3.4761	0.5347	0.2153	0.2497
	2	1.5671	3.3901	0.5260	0.2492	0.2105
	3	1.5848	3.3256	0.5185	0.2746	0.1814
3.0	1	0.3425	6.3985	0.4140	0.4640	0.6263
	2	0.1684	5.9509	0.4010	0.5498	0.5287
	3	0.0154	5.6298	0.3880	0.6145	0.4538
4.0	1	-0.1789	9.6225	0.3560	0.7167	1.0885
	2	-0.4575	8.5533	0.3402	0.8620	0.9180
	3	-0.7086	7.8304	0.3233	0.9712	0.7841

The values f_n and φ_n depend on the component number n of the model and the universal value x^* which is a solution of the nonlinear equation

$$s^{4+d} \varphi_n(y(x^*)) = \varphi_n(x^*). \quad (2.31)$$

The values f_n and φ_n for different n and s are presented in Table I.

The presence of the fixed point in RR (2.25) allows us to write them in the linearized form

$$\begin{pmatrix} r_{l+1}^{(n)} - r_n^* \\ u_{l+1}^{(n)} - u_n^* \end{pmatrix} = \text{Re} \begin{pmatrix} r_l^{(n)} - r_n^* \\ u_l^{(n)} - u_n^* \end{pmatrix}. \quad (2.32)$$

In calculating the matrix elements of the Re matrix we restrict our consideration to a linear term on $(x_l - x^*)$. As a result the following expressions for the matrix elements⁵⁴ are obtained:

$$R_{11} = s^2 \sqrt{3} \mu_1, \quad R_{12} = \frac{s^2}{2} (\mu_0 - \mu_1 x^*) (u_n^*)^{-1/2},$$

$$R_{21} = s^{4-d} \sqrt{3} u_n^* \omega_1, \quad R_{22} = s^{4-d} \left(\omega_0 - \frac{\omega_1 x^*}{2} \right). \quad (2.33)$$

It should be pointed out that in Eq. (2.33) we introduce the following definition:

$$\mu_1 = \mu_0 \left(a_1 - \frac{q_1}{2} \right); \quad \mu_0 = \frac{s^{d/2} \sqrt{n+2} U_n(y^*)}{\sqrt{3} \varphi_n^{1/2}(x^*)},$$

$$\omega_0 = \frac{s^{2d} \varphi_n(y^*)}{\varphi_n(x^*)}; \quad \omega_1 = \omega_0 (b_1 - q_1),$$

$$a_1 = \tilde{P}_1 y^* r_1, \quad r_1 = \partial_1 - \frac{q_1}{2},$$

$$\tilde{P}_m = \frac{1}{U_n(y^*)} \left(\frac{d^m U_n(y_l)}{dy_l^m} \right)_{y^*},$$

$$b_1 = \tilde{Q}_1 y^* r_1, \quad \tilde{Q}_m = \frac{1}{\varphi_n(y^*)} \left(\frac{d^m \varphi_n(y_l)}{dy_l^m} \right)_{y^*},$$

$$R_{12}^{(0)} = R_{12}(u_n^*)^{1/2}, \quad R_{21}^{(0)} = R_{21}(u_n^*)^{-1/2}.$$

The eigenvalues E_1 and E_2 of the matrix Re are universal values,^{54,59,60}

$$E_{1,2} = \frac{1}{2} \{ R_{11} + R_{22} \pm [(R_{11} - R_{22})^2 + 4R_{12}^{(0)}R_{21}^{(0)}]^{1/2} \}. \tag{2.34}$$

As is obvious from Table I, we have a saddle-type fixed point ($E_1 > 1, E_2 < 1$) for all values n and s . According to Refs. 59 and 60 the bigger eigenvalue E_1 defines the critical exponent ν for the correlation length

$$\nu = \frac{\ln s}{\ln E_1}. \tag{2.35}$$

Since E_1 is a universal value, the critical exponents are also universal and do not depend on the microscopic characteristics of the system. As we can see from Eqs. (2.33) and (2.34), they only depend on the dimensionality of space d and the n spin component number. The results of calculating the critical exponents of the model in the framework of this approach were shown in Refs. 61 and 62. Thus in the case $d=3, n=3$ the values $\nu=0.674, \alpha=-0.021, \gamma=1.347$ were obtained. These values of the critical exponents correspond to the ρ^4 model approximation which gives a good qualitative description of the critical behavior of the n -vector model (see Appendix C).

As is known,¹¹ good quantitative results for the critical exponents can be obtained in the framework of the ρ^6 model approximation. For example, the value of the ν critical exponent in the ρ^6 model approximation increases and practically remains unchanged with the increase of the m order of the ρ^{2m} model. Obtaining the eigenvectors of the transform matrix Re from Eq. (2.32) is an essential aspect of the investigation of the RR. They can be represented as follows:^{1,54}

$$w_1 = w_{11} \begin{pmatrix} 1 \\ R_1 \end{pmatrix}, \quad w_2 = w_{22} \begin{pmatrix} R \\ 1 \end{pmatrix}, \tag{2.36}$$

where

$$R_1 = \frac{R_{21}}{E_1 - R_{22}} = \frac{E_1 - R_{11}}{R_{12}}, \tag{2.37}$$

$$R = \frac{R_{12}}{E_2 - R_{11}} = \frac{E_2 - R_{22}}{R_{21}}. \tag{2.38}$$

The conjugate vectors v_1 and v_2 are written in the form

$$v_1 = v_{11} \begin{pmatrix} 1 & R_{12} \\ E_1 - R_{22} & \end{pmatrix}, \quad v_2 = v_{22} \begin{pmatrix} E_2 - R_{22} & \\ R_{12} & 1 \end{pmatrix}. \tag{2.39}$$

The normalization conditions $w_1 v_1 = 1, w_2 v_2 = 1$ give the relations for obtaining the coefficients $w_{ii}, v_{ii} (i=1,2)$. Proceeding from Eqs. (2.32) and (2.36) the RR (2.25) can be written in the form

$$\begin{aligned} r_l^{(n)} &= r_n^* + c_1 E_1^l + c_2 R E_2^l, \\ u_l^{(n)} &= u_n^* + c_1 R_1 E_1^l + c_2 E_2^l, \end{aligned} \tag{2.40}$$

where (see Appendix D)

$$\begin{aligned} c_1 &= \beta \Phi(0) \tau (c_{1k} + c_{1k1} \tau), \\ c_2 &= [\beta \Phi(0)]^2 (c_{2k} + \tau c_{2k1} + \tau^2 c_{2k}). \end{aligned} \tag{2.41}$$

The calculation of the partial partition functions (2.18) and (2.19) is connected with the employment of common RR (2.21). In the vicinity of the fixed point (2.29) they can be replaced by the approximate relations (2.40) which are exact for $T=T_c$. The question arises under what conditions the relations (2.40) can be made use of instead of common RR (2.21). It is obvious that the system of the relations

$$\begin{aligned} |r_l^{(n)} - r_n^*| &\leq |r_n^*|, \\ |u_l^{(n)} - u_n^*| &\leq u_n^* \end{aligned} \tag{2.42}$$

is a condition of the applicability of the approximate relations (2.40).

The magnitudes which from Eq. (2.42) are connected with the value of the n spin component number and the value of the iteration number l . The main reason for the deviation of the values $r_l^{(n)}$ and $u_l^{(n)}$ from their fixed values is the availability of the terms proportional to $c_1 E_1^l$ in the solutions (2.40). For small values l the contribution of these terms is small as compared with r_n^* and u_n^* , as $c_1 \sim \tau$. But in the case $T \neq T_c$ there always exists such a value as $l = m_\tau$ so that the contribution will be of the order r_n^* or u_n^* . With $l > m_\tau$ the deviation will become considerable and Eqs. (2.40) cannot be used for the description of common RR (2.21). It is necessary to use the first equation in Eq. (2.40) for determining the value m_τ ,⁶⁵

$$r_{m_\tau+1} - r_n^* = \delta r_n^*, \tag{2.43}$$

where δ is a certain constant value ($\delta \leq 1$). Since we will further compare the results obtained in the case of $T > T_c$ with those obtained for $T < T_c$, we assume that $\delta = 1$ with $T < T_c$ and $\delta = -1$ with $T > T_c$. The condition similar to Eq. (2.43) was employed in Ref. 11. In the first approximation on $(E_2/E_1)^{m_\tau}$ for m_τ we have

$$m_\tau = - \frac{\ln |\tau|}{\ln E_1} + m_0 - 1, \tag{2.44}$$

where

$$m_0 = m_c + m_1 \tau.$$

For the coefficients m_c and m_1 the following relations take place:

$$m_c = \frac{\ln(f_n \delta / c_{1k})}{\ln E_1}, \quad m_1 = - \frac{c_{1k1}}{c_{1k} \ln E_1}.$$

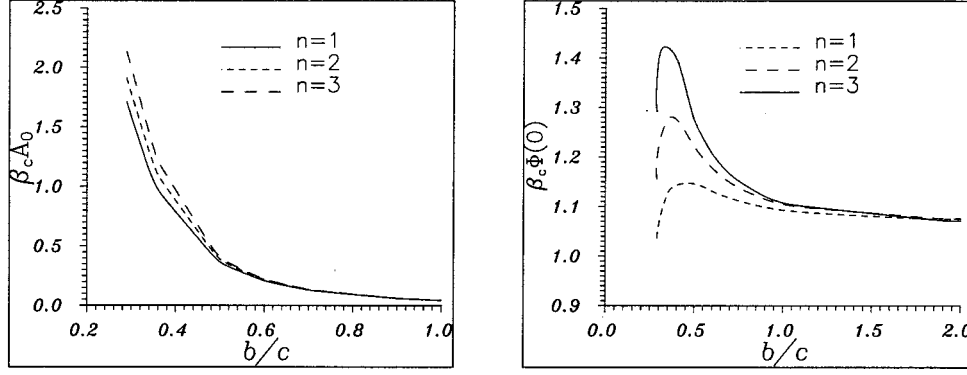


FIG. 1. The dependence of the PT temperature on the ratio of the effective range b of the interaction potential to the lattice constant c for different values of the n component number of the model.

The obtained value of m_τ defines the point of exit of the system from the critical region

$$B_{m_\tau} = B' s^{-m_\tau}.$$

The analysis of the RR shows that in the vicinity of the PT point two different fluctuation processes take place. The first one corresponds to the index values $l \in (0, m_\tau)$ and describes the renormalization-group symmetry. It is the so-called critical regime (CR). The second one corresponds to the index values $l > m_\tau$ and describes the long-wavelength fluctuations (LWF) of the spin and is valid both near and far from the PT point. It is characterized by Gaussian distribution with dispersion depending on the availability of the CR. It is the so-called Gaussian regime (GR) for $T > T_c$ and the inverse Gaussian regime (IGR) for $T < T_c$.

The calculation of the PT temperature is a significant moment in the investigation of the critical behavior of the model. As was shown in Refs. 1 and 11, the critical temperature is the point where GR is absent and subsequent relations occur:

$$\begin{aligned} \lim_{l \rightarrow \infty} r_{l+1}^{(n)}(T_c) &= \lim_{l \rightarrow \infty} r_l^{(n)}(T_c) = r_n^* = \text{const}, \\ \lim_{l \rightarrow \infty} u_{l+1}^{(n)}(T_c) &= \lim_{l \rightarrow \infty} u_l^{(n)}(T_c) = u_n^* = \text{const}. \end{aligned} \quad (2.45)$$

In accordance with Eq. (2.40), this condition is realized only in the case

$$c_1(T_c) = 0. \quad (2.46)$$

With Eq. (D1) taken into account the explicit equation for critical temperature was obtained:

$$\begin{aligned} [\beta_c \Phi(0)]^2 (1 - f_n - \varphi_n^{1/2} R^*) - a_2^{(n,0)} \beta_c \Phi(0) \\ = -a_4^{(n,0)} R^* \varphi_n^{-1/2}, \end{aligned} \quad (2.47)$$

where $R^* = R \sqrt{u_n^*}$, and $a_2^{(n,0)}$, $a_4^{(n,0)}$ are functions of the initial interaction potential (2.14).⁶⁶ In this paper we present the results of calculating the PT temperature with the interaction potential of the Eq. (2.14) type. As follows from Eq. (2.14), the obtaining of the concrete calculation results is connected with the choice of the value $\bar{\Phi}$. The correction considering the presence of the Fourier transform of the po-

tential in the interval $k \in [B', B)$ makes the results of the calculation more precise. Let us choose the next form for $\bar{\Phi}$,

$$\bar{\Phi} = \langle \Phi(k) \rangle + \Phi_\infty, \quad (2.48)$$

where

$$\langle \Phi(k) \rangle = \frac{\int_{B'}^B dk \Phi(k) k^2}{\int_{B'}^B dk k^2}. \quad (2.49)$$

The results obtained for the temperature in the limit $b/c \rightarrow \infty$ must be in agreement with the mean-field theory results, i.e.,

$$\beta_c \Phi(0) = \frac{n}{m^2}.$$

Taking into account this condition and the equation for the temperature T_c (2.47), we obtain the equation for defining the Φ_∞ . The solution of this equation is written as

$$\Phi_\infty = -\frac{(n+2)(f_n + \varphi_n^{1/2} R^*)}{3n(1 - s_0^{-d})}. \quad (2.50)$$

The results of calculating the PT temperature of the n -vector model in the case $m^2 = n$ are represented in Fig. 1.

As we can see from this figure, the PT temperature in the $\beta_c A_0$ units [where A_0 is a constant; see Eq. (2.2)] grows with the increase of the n component number of the model. The PT temperature decreases and strives to the mean-field theory results in the case of the increase of the effective range of the interaction potential b .

III. CALCULATION OF THE FREE ENERGY OF THE n -VECTOR MAGNETIC MODEL

The calculation of the free energy of the system can be performed in accordance with Eq. (2.24). The given analysis of the RR and the definition of the region of the availability of their approximate solutions enable us to present the free energy of the system in the vicinity of the PT point in the form

$$F = F_0 + F_{\text{CR}} + F_{\text{LWF}}, \quad (3.1)$$

where F_0 is the free energy of the noninteracting spins

TABLE II. The dependence of the coefficients of the free energy on the microscopic parameters of the interaction potential and the characteristics of the crystal lattice for a different n component number of the model are shown.

b/c	n	γ'_{01}	γ_1	γ_2	γ_{10}^+	γ_{10}^-	γ_0	γ_3^+	γ_3^-
0.2887	1	0.349	-0.500	-0.459	-0.538	2.737	1.811	1.283	2.726
	2	0.727	-0.976	-4.427	3.315	0.368	5.335	5.795	6.294
	3	1.099	-1.435	24.497	-25.359	30.049	9.488	-22.603	-22.530
$b=c$	1	0.297	-0.521	-0.122	-0.448	2.276	61.085	1.066	2.266
	2	0.620	-1.011	-3.200	2.722	0.303	192.194	4.759	5.170
	3	0.938	-1.470	21.176	-21.397	25.358	349.648	-19.072	-19.013

$$F_0 = -kTN \ln \left[\frac{(2\pi)^{n/2} m^{n-1}}{\Gamma(n/2)} \right], \quad (3.2)$$

F_{LWF} is the LWF free energy and F_{CR} is part of the free energy corresponding to the CR. The expression of the F_{LWF} for the case $T > T_c$ is presented in Eq. (3.13) and the expression of the F_{LWF} for the case $T < T_c$ is presented in Eq. (3.14). For F_{CR} we have

$$F_{CR} = -kT \sum_{l=0}^{m_\tau} F_l, \quad (3.3)$$

where

$$F_l = N_l f_l, \quad (3.4)$$

$$f_l = \frac{n}{4} \ln \left(\frac{n+2}{\varphi_n(y_l-1)} \right) + \ln U \left(\frac{n-1}{2}, x_l \right) + \ln U \left(\frac{n-1}{2}, y_{l-1} \right) + \frac{x_l^2}{4} + \frac{y_{l-1}^2}{4}.$$

In the case $l=0$ for f_l the following relation takes place:

$$f_0 = \frac{n}{4} \ln \left(\frac{3}{u'_4} \right) + u'_0 + \frac{3}{4} \frac{(u'_2)^2}{u'_4} + \ln U \left(\frac{n-1}{2}, z' \right) + \frac{n}{4} \ln \left(\frac{3}{u_0^{(n)}} \right) + \frac{x_0^2}{4} + \ln U \left(\frac{n-1}{2}, x_0 \right). \quad (3.5)$$

The employment of the RR solutions (2.40) enables us to select in f_l the explicit dependence on the number of the phase layer l . Having performed the summation along the layers of the CV phase space to the point m_τ of the exit of the system from the CR according to Eq. (3.3), for the free energy of the CR we obtain

$$E_{CR}^\pm = -kTN' [\gamma'_{01} + \gamma_1 \tau + \gamma_2 \tau^2 - \gamma_{10}^\pm |\tau|^{d\nu}]. \quad (3.6)$$

Let us note that the signs “+” and “-” correspond to the cases $T > T_c$ and $T < T_c$, respectively. The coefficients $\gamma'_{01}, \gamma_1, \gamma_2, \gamma_{10}^\pm$ are constants and do not depend on the temperature (see Appendix E). The analytical part of the CR free energy is connected with the coefficients $\gamma'_{01}, \gamma_1, \gamma_2$. It should be mentioned that the expressions of these coefficients coincide at the temperatures above and below the critical temperature. The dependence of γ_l on the microscopic parameters of the interaction potential and the n component number of the model are shown in Table II.

The nonanalytical part characterizing the temperature dependence of the specific heat in the vicinity of the PT point is connected with the term $\gamma_{10}^\pm \tau^{d\nu}$, where

$$\gamma_{10}^\pm = \bar{\gamma}' s^{-dm_0}, \quad (3.7)$$

$$\bar{\gamma}' = \frac{f_{CR}^*}{1-s^{-d}} - \frac{f_n \delta d_1}{1-s^{-d} E_1} + \frac{f_n^2 \delta^2 d_3}{1-s^{-d} E_1^2}, \quad (3.8)$$

and the following definition is introduced:

$$f_n = \tau E_1^{m_\tau+1} c_{1k}.$$

For f_{CR}^* we have

$$f_{CR}^* = \frac{n}{2} \ln y^* + \bar{\alpha} (y^*)^{-2} + \frac{(x^*)^2}{4} + \ln U \left(\frac{n-1}{2}, x^* \right). \quad (3.9)$$

The values of d_m are given in Appendix F. In Table II the dependence of γ_{10}^\pm on the component number n of the model for different ratios b/c is shown. The expression (3.6) describes the contribution of the region of the renormalization-group symmetry to the free energy of the system. It allows us to obtain the respective contributions to the specific heat of the system at $T < T_c$ and $T > T_c$,

$$C_{CR}^\pm = kN' [c^{(0)} - c_{CR}^\pm |\tau|^{-\alpha}], \quad (3.10)$$

where

$$\alpha = 2 - d\nu,$$

$$c^{(0)} = 2(\gamma_1 + \gamma_2),$$

$$c_{CR}^\pm = (1 - \alpha) u_{CR}^\pm,$$

$$u_{CR}^\pm = d\nu \gamma_{10}^\pm. \quad (3.11)$$

The curves 1 in Fig. 2 correspond to the contribution of the CR to the specific heat at $T < T_c$ and $T > T_c$, respectively. The negative value of the specific-heat amplitude that corresponds to the contribution of the CR testifies to the nonstability of the contribution of the short-wavelength fluctuations (SWF) of the spin moment density. Considering the contribution of the region of the LWF of the spin moment density in calculating the thermodynamic characteristics of the system is a topical problem of today.

The regions of GR for $T > T_c$ (and IGR for $T < T_c$) correspond to the LWF of the spin moment density. The increase

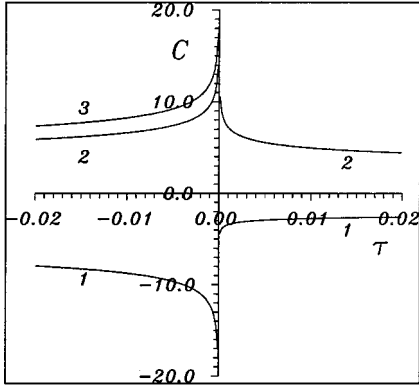


FIG. 2. The temperature dependence of the specific heat. The comparison of the contribution of the CR and the region of the LWF. Notes: 1 corresponds to the CR, 2 to the limit GR ($\tau > 0$) and IGR ($\tau < 0$), 3 to the contribution to the specific heat due to the rise of the ordering in the system.

of the basic x_l and the intermediate y_l variables as functions of l is a typical peculiarity of the limit GR (LGR) and IGR. In this connection the contribution of these regions to the free energy can be calculated in the Gaussian measure density approximation as in this region of the wave vectors the term proportional to the fourth power under the exponent of the distribution functions becomes much smaller than the square term. Since the increase of x_l is gradual, there exists the so-called transition region (TR) where it is necessary to keep the fourth power of the ρ_k variables in the distribution function. The value of the TR is defined by a certain number of the CV phase space layers m'' following the point m_τ of the exit of the system from the CR. The value of the TR is defined by the condition

$$|x_{m_r+m''_0}| = \frac{\alpha_m}{1-s^{-d}}, \quad (3.12)$$

where α_m is a constant ($\alpha_m \geq 10$). The arguments mentioned above enable us to write the contribution of the LWF at $T > T_c$ to the free energy of the system in the form

$$F_{\text{LGR}}^+ = -kTN' f_{\text{LWF}}^+ \tau^{3\nu} - \beta \mu_B^2 H^2 N \gamma_4 \tau^{-2\nu}, \quad (3.13)$$

where μ_B is Bohr's magneton and

$$f_{\text{LWF}}^+ = f_{\text{TR}} + f'_*.$$

f_{TR} corresponds to the contribution of the TR and f'_* corresponds to the contribution to the free energy of the CV's from the wave-vectors region with $k < B' s^{-(m_\tau+m''+1)}$. The explicit analytical expressions of these coefficients were shown in Ref. 61. The contribution of the region of the LWF of the spin moment density at $T < T_c$ to the free energy of the system is described by the value F_{IGR}^- . The value F_{IGR}^- corresponds to the IGR. The calculation of the IGR contribution has its own peculiarities. In the temperature region $T < T_c$ large scale fluctuations of the spin moment density are described by the non-Gaussian distribution in which the coefficient near the square term becomes negative. This indicates the appearance of the nonzero order parameter of the system. After selecting the ordering free energy the distribution of

the fluctuations (2.17) becomes Gaussian (see Appendix G). As a result, for F_{IGR}^- we obtain

$$F_{\text{IGR}}^- = -kTN' |\tau|^{3\nu} \gamma_{\text{LWF}}^-, \quad (3.14)$$

where

$$\gamma_{\text{LWF}}^- = \gamma_3^{(\mu_\tau)} + \gamma_3^{(\sigma)},$$

$$\gamma_3^{(\mu_\tau)} = \gamma_g + \gamma_\rho, \quad \gamma_3^{(\sigma)} = c_\nu^d \bar{\gamma}_3^{(\sigma)}, \quad \bar{\gamma}_3^{(\sigma)} = s_0^d E'_0. \quad (3.15)$$

The value $\gamma_3^{(\sigma)}$ corresponds to the contribution from the ordering in the system. The coefficients γ_g and γ_ρ are written in the form

$$\gamma_g = \bar{\gamma}_g c_\nu^d,$$

$$\bar{\gamma}_g = \ln \left[\left(\frac{s^{d+4} (n+2) \bar{u}_{m_\tau}}{3 \pi^2 \varphi_n(x_{m_\tau})} \right)^{n/4} e^{y_{m_\tau}^2/4} U \left(\frac{n-1}{2}, y_{m_\tau} \right) \right], \quad (3.16)$$

$$\gamma_\rho = \bar{\gamma}_\rho c_\nu^d,$$

$$\begin{aligned} \bar{\gamma}_\rho = & \frac{5}{12} n L(x) - \frac{n}{2} \ln \left(\frac{1+2\bar{\tau}_{m_\tau}}{\pi} \right) + \frac{n}{3} - \frac{\bar{u}_{\mu_\tau+1}}{8} [\bar{\alpha}_1^2 n^2 \\ & + 3n^3 L(x) \bar{\alpha}_2] + \frac{\bar{u}_{m_\tau}^2}{48} n^4 (\bar{\alpha}_4 + 3\bar{\alpha}_1^2 \bar{\alpha}_2) + \frac{9}{4} n^2 \bar{\alpha}_2 \bar{r}_{m_\tau}^2. \end{aligned} \quad (3.17)$$

It should be pointed out that the following definitions are introduced here:

$$\bar{r}_{m_r+1} = f_n (1 + \delta), \quad \bar{u}_{m_r+1} = \varphi_n - f_n \varphi_n^{1/2} R_1^* \delta, \quad (3.18)$$

$$L(x) = 3 \left(\frac{x - \arctan x}{x^3} \right), \quad x = \frac{1}{\sqrt{2\bar{r}_{m_r+1}}}. \quad (3.19)$$

Besides, $c_\nu = (c_{1T}/f_n \delta)^\nu$ is a nonuniversal value connected with the microscopic parameters of the initial Hamiltonian. According to Eqs. (3.1), (3.6), (3.13), and (3.14) the complete expression of the free energy of the three-dimensional n -vector magnetic model in the absence of the external field can be written as

$$F = -kTN' [\gamma_0 - \gamma_1 |\tau| + \gamma^2 |\tau|^2 + \gamma_3^\pm |\tau|^{3\nu}], \quad (3.20)$$

where

$$\gamma_0 = \gamma'_{01} + s_0^3 \ln \left[\frac{(2\pi)^{n/2} m^{n-1}}{\Gamma(n/2)} \right], \quad (3.21)$$

$$\gamma_3^\pm = \gamma_{\text{LWF}}^\pm - \gamma_{10}^\pm. \quad (3.22)$$

The coefficient γ_3^\pm includes the contribution of the CR and the region of the LWF of the spin moment density at the temperatures above and below the critical. It describes the singular behavior of the specific heat in the vicinity of the PT point. The dependence of the coefficients γ_0, γ_3^\pm on the microscopic parameters of the interaction potential and the

TABLE III. The dependence of the amplitudes of the thermodynamic functions on the microscopic parameters of the interaction potential and the characteristics of the crystal lattice for a different n component number of the model.

b/c	n	S^0	S^1	u_3^+	u_3^-	$C^{(0)}$	C_1^+	C_1^-
0.2887	1	1.311	-1.917	2.355	-5.007	-1.917	1.972	4.190
	2	4.359	-10.805	11.226	-12.196	-10.805	10.529	11.436
	3	8.053	46.124	-45.677	45.530	46.124	-46.629	-46.478
$b=c$	1	60.564	-1.286	1.958	-4.163	-1.286	1.639	3.484
	2	191.183	-8.421	9.220	-10.017	-8.421	8.646	9.393
	3	348.178	39.412	-38.540	38.422	39.412	-39.344	-39.223

characteristics of the crystal lattice for different n component number of the model is shown in Table II.

IV. THERMODYNAMIC FUNCTIONS OF THE n -VECTOR MAGNETIC MODEL IN THE FRAMEWORK OF THE ρ^4 MODEL APPROXIMATION

The complete expression obtained for the free energy of the n -vector magnetic model (3.20) in the ρ^4 model approximation allows us to calculate other thermodynamic functions in the vicinity of the phase-transition point. As was observed above [see Eq. (3.10) and Fig. 2], considering the contribution of the LWF of the spin moment density is especially significant in calculating the thermodynamic functions of the system. So, differentiating the expression of the free energy by the temperature, we obtain the expression for the entropy,

$$S = kN[S^0 + S^1\tau + u_3^\pm |\tau|^{3\nu-1}], \quad (4.1)$$

where

$$S^0 = \gamma_0 + \gamma_1, \quad S^1 = 2(\gamma_1 + \gamma_2), \quad u_3^\pm = \pm 3\nu\gamma_3^\pm.$$

The values of the coefficients S^0, S^1, u_3^\pm for different n values are shown in Table III.

It should be mentioned that the correct temperature behavior of the specific-heat curves is ensured by considering the region of the LWF of the spin moment density, i.e., the region of LGR at $T > T_c$ and the region of IGR at $T < T_c$. The significant characteristic of the system is the specific heat for which we obtain

$$C = kN'[C^{(0)} + C_1^\pm |\tau|^{-\alpha}], \quad (4.2)$$

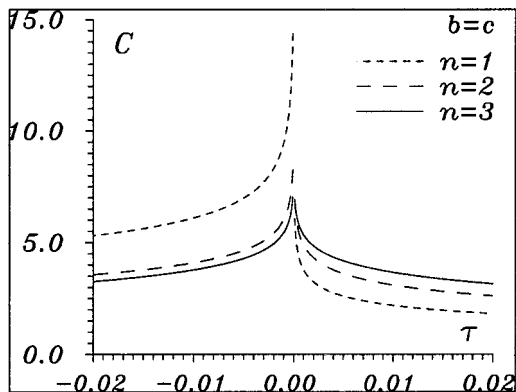


FIG. 3. The temperature dependence of the specific heat for a different n component number of the model.

where

$$\alpha = 2 - 3\nu, \quad C^{(0)} = 2(\gamma_1 + \gamma_2), \quad C_1^\pm = 3\nu(1 - \alpha)\gamma_3^\pm.$$

The second term in Eq. (4.2) describes the main peculiarity of the specific-heat behavior in the vicinity of the PT point. As we can see from Eq. (4.2), the coefficient C_1^\pm includes the contributions of the CR and the region of the LWF of the spin moment density. We can see from Fig. 2 that considering the influence of the regions of LWF (curves 2) provides the positivity of the specific heat and the system stability, respectively. The dependence of the coefficients $C^{(0)}$ and C_1^\pm on the microscopic parameters of the Hamiltonian, i.e., from the b/c ratio for a different n is exhibited in Table III.

In Fig. 3 the temperature dependence of the specific heat for different n is shown. As was noted above, in the case $n = 3$ the critical exponent α , which describes the singularity of the specific heat becomes negative $\alpha = -0.021$.^{61,62} The analysis of the expression (4.2) and the obtained values of the specific-heat amplitudes (see Table III) shows that the specific heat in the case $n = 3$ does not diverge and receives a concrete finite value (see Fig. 3).

The curve of the dependence of the specific heat maximum at $T = T_c$ in the case $n = 3$ on the ratio of the effective range b of the interaction potential to the lattice constant c is shown in Fig. 4. One can see from this figure that the value of the specific-heat maximum decreases and tends to a constant value as the effective range b of the interaction potential increases. This agrees with the results of the mean-field theory.

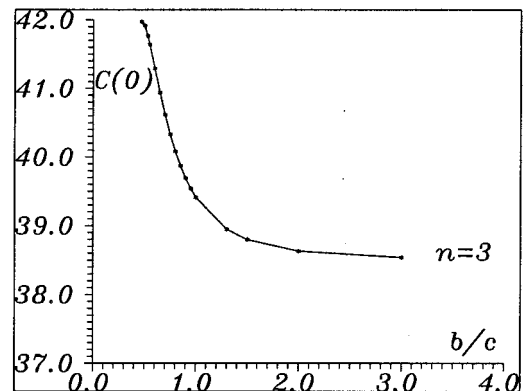


FIG. 4. The dependence of the maximum of the specific heat on the ratio of the effective range b of the interaction potential to the crystal lattice constant c in the case $n = 3$ and $T = T_c$.

TABLE IV. The dependence of the ratio A of the specific heat critical amplitudes at $T > T_c$ and $T < T_c$ on the n component number of the model.

n	Present work	Lattice series expansions	Field theory	1/s-exp (Ref. 47)	Experiment
1	0.470	0.523 ± 0.009 (Ref. 33)	0.524 ± 0.010 (Ref. 29) 0.55 (Ref. 22) 0.541 ± 0.014 (Ref. 68) 0.540 ± 0.011 (Ref. 48)	0.519	0.538 (Ref. 67) 0.53 (Ref. 71)
2	0.921	1.08 (Ref. 69)	1.029 ± 0.013 (Ref. 29) 0.99 (Ref. 22) 1.05 (Ref. 70) 1.056 ± 0.004 (Ref. 48)	0.888	1.067 (Ref. 67) 1.054 ± 0.001 (Ref. 72) 1.088 ± 0.007 (Ref. 73)

According to Eq. (4.2) the ratio of the critical amplitudes of the leading singular terms of the specific heat at $T > T_c$ and $T < T_c$ can be written in the form

$$A = \frac{\gamma_3^+}{\gamma_3^-}. \quad (4.3)$$

The comparison of the results obtained for the ratio of the critical amplitudes of the specific-heat leading singular terms with results obtained by other methods is shown in Table IV.

V. CONCLUSIONS

In general, it should be noted that separate accounting of the contributions of the short- and long-wavelength fluctuations of the spin moment density in the expression of the free energy of the system in the vicinity of the PT temperature allows us to find the explicit analytical expressions for the thermodynamic functions as functions of the temperature. The proposed method enables us to investigate the dependence of the critical amplitudes of the thermodynamic functions on the microscopic parameters of the interaction potential and the characteristics of the crystal lattice. The results obtained for the critical exponents and the ratio of the critical amplitudes agree with those achieved by other methods. The negligible deviation of the obtained results from the experimental data and the results of the numerical calculations is connected with the restriction in the calculation by the ρ^4 model approximation. As was seen in Refs. 11 and 74, the employment of the ρ^6 measure density for the investigation of the PT in the case $n=1$ gives a more precise definition of the calculation results of the universal and nonuniversal characteristics of the system. The extension of the suggested method to the investigation of the critical behavior of the n -vector model in the frame of the ρ^6 model approximation does not require any principal changes. To be brief, in the present paper we do not give enough attention to calculating the scaling corrections. In the case $n=1$ such calculations were made in Ref. 11. Besides, in the common case the critical exponent of the correlation function is $\eta \neq 0$. Such values of the correlation function critical exponent can be obtained by the method we propose if we take into account the correction on the averaging of the interaction potential in each layer of the CV. We are going to perform such investigations in our subsequent papers.

APPENDIX A

The $\rho_{\mathbf{k}}$ CV are introduced by means of the functional representation for the operators of the spin-density fluctuation $\hat{\rho}$,

$$\hat{\rho}_{\mathbf{k}} = \int \rho_{\mathbf{k}} J(\rho - \hat{\rho}) (d\rho_{\mathbf{k}})^N, \quad \hat{\rho}_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} \hat{S}_{\mathbf{R}} \exp(-i\mathbf{k}\mathbf{R}),$$

where

$$J(\rho - \hat{\rho}) = \left[\prod_{\mathbf{k}}' \delta(\rho_{\mathbf{k}}^c - \hat{\rho}_{\mathbf{k}}^c) \delta(\rho_{\mathbf{k}}^s - \hat{\rho}_{\mathbf{k}}^s) \right] \delta(\rho_0 - \hat{\rho}_0)$$

is the transition operator. For the $\rho_{\mathbf{k}}$ CV the following relations come into being:

$$\rho_{\mathbf{k}} = \rho_{\mathbf{k}}^c - i\rho_{\mathbf{k}}^s, \quad \rho_{\mathbf{k}}^c = \rho_{-\mathbf{k}}^c, \quad \rho_{\mathbf{k}}^s = -\rho_{-\mathbf{k}}^s.$$

The Jacobian of the transition from spins to CV has the form^{11,54}

$$J[\rho] = \tilde{Z}_0 \int \exp\left(2i\pi \sum_{\mathbf{k}} \rho_{\mathbf{k}} \omega_{\mathbf{k}} + \bar{D}[\omega]\right) (d\omega_{\mathbf{k}})^N, \quad (A1)$$

where for $\omega_{\mathbf{k}}$ variables conjugate to $\rho_{\mathbf{k}}$ variables we have

$$\omega_{\mathbf{k}} = \frac{1}{2}(\omega_{\mathbf{k}}^c + i\omega_{\mathbf{k}}^s), \quad \omega_{\mathbf{k}}^c = \omega_{-\mathbf{k}}^c, \quad \omega_{\mathbf{k}}^s = -\omega_{-\mathbf{k}}^s,$$

$$(d\omega_{\mathbf{k}})^N = \prod_{a=1}^n d\omega_0^a \prod_{\mathbf{k}}' d\omega_{\mathbf{k}}^{a,c} d\omega_{\mathbf{k}}^{a,s}.$$

APPENDIX B

For the coefficients a_{2l} the following expressions are available:

$$a_2 = \frac{n}{m^2} s_0^{d/2} \left[\frac{1}{1 - \frac{20m^2}{(n+4)} \sum_{k \in \Delta} \frac{\beta\Phi(k)}{N}} \right]^{1/2} U_0,$$

$$a_4 = -\frac{3n^2}{m^4} s_0^d \left[\frac{1}{1 - \frac{20m^2}{(n+4)} \sum_{k \in \Delta} \frac{\beta\Phi(k)}{N}} \right] \times [1 - z' U_n(z') - U_0^2], \quad (\text{B1})$$

Here subsequent definitions are introduced:

$$U_0 = \sqrt{\frac{n+2}{2}} U_n(z'), \quad \Delta = [B', B], \quad (\text{B2})$$

$$U_n(z') = \frac{U((n+1)/2, z')}{U((n-1)/2, z')}, \quad z' = \sqrt{\frac{3}{u_4'}} u_2', \quad (\text{B3})$$

where $U(a, x) = D_{-a-1/2}(x)$ are the Weber cylinder parabolic functions. The renormalized u_{2l} cumulants considering the availability of $\Phi(k)$ for the large values of k have the form

$$u_0' = s_0^d \frac{u_2 n}{2N} \sum_{k \in \Delta} \beta\Phi(k), \quad u_2' = u_2 - \frac{|u_4|n}{2N} \sum_{k \in \Delta} \beta\Phi(k),$$

$$u_4' = \left[|u_4| - \frac{u_6 n}{2N} \sum_{k \in \Delta} \beta\Phi(k) \right] s_0^{-d}. \quad (\text{B4})$$

The coefficients u_{2l} have the following expressions:⁵⁰

$$u_2 = \frac{m^2}{n}, \quad u_4 = -\frac{6m^4}{n^2(n+2)},$$

$$u_6 = 15m^6 \left[\frac{1}{n(n+2)(n+4)} - \frac{3}{n^2(n+2)} + \frac{2}{n^3} \right]. \quad (\text{B5})$$

In the case $n \rightarrow \infty$ the behavior of the coefficients u_{2l} were represented in Appendix C.

APPENDIX C

In the marginal case of the larger $n \rightarrow \infty$, the cumulants u_{2l} strive for their limit values

$$\lim_{n \rightarrow \infty} u_2 = 1, \quad \lim_{n \rightarrow \infty} u_4 = \lim_{n \rightarrow \infty} \frac{6}{n+2} \rightarrow 0,$$

$$\lim_{n \rightarrow \infty} u_{2l} = 0, \quad l = 3, 4, \dots$$

(in normalizing the spin dimensionality $m^2 = n$). Considering only the leading members by order of the value $1/n$ in the process of integration of the partition functions enables us to employ the method of g expansion.^{50,56,58} In this case the values

$$g_{2l} = \frac{u_{2l}}{(2l)!} \left/ \left(\frac{d(B_1, B')}{2} \right)^l \right., \quad \mathbf{g} = (g_4, g_6, \dots)$$

are small. It allows obtaining the next relations for the correlation length critical exponent (in the case $\eta = 0$)

TABLE V. The dependence of the temperature critical region $\tau_{1,2}^*$ on the n spin component number of the model.

n	τ_1^*	γ_2^*
1	0.0286	0.3449
2	0.0371	0.3448
3	0.0424	0.3270

$$g_1^* = 0, \quad \nu = \frac{1}{2}, \quad \text{at } d > 4;$$

$$g_2^* = \frac{1 - s^{d-4}}{(n+8)(1-s^{-d})},$$

$$\nu = \left[2 + \frac{\ln\{1 + [(n+2)/(n+8)](s^{d-4} - 1)\}}{\ln s} \right]^{-1}, \quad \text{at } d < 4,$$

where g_i^* are the fixed points. But, starting from the type of fixed point we have certain restrictions on the s value ($1 \leq s < 2$). In the limit $n \rightarrow \infty$ for $d < 4$ we obtain $\nu = 1$, which is in agreement with the Berlin-Kac spherical model.⁵¹ Analogical expressions for ν were obtained in a series of works.^{50,56,58,63,64}

APPENDIX D

From the initial conditions at $l = 0$

$$r_0^{(n)} = a_2^{(n,0)} - \beta\Phi(0), \quad u_0^{(n)} = a_4^{(n,0)}$$

the following expressions for the coefficients c_1, c_2 were found:

$$c_1 = \{r_0^{(n)} - r_n^* + (a_4^{(n,0)} - u_n^*)(-R)\} D^{-1},$$

$$c_2 = \{a_4^{(n,0)} - u_n^* + (r_0^{(n)} - u_n^*)(-R_1)\} D^{-1}, \quad (\text{D1})$$

where $D = (E_1 - E_2)/(R_{11} - E_2)$. For temperatures close to T_c the coefficients c_1 and c_2 can be represented as follows:

$$c_1(T) = c_{1T} \tau \beta\Phi(0),$$

$$c_2(T) = c_{2T} [\beta\Phi(0)]^2. \quad (\text{D2})$$

Having applied these relations we evaluate the critical region of the temperatures $\tau < \tau^*$ in which the solutions of RR (2.40) are valid. For the critical region to exist it is necessary that the ‘‘exit’’ from this region at $l \rightarrow 1$ should not exceed the ‘‘entrance.’’ It means that the value τ^* is equal to the smaller root of the two equations

$$c_2 R E_2 = c_1 E_1, \quad c_1 R_1 E_1 = c_2 E_2.$$

Taking into account Eq. (D2) we obtain for $\tau_{1,2}^*$

$$\tau_1^* = \left| \frac{c_{2T} R E_2 \beta(0)}{c_{1T} E_1} \right|, \quad \tau_2^* = \left| \frac{c_{2T} E_2 \beta(0)}{c_{1T} E_1 R_1} \right|.$$

The results of calculating $\tau_{1,2}^*$ in the case $s = 4$ are shown in Table V.

As $c_1(T) \sim \tau$, the value c_{1T} can be represented in the following approximation:

$$c_{1T} = c_{1k} + c_{1k1} \tau + O(\tau^2), \quad (\text{D3})$$

where

$$c_{1k} = \left[c_{11} + \frac{c_{12}}{[\beta_c \Phi(0)]^2} \right] D^{-1},$$

$$c_{1k1} = \frac{c_{12}}{[\beta_c \Phi(0)]^2} D^{-1}, \quad (\text{D4})$$

with

$$c_{11} = 1 - f_n - R^* \varphi_n^{1/2},$$

$$c_{12} = -a_4^{(n,0)} R^* \varphi_n^{-1/2}. \quad (\text{D5})$$

In accordance with Eq. (D2) for c_{2T} we consider only the terms proportional to τ^2 ,

$$c_{2T} = c_{2k} + \tau c_{2k1} + \tau^2 c_{2k2} + O(\tau^3), \quad (\text{D6})$$

where the following definitions are introduced:

$$c_{2k} = \left[c_{23} + \frac{c_{22}}{\beta_c \Phi(0)} + \frac{c_{21}}{[\beta_c \Phi(0)]^2} \right] D^{-1},$$

$$c_{2k1} = \left[\frac{c_{22}}{\beta_c \Phi(0)} + \frac{2c_{21}}{[\beta_c \Phi(0)]^2} \right] D^{-1}, \quad (\text{D7})$$

$$c_{2k2} = \frac{c_{21}}{[\beta_c \Phi(0)]^2} D^{-1}$$

and

$$c_{21} = a_4^{(n,0)}, \quad c_{22} = -a_2^{(n,0)} R_1^* \varphi_n^{1/2},$$

$$c_{23} = R_1^* \varphi_n^{1/2} (1 - f_n) - \varphi_n,$$

$$R_1^* = R_1 (u_n^*)^{-1/2}, \quad R^* = R (u_n^*)^{1/2}.$$

APPENDIX E

The coefficients $\gamma'_{01}, \gamma_1, \gamma_2$ are expressed in the form

$$\gamma'_{01} = \bar{a}_0 + \gamma_{01},$$

$$\gamma_1 = \bar{a}_1 + \gamma_{02},$$

$$\gamma_2 = \bar{a}_2 + \gamma_{03},$$

where

$$\bar{a}_0 = a'_0 + \frac{n}{2} \ln 2\pi + \frac{n}{4} \ln \left(\frac{3}{a_4^{(n,0)}} \right) + \frac{(x^{(0)})^2}{4}$$

$$+ \ln U \left(\frac{n-1}{2}, x^{(0)} \right),$$

$$a'_0 = \ln \left(\frac{m^{n-1}}{\Gamma \left(\frac{n}{2} \right)} \right) + \frac{n}{4} \ln \left(\frac{3}{u'_4} \right) + \frac{3(u'_2)^2}{4u'_4}$$

$$+ \ln U \left(\frac{n-1}{2}, \sqrt{\frac{n+2}{2}} \right),$$

$$\bar{a}_1 = -n T_c U_n(x^{(0)}) \left(\frac{dx^{(0)}}{dT} \right)_{T=T_c},$$

$$\bar{a}_2 = -\frac{n}{4} T_c^2 \left\{ U_n(x^{(0)}) \left(\frac{d^2 x^{(0)}}{dT^2} \right)_{T=T_c} \right.$$

$$\left. + \left[\frac{dU_n(x^{(0)})}{dx^{(0)}} \left(\frac{dx^{(0)}}{dT} \right)^2 \right]_{T=T_c} \right\}$$

and

$$x^{(0)} = \sqrt{3} d_{2c} (a_{4c})^{-1/2},$$

$$d_{2c} = \bar{q} - f_0 + c_{2k} R^{(0)} \varphi_0^{-1/2},$$

$$a_{4c} = \varphi_0 + c_{2k}.$$

For the γ_{0i} coefficients we have

$$\gamma_{01} = s^{-d} \left(\frac{f^*}{1-s^{-d}} + \frac{c_{2k} d_2 E_2}{1-s^{-d} E_2} + \frac{c_{2k}^2 d_4 E_2^2}{1-s^{-d} E_2^2} \right),$$

$$\gamma_{02} = s^{-d} \left(\frac{c_{2k1} d_2 E_2}{1-s^{-d} E_2} + \frac{b_1 d_4 E_2^2}{1-s^{-d} E_2^2} + \frac{c_{1k} d_1 E_1}{1-s^{-d} E_1} \right.$$

$$\left. + \frac{c_{1k} c_{2k} d_5 E_1 E_2}{1-s^{-d} E_1 E_2} + \frac{c_{1k} b_0 d_7 E_2^2 E_1}{1-s^{-d} E_1 E_2^2} \right),$$

$$\gamma_{03} = s^{-d} \left(\frac{c_{2k2} d_2 E_2}{1-s^{-d} E_2} + \frac{(c_{1k} c_{2k1} + c_{2k} c_{1k1}) d_5 E_1 E_2}{1-s^{-d} E_1 E_2} \right.$$

$$\left. + \frac{c_{1k1} d_1 E_1}{1-s^{-d} E_1} + \frac{b_2 d_4 E_2^2}{1-s^{-d} E_2^2} + \frac{(c_{1k} b_1 + c_{1k1} b_0) d_7 E_1 E_2^2}{1-s^{-d} E_1 E_2^2} \right.$$

$$\left. + \frac{c_{1k}^2 d_3 E_1^2}{1-s^{-d} E_1^2} + \frac{c_{1k}^2 c_{2k} d_6 E_1^2 E_2}{1-s^{-d} E_1^2 E_2} + \frac{c_{1k}^2 b_0 d_8 E_1^2 E_2^2}{1-s^{-d} E_1^2 E_2^2} \right),$$

where

$$b_0 = c_{2k}^2, \quad b_1 = 2c_{2k} c_{2k1}, \quad b_2 = c_{2k1}^2 + 2c_{2k} c_{2k2}.$$

For γ' we have

$$\gamma' = \frac{f^*}{1-s^{-d}} + \frac{f_n \delta d_1}{1-s^{-d} E_1} + \frac{f_n^2 \delta^2 d_3}{1-s^{-d} E_1^2}.$$

The values of d_m are given in Appendix F. For γ_4 we have

$$\gamma_4 = s^{2m''} \left(\frac{f_n \delta}{c_{1T}} \right)^{2\nu} \frac{1}{2\beta \Phi(0) g_0}, \quad (\text{E1})$$

where g_0 is a complex function of $x_{m'_\tau}^*$ with $m'_\tau = m_\tau + m'' + 2$ (see Ref. 61).

APPENDIX F

For the coefficients d_i the following expressions are valid:

$$d_1 = B_3 \left(A_3 + \frac{A_1}{E_1} \right), \quad d_2 = B_1 \left(A_3 + \frac{A_1}{E_2} \right),$$

$$d_3 = B_6 \left(A_3 + \frac{A_1}{E_1^2} \right) + B_3^2 \left(A_4 + \frac{A_2}{E_1^2} \right),$$

$$d_4 = B_2 \left(A_3 + \frac{A_1}{E_2^2} \right) + B_1^2 \left(A_4 + \frac{A_2}{E_2^2} \right),$$

$$d_5 = B_4 \left(A_3 + \frac{A_1}{E_1 E_2} \right) + 2B_1 B_3 \left(A_4 + \frac{A_2}{E_1 E_2} \right),$$

$$d_6 = B_7 \left(A_3 + \frac{A_1}{E_1 E_2^2} \right) + 2(B_1 B_6 + B_3 B_4) \left(A_4 + \frac{A_2}{E_1 E_2^2} \right),$$

$$d_7 = B_5 \left(A_3 + \frac{A_1}{E_1 E_2^2} \right) + 2(B_1 B_4 + B_2 B_3) \left(A_4 + \frac{A_2}{E_1 E_2^2} \right),$$

$$d_8 = B_8 \left(A_3 + \frac{A_1}{E_1^2 E_2^2} \right) + 2 \left(B_1 B_7 + B_2 B_6 + B_3 B_5 + \frac{B_4^2}{2} \right) \\ \times (A_4 + A_2 E_1^{-2} E_2^{-2}),$$

where the coefficients A_i, B_j are universal constants and are defined by the fixed-point coordinates. For the B_j coefficients we have

$$B_1 = \varphi_n^{-1} \left(R^* \sqrt{3} - \frac{x^*}{2} \right), \quad B_2 = \varphi_n^{-2} \left(\frac{3}{8} x^* - \frac{\sqrt{3}}{2} R^* \right),$$

$$B_3 = \varphi_n^{-1/2} \left(\sqrt{3} - \frac{R_1^* x^*}{2} \right),$$

$$B_4 = \varphi_n^{-3/2} \left(-\frac{\sqrt{3}}{2} R_1^* R^* - \frac{\sqrt{3}}{2} + \frac{3}{4} R_1^* x^* \right),$$

$$B_5 = \varphi_n^{-5/2} \frac{3\sqrt{3}}{4} \left(R_1^* R^* + \frac{1}{2} - \frac{5}{4\sqrt{3}} R_1^* x^* \right),$$

$$B_6 = \varphi_n^{-1} R_1^* \left(\frac{3}{8} x^* R_1^* - \frac{\sqrt{3}}{2} \right),$$

$$B_7 = \varphi_n^{-2} \frac{3\sqrt{3}}{4} R_1^* \left(1 + \frac{R_1^* R^*}{2} - \frac{5R_1^* x^*}{4\sqrt{3}} \right),$$

$$B_8 = \frac{\varphi_n^{-3} 15\sqrt{3} R_1^*}{16} \left(\frac{7x^* R_1^*}{4\sqrt{3}} - 1 + R^* R_1^* \right).$$

The coefficients A_i are written in the form

$$A_1 = \frac{n}{2} r_1 - \frac{2r_1 \bar{\alpha}}{(y^*)^2}, \quad A_2 = \frac{n}{2} r_2 - \frac{n}{4} r_1^2 + \frac{\bar{\alpha}(3r_1^2 - 2r_2)}{(y^*)^2},$$

$$A_3 = -\frac{n}{2} U_n(x^*), \quad A_4 = -\frac{n}{4} U'(x^*),$$

where the following definitions are introduced:

$$\bar{\alpha} = \frac{(5n+16)n}{8} - \frac{n/2(n/2+1)}{2}, \quad U_n'(x^*) = \left(\frac{dU_n(x_l)}{dx_l} \right)_{x^*},$$

$$r_1 = \bar{d}_1 - \frac{q_1}{2}, \quad r_2 = \frac{1}{2} \bar{d}_2 - \frac{1}{2} \bar{d}_1 q_1 + \frac{3}{8} q_1^2 - \frac{1}{4} q_2,$$

$$\bar{d}_i = \frac{1}{U_n(x^*)} \left(\frac{d^i U_n(x_l)}{dx_l^i} \right)_{x^*}, \quad q_i = \frac{1}{\varphi_n(x^*)} \left(\frac{d^i \varphi_n(x_l)}{dx_l^i} \right)_{x^*}.$$

APPENDIX G

The contribution of the IGR to the free energy can be written in the form

$$F_{\text{IGR}}^- = -kTN' s^{-d(m_\tau+1)} \ln[2^{n/2} Q(P_{m_\tau})] - kT \ln Z_{m_\tau+1}, \quad (\text{G1})$$

where

$$Z_{m_\tau+1} = \int \exp \left[-\frac{1}{2} \sum_{k \leq B_{m_\tau+1}} d^{(n, m_\tau+1)}(k) \boldsymbol{\rho}_k \boldsymbol{\rho}_{-k} - \frac{a_4^{(n, m_\tau+1)}}{4! N_{m_\tau+1}} \right. \\ \left. \times \sum_{\substack{\mathbf{k}_1, \dots, \mathbf{k}_4 \\ k_i \leq B_{m_\tau+1}}} \boldsymbol{\rho}_{\mathbf{k}_1} \cdots \boldsymbol{\rho}_{\mathbf{k}_4} \delta_{\mathbf{k}_1 + \dots + \mathbf{k}_4} \right] (d\boldsymbol{\rho})^{N_{m_\tau+1}},$$

$$Q(P_{m_\tau}) = (2\pi)^{-n/2} \left\{ \frac{n+2}{3} s^d \frac{a_4^{(n, m_\tau-1)}}{\varphi_n(x_{m_\tau-1})} \right\}^{n/4} \\ \times U \left(\frac{n-1}{2}, y_{m_\tau-1} \right) \exp \left(\frac{y_{m_\tau-1}^2}{4} \right). \quad (\text{G2})$$

After the separation of the ordering free energy in $Z_{m_\tau+1}$ the coefficient at the square term becomes positive. It allows us to use the Gaussian measure density as basic under the integration of $Z_{m_\tau+1}$ by the variables $\boldsymbol{\rho}_k$ with $\mathbf{k} \neq 0$. After the integration for $Z_{m_\tau+1}$ we obtain

$$Z_{m_\tau+1} = e^{-\beta F_{m_\tau+1}} \int \exp \left(\beta \sqrt{N} \mu_B \mathbf{H} \boldsymbol{\rho}_0 + B \boldsymbol{\rho}_0^2 - \frac{G}{N} \boldsymbol{\rho}_0^4 \right) d\boldsymbol{\rho}_0. \quad (\text{G3})$$

The value $F_{m_\tau+1}$ corresponds to the contribution of the LWF region of the spin moment density (i.e., from the variables $\boldsymbol{\rho}_k$ with $k \rightarrow 0$, but $k \neq 0$) to the free energy of the system

$$-\beta F_{m_\tau+1} = N_{m_\tau+1} \left\{ \frac{3}{2} |d^{(n, m_\tau+1)}(0)| I_1 - \frac{n}{2} \frac{1}{N_{m_\tau+1}} \right. \\ \times \sum'_{k \leq B_{m_\tau+1}} \ln \left(\frac{\overline{d_2(k)}}{\pi} \right) - \frac{a_4^{(n, m_\tau+1)} I_1^2}{8} \\ + \frac{a_4^{2(n, m_\tau+1)}}{48} (I_4 + 3I_1^2 I_2) + \frac{9}{4} |d^{(n, m_\tau)}(0)|^2 I_2 \\ \left. - \frac{b^{2(n, m_\tau)}}{8} I_1 I_2 \right\}. \quad (\text{G4})$$

For $I_i (i=1, \dots, 4)$ the next relations take place:

$$\begin{aligned}
I_1 &= n\bar{\alpha}_1 \frac{s^{2(m_\tau)}}{\beta\Phi(0)}, \quad \bar{\alpha}_1 = \frac{L(x)}{2\bar{r}_{m_\tau}}, \\
I_2 &= n^2\bar{\alpha}_2 \left[\frac{s^{2(m_\tau)}}{\beta\Phi(0)} \right]^2, \quad \bar{\alpha}_2 = [\bar{\alpha}_1^2 + 6e_1^2(1 + e_2^2)], \\
I_3 &= n^3\bar{\alpha}_3 \left[\frac{s^{2(m_\tau)}}{\beta\Phi(0)} \right]^3, \quad \bar{\alpha}_3 = \bar{\alpha}_1^3 + 6e_1^3 \left(1 + \frac{e_2^3}{\sqrt{2}} \right), \\
I_4 &= n^4\bar{\alpha}_4 \left[\frac{s^{2(m_\tau)}}{\beta\Phi(0)} \right]^4, \quad \bar{\alpha}_4 = \bar{\alpha}_1^4 + 6e_1^4 \left(1 + \frac{e_2^4}{\sqrt{2}} \right). \quad (G5)
\end{aligned}$$

It should be mentioned that

$$\begin{aligned}
e_1 &= \frac{15}{\pi^2[3 + 10\bar{r}_{m_\tau}]}, \\
e_2 &= \frac{1}{2\pi} \{ \sin(\pi\sqrt{2}) - \pi\sqrt{2} \cos(\pi\sqrt{2}) \}. \quad (G6)
\end{aligned}$$

The variable ρ_0 in Eq. (G3) is connected with order parameter. Its mean value is proportional to the spin density of the system. For the values B and G we obtain

$$\begin{aligned}
B &= |\tau|^{2\nu} B_0, \quad B_0 = \beta\Phi(0)B^{(0)}, \\
B^{(0)} &= c_{\nu n}^2 \frac{1 + \delta}{2} B_1^{(0)}, \\
B_1^{(0)} &= 1 - \alpha_{11}\bar{u}_{m_\tau} + \alpha_{22} \frac{\bar{u}_{m_\tau}^2}{2\bar{r}_{m_\tau}}, \quad (G7)
\end{aligned}$$

$$\begin{aligned}
G &= |\tau|^\nu G_0, \quad G_0 = [\beta\Phi(0)]^2 G^{(0)}, \\
G^{(0)} &= c_{\nu} \frac{s_0^3}{24} \bar{u}_{m_\tau} g^{(0)}, \quad g^{(0)} = 1 - \frac{3}{2} n^2 \bar{\alpha}_2 \bar{u}_{m_\tau}, \quad (G8)
\end{aligned}$$

where

$$\alpha_{11} = \frac{n}{2} \frac{\bar{\alpha}_1}{\bar{r}_{m_\tau}} + \frac{3}{2} n^2 \bar{\alpha}_2, \quad \alpha_{22} = n^3 \left\{ \frac{\bar{\alpha}_1 \bar{\alpha}_2}{2} + \frac{\bar{\alpha}_3}{3} \right\}. \quad (G9)$$

The variable ρ_0 is a macroscopic value, so we can accept that

$$\rho_0 = \sqrt{N} \rho. \quad (G10)$$

It makes it possible for us to apply the saddle-point method for the calculation of $Z_{m_\tau+1}$ in Eq. (G3). As a result we find

$$Z_{m_\tau+1} = \sqrt{\frac{2\pi}{E_0''(\langle \rho \rangle)}} \exp\{-\beta F_{m_\tau+1} - N E_0(\langle \rho \rangle)\}, \quad (G11)$$

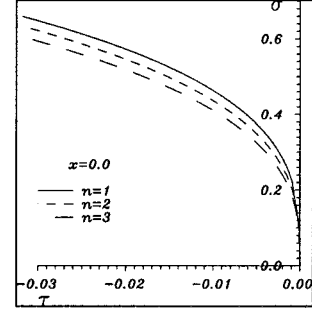


FIG. 5. The temperature dependence of the order parameter for different values of the n -component number of the model in the case $\mathbf{H}=0$ (with $b=c$).

where $\langle \rho \rangle$ is an extreme point of expression

$$E_0(\rho) = G\rho^4 - B\rho^2 - \beta\mu\mathbf{H}\rho, \quad (G12)$$

which arises in Eq. (G3) with the change of variables (G10). The variable ρ_0 corresponds to the operator $\hat{\rho}_0 = (1/\sqrt{N})\sum_i \hat{\sigma}_i$, the mean value of which is connected with the equilibrium value of the order parameter σ . In the case of $\mathbf{H}=0$ we find for $\langle \rho \rangle$ the following solutions:

$$\langle \rho_{1,2} \rangle = \pm \sqrt{\frac{B}{2G}}, \quad \langle \rho_3 \rangle = 0. \quad (G13)$$

The solutions $\langle \rho_{1,2} \rangle$ and $\langle \rho_3 \rangle$ correspond to extreme value of the functional $E_0(\rho)$ (G12). The presence of the nonzero mean spin moment at the temperatures $T < T_c$ testifies to the appearance of spontaneous magnetization in the system in the absence of the external field. Figure 5 shows the temperature dependence of the order parameter σ for different values of n component number of the model in the absence of the external magnetic field.

In accordance with the above for $E_0(\langle \rho \rangle)$ we obtain

$$E_0(\langle \rho \rangle) = -\frac{B^2}{4G} = E_0' |\tau|^{3\nu}, \quad (G14)$$

where

$$E_0' = \frac{3}{2} \frac{\bar{r}_{m_\tau}^2 (B_1^{(0)})^2}{\bar{u}_{m_\tau} s_0^3 g^{(0)}}. \quad (G15)$$

All this enables us to obtain the explicit analytical expression for the IGR free energy. Summarizing the expression (G4) by the variables $k \leq B_{m_\tau}$ ($k \neq 0$) and considering the contribution of the ρ_0 variables in accordance with Eqs. (G11)–(G15), for F_{IGR}^- we obtain the expression (3.14).

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