Study of the critical behaviour of three-dimensional Ising-like systems on the basis of the ρ^6 model with allowance for microscopic parameters: I. High-temperature region

2002 J. Phys.: Condens. Matter 14 10113

(http://iopscience.iop.org/0953-8984/14/43/310)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **14** (2002) 10113–10129 PII: S0953-8984(02)52286-4

Study of the critical behaviour of three-dimensional Ising-like systems on the basis of the ρ^6 model with allowance for microscopic parameters: I. High-temperature region

I R Yukhnovskii, I V Pylyuk[1] and M P Kozlovskii

Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, 1 Svientsitskii Str., Lviv 79011, Ukraine

E-mail: piv@icmp.lviv.ua

Received 13 August 2002
Published 18 October 2002
Online at stacks.iop.org/JPhysCM/14/10113

Abstract

The behaviour of a three-dimensional Ising-like system at temperatures above the critical value of T_c is studied in the approximation of the sextic distribution for modes of spin density oscillations (ρ^6 model). The original collective variables method is developed in this higher non-Gaussian approximation for calculating the thermodynamic characteristics of the system near T_c taking into account the first confluent correction. The calculations are illustrated by an example of a simple cubic lattice and an exponentially decreasing interaction potential. The main distinctive feature of the method is the separate inclusion of the contributions to the thermodynamic functions from the short-wave and long-wave spin density oscillation modes. The dependences of the phase transition temperature, leading critical amplitudes, and correction-to-scaling amplitudes for the specific heat and susceptibility on the microscopic parameters of the system are investigated.

1. Introduction

The description of phase transitions and critical phenomena, i.e., the construction of a microscopic theory of phase transitions, is one of the central problems in statistical physics. Persistent scientific interest in phase transitions is stimulated by the exceptional significance of these phenomena for modern technology, their complexity near the phase transition point, and the difficulties of their theoretical and experimental investigation in view of the increasing role of large-scale fluctuations and large relaxation times. Comprehensive and intensive studies of phase transitions have made it possible to formulate new concepts revealing the essence of

[1] Author to whom any correspondence should be addressed.

0953-8984/02/4310113+17$30.00

critical phenomena and to develop a powerful mathematical apparatus for their description. These questions have been considered in a number of books (see, for example, [1–4]) and articles (for example, [5–8]). In most papers devoted to the theory of phase transitions, attention is primarily paid to determining the universality class of the systems, investigating symmetry properties irrespective of the seed parameters in the initial Hamiltonian, solving recurrence relations (RR), and calculating critical exponents. Important experimental results are obtained. Universal ratios and combinations of critical amplitudes for thermodynamic characteristics are calculated for spin systems, in particular, for the three-dimensional (3D) Ising model. The problem of the dependence of critical amplitudes on the microscopic parameters of the system required a consistent analysis and could be solved successfully together with the main problem in the theory of phase transitions, i.e., the derivation of explicit expressions for thermodynamic characteristics of the system near the phase transition point as functions of temperature and microscopic parameters. Considerable progress in the solution of this problem was made by using the method of collective variables (CV) generalized by Yukhnovskii [9–12] to the case of spin systems. The term 'CV' is applied to a special class of variables specific to each individual physical system. The set of CV contains variables associated with order parameters. For this reason, the phase space of CV is the most natural one to use for describing a phase transition. For magnetic systems, the CV ρ_k are the variables associated with modes of spin moment density oscillations, while the order parameter is associated with the variable ρ_0, in which the subscript '0' corresponds to the peak of the Fourier transform of the interaction potential. The recent results from investigating the critical behaviour of 3D Ising-like systems using the CV method are presented in [13].

This paper supplements the previous study [14] based on the CV method. In [14], the thermodynamic functions of the classical n-vector 3D magnetic model near T_c were calculated in the approximation of the quartic distribution for the spin density oscillation modes (ρ^4 model) without taking into account confluent corrections (corrections to scaling). In the present publication, the results of calculating the thermodynamic characteristics of a 3D Ising ferromagnet are obtained using the higher non-Gaussian distribution (ρ^6 model). In the process of determining these characteristics, a technique for calculating correction-to-scaling terms is elaborated. The employment of the ρ^6 model for the investigation of the phase transition by the CV method gives a more precise definition of the calculation results and provides the basis for quantitative analysis of the critical behaviour of 3D Ising-like systems including the nonuniversal characteristics. On the other hand, the dependence of nonuniversal quantities on the microscopic parameters of the system has not been studied deeply enough so far. Such a study is our aim in this research. The results obtained can be used for interpreting experimental results concerning the behaviour of real materials in the vicinity of the second-order phase transition point, and the computational technique proposed here for thermodynamic characteristics can be used for calculating their thermodynamic functions in the critical region.

2. Method of the calculation

We consider a 3D Ising-like system on a simple cubic lattice with period c. The Hamiltonian of such a system has the form

$$H = -\tfrac{1}{2}\sum_{j,l}\Phi(|\boldsymbol{j}-\boldsymbol{l}|)\sigma_j\sigma_l \tag{1}$$

where $\Phi(|\boldsymbol{j}-\boldsymbol{l}|)$ is the potential of interaction of particles at sites $\boldsymbol{j}$ and $\boldsymbol{l}$, and σ_j is the operator of the z-component of spin at the $\boldsymbol{j}$th site, having two eigenvalues +1 and −1. The interaction

potential is an exponentially decreasing function

$$\Phi(r_{jl}) = A \exp\left(-\frac{r_{jl}}{b}\right). \tag{2}$$

Here A is a constant, r_{jl} is the interparticle distance, and b is the radius of effective interaction. The approximation for the Fourier transform of the interaction potential is taken in the form [11]

$$\tilde{\Phi}(k) = \begin{cases} \tilde{\Phi}(0)(1 - 2b^2k^2) & k \leqslant B' \\ 0 & B' < k \leqslant B \end{cases} \tag{3}$$

where B is the boundary of the Brillouin half-zone ($B = \pi/c$), $B' = (b\sqrt{2})^{-1}$, $\tilde{\Phi}(0) = 8\pi A(b/c)^3$.

We shall use here the method of CV [11], which allows us to calculate approximately the expression for the partition function and to obtain complete expressions for the thermodynamic functions near the phase transition temperature T_c in addition to universal quantities (critical exponents).

In the CV representation for the partition function of the 3D Ising model, we have

$$Z = \int \exp\left[\tfrac{1}{2}\sum_{\boldsymbol{k}} \beta\tilde{\Phi}(k)\rho_{\boldsymbol{k}}\rho_{-\boldsymbol{k}}\right] J(\rho)\,(\mathrm{d}\rho)^N. \tag{4}$$

Here the summation over the wavevectors $\boldsymbol{k}$ is carried out within the first Brillouin zone, $\beta = 1/(kT)$ is the inverse temperature, the CV $\rho_{\boldsymbol{k}}$ are introduced by means of the functional representation for operators of spin density oscillation modes $\hat{\rho}_{\boldsymbol{k}} = (\sqrt{N})^{-1}\sum_l \sigma_l \exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{l})$,

$$J(\rho) = 2^N \int \exp\left[2\pi\mathrm{i}\sum_{\boldsymbol{k}} \omega_{\boldsymbol{k}}\rho_{\boldsymbol{k}} + \sum_{n=1}^{\infty}(2\pi\mathrm{i})^{2n}N^{1-n} \times \frac{\mathcal{M}_{2n}}{(2n)!}\sum_{\boldsymbol{k}_1,\ldots,\boldsymbol{k}_{2n}} \omega_{\boldsymbol{k}_1}\cdots\omega_{\boldsymbol{k}_{2n}}\delta_{\boldsymbol{k}_1+\cdots+\boldsymbol{k}_{2n}}\right](\mathrm{d}\omega)^N \tag{5}$$

is the Jacobian of transition from the set of N spin variables σ_l to the set of CV $\rho_{\boldsymbol{k}}$, and $\delta_{\boldsymbol{k}_1+\cdots+\boldsymbol{k}_{2n}}$ is the Kronecker symbol. The variables $\omega_{\boldsymbol{k}}$ are conjugate to $\rho_{\boldsymbol{k}}$, and the cumulants $\mathcal{M}_{2n}$ assume constant values (see [11]). The expression for the partition function (4) cannot be calculated exactly due to the presence of an infinitely large number of terms in the exponent (5). For this reason, approximations limiting the number of terms in the exponent of the integrand in (5) are used. A certain approximation of the integrand in the expression for $J(\rho)$ used when calculating the explicit form of the Jacobian of the transition determines the choice of the model (models ρ^4, ρ^6, etc). For $n = 1$, we obtain the Gaussian approximation. It leads to classical values of critical exponents. An important condition in describing the critical properties of the Ising model is the use of non-Gaussian densities of measures. The approximation corresponding to $n = 2$ is based on a quartic density of measure (the ρ^4 model). This approximation is used for calculating the critical exponents of thermodynamic characteristics, complete expressions for these characteristics taking into account confluent corrections, and for analysing the relation for critical amplitudes (see, for example, [15–17]). In view of the approximate calculation of the partition function, confined to the ρ^4 model, the results obtained (critical exponents, amplitudes, and thermodynamic functions) contain a certain dependence on the renormalization group (RG) parameter s. This dependence becomes much weaker as the form of the non-Gaussian density of measure becomes more complicated (transition to the more complicated models ρ^6 ($n = 3$; see (5)), ρ^8, and ρ^{10}). This is confirmed by an analysis of the behaviour of the critical exponent of the correlation length ν for the models ρ^{2m} ($m = 3, 4, 5$) [18–20] as well as by a direct comparison of the curves describing the

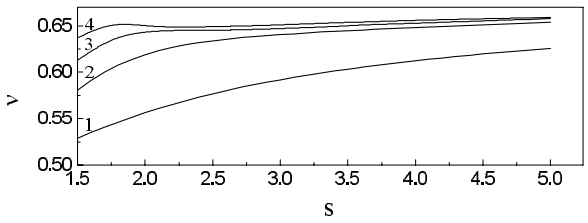

Figure 1. Evolution of the critical exponent of the correlation length ν with increasing parameter of division of the CV phase space into layers s. Curves 1, 2, 3 and 4 correspond to the ρ^4, ρ^6, ρ^8 and ρ^{10} models, respectively.

temperature dependences of the thermodynamic characteristics calculated for the models ρ^4 and ρ^6 at different values of the parameter s [21, 22]. For each of the ρ^{2m} models, there exists a preferred value of the parameter $s = s^*$ ($s^* = 3.5862$ for the ρ^4 model, $s^* = 2.7349$ for the ρ^6 model, $s^* = 2.6511$ for the ρ^8 model, and $s^* = 2.6108$ for the ρ^{10} model) nullifying the average value of the coefficient in the term with the second power in the effective density of measure at a fixed point. The values of s close to s^* are optimal for the given method of calculations. The difference form of the RR between the coefficients of effective non-Gaussian densities of measures (expansions for the functions appearing in these relations) operates successfully just in this region of s.

It was established [18–20] that as the form of the density of measure becomes more complicated, the dependence of the critical exponent ν on the RG parameter s becomes gradually weaker, and, starting from the sextic density of measure, the value of the exponent ν, having a tendency to saturation with increasing m (which characterizes the order of the ρ^{2m} model or determines the summation limit in formula (5), $m = 2, 3, 4, 5$), changes insignificantly (see figures 1 and 2). The point $s \approx s^*$ in figure 1 corresponds to the beginning of the $\nu(s)$ curve stabilization for each of the ρ^{2m} models. The value of the exponent ν in figure 2 is calculated for $s = s^*$. The ρ^2 model (Gaussian approximation) leads to the classical value $\nu = 0.500$. In the case when $s = s^*$, we have $\nu = 0.605$ for the ρ^4 model and $\nu = 0.637$ for the ρ^6 model. The value of the critical exponent ν for the ρ^6 model agrees more closely with other authors' data for the 3D Ising model than the estimate in the ρ^4 model approximation (e.g., with the recent values determined using the fixed-dimension perturbative RG ($\nu = 0.6304(13)$ [23]), high-temperature series ($\nu = 0.630\,02(23)$ [8]), and Monte Carlo simulations ($\nu = 0.6296(7)$ [24])). The Ising model corresponds to the ρ^{2m} model approximation, where the order of the model $2m \geqslant 4$. The ρ^4 model allows us to go beyond the classical analysis and to describe all qualitative aspects of the second-order phase transition. As is seen from figures 1 and 2, the critical behaviour of a 3D Ising-like system within the CV method can be described quantitatively at $2m \geqslant 6$, and, in particular, at $2m = 6$.

The correctness of the choice of the ρ^6 model for investigations is confirmed in [25, 26], where the effective potential is studied for the scalar field theory in three dimensions in the symmetric and spontaneously broken phases, respectively. In this case, probability distributions of average magnetization in the 3D Ising model in an external field obtained with the help of the Monte Carlo method were used. Tsypin [25, 26] proved that the term with the sixth power of the variable in the effective potential plays an important role.

In this paper, the ρ^6 model is used for developing the method of calculation of expressions for thermodynamic functions of the 3D Ising system taking into account the terms determining the correction to scaling. The calculations are made for above the phase transition temperature T_c (high-temperature region). The expressions obtained for the leading critical amplitudes and

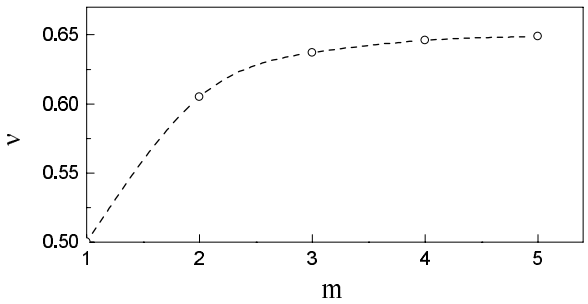

Figure 2. Saturation of the critical exponent ν with increasing order of the ρ^{2m} model.

Table 1. Values of coefficients a'_{2l} for various values of b.

b	b_{I}	b_{II}	b_{III}	c	$2c$	$5c$	$7c$
a'_0	−1.0196	−0.9863	−0.9764	−0.9218	−0.9193	−0.9190	−0.9189
a'_2	0.7023	0.7820	0.8083	0.9887	0.9986	0.9999	1.0000
a'_4	0.2212	0.2163	0.2086	0.0220	0.0028	0.0002	0.0000
a'_6	0.4379	0.3895	0.3547	0.0031	0.0000	0.0000	0.0000

the amplitudes of the first confluent correction make it possible to analyse their dependence on microscopic parameters of the system (the range b of potential and the lattice constant c).

We shall proceed from the expression for the partition function in the approximation of the ρ^6 model. Putting $n = 3$ in (5) and carrying out integration in (4) with respect to the variables ρ_k and ω_k with indices $B' < k \leqslant B$, followed by integration with respect to the N' variables ω_k, we obtain

$$Z = 2^N 2^{(N'-1)/2} \mathrm{e}^{a'_0 N'} \int \exp\Bigg[-\frac{1}{2} \sum_{k \leqslant B'} d'(k) \rho_k \rho_{-k} - \sum_{l=2}^{3} \frac{a'_{2l}}{(2l)!(N')^{l-1}} \times \sum_{k_1,\ldots,k_{2l} \leqslant B'} \rho_{k_1} \cdots \rho_{k_{2l}} \delta_{k_1+\cdots+k_{2l}} \Bigg] (\mathrm{d}\rho)^{N'}. \tag{6}$$

Here $N' = N s_0^{-3}$, $s_0 = B/B' = \pi\sqrt{2}b/c$, and

$$d'(k) = a'_2 - \beta\tilde{\Phi}(k). \tag{7}$$

The coefficients a'_{2l} are defined as

$$\begin{aligned} a'_0 &= \ln Q(\mathcal{M}) \qquad Q(\mathcal{M}) = (12 s_0^3)^{1/4} \pi^{-1} I_0(\eta', \xi') \\ a'_2 &= (12 s_0^3)^{1/2} F_2(\eta', \xi') \\ a'_4 &= 12 s_0^3 C(\eta', \xi') \\ a'_6 &= (12 s_0^3)^{3/2} N(\eta', \xi') \end{aligned} \tag{8}$$

and are functions of s_0, i.e., of the ratio b/c (see table 1). In this expressions, the role of the arguments is played by the quantities

$$\eta' = \sqrt{3} s_0^{3/2} \qquad \xi' = \frac{8\sqrt{3}}{15 s_0^{3/2}}. \tag{9}$$

The special functions $C(\eta', \xi')$ and $N(\eta', \xi')$ have the forms

$$\begin{aligned} C(\eta', \xi') &= -F_4(\eta', \xi') + 3F_2^2(\eta', \xi') \\ N(\eta', \xi') &= F_6(\eta', \xi') - 15F_4(\eta', \xi')F_2(\eta', \xi') + 30F_2^3(\eta', \xi') \end{aligned} \tag{10}$$

where

$$F_{2l}(\eta', \xi') = I_{2l}(\eta', \xi')/I_0(\eta', \xi')$$
$$I_{2l}(\eta', \xi') = \int_0^\infty t^{2l} \exp(-\eta' t^2 - t^4 - \xi' t^6)\, \mathrm{d}t. \tag{11}$$

The value of $b = b_{\mathrm{I}} = c/(2\sqrt{3})$ in table 1 corresponds to the interaction between nearest neighbours, $b = b_{\mathrm{II}} = 0.3379c$ to the interaction between the nearest and next-nearest neighbours, and $b = b_{\mathrm{III}} = 0.3584c$ to the nearest, next-nearest, and third neighbours [27]. At these values of b and small values of the wavevectors $\boldsymbol{k}$, the parabolic approximation of the Fourier transform of the exponentially decreasing interaction potential corresponds to the analogous approximation of the Fourier transform for the interaction potentials of the above-mentioned neighbours.

We shall use the method of 'layer-by-layer' integration of (6) with respect to variables $\rho_{\boldsymbol{k}}$ proposed by Yukhnovskii [10]. The integration begins from the variables $\rho_{\boldsymbol{k}}$ with a large value of k (of the order of the Brillouin half-zone boundary) and terminates at $\rho_{\boldsymbol{k}}$ with $k \to 0$. For this purpose, we divide the phase space of the CV $\rho_{\boldsymbol{k}}$ into layers with the division parameter s. In each nth layer (corresponding to the region of wavevectors $B_{n+1} < k \leqslant B_n$, $B_{n+1} = B_n/s$, $s > 1$), the Fourier transform of the potential $\tilde{\Phi}(k)$ is replaced by its average value (the arithmetic mean in the case given). To simplify the presentation, we assume that the correction for the potential averaging is zero, although it can be taken into account if necessary [11]. Including this correction leads to a nonzero value of the critical exponent η characterizing the behaviour of the pair correlation function for $T = T_c$. The formal part of the procedure has already been presented for the simpler ρ^4 model in [14]. In the case of the ρ^6 model, we exploit more complicated special functions of two arguments than the parabolic cylinder functions for the ρ^4 model. After the integration over $n+1$ layers of the CV space, we obtain

$$Z = 2^N 2^{(N_{n+1}-1)/2} Q_0 Q_1 \cdots Q_n [Q(P_n)]^{N_{n+1}} \int \mathcal{W}_6^{(n+1)}(\rho)\, (\mathrm{d}\rho)^{N_{n+1}}. \tag{12}$$

Here $N_{n+1} = N' s^{-3(n+1)}$ and

$$Q_0 = [\mathrm{e}^{a_0'} Q(d)]^{N'} \qquad Q_1 = [Q(P)Q(d_1)]^{N_1} \qquad \cdots$$
$$Q_n = [Q(P_{n-1})Q(d_n)]^{N_n}$$
$$Q(d_n) = 2(24/a_4^{(n)})^{1/4} I_0(h_n, \alpha_n) \tag{13}$$
$$Q(P_n) = \pi^{-1}(s^3 a_4^{(n)}/C(h_n, \alpha_n))^{1/4} I_0(\eta_n, \xi_n).$$

The basic arguments

$$h_n = d_n(B_{n+1}, B_n)(6/a_4^{(n)})^{1/2} \qquad \alpha_n = \frac{\sqrt{6}}{15} a_6^{(n)}/(a_4^{(n)})^{3/2} \tag{14}$$

are determined by the mean value of the coefficient $d_n(k)$ in the nth layer of the phase space of CV, i.e., by $d_n(B_{n+1}, B_n)$ as well as the quantities $a_4^{(n)}$ and $a_6^{(n)}$. The effective sextic density of measure of the $(n+1)$th block structure $\mathcal{W}_6^{(n+1)}(\rho)$ has the form

$$\mathcal{W}_6^{(n+1)}(\rho) = \exp\Bigg[-\frac{1}{2}\sum_{k \leqslant B_{n+1}} d_{n+1}(k)\rho_{\boldsymbol{k}}\rho_{-\boldsymbol{k}}$$
$$- \sum_{l=2}^{3} \frac{a_{2l}^{(n+1)}}{(2l)!\, N_{n+1}^{l-1}} \sum_{k_1, \ldots, k_{2l} \leqslant B_{n+1}} \rho_{\boldsymbol{k}_1} \cdots \rho_{\boldsymbol{k}_{2l}} \delta_{\boldsymbol{k}_1 + \cdots + \boldsymbol{k}_{2l}} \Bigg]. \tag{15}$$

Table 2. Quantities f_0, φ_0, and ψ_0 (which characterize the coordinates of the fixed point) and eigenvalues E_l ($l = 1, 2, 3$) of the RG transformation matrix for some optimal values of the RG parameter s.

s	f_0	φ_0	ψ_0	E_1	E_2	E_3
2.0000	0.4212	0.3620	0.3805	3.0649	0.4811	0.0035
2.7349	0.5668	0.5647	0.4870	4.8468	0.4367	0.0032
3.0000	0.6166	0.6426	0.5178	5.5581	0.4221	0.0030

Here $B_{n+1} = B's^{-(n+1)}$, $d_{n+1}(k) = a_2^{(n+1)} - \beta\tilde{\Phi}(k)$, $a_{2l}^{(n+1)}$ are renormalized values of the coefficients a'_{2l} after integration over $n+1$ layers of the phase space of CV. The intermediate variables η_n, ξ_n are functions of h_n and α_n and are defined as

$$\begin{aligned} \eta_n &= (6s^3)^{1/2} F_2(h_n, \alpha_n)[C(h_n, \alpha_n)]^{-1/2} \\ \xi_n &= \frac{\sqrt{6}}{15} s^{-3/2} N(h_n, \alpha_n)[C(h_n, \alpha_n)]^{-3/2} \end{aligned} \tag{16}$$

where the forms of the special functions $C(h_n, \alpha_n)$ and $N(h_n, \alpha_n)$ are given by (10). The coefficients $d_n(B_{n+1}, B_n)$, $a_4^{(n)}$, and $a_6^{(n)}$ are connected with the coefficients for the $(n+1)$th layer through the RR [19, 28] whose solutions [28–30]

$$\begin{aligned} r_n &= r^{(0)} + c_1 E_1^n + c_2 w_{12}^{(0)} (u^{(0)})^{-1/2} E_2^n + c_3 w_{13}^{(0)} (u^{(0)})^{-1} E_3^n \\ u_n &= u^{(0)} + c_1 w_{21}^{(0)} (u^{(0)})^{1/2} E_1^n + c_2 E_2^n + c_3 w_{23}^{(0)} (u^{(0)})^{-1/2} E_3^n \\ w_n &= w^{(0)} + c_1 w_{31}^{(0)} u^{(0)} E_1^n + c_2 w_{32}^{(0)} (u^{(0)})^{1/2} E_2^n + c_3 E_3^n \end{aligned} \tag{17}$$

are used for calculating the free energy of the system. Here $r_n = s^{2n} d_n(0)$, $u_n = s^{4n} a_4^{(n)}$, $w_n = s^{6n} a_6^{(n)}$. The quantities $r^{(0)} = -f_0 \beta\tilde{\Phi}(0)$, $u^{(0)} = \varphi_0(\beta\tilde{\Phi}(0))^2$, $w^{(0)} = \psi_0(\beta\tilde{\Phi}(0))^3$ are the fixed-point coordinates. The temperature-independent quantities $w_{il}^{(0)}$ determine the eigenvectors of the RG linear transformation matrix. The above solutions (17) naturally have the general form of the RG solutions. A peculiar feature of the solutions is the presence of explicit expressions for the coefficients c_l. The coefficients $c_1 = \tilde{c}_1 \beta\tilde{\Phi}(0)\tau$, $c_2 = c_{20}(\beta\tilde{\Phi}(0))^2$, $c_3 = c_{30}(\beta\tilde{\Phi}(0))^3$, where $\tilde{c}_1 = \tilde{c}_1^{(0)} + \tilde{c}_1^{(1)}\tau$, $c_{20} = c_{20}^{(0)} + c_{20}^{(1)}\tau + c_{20}^{(2)}\tau^2$, $c_{30} = c_{30}^{(0)} + c_{30}^{(1)}\tau + c_{30}^{(2)}\tau^2$, $\tau = (T - T_c)/T_c$, are determined by the eigenvalues E_l and elements of the RG transformation matrix, coordinates of the fixed point, and initial coefficients a'_{2l}. The quantities f_0, φ_0, ψ_0 and the eigenvalues E_l are given in table 2 for some optimal values of s. For $s = 2.7349$, the value of the basic variable at a fixed point satisfies the condition $h^{(0)} \approx 0$ (see, for example, [13]).

The basic idea of the calculation of explicit expressions for free energy and other thermodynamic functions of the system near T_c on a microscopic level lies in the separate inclusion of contributions from short-wave and long-wave modes of spin moment density oscillations [11, 14, 31]. Short-wave modes are characterized by a RG symmetry and are described by a non-Gaussian density of measure. In this case, the RG method is used (see, for example, [32]). The inclusion of short-wave oscillation modes leads to a renormalization of the dispersion of the distribution describing long-wave modes. The way in which the contribution from long-wave modes of oscillations to the free energy of the system is taken into account differs qualitatively from the method of calculating the short-wave part of the partition function. The calculation of this contribution is based on the use of the Gaussian density of measure as the basis density. We have developed a direct method of calculation with the results obtained by taking into account the short-wave modes as initial parameters.

Calculating separately the contributions F_{CR} and F_{LGR} to the free energy from short-wave (the region of the critical regime (CR)) and long-wave (the region of the limiting Gaussian regime (LGR)) modes of spin moment density oscillations at $T > T_c$, we can obtain the complete expression for the free energy of the system:

$$F = F_0 + F_{CR} + F_{LGR}. \tag{18}$$

Here $F_0 = -kTN \ln 2$ is the free energy of N noninteracting spins. Let us calculate the contributions F_{CR} and F_{LGR}.

3. Thermodynamic functions of the system in the critical regime region

It is convenient to write the partition function of the model in the form [21]

$$Z = 2^N Z_{CR} Z_{LGR} \tag{19}$$

where the first factor corresponds to noninteracting spins. The quantity Z_{CR} describes the contribution of short-wave fluctuations of $\rho_{\boldsymbol{k}}$ with $k \in [B_{m_\tau}, B']$ (the CR region). The number m_τ of the layer in the CV space appearing in the expression $B_{m_\tau} = B's^{-m_\tau}$ determines the point of exit of the system from the CR at $T > T_c$. The quantity m_τ can be obtained from the condition [29, 30]

$$\frac{r_{m_\tau+1} - r^{(0)}}{r^{(0)}} = -\delta \tag{20}$$

where δ is a constant ($\delta \leqslant 1$), $r^{(0)}$ is a coordinate of the fixed point, and r_n characterizes the coefficient of the sextic density of measure of the nth block structure in the term with the second power of the variable and is determined with the help of solutions of RR (17). In our numerical calculations, we shall put $\delta = 1$. In this case, $r_{m_\tau+1} = 0$ or $d_{m_\tau+1}(0) = r_{m_\tau+1}s^{-2(m_\tau+1)} = 0$ and the curves $d_n(k)$ are situated above the abscissa axis for all $n > m_\tau$. The factor Z_{LGR} in (19) contains contributions from long-wave fluctuations with $k \in [0, B_{m_\tau})$ and corresponds to the LGR.

The calculation of the expression describing the contribution from short-wave modes of spin moment density oscillations to the free energy involves the summation of partial free energies over the layers of the phase space of CV up to the point at which the system leaves the CR region. The main task is to obtain an explicit dependence on the number of the layer. For this purpose, the solutions of RR (17) are used.

A typical feature of the solutions of RR is a specific temperature dependence of the coefficient c_1 ($c_1 \sim \tau$). Taking into account the larger eigenvalue ($E_1 > 1$) of the RG linear transformation matrix, we can describe the main singularity for specific heat near T_c. Smaller eigenvalues ($E_2 < 1$ and $E_3 < 1$) are responsible for the emergence of corrections to scaling. Equations (17) are valid for temperatures close to T_c and, in particular, at $T = T_c$. In this case, we encounter a special behaviour related to the approach of the coefficients r_n, u_n, and w_n to their fixed values as $n \to \infty$:

$$\begin{aligned} &\lim_{n\to\infty} r_n = r^{(0)} \\ &\lim_{n\to\infty} u_n = u^{(0)} \\ &\lim_{n\to\infty} w_n = w^{(0)}. \end{aligned} \tag{21}$$

This is possible only under the condition

$$c_1(T_c) = 0. \tag{22}$$

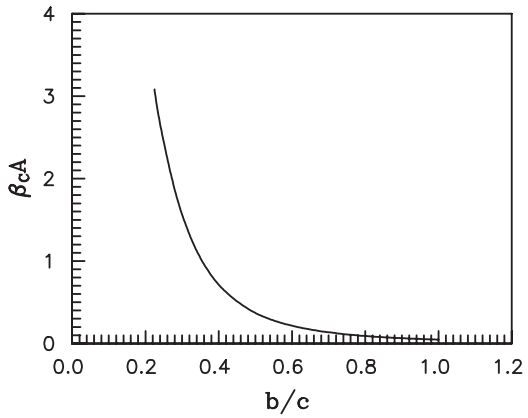

Figure 3. The dependence of the inverse phase transition temperature on the ratio of the interaction potential range to the lattice constant.

Equation (22) determines the phase transition temperature T_c. On the basis of (22), it is possible to find an explicit equation for the quantity $\beta_c\tilde{\Phi}(0)$ determining the critical temperature in the case of the ρ^6 model [28]:

$$D_3(\beta_c\tilde{\Phi}(0))^3 + D_2(\beta_c\tilde{\Phi}(0))^2 + D_1\beta_c\tilde{\Phi}(0) + D_0 = 0. \tag{23}$$

Solving the equation (23) and taking into account the dependence on the ratio b/c in the expressions for coefficients D_i and $\tilde{\Phi}(0) = 8\pi A(b/c)^3$, we obtain the values of the critical temperature $\beta_c A$ presented in figure 3 for $s = 3$. The quantity A is the constant appearing in an exponentially decreasing interaction potential (2). In this paper, we use the potential approximation (3), where $\tilde{\Phi}(k) = 0$ at $B' < k \leqslant B$. Then we have $\beta_c\tilde{\Phi}(0) = 0.9649$ (ρ^4 model, $s = 3$) and $\beta_c\tilde{\Phi}(0) = 1.0419$ (ρ^6 model, $s = 3$) for the effective interaction radius $b = b_{\mathrm{I}}$. The correction considering the presence of the Fourier transform of the potential in the interval $k \in (B', B]$ ($\tilde{\Phi}(k)$ is the small constant $\bar{\Phi}$ at $B' < k \leqslant B$) makes the results of the calculation more precise. A direct analytic method for calculating the phase transition temperature in the ρ^4 model approximation at $\bar{\Phi} \neq 0$ was developed in our earlier publications [27, 33]. When we consider in our calculations the 'tail-end' of the Fourier transform of the potential ($\bar{\Phi} \neq 0$), we find for the phase transition temperature a value which essentially approximates to the corresponding values of the critical temperature obtained by special methods. For example, our numerical value $\beta_c\tilde{\Phi}(0) = 1.2649$ or $\beta_c J = 0.211$ [27] for the ρ^4 model in the case where the potential parameters correspond to the nearest-neighbour interaction with the constant J accords with the value $(\beta_c J)^{-1} = 4.5103$ [34, 35] or $\beta_c J = 0.221\,654(1)$ [36] calculated using the high-temperature series data. Similar values are also obtained using the real-space RG method based on the cumulant expansion ($\beta_c J = 0.224\,01$ [37]) and the Monte Carlo method ($\beta_c J = 0.221\,654 \pm 0.000\,006$ [38], $\beta_c J = 0.221\,6595 \pm 0.000\,0026$ [39–41]). Liu and Fisher [42] preferred $\beta_c J = 0.221\,692$, 0.221 630, and 0.221 620 for the simple cubic Ising lattice and three selected values of the susceptibility exponent γ ($\gamma = 1.250$, 1.2395, and 1.237, respectively).

A calculation technique based on the ρ^6 model for the contribution to the free energy of the system from short-wave oscillation modes is elaborated in detail in [13, 22, 30]. In our calculations, we take into account only the first confluent correction (which is determined by the term proportional to τ^{Δ_1}, $\Delta_1 = -\ln E_2/\ln E_1$) and disregard the second confluent correction (which is determined by the term proportional to τ^{Δ_2}, $\Delta_2 = -\ln E_3/\ln E_1$). This

Table 3. The nonuniversal quantities c_ν, c_{Δ_1} and coefficients $\gamma_0^{(CR)}$, γ_0, γ_1, γ_2 in the expressions for F_{CR} (24) and F (34).

b	b_{I}	b_{II}	b_{III}	c	$2c$
			$s = 2.0000$		
c_ν	1.7006	1.6514	1.6318	1.4412	1.4303
c_{Δ_1}	−0.1130	−0.1637	−0.1828	−0.3386	−0.3464
$\gamma_0^{(CR)}$	0.4135	0.4018	0.3985	0.3915	0.3923
γ_0	1.8758	2.7464	3.1962	61.1798	486.699
γ_1	−0.8032	−0.7759	−0.7651	−0.6734	−0.6701
γ_2	−4.4816	−3.9551	−3.7548	−2.0482	−1.9599
			$s = 2.7349$		
c_ν	1.4168	1.3764	1.3605	1.2097	1.2011
c_{Δ_1}	−0.2671	−0.3075	−0.3227	−0.4468	−0.4530
$\gamma_0^{(CR)}$	0.4153	0.4050	0.4023	0.4047	0.4066
γ_0	1.8776	2.7496	3.2000	61.1930	486.713
γ_1	−0.7063	−0.6952	−0.6913	−0.6924	−0.6978
γ_2	−4.6948	−4.1735	−3.9764	−2.2672	−2.1665
			$s = 3.0000$		
c_ν	1.3373	1.2997	1.2849	1.1462	1.1383
c_{Δ_1}	−0.3243	−0.3629	−0.3774	−0.4952	−0.5012
$\gamma_0^{(CR)}$	0.4166	0.4070	0.4046	0.4116	0.4140
γ_0	1.8789	2.7516	3.2023	61.1999	486.720
γ_1	−0.6867	−0.6795	−0.6773	−0.7020	−0.7100
γ_2	−4.5304	−4.0342	−3.8466	−2.1971	−2.0936

Table 4. Universal factors of coefficients appearing in the nonanalytic components of F_{CR} (24) and F (34).

s	$\bar\gamma_3^{(CR)(0)+}$	$\bar\gamma_3^{(CR)(1)+}$	$\bar\gamma_3^{(0)+}$	$\bar\gamma_3^{(1)+}$
2.0000	−0.3170	−4.6451	0.9699	0.6508
2.7349	−0.9831	−4.0744	1.8654	0.7263
3.0000	−1.2229	−3.8409	2.1770	0.7162

is due to the fact that the contribution from the first confluent correction to thermodynamic functions of the model near T_c is more significant than the small contribution from the second correction ($\tau \ll 1$, Δ_1 is of the order of 0.5, and $\Delta_2 > 2$; see [21, 22]). The final expression for the free energy of the CR assumes the following form:

$$\begin{aligned} &F_{CR} = -kTN'[\gamma_0^{(CR)} + \gamma_1\tau + \gamma_2\tau^2 - \gamma_3^{(CR)(0)+}\tau^{3\nu} - \gamma_3^{(CR)(1)+}\tau^{3\nu+\Delta_1}] \\ &\gamma_0^{(CR)} = \gamma_0^{(0)} + \delta_0^{(0)} \\ &\gamma_k = \gamma_0^{(k)} + \delta_0^{(k)} \qquad k = 1, 2 \\ &\gamma_3^{(CR)(l)+} = c_\nu^3 c_{\Delta_1}^l \bar\gamma_3^{(CR)(l)+} \qquad l = 0, 1. \end{aligned} \tag{24}$$

Here $\nu = \ln s / \ln E_1$ is the critical exponent of the correlation length. The coefficients $\gamma_0^{(CR)}$, γ_1, and γ_2 (see table 3) are not universal, since they depend on microscopic parameters of the Hamiltonian. Explicit expressions for the temperature-independent components of the coefficients $\gamma_0 = \gamma_0^{(0)} + \gamma_0^{(1)}\tau + \gamma_0^{(2)}\tau^2$ and $\delta_0 = \delta_0^{(0)} + \delta_0^{(1)}\tau + \delta_0^{(2)}\tau^2$ are given in [22]. The coefficients $\gamma_3^{(CR)(l)+}$ ($l = 0, 1$) are written as the product of the universal factor $\bar\gamma_3^{(CR)(l)+}$, independent of microscopic parameters, and the nonuniversal factor $c_\nu^3 c_{\Delta_1}^l$, which depends on

these parameters. The values of $c_\nu = [\tilde{c}_1^{(0)}/(f_0\delta)]^\nu$ and $c_{\Delta_1} = c_{20}^{(0)}[\tilde{c}_1^{(0)}/(f_0\delta)]^{\Delta_1}$ are presented in table 3 for different values of the parameter s and the effective range b of the potential, while the values of $\bar{\gamma}_3^{(CR)(l)+}$ are given in table 4.

Using F_{CR}, we can calculate other thermodynamic functions of the system in the CR region at $T > T_c$. For the entropy $S_{CR} = -\partial F_{CR}/\partial T$, internal energy $U_{CR} = F_{CR} + TS_{CR}$, and specific heat $C_{CR} = T\,\partial S_{CR}/\partial T$, we have

$$\begin{aligned} S_{CR} &= kN'[s^{(CR)(0)} + c_0\tau + u_3^{(CR)(0)+}\tau^{1-\alpha} + u_3^{(CR)(1)+}\tau^{1-\alpha+\Delta_1}] \\ U_{CR} &= kTN'[\gamma_1 + u_1\tau + u_3^{(CR)(0)+}\tau^{1-\alpha} + u_3^{(CR)(1)+}\tau^{1-\alpha+\Delta_1}] \\ C_{CR} &= kN'[c_0 + c_3^{(CR)(0)+}\tau^{-\alpha} + c_3^{(CR)(1)+}\tau^{\Delta_1-\alpha}] \end{aligned} \tag{25}$$

where

$$\begin{aligned} &s^{(CR)(0)} = \gamma_0^{(CR)} + \gamma_1 \qquad c_0 = 2(\gamma_1 + \gamma_2) \\ &u_3^{(CR)(l)+} = c_\nu^3 c_{\Delta_1}^l \bar{u}_3^{(CR)(l)+} \qquad l = 0, 1 \\ &\bar{u}_3^{(CR)(0)+} = -3\nu\bar{\gamma}_3^{(CR)(0)+} \\ &\bar{u}_3^{(CR)(1)+} = -(3\nu + \Delta_1)\bar{\gamma}_3^{(CR)(1)+} \\ &u_1 = \gamma_1 + 2\gamma_2 \\ &c_3^{(CR)(l)+} = c_\nu^3 c_{\Delta_1}^l \bar{c}_3^{(CR)(l)+} \\ &\bar{c}_3^{(CR)(0)+} = -3\nu(3\nu - 1)\bar{\gamma}_3^{(CR)(0)+} \\ &\bar{c}_3^{(CR)(1)+} = -(3\nu + \Delta_1)(3\nu + \Delta_1 - 1)\bar{\gamma}_3^{(CR)(1)+}. \end{aligned} \tag{26}$$

Here $\alpha = 2 - 3\nu$ is the critical exponent of the specific heat.

4. Thermodynamic functions of the system in the limiting Gaussian regime region

The contribution of long-wave modes of spin moment density oscillations to the free energy of the 3D Ising model ($k < B's^{-m_\tau}$) taking into account the first confluent correction is calculated according to the scheme proposed in [11, 22]. After the exit from the CR, the system goes over to the LGR. In this case, while calculating the partition function component Z_{LGR} from (19), it is convenient to single out two regions of values of wavevectors. The first is the transition region (TR) corresponding to values of $\boldsymbol{k}$ close to B_{m_τ}, while the second is the Gaussian region corresponding to small values of the wavevector ($k \to 0$). After the integration of the partition function in several layers of the phase space of CV, which follow the point of exit from the CR and determine the size of the TR, the system is described by a Gaussian density of measure. Thus, we can write

$$Z_{LGR} = Z_{LGR}^{(1)} Z_{LGR}^{(2)}. \tag{27}$$

4.1. Transition region (TR)

The TR corresponds to $\tilde{m}_0$ layers of the phase space of CV. The lower boundary of the TR is determined by the point of exit of the system from the CR region ($n = m_\tau + 1$). The upper boundary corresponds to the layer $m_\tau + \tilde{m}_0 + 1$. The latter determines the beginning of the Gaussian region in which the Gaussian distribution of spin density oscillation modes is observed. A transition of the system to the LGR region is accompanied by an increase in the value of h_n as a function of n. Consequently, the condition for obtaining $\tilde{m}_0$ is the equality

$$|h_{m_\tau + \tilde{m}_0'}| = \frac{A_0}{1 - s^{-3}} \tag{28}$$

Table 5. Universal parts of coefficients in $F^{(1)}_{LGR}$ (29) and $F^{(2)}_{LGR}$ (30).

s	$\bar{f}^{(0)}_{TR}$	$\bar{f}^{(1)}_{TR}$	$\bar{f}^{(0)'}$	$\bar{f}^{(1)'}$	$\bar{\gamma}^{+}_{4}$
2.0000	0.6529	−3.9942	0.4749×10^{-5}	-0.3800×10^{-4}	2.7055
2.7349	0.8824	−3.3481	0.2155×10^{-5}	-0.1107×10^{-4}	2.1737
3.0000	0.9541	−3.1247	0.6587×10^{-6}	-0.2945×10^{-5}	2.1841

where A_0 is a large number ($A_0 \geqslant 10$). The value of $\tilde{m}'_0$ determined from (28) actually determines the number $\tilde{m}_0$ (see [22, 30]). It follows from [11, 43–46] containing the results of numerical calculation of the partition function for the Ising model as well as the results of analysis of RR that the evolution of the coefficients of effective densities of measures with increasing number of the layer in the TR is successfully described by solutions of the RG type. Consequently, $F^{(1)}_{LGR}$ can be calculated by using the solutions of RR. The free energy contribution $F^{(1)}_{LGR}$ corresponding to $Z^{(1)}_{LGR}$ from (27) is defined as

$$\begin{aligned}
&F^{(1)}_{LGR} = -kTN'[f^{(0)}_{TR}\tau^{3\nu} + f^{(1)}_{TR}\tau^{3\nu+\Delta_1}] \\
&f^{(l)}_{TR} = c^3_\nu c^l_{\Delta_1}\bar{f}^{(l)}_{TR} \qquad l = 0, 1 \\
&\bar{f}^{(0)}_{TR} = \sum_{m=0}^{\tilde{m}_0} s^{-3m} f^{(0)}_{LGR_1}(m) \\
&\bar{f}^{(1)}_{TR} = \bar{f}_{TR1} + 3\nu\Phi_0\bar{f}^{(0)}_{TR} \qquad \bar{f}_{TR1} = c^{-1}_{\Delta_1}\sum_{m=0}^{\tilde{m}_0} s^{-3m} f^{(1)}_{LGR_1}(m)
\end{aligned} \tag{29}$$

where $\Phi_0 = w^{(0)}_{12}/(f_0\delta\sqrt{\varphi_0})$. The coefficients $f^{(l)}_{LGR_1}(m)$ ($l = 0, 1$) appearing in $\bar{f}^{(l)}_{TR}$ are given in [22, 30]. The quantities $\bar{f}^{(l)}_{TR}$ (see table 5) do not depend on microscopic parameters.

4.2. Region of small values of wavevector ($k \to 0$)

Introducing an infinitely weak external magnetic field $\mathcal{H}$ (or $h = \mu_B\mathcal{H}$, where μ_B is the Bohr magneton), we obtain the following expression for the free energy component $F^{(2)}_{LGR}$ corresponding to $Z^{(2)}_{LGR}$ from (27) (see [13, 30]):

$$\begin{aligned}
&F^{(2)}_{LGR} = -kTN'[f^{(0)'}\tau^{3\nu} + f^{(1)'}\tau^{3\nu+\Delta_1}] - \beta N\gamma^{+}_{4}h^2\tau^{-2\nu}(1 + a^{+}_{\chi}\tau^{\Delta_1}) \\
&f^{(l)'} = c^3_\nu c^l_{\Delta_1}\bar{f}^{(l)'} \qquad l = 0, 1 \\
&\bar{f}^{(0)'} = s^{-3(\tilde{m}_0+1)} f^{(0)} \\
&\bar{f}^{(1)'} = \bar{f}_{1'} + 3\nu\Phi_0\bar{f}^{(0)'} \qquad \bar{f}_{1'} = c^{-1}_{\Delta_1} s^{-3(\tilde{m}_0+1)} f^{(1)} \\
&\gamma^{+}_{4} = c^{-2}_\nu\bar{\gamma}^{+}_{4}/(\beta\tilde{\Phi}(0)) \\
&\bar{\gamma}^{+}_{4} = s^{2\tilde{m}_0}/(2g_0) \\
&a^{+}_{\chi} = -g_1 - 2\nu c_{\Delta_1}\Phi_0.
\end{aligned} \tag{30}$$

Here $f^{(0)}$ and $f^{(1)}$ can be presented in terms of coefficients g_0 and g_1 determining the quantity $\tilde{d}_{m'_\tau}(k) = s^{-2(m'_\tau-1)}\beta\tilde{\Phi}(0)g_0(1 + g_1\tau^{\Delta_1}) + 2\beta\tilde{\Phi}(0)b^2k^2$ in the expression for the long-wave part $Z^{(2)}_{LGR}$ of the partition function. The coefficients $\bar{f}^{(l)'}$ and $\bar{\gamma}^{+}_{4}$ are contained in table 5.

On the basis of (29) and (30), the general expression $F_{LGR} = F^{(1)}_{LGR} + F^{(2)}_{LGR}$ corresponding to the contribution to the free energy from long-wave modes of spin moment density oscillations

takes the form

$$\begin{aligned} F_{LGR} &= -kTN'[f_{LGR}^{(0)}\tau^{3\nu} + f_{LGR}^{(1)}\tau^{3\nu+\Delta_1}] - \beta N\gamma_4^+ h^2\tau^{-2\nu}(1 + a_\chi^+\tau^{\Delta_1}) \\ f_{LGR}^{(l)} &= c_\nu^3 c_{\Delta_1}^l \bar{f}_{LGR}^{(l)} \\ \bar{f}_{LGR}^{(l)} &= \bar{f}_{TR}^{(l)} + \bar{f}^{(l)'} \qquad l = 0, 1. \end{aligned} \tag{31}$$

In view of the very small values of the universal quantities $\bar{f}^{(l)'}$, the values of $\bar{f}_{LGR}^{(l)}$ practically coincide with the values of $\bar{f}_{TR}^{(l)}$ (see table 5).

For $\mathcal{H} = 0$, the entropy, internal energy, and specific heat of the system corresponding to LGR are defined by the following relations:

$$\begin{aligned} S_{LGR} &= kN'[u_3^{(LGR)(0)}\tau^{1-\alpha} + u_3^{(LGR)(1)}\tau^{1-\alpha+\Delta_1}] \\ U_{LGR} &= kTN'[u_3^{(LGR)(0)}\tau^{1-\alpha} + u_3^{(LGR)(1)}\tau^{1-\alpha+\Delta_1}] \\ C_{LGR} &= kN'[c_3^{(LGR)(0)}\tau^{-\alpha} + c_3^{(LGR)(1)}\tau^{\Delta_1-\alpha}] \end{aligned} \tag{32}$$

where

$$\begin{aligned} u_3^{(LGR)(l)} &= c_\nu^3 c_{\Delta_1}^l \bar{u}_3^{(LGR)(l)} \qquad l = 0, 1 \\ \bar{u}_3^{(LGR)(0)} &= 3\nu\bar{f}_{LGR}^{(0)} \\ \bar{u}_3^{(LGR)(1)} &= (3\nu + \Delta_1)\bar{f}_{LGR}^{(1)} \\ c_3^{(LGR)(l)} &= c_\nu^3 c_{\Delta_1}^l \bar{c}_3^{(LGR)(l)} \\ \bar{c}_3^{(LGR)(0)} &= 3\nu(3\nu - 1)\bar{f}_{LGR}^{(0)} \\ \bar{c}_3^{(LGR)(1)} &= (3\nu + \Delta_1)(3\nu + \Delta_1 - 1)\bar{f}_{LGR}^{(1)}. \end{aligned} \tag{33}$$

Let us now write out the complete expressions for the free energy and other thermodynamic functions of the 3D Ising model near the phase transition point.

5. Total thermodynamic characteristics of Ising-like system for $T > T_c$ taking into account first confluent correction

In accordance with (18), the total free energy of the system in zero external field reads

$$\begin{aligned} F &= -kTN'[\gamma_0 + \gamma_1\tau + \gamma_2\tau^2 + \gamma_3^{(0)+}\tau^{3\nu} + \gamma_3^{(1)+}\tau^{3\nu+\Delta_1}] \\ \gamma_0 &= s_0^3 \ln 2 + \gamma_0^{(CR)} \\ \gamma_3^{(l)+} &= c_\nu^3 c_{\Delta_1}^l \bar{\gamma}_3^{(l)+} \\ \bar{\gamma}_3^{(l)+} &= -\bar{\gamma}_3^{(CR)(l)+} + \bar{f}_{LGR}^{(l)} \qquad l = 0, 1. \end{aligned} \tag{34}$$

The coefficients γ_1 and γ_2 are defined in (24). The terms proportional to integral powers of τ in (34) appear exclusively due to the inclusion of short-wave modes of oscillations. The terms proportional to $\tau^{3\nu}$ and $\tau^{3\nu+\Delta_1}$ (the nonanalytic component of the free energy) are formed as a result of inclusion of short-wave as well as long-wave modes of oscillations. The first confluent correction appears due to the smaller eigenvalue E_2 of the RG linear transformation matrix taken into account in the solutions of RR.

The main advantage of the expression for F is the presence of relations connecting its coefficients with microscopic parameters of the system and the coordinates of a fixed point of RR. The coefficients $\gamma_3^{(l)+}$ ($l = 0, 1$) are presented in the form of the product of the universal component $\bar{\gamma}_3^{(l)+}$ and the nonuniversal factor depending on microscopic parameters through c_ν and c_{Δ_1} (see (34)). The leading critical amplitudes and the amplitudes of the confluent

correction for the specific heat and other thermodynamic characteristics of the system can be presented in a similar way.

The coefficient γ_0 as well as γ_1 and γ_2 are given in table 3. Numerical values of $\bar{\gamma}_3^{(l)+}$ are contained in table 4. The coefficients of the entropy S, internal energy U, and specific heat C can be expressed in terms of the coefficients of the free energy. Taking into account the first confluent correction, we arrive at the expressions

$$\begin{aligned} S &= kN'[s^{(0)} + c_0\tau + u_3^{(0)+}\tau^{1-\alpha} + u_3^{(1)+}\tau^{1-\alpha+\Delta_1}] \\ U &= kTN'[\gamma_1 + u_1\tau + u_3^{(0)+}\tau^{1-\alpha} + u_3^{(1)+}\tau^{1-\alpha+\Delta_1}] \\ C &= kN'[c_0 + c_3^{(0)+}\tau^{-\alpha} + c_3^{(1)+}\tau^{\Delta_1-\alpha}]. \end{aligned} \tag{35}$$

Here

$$\begin{aligned} s^{(0)} &= \gamma_0 + \gamma_1 \\ u_3^{(l)+} &= c_\nu^3 c_{\Delta_1}^l \bar{u}_3^{(l)+} \qquad l = 0, 1 \\ \bar{u}_3^{(0)+} &= 3\nu\bar{\gamma}_3^{(0)+} \\ \bar{u}_3^{(1)+} &= (3\nu + \Delta_1)\bar{\gamma}_3^{(1)+} \\ c_3^{(l)+} &= c_\nu^3 c_{\Delta_1}^l \bar{c}_3^{(l)+} \\ \bar{c}_3^{(0)+} &= 3\nu(3\nu - 1)\bar{\gamma}_3^{(0)+} \\ \bar{c}_3^{(1)+} &= (3\nu + \Delta_1)(3\nu + \Delta_1 - 1)\bar{\gamma}_3^{(1)+}. \end{aligned} \tag{36}$$

The coefficients c_0 and u_1 are given in (26).

The formula for the specific heat (see (35)) for the model under investigation can be written in the form [47, 48]

$$\begin{aligned} \frac{C}{kN'} &= \frac{A^+}{\alpha}\tau^{-\alpha}(1 + \alpha a_c^+\tau^{\Delta_1}) + B^+ \\ A^+ &= c_\nu^3\alpha\bar{c}_3^{(0)+} \qquad a_c^+ = \frac{c_{\Delta_1}}{\alpha}\frac{\bar{c}_3^{(1)+}}{\bar{c}_3^{(0)+}} \qquad B^+ = c_0. \end{aligned} \tag{37}$$

Such an important characteristic of the system as the susceptibility per particle

$$\chi = -\frac{1}{N}\frac{\partial^2 F_{LGR}}{\partial\mathcal{H}^2} \tag{38}$$

can be calculated using (31). For infinitely small values of the external field $\mathcal{H}$ near T_c, it is defined as

$$\begin{aligned} \chi &= \Gamma^+\tau^{-\gamma}(1 + a_\chi^+\tau^{\Delta_1})\frac{\mu_B^2}{\tilde{\Phi}(0)} \\ \Gamma^+ &= 2c_\nu^{-2}\bar{\gamma}_4^+ \\ a_\chi^+ &= c_{\Delta_1}\bar{a}_\chi^+ \\ \bar{a}_\chi^+ &= -\bar{g}_1 - 2\nu\Phi_0. \end{aligned} \tag{39}$$

Here $\gamma = 2\nu$ is the critical exponent of the susceptibility. The value of $\bar{g}_1$ does not depend on microscopic parameters and can be obtained as a result of the elimination of the nonuniversal factor c_{Δ_1} from g_1.

The coefficients for the specific heat C/kN' (37) and susceptibility χ (39) are given in table 6. It should be emphasized that the calculated amplitudes a_c^+ and a_χ^+ of the confluent corrections are in accord with the results obtained by Liu and Fisher [49] who considered

Table 6. Values of coefficients in the expressions (37) for the specific heat C/kN' and (39) for the susceptibility χ.

b	b_{I}	b_{II}	b_{III}	c	$2c$
			$s = 2.0000$		
A^+	1.0876	0.9960	0.9609	0.6620	0.6471
a_c^+	−1.2609	−1.8262	−2.0389	−3.7773	−3.8634
B^+	−10.5696	−9.4620	−9.0397	−5.4430	−5.2601
Γ^+	1.8711	1.9842	2.0321	2.6052	2.6450
a_χ^+	−0.0691	−0.1001	−0.1118	−0.2071	−0.2118
			$s = 2.7349$		
A^+	0.8113	0.7439	0.7184	0.5050	0.4944
a_c^+	−2.3816	−2.7420	−2.8773	−3.9838	−4.0397
B^+	−10.8022	−9.7375	−9.3355	−5.9193	−5.7286
Γ^+	2.1659	2.2948	2.3488	2.9709	3.0134
a_χ^+	−0.1177	−0.1355	−0.1422	−0.1969	−0.1996
			$s = 3.0000$		
A^+	0.7238	0.6644	0.6420	0.4558	0.4465
a_c^+	−2.6494	−2.9650	−3.0832	−4.0460	−4.0947
B^+	−10.4343	−9.4274	−9.0478	−5.7981	−5.6074
Γ^+	2.4427	2.5860	2.6459	3.3248	3.3710
a_χ^+	−0.1291	−0.1445	−0.1502	−0.1971	−0.1995

leading corrections to scaling amplitudes for Ising models with the interaction between nearest neighbours on sc (simple cubic), bcc (body-centred cubic), and fcc (face-centred cubic) lattices. It was proved in [49] that the amplitudes of these corrections for susceptibility, correlation length, specific heat, and spontaneous magnetization have negative sign for all three lattices. Liu and Fisher also noted the agreement between the results obtained, the results from other high-temperature expansions, and the results of the field-theory analysis. Our values $\Gamma^+ = 1.8711$, $a_\chi^+ = -0.0691$ (see table 6, $s = 2.0000$, $b = b_{\mathrm{I}}$), for example, accord with the recent high-temperature estimates $\Gamma^+ = 1.111(1)$, $a_\chi^+ = -0.10(3)$ obtained by Butera and Comi [50].

6. Conclusions

The analytic method for calculating the thermodynamic functions of 3D Ising-like systems above the critical temperature T_c is briefly presented in the higher non-Gaussian approximation (ρ^6 model) taking into account the first confluent correction. The starting point of the problem statement in the CV method under study is the Hamiltonian of the 3D Ising model. After passing to the CV set, the Jacobian of the transition from the spin variables to the CV is calculated to obtain a partition function functional similar to the Ginzburg–Landau functional. The partition function of the spin system is integrated over the layers of the CV phase space. The corresponding RG transformation can be related to one of Wilson type. Although the CV method like the Wilson approach exploits RG ideas, it is based on the use of a non-Gaussian density of measure. The main feature is the integration of short-wave spin density oscillation modes, which is generally done without using perturbation theory. The short-wave modes are characterized by the presence of RG symmetry and are described by a non-Gaussian measure density. These modes are responsible for the formation of critical exponents and for renormalization of the coefficient of the distribution describing the long-wave modes. The calculation for long-wave modes of spin moment density oscillations is based on using the

Gaussian density of measure as the basis density. The contributions to the thermodynamic functions of an Ising ferromagnet (free energy, entropy, internal energy, and specific heat) from the short-wave and long-wave modes are calculated separately. A calculation technique for confluent corrections is elaborated in the course of determining the thermodynamic functions.

The CV method allows one to calculate the partition function of the system and to obtain not only the universal quantities (critical exponents) but also the nonuniversal characteristics. The advantage of the proposed method is the possibility of deriving analytic expressions for the phase transition temperature and the amplitudes of thermodynamic characteristics as functions of microscopic parameters of the initial system (the lattice constant and parameters of the interaction potential), which makes this method useful in describing the phase transitions in a wide class of 3D systems. A nonuniversal factor determined by microscopic parameters of the system is singled out in the expressions for leading critical amplitudes and correction-to-scaling amplitudes of the thermodynamic characteristics. These amplitudes for the specific heat and susceptibility as well as the phase transition temperature are obtained for various interaction potential ranges.

The 3D Ising-like system thermodynamics at $T < T_c$ (the ρ^6 model approximation) and plots of the temperature dependences of the entropy, specific heat, and other thermodynamic characteristics near T_c (above and below T_c) for various values of the effective radius of the exponentially decreasing interaction potential will be the subject of the following paper.

References

[1] Stanley H E 1971 *Introduction to Phase Transitions and Critical Phenomena* (Oxford: Clarendon)
[2] Amit D J 1984 *Field Theory, the Renormalization Group, and Critical Phenomena* (Singapore: World Scientific)
[3] Zinn-Justin J 1996 *Quantum Field Theory and Critical Phenomena* (Oxford: Clarendon)
[4] Kleinert H and Schulte-Frohlinde V 2001 *Critical Properties of φ^4-Theories* (Singapore: World Scientific)
[5] Wilson K G and Kogut J 1974 *Phys. Rep.* C **12** 75
[6] Binder K 1985 *J. Comput. Phys.* **59** 1
[7] Fisher M E 1998 *Rev. Mod. Phys.* **70** 653
[8] Campostrini M, Pelissetto A, Rossi P and Vicari E 1999 *Phys. Rev.* E **60** 3526
[9] Yukhnovskii I R 1977 *Dokl. Akad. Nauk SSSR* **232** 312 (Engl. transl. 1977 *Sov. Phys.–Dokl.* **22** 18)
[10] Yukhnovskii I R 1978 *Teor. Mat. Fiz.* **36** 373
[11] Yukhnovskii I R 1987 *Phase Transitions of the Second Order. Collective Variables Method* (Singapore: World Scientific)
[12] Yukhnovskii I R 1989 *Riv. Nuovo Cimento* **12** 1
[13] Yukhnovskii I R, Kozlovskii M P and Pylyuk I V 2001 *Microscopic Theory of Phase Transitions in the Three-Dimensional Systems* (Lviv: Eurosvit) (in Ukrainian)
[14] Usatenko Z E and Kozlovskii M P 2000 *Phys. Rev.* B **62** 9599
[15] Yukhnovskii I R, Kozlovskii M P and Pylyuk I V 1991 *Z. Naturf.* a **46** 1
[16] Kozlovskii M P, Pylyuk I V and Yukhnovskii I R 1991 *Teor. Mat. Fiz.* **87** 293
[17] Kozlovskii M P, Pylyuk I V and Yukhnovskii I R 1991 *Teor. Mat. Fiz.* **87** 434
[18] Kozlovskii M P and Pylyuk I V 1987 *Proc. All-Union Conf. on Modern Problems in Statistical Physics (L'vov, Feb. 1987)* vol 2 (Kiev: Naukova Dumka) p 50 (in Russian)
[19] Kozlovskii M P 1989 *Teor. Mat. Fiz.* **78** 422
[20] Kozlovskii M P and Pylyuk I V 1990 *Ukr. Fiz. Zh.* **35** 146 (in Ukrainian)
[21] Kozlovskii M P, Pylyuk I V and Dukhovii V V 1997 *Condens. Matter Phys.* **11** 17
[22] Kozlovskii M P, Pylyuk I V and Dukhovii V V 1999 *Preprint* cond-mat/9907468
[23] Guida R and Zinn-Justin J 1998 *J. Phys. A: Math. Gen.* **31** 8103
[24] Hasenbusch M 1999 *J. Phys. A: Math. Gen.* **32** 4851
[25] Tsypin M M 1994 *Phys. Rev. Lett.* **73** 2015
[26] Tsypin M M 1997 *Phys. Rev.* B **55** 8911
[27] Kozlovskii M P, Pylyuk I V and Usatenko Z E 1996 *Phys. Status Solidi* b **197** 465
[28] Kozlovskii M P 1984 *Preprint* ITP-84-35R (Inst. Theor. Phys., Acad. Sci. Ukr. SSR, Kiev) (in Russian)
[29] Dukhovii V V, Kozlovskii M P and Pylyuk I V 1996 *Teor. Mat. Fiz.* **107** 288

[30] Pylyuk I V and Kozlovskii M P 1997 *Preprint* ICMP-97-06U (Inst. Cond. Matt. Phys., Natl Acad. Sci. Ukraine, Lviv) (in Ukrainian)
[31] Kozlovskii M P and Pylyuk I V *Preprint* 1985 ITP-85-23E (Inst. Theor. Phys., Acad. Sci. Ukr. SSR, Kiev) (in English)
[32] Ma S 1976 *Modern Theory of Critical Phenomena* (Reading, MA: Benjamin)
[33] Kozlovskii M P, Dukhovii V V and Pylyuk I V 2000 *Condens. Matter Phys.* **3** 727
[34] Moore M A, Jasnov D and Wortis M 1969 *Phys. Rev. Lett.* **22** 940
[35] Ferer M and Wortis M 1972 *Phys. Rev.* B **6** 3426
[36] Butera P and Comi M 2000 *Phys. Rev.* B **62** 14837
[37] Reich W 1984 *J. Phys. A: Math. Gen.* **17** 3553
[38] Pawley G S, Swendsen R H, Wallace D J and Wilson K G 1984 *Phys. Rev.* B **29** 4030
[39] Ferrenberg A M and Landau D P 1991 *Phys. Rev.* B **44** 5081
[40] Landau D P and Ferrenberg A M 1993 *J. Kor. Phys. Soc.* **26** S371
[41] Landau D P 1994 *Physica* A **205** 41
[42] Liu A J and Fisher M E 1989 *Physica* A **156** 35
[43] Yukhnovskii I R, Kozlovskii M P and Kolomiets V A 1982 *Ukr. Fiz. Zh.* **27** 925 (in Russian)
[44] Yukhnovskii I R, Kozlovskii M P and Kolomiets V A 1982 *Ukr. Fiz. Zh.* **27** 930 (in Russian)
[45] Yukhnovskii I R, Kozlovskii M P and Kolomiets V A 1982 *Ukr. Fiz. Zh.* **27** 1399 (in Russian)
[46] Kozlovskii M P, Pylyuk I V and Kolomiets V A 1984 *Preprint* ITP-84-177R (Inst. Theor. Phys., Acad. Sci. Ukr. SSR, Kiev) (in Russian)
[47] Bagnuls C and Bervillier C 1981 *Phys. Rev.* B **24** 1226
[48] Nicoll J F and Albright P C 1986 *Phys. Rev.* B **34** 1991
[49] Liu A J and Fisher M E 1990 *J. Stat. Phys.* **58** 431
[50] Butera P and Comi M 1998 *Phys. Rev.* B **58** 11552