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

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Abstract

A microscopic approach to the investigation of the three-dimensional Ising-like system thermodynamics below the phase transition temperature T_c is schematically presented within the framework of the higher non-Gaussian approximation (ρ^6 model) taking into account the corrections to scaling. A microscopic analogue of the Landau free energy is calculated. Explicit expressions for the thermodynamic characteristics are obtained as functions of the temperature and microscopic parameters of the system. The thermodynamic characteristics near T_c and their amplitudes are given for various values of the effective radius of the exponentially decreasing interaction potential (including the values corresponding to the nearest-neighbour interaction, the interaction between the nearest and next-nearest neighbours, and that between the nearest, next-nearest, and third neighbours). The evolutions of the free energy of the system at the phase transition point, average spin moment, and specific heat with increasing ratio of the potential effective radius to the simple cubic lattice constant are plotted. The results of calculations and their comparison with other authors' data show that the ρ^6 model provides a better quantitative description of the critical behaviour of a three-dimensional Ising magnetic than the ρ^4 model.

1. Introduction

This research is devoted to the theory of phase transitions and critical phenomena, which remain the subjects of wide-ranging studies (see, for example, [1–5]). The approach to the description

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

of second-order phase transitions based on the method of collective variables (CV) [6] has been developed further. The object of investigation is a three-dimensional (3D) Ising-like system on a simple cubic lattice with an exponentially decreasing interaction potential (see, for example, [7, 8]). The Ising model, which is simple and convenient for mathematical analysis, is widely used in the theory of phase transitions for analysis of properties of various magnetic and nonmagnetic systems (ferromagnets, antiferromagnets, ferroelectrics, binary mixtures, lattice models of liquids, etc). The partition function of the spin system in the CV representation is written in the form of an integral with respect to these CV [6, 8, 9]. An important factor in describing the system behaviour near the phase transition temperature T_c by the CV method is the use of non-Gaussian measure densities. A non-Gaussian density of measure at a zero external field is represented as an exponential function of the CV ρ_k, the argument of which contains, along with the quadratic term, higher even powers of the variable with the corresponding coupling constants. The simplest non-Gaussian measure density is the quartic one (the ρ^4 model) with the second and the fourth powers of the variable in the exponent. The sextic measure density (the ρ^6 model) includes the sixth power of the variable in addition to the second and fourth powers, etc.

The present publication complements our previous works [8, 9], in which the study was based on the CV method. In [9], the ρ^4 model was used for calculating the thermodynamic functions of the classical n-vector 3D magnetic model without taking into account confluent corrections (corrections to scaling). The crossover from Gaussian or non-Gaussian to Ising forms was discussed in [8], where the influence of the complication of the measure density on the behaviour of the critical exponent of the correlation length was considered. The simple ρ^4 model describes the main features of the second-order phase transition [10–13]. A more correct quantitative description of critical properties of a 3D Ising ferromagnet by the CV method can be given using the sextic measure density [8, 14, 15]. The analytic method for calculating the 3D Ising-like system thermodynamics below T_c (the low-temperature region) is developed in the present paper on the basis of this higher non-Gaussian approximation (the ρ^6 model). A technique for taking into account the first confluent correction is elaborated in the course of calculation of thermodynamic characteristics. The dependences of these characteristics on temperature and microscopic parameters of the system are plotted. The case of $T > T_c$ was considered in [8].

The real task of the critical phenomena physics at the present time is elaborating the methods giving quantitative descriptions of the critical behaviour of the system without using any adjustable parameters. The approach suggested in the present paper allows us to perform the calculations for an Ising ferromagnet in real 3D space on the microscopic level without any adjustable parameters. In this case, the new special functions [8, 14–17] appearing in the construction of the phase transition theory using the sextic measure density are exploited. We hope that our explicit representations and plots will provide useful benchmarks in studying the dependence of the thermodynamic functions of 3D Ising-like systems on the parameters of the interaction potential and characteristics of the crystal lattice.

2. Calculation scheme for the free energy of the system below the phase transition temperature

As in the case of $T > T_c$ [8], we shall calculate the free energy of the system by separating the contributions from short- and long-wave modes of spin moment density oscillations. For $T < T_c$, we have

$$F = F_0 + F_{CR} + F_{IGR} \tag{1}$$

where $F_0 = -kTN\ln 2$ corresponds to the free energy of N noninteracting spins, F_{CR} to the contribution of short-wave oscillation modes to the free energy of the system (the critical regime (CR) region), and F_{IGR} to the contribution of long-wave oscillation modes (the region of the inverse Gaussian regime (IGR)).

While calculating the free energy of the system, we shall use extensively the solutions of recurrence relations (RR) between the coefficients of effective sextic distributions (see, for example, [8, 18]). In the CR region, the solutions of RR of the renormalization group (RG) type are valid. In contrast to the limiting Gaussian regime (LGR) observed for $T > T_c$, the IGR is described by a non-Gaussian density of measure. It should be emphasized that at $T < T_c$, the system acquires a nonzero order parameter. It is not introduced as an independent quantity, but is determined as a result of direct calculation. This is possible since the set of CV contains the variable ρ_0 associated with the order parameter. The distribution acquires a Gaussian form only as a result of separating the free energy of the ordering.

Calculating the partition function of the Ising model, we divide the CV phase space into layers with the division parameter s and use the average value of the Fourier transform of the interaction potential (the arithmetic mean in the case given) corresponding to the given layer [6, 9]. Short- and long-wave modes of spin density oscillations at $T < T_c$ are separated by the layer number μ_τ. The CR takes place for layers of the CV phase space with $n \leqslant \mu_\tau$, while the IGR is observed for $n > \mu_\tau$. The condition for determining μ_τ is the equality [7, 15, 19]

$$\frac{r_{\mu_\tau+1} - r^{(0)}}{r^{(0)}} = \delta. \tag{2}$$

Here δ is a constant quantity ($\delta \leqslant 1$), $r_{\mu_\tau+1}$ is determined from the solutions of RR, and $r^{(0)}$ corresponds to a coordinate of the fixed point [8, 18]. In numerical calculations, we shall put $\delta = 1$, which is in accord with the condition for δ used by us for $T > T_c$ [8]. In analogy with the case $T > T_c$, we obtain the following expression for μ_τ:

$$\mu_\tau = \mu_\tau^{(0)} - m_{\Delta_1}|\tau|^{\Delta_1} \qquad \mu_\tau^{(0)} = -\frac{\ln|\tau|}{\ln E_1} + \mu_0 - 1 \qquad \mu_0 = m_c. \tag{3}$$

The quantities m_{Δ_1}, Δ_1, and m_c coincide with the corresponding quantities for $T > T_c$ [18], $\tau = (T - T_c)/T_c$, and E_1 is the largest eigenvalue of the matrix of the RG linear transformation.

The expression for the layer μ_τ determining the point of exit of the system from the CR region at $T < T_c$ makes it possible to find F_{CR} as well as F_{IGR}. We shall consider these calculations schematically. The free energy of the system is obtained by using the values of the critical temperature depending on microscopic parameters. The equation for the critical temperature in the case of the ρ^6 model as well as the variation of this temperature with increasing ratio of the potential effective radius to the lattice constant are given in [8]. It should be noted that the thermodynamic characteristics are calculated taking into account the term proportional to $|\tau|^{\Delta_1}$ and determining the first confluent correction.

3. Contribution to the thermodynamic functions of the system from the critical regime region

As in the case of $T > T_c$, the contribution F_{CR} to the free energy of the system from the CR region is calculated through the summation of partial free energies over the layers of the CV phase space. Using formulae (3) and singling out temperature explicitly in the calculations, we arrive at the following expression:

$$F_{CR} = -kTN'[\gamma_0^{(CR)} - \gamma_1|\tau| + \gamma_2|\tau|^2 - \gamma_3^{(CR)(0)-}|\tau|^{3\nu} - \gamma_3^{(CR)(1)-}|\tau|^{3\nu+\Delta_1}] \tag{4}$$

Table 1. Universal factors occurring in the expressions for the coefficients $\gamma_3^{(CR)(l)-}$, $\gamma_{IGR}^{(l)}$, and $\gamma_3^{(l)-}$ $(l = 0, 1)$.

s	$\bar{\gamma}_3^{(CR)(0)-}$	$\bar{\gamma}_3^{(CR)(1)-}$	$\bar{\gamma}_{IGR}^{(0)}$	$\bar{\gamma}_{IGR}^{(1)}$	$\bar{\gamma}_3^{(0)-}$	$\bar{\gamma}_3^{(1)-}$
2.0000	0.7382	6.7881	2.4980	−0.0087	1.7599	−6.7968
2.7349	0.4188	5.6159	3.1838	1.9416	2.7650	−3.6743
3.0000	0.2899	5.2219	3.3972	2.1505	3.1073	−3.0714

where $\nu = \ln s / \ln E_1$ is the critical exponent of the correlation length, N', $\gamma_0^{(CR)}$, γ_1, and γ_2 (which are functions of microscopic parameters of the system) are the same as for $T > T_c$ [8, 18]. We present the coefficients $\gamma_3^{(CR)(l)-}$ in the form in which the universal factor $\bar{\gamma}_3^{(CR)(l)-}$ independent of microscopic parameters of the system is separated. The latter parameters in our case include the parameters of the exponentially decreasing interaction potential (the effective radius b of the potential and its Fourier transform $\tilde{\Phi}(0)$ for zero value of the wavevector) as well as the constant c of the simple cubic lattice. We have

$$\begin{aligned} &\gamma_3^{(CR)(l)-} = c_\nu^3 c_{\Delta_1}^l \bar{\gamma}_3^{(CR)(l)-} \qquad l = 0, 1 \\ &\bar{\gamma}_3^{(CR)(0)-} = \gamma^- \qquad \bar{\gamma}_3^{(CR)(1)-} = \gamma_{\Delta_1}^- - \Phi_0(\gamma_{11}^- + 3\nu\gamma^-). \end{aligned} \tag{5}$$

Here

$$\begin{aligned} \gamma^- &= \frac{f_{CR}^{(0)}}{1 - s^{-3}} - \frac{f_{CR}^{(1)} \varphi_0^{-1/2} f_0 \delta}{1 - E_1 s^{-3}} + \frac{f_{CR}^{(7)} \varphi_0^{-1} (f_0\delta)^2}{1 - E_1^2 s^{-3}} \\ \gamma_{\Delta_1}^- &= \frac{f_{CR}^{(2)} \varphi_0^{-1}}{1 - E_2 s^{-3}} - \frac{f_{CR}^{(4)} \varphi_0^{-3/2} f_0 \delta}{1 - E_1 E_2 s^{-3}} + \frac{f_{CR}^{(8)} \varphi_0^{-2} (f_0\delta)^2}{1 - E_1^2 E_2 s^{-3}} \\ \gamma_{11}^- &= \frac{f_{CR}^{(1)} \varphi_0^{-1/2} f_0 \delta}{1 - E_1 s^{-3}} - \frac{2 f_{CR}^{(7)} \varphi_0^{-1} (f_0\delta)^2}{1 - E_1^2 s^{-3}}. \end{aligned} \tag{6}$$

The nonuniversal factors c_ν, c_{Δ_1}, the factor Φ_0, the eigenvalues E_l of the matrix of the RG transformation, three coordinates of the fixed point and the quantities characterizing them (including f_0 and φ_0), as well as the quantities $f_{CR}^{(i)}$ depending on the values of the variables at the fixed point, are presented in [8, 18]. The universal factors $\bar{\gamma}_3^{(CR)(l)-}$ $(l = 0, 1)$ of the coefficients $\gamma_3^{(CR)(l)-}$ are given in table 1 for some optimal values of the RG parameter s [8, 14]. For $s = s^* = 2.7349$, the average value of the coefficient in the term with the second power of the variable in the expression for the effective measure density is equal to zero at a fixed point (in the ρ^4 model, this corresponds to $s^* = 3.5862$).

Differentiating expression (4) for F_{CR} with respect to temperature, we obtain the following expressions for the entropy S_{CR}, internal energy U_{CR}, and specific heat C_{CR} in the CR region:

$$\begin{aligned} S_{CR} &= kN'[s^{(CR)(0)} - c_0|\tau| + u_3^{(CR)(0)-}|\tau|^{1-\alpha} + u_3^{(CR)(1)-}|\tau|^{1-\alpha+\Delta_1}] \\ U_{CR} &= kTN'[\gamma_1 - u_1|\tau| + u_3^{(CR)(0)-}|\tau|^{1-\alpha} + u_3^{(CR)(1)-}|\tau|^{1-\alpha+\Delta_1}] \\ C_{CR} &= kN'[c_0 - c_3^{(CR)(0)-}|\tau|^{-\alpha} - c_3^{(CR)(1)-}|\tau|^{\Delta_1-\alpha}] \end{aligned} \tag{7}$$

where $\alpha = 2 - 3\nu$ is the critical exponent of the specific heat, and

$$\begin{aligned}
u_3^{(CR)(l)-} &= c_\nu^3 c_{\Delta_1}^l \bar{u}_3^{(CR)(l)-} \qquad l = 0, 1\\
\bar{u}_3^{(CR)(0)-} &= 3\nu\bar{\gamma}_3^{(CR)(0)-}\\
\bar{u}_3^{(CR)(1)-} &= (3\nu + \Delta_1)\bar{\gamma}_3^{(CR)(1)-}\\
c_3^{(CR)(l)-} &= c_\nu^3 c_{\Delta_1}^l \bar{c}_3^{(CR)(l)-}\\
\bar{c}_3^{(CR)(0)-} &= 3\nu(3\nu - 1)\bar{\gamma}_3^{(CR)(0)-}\\
\bar{c}_3^{(CR)(1)-} &= (3\nu + \Delta_1)(3\nu + \Delta_1 - 1)\bar{\gamma}_3^{(CR)(1)-}.
\end{aligned} \tag{8}$$

The remaining coefficients are defined by corresponding expressions obtained from an analysis of temperatures above T_c [8, 18].

4. Contribution to the thermodynamic functions of the system from the region of the inverse Gaussian regime

We shall write the final result for the contribution of the IGR region

$$F_{IGR} = -kTN's^{-3(\mu_\tau+1)}\ln[\sqrt{2}Q(P_{\mu_\tau})] - kT\ln Z_{\mu_\tau+1} \tag{9}$$

to the free energy of the system. The calculations of the first and second terms in (9) associated with the calculations of

$$\sqrt{2}Q(P_{\mu_\tau}) = \left(\frac{4s^3 u_{\mu_\tau} s^{-4\mu_\tau}}{\pi^4 C(h_{\mu_\tau}, \alpha_{\mu_\tau})}\right)^{1/4} I_0(\eta_{\mu_\tau}, \xi_{\mu_\tau}) \tag{10}$$

and

$$\begin{aligned}
Z_{\mu_\tau+1} = \int \exp\Bigg[&-\frac{1}{2}\sum_{k\leqslant B_{\mu_\tau+1}} d_{\mu_\tau+1}(k)\rho_{\boldsymbol{k}}\rho_{-\boldsymbol{k}}\\
&- \sum_{l=2}^{3}\frac{a_{2l}^{(\mu_\tau+1)}}{(2l)!N_{\mu_\tau+1}^{l-1}}\sum_{k_1,\ldots,k_{2l}\leqslant B_{\mu_\tau+1}}\rho_{\boldsymbol{k}_1}\cdots\rho_{\boldsymbol{k}_{2l}}\delta_{\boldsymbol{k}_1+\cdots+\boldsymbol{k}_{2l}}\Bigg](\mathrm{d}\rho)^{N_{\mu_\tau+1}}
\end{aligned} \tag{11}$$

are described in detail in [15, 19] (see [12] for the ρ^4 model). We obtain

$$\begin{aligned}
F_{IGR} &= -kTN'[\gamma_{IGR}^{(0)}|\tau|^{3\nu} + \gamma_{IGR}^{(1)}|\tau|^{3\nu+\Delta_1}]\\
\gamma_{IGR}^{(l)} &= \gamma_3^{(l)(\mu_\tau)} + \gamma_3^{(l)\langle\sigma\rangle} \qquad l = 0, 1.
\end{aligned} \tag{12}$$

The term $\gamma_3^{(l)(\mu_\tau)}$ defines the free energy after the exit from the CR, and $\gamma_3^{(l)\langle\sigma\rangle}$ defines the free energy of ordering. These terms can be determined by the formulae

$$\begin{aligned}
\gamma_3^{(l)(\mu_\tau)} &= \gamma_g^{(l)} + \gamma_\rho^{(l)} \qquad & \gamma_g^{(l)} &= c_\nu^3 c_{\Delta_1}^l \bar{\gamma}_g^{(l)}\\
\gamma_\rho^{(l)} &= c_\nu^3 c_{\Delta_1}^l \bar{\gamma}_\rho^{(l)} & \gamma_3^{(l)\langle\sigma\rangle} &= c_\nu^3 c_{\Delta_1}^l \bar{\gamma}_3^{(l)\langle\sigma\rangle}.
\end{aligned} \tag{13}$$

The expressions for the quantities $\bar{\gamma}_g^{(l)}$, $\bar{\gamma}_\rho^{(l)}$, $\bar{\gamma}_3^{(l)\langle\sigma\rangle}$ independent of the microscopic parameters are given in [19]. The values of these quantities are contained in tables 2 and 3.

The entropy S_{IGR}, internal energy U_{IGR}, and specific heat C_{IGR} corresponding to the IGR can be written in the form

$$S_{IGR} = S_{\mu_\tau} + S_{\langle\sigma\rangle} \qquad U_{IGR} = U_{\mu_\tau} + U_{\langle\sigma\rangle} \qquad C_{IGR} = C_{\mu_\tau} + C_{\langle\sigma\rangle}. \tag{14}$$

Table 2. The universal parts $\bar{\gamma}_g^{(l)}$ and $\bar{\gamma}_\rho^{(l)}$ of the coefficients $\gamma_g^{(l)}$ and $\gamma_\rho^{(l)}$ (see (13)).

s	$\bar{\gamma}_g^{(0)}$	$\bar{\gamma}_g^{(1)}$	$\bar{\gamma}_\rho^{(0)}$	$\bar{\gamma}_\rho^{(1)}$
2.0000	−0.3024	−1.2299	1.0386	5.2424
2.7349	0.0039	0.1930	1.0227	3.3225
3.0000	0.0986	0.4368	1.0179	2.8748

Table 3. Values of the universal quantities $\bar{\gamma}_3^{(l)(\mu_\tau)}$ and $\bar{\gamma}_3^{(l)\langle\sigma\rangle}$.

s	$\bar{\gamma}_3^{(0)(\mu_\tau)}$	$\bar{\gamma}_3^{(1)(\mu_\tau)}$	$\bar{\gamma}_3^{(0)\langle\sigma\rangle}$	$\bar{\gamma}_3^{(1)\langle\sigma\rangle}$
2.0000	0.7362	4.0126	1.7618	−4.0212
2.7349	1.0265	3.5155	2.1572	−1.5739
3.0000	1.1164	3.3116	2.2808	−1.1610

The components of these thermodynamic characteristics satisfy the following relations:

$$\begin{aligned}
&S_\eta = -kN'[u_3^{(0)(\eta)}|\tau|^{1-\alpha} + u_3^{(1)(\eta)}|\tau|^{1-\alpha+\Delta_1}]\\
&U_\eta = -kTN'[u_3^{(0)(\eta)}|\tau|^{1-\alpha} + u_3^{(1)(\eta)}|\tau|^{1-\alpha+\Delta_1}]\\
&C_\eta = kN'[c_3^{(0)(\eta)}|\tau|^{-\alpha} + c_3^{(1)(\eta)}|\tau|^{\Delta_1-\alpha}]\\
&u_3^{(l)(\eta)} = c_\nu^3 c_{\Delta_1}^l \bar{u}_3^{(l)(\eta)} \qquad l = 0, 1\\
&\bar{u}_3^{(0)(\eta)} = 3\nu\bar{\gamma}_3^{(0)(\eta)} \qquad \bar{u}_3^{(1)(\eta)} = (3\nu+\Delta_1)\bar{\gamma}_3^{(1)(\eta)}\\
&c_3^{(l)(\eta)} = c_\nu^3 c_{\Delta_1}^l \bar{c}_3^{(l)(\eta)}\\
&\bar{c}_3^{(0)(\eta)} = 3\nu(3\nu-1)\bar{\gamma}_3^{(0)(\eta)}\\
&\bar{c}_3^{(1)(\eta)} = (3\nu+\Delta_1)(3\nu+\Delta_1-1)\bar{\gamma}_3^{(1)(\eta)}.
\end{aligned} \tag{15}$$

The exponent η can assume two values: μ_τ and $\langle\sigma\rangle$. The quantities $\bar{\gamma}_3^{(l)(\mu_\tau)} = \bar{\gamma}_g^{(l)} + \bar{\gamma}_\rho^{(l)}$ ($l = 0, 1$) are presented in table 3. The coefficients $\bar{\gamma}_3^{(l)\langle\sigma\rangle}$ are universal factors appearing in $\gamma_3^{(l)\langle\sigma\rangle}$ (see (13) and table 3).

Thus, we have calculated free energy in the IGR region. The values of the universal factors $\bar{\gamma}_{IGR}^{(l)} = \bar{\gamma}_3^{(l)(\mu_\tau)} + \bar{\gamma}_3^{(l)\langle\sigma\rangle}$ of the coefficients $\gamma_{IGR}^{(l)} = c_\nu^3 c_{\Delta_1}^l \bar{\gamma}_{IGR}^{(l)}$ in F_{IGR} (12) are given in table 1. Proceeding from the expression (12) for F_{IGR}, we have obtained other thermodynamic functions corresponding to the IGR. The expression (12) contains the free energy of ordering determined by integration with respect to CV ρ_0, whose average value is proportional to the order parameter which is an important characteristic of the phase transition.

5. Microscopic analogue of the Landau free energy and order parameter of a 3D Ising-like system

The role of the order parameter for the system under investigation is played by the average spin moment. It is associated with the existence of a nonzero value $\bar{\rho}_0$ below the phase transition temperature, for which the integrand of the expression

$$Z_{\mu_\tau+1} = \mathrm{e}^{-\beta F'_{\mu_\tau+1}} \int \exp\left[\beta\sqrt{N}\rho_0 h + \tilde{B}\rho_0^2 - \frac{G}{N}\rho_0^4 - \frac{D}{N^2}\rho_0^6\right] \mathrm{d}\rho_0 \tag{16}$$

attains its extremum value. Here $\beta = 1/(kT)$ is the inverse temperature; h is determined by the value of the constant external magnetic field $\mathcal{H}$ introduced in our analysis ($h = \mu_B\mathcal{H}$, μ_B

being the Bohr magneton). The expression for $-\beta F'_{\mu_\tau+1}$ corresponding to the contribution to the free energy of the system from CV ρ_k with the values of wavevectors $k \to 0$ (but not equal to zero) as well as the coefficients

$$\begin{aligned} \tilde{B} &= \tilde{B}^{(0)}|\tau|^{2\nu}\beta\tilde{\Phi}(0)(1+\tilde{B}^{(1)}|\tau|^{\Delta_1}) \\ G &= G^{(0)}|\tau|^{\nu}(\beta\tilde{\Phi}(0))^2(1+G^{(1)}|\tau|^{\Delta_1}) \\ D &= D^{(0)}(\beta\tilde{\Phi}(0))^3(1+D^{(1)}|\tau|^{\Delta_1}) \end{aligned} \tag{17}$$

are given in [19]. Carrying out in (16) the substitution of the variable

$$\rho_0 = \sqrt{N}\rho \tag{18}$$

we obtain

$$Z_{\mu_\tau+1} = \mathrm{e}^{-\beta F'_{\mu_\tau+1}}\sqrt{N}\int \mathrm{e}^{-NE_0(\rho)}\,\mathrm{d}\rho \tag{19}$$

and the evaluation of the order parameter is reduced to determining the extremum point $\bar{\rho}$ of the expression

$$E_0(\rho) = D\rho^6 + G\rho^4 - \tilde{B}\rho^2 - \beta h\rho. \tag{20}$$

The value of $\bar{\rho}$ coincides with the average value of ρ corresponding to the equilibrium value of the order parameter [6, 14, 15]. The expression for $E_0(\rho)$ defines the fraction of free energy associated with the order parameter. It corresponds to a microscopic analogue of the Landau free energy. The quantity $Z_{\mu_\tau+1}$ will be expressed in terms of $E_0(\bar{\rho})$ (coinciding in form with the expansion of the free energy into a power series in the order parameter) by using the steepest descent method for evaluating the integral (19) (see [19]).

The expression (20) was derived by successive elimination of 'insignificant' variables ρ_k with $k \neq 0$, which allowed us to calculate the coefficients of $E_0(\rho)$ (see table 4). Numerical values in table 4 are given for some values of the effective radius b of the potential and optimal values of the RG parameter s. As in the case of $T > T_c$ [8, 18], the parabolic approximation of the Fourier transform of the exponentially decreasing potential of interaction in the region of small values of wavevectors for $b = b_{\mathrm{I}} = c/(2\sqrt{3})$ corresponds to the analogous approximation of the Fourier transform for the potential of interaction between nearest neighbours, nearest and next-nearest neighbours for $b = b_{\mathrm{II}} = 0.3379c$, and first, second, and third neighbours for $b = b_{\mathrm{III}} = 0.3584c$. Thus, there is no need to postulate a temperature dependence of the coefficients in formula (20) (as in the case of the Landau expansion) since the analytic form of their dependence on the temperature and microscopic parameters of the system has been obtained as a result of direct calculations. In contrast to case for the Landau theory, the temperature dependence of these coefficients is nonanalytic (see (17)).

Let us go over to direct calculation of the average spin moment. The point $\bar{\rho}$ can be determined from the condition for the extremum $\partial E_0(\rho)/\partial\rho = 0$ or

$$6D\bar{\rho}^5 + 4G\bar{\rho}^3 - 2\tilde{B}\bar{\rho} - \frac{h}{kT} = 0. \tag{21}$$

For $h = 0$, we obtain the biquadratic equation

$$6D\bar{\rho}^4 + 4G\bar{\rho}^2 - 2\tilde{B} = 0 \tag{22}$$

in which the substitution of the variable

$$\bar{\rho}^2 = y \tag{23}$$

leads to the equation

$$6Dy^2 + 4Gy - 2\tilde{B} = 0. \tag{24}$$

Table 4. Values of quantities determining the coefficients in the expression for a microscopic analogue of the Landau free energy.

b	b_{I}	b_{II}	b_{III}	c	$2c$
			$s = 2.0000$		
$\tilde{B}^{(0)}$	1.0106	0.9530	0.9305	0.7258	0.7149
$\tilde{B}^{(1)}$	−0.2733	−0.3959	−0.4420	−0.8188	−0.8375
$G^{(0)}$	0.0550	0.0857	0.1010	1.9382	15.3880
$G^{(1)}$	−0.8919	−1.2918	−1.4423	−2.6720	−2.7330
$D^{(0)}$	0.0009	0.0023	0.0033	1.5614	99.9318
$D^{(1)}$	−0.6952	−0.9377	−1.0470	−1.9396	−1.9839
			$s = 2.7349$		
$\tilde{B}^{(0)}$	0.9417	0.8888	0.8683	0.6865	0.6768
$\tilde{B}^{(1)}$	−0.4451	−0.5124	−0.5377	−0.7445	−0.7550
$G^{(0)}$	0.0690	0.1074	0.1267	2.4478	19.4434
$G^{(1)}$	−1.1718	−1.3491	−1.4157	−1.9601	−1.9876
$D^{(0)}$	0.0012	0.0031	0.0044	2.0825	133.281
$D^{(1)}$	−0.8853	−1.0193	−1.0696	−1.4809	−1.5017
			$s = 3.0000$		
$\tilde{B}^{(0)}$	0.9115	0.8610	0.8415	0.6697	0.6605
$\tilde{B}^{(1)}$	−0.4755	−0.5321	−0.5533	−0.7261	−0.7348
$G^{(0)}$	0.0732	0.1141	0.1346	2.6087	20.7264
$G^{(1)}$	−1.1967	−1.3392	−1.3926	−1.8275	−1.8495
$D^{(0)}$	0.0013	0.0033	0.0047	2.2185	141.986
$D^{(1)}$	−0.9113	−1.0199	−1.0606	−1.3918	−1.4085

Table 5. Coefficients of the average spin moment $\langle\sigma\rangle$ in (25) for some values of the effective radius b of the potential and the RG parameter s.

b	b_{I}	b_{II}	b_{III}	c	$2c$
			$s = 2.0000$		
$\langle\sigma\rangle^{(0)}$	2.7329	2.0684	1.8700	0.3747	0.1321
$\langle\sigma\rangle^{(1)}$	0.2499	0.3619	0.4040	0.7485	0.7656
			$s = 2.7349$		
$\langle\sigma\rangle^{(0)}$	2.3854	1.8027	1.6288	0.3248	0.1145
$\langle\sigma\rangle^{(1)}$	0.3034	0.3493	0.3666	0.5076	0.5147
			$s = 3.0000$		
$\langle\sigma\rangle^{(0)}$	2.2861	1.7269	1.5600	0.3107	0.1095
$\langle\sigma\rangle^{(1)}$	0.3046	0.3409	0.3545	0.4651	0.4707

Solving this equation and separating temperature explicitly, we arrive at the following formula for the average spin moment $\langle\sigma\rangle = \bar{\rho} = \sqrt{y}$:

$$\langle\sigma\rangle = \langle\sigma\rangle^{(0)}|\tau|^{\beta}(1 + \langle\sigma\rangle^{(1)}|\tau|^{\Delta_1}). \tag{25}$$

Here $\beta = \nu/2$ is the critical exponent of the average spin moment, and the coefficients $\langle\sigma\rangle^{(l)}$ [19] are given in table 5.

The curves describing the dependence of $\langle\sigma\rangle$ on τ for various values of b are shown in figure 1. Here and below, the curves are plotted for the RG parameter $s = 3$.

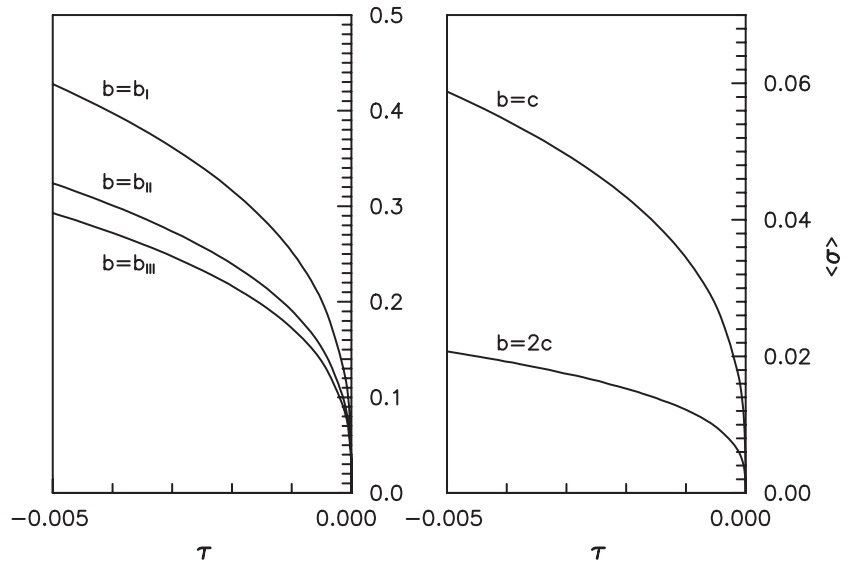

Figure 1. The temperature dependence of the average spin moment of the system in the ρ^6 model approximation for various values of the effective radius b of the potential: $b_{\rm I} = c/(2\sqrt{3})$; $b_{\rm II} = 0.3379c$; $b_{\rm III} = 0.3584c$; c; and $2c$.

6. Thermodynamic characteristics as functions of temperature and microscopic parameters of the system

Let us now find total expressions for the thermodynamic functions of an Ising-like system at $T < T_c$ in the approximation of the ρ^6 model taking into account the first confluent correction (the case $\mathcal{H} = 0$).

The contributions from the CR and IGR regions to the free energy of the 3D Ising model near T_c obtained above allow us to write its total free energy (1) in the form

$$F = -kTN'[\gamma_0 - \gamma_1|\tau| + \gamma_2|\tau|^2 + \gamma_3^{(0)-}|\tau|^{3\nu} + \gamma_3^{(1)-}|\tau|^{3\nu+\Delta_1}]. \tag{26}$$

All the coefficients in expression (26) are functions of microscopic parameters of the system, i.e., the effective radius b of the potential, the Fourier transform $\tilde{\Phi}(0)$ of the potential, and the lattice constant c. The coefficients γ_0, γ_1, and γ_2 can be determined from expressions for corresponding quantities in the high-temperature region (see [8, 18]). In contrast to $\gamma_3^{(l)-}$ $(l = 0, 1)$, their values are independent of whether calculations are made for a temperature above or below the phase transition point. The coefficients $\gamma_3^{(l)-}$ have the form of a product of the quantity $\bar{\gamma}_3^{(l)-}$, which is universal relative to microscopic parameters, and the nonuniversal factor $c_\nu^3 c_{\Delta_1}^l$, which is a function of these parameters:

$$\begin{aligned} &\gamma_3^{(l)-} = c_\nu^3 c_{\Delta_1}^l \bar{\gamma}_3^{(l)-} \qquad l = 0, 1 \\ &\bar{\gamma}_3^{(l)-} = -\bar{\gamma}_3^{(CR)(l)-} + \bar{\gamma}_{IGR}^{(l)} \qquad \bar{\gamma}_{IGR}^{(l)} = \bar{\gamma}_g^{(l)} + \bar{\gamma}_\rho^{(l)} + \bar{\gamma}_3^{(l)\langle\sigma\rangle}. \end{aligned} \tag{27}$$

Numerical values of the coefficients $\bar{\gamma}_3^{(l)-}$ are given in table 1.

Proceeding from the expression (26) for free energy F, we can find other thermodynamic functions for $T < T_c$. For example, the following expressions are valid for the entropy S,

internal energy U, and specific heat C:

$$\begin{aligned} S &= kN'[s^{(0)} - c_0|\tau| - u_3^{(0)-}|\tau|^{1-\alpha} - u_3^{(1)-}|\tau|^{1-\alpha+\Delta_1}] \\ U &= kTN'[\gamma_1 - u_1|\tau| - u_3^{(0)-}|\tau|^{1-\alpha} - u_3^{(1)-}|\tau|^{1-\alpha+\Delta_1}] \\ C &= kN'[c_0 + c_3^{(0)-}|\tau|^{-\alpha} + c_3^{(1)-}|\tau|^{\Delta_1-\alpha}] \end{aligned} \tag{28}$$

where $s^{(0)}$, c_0, and u_1 coincide with the corresponding quantities for $T > T_c$ [8, 18], while the structure of the remaining coefficients in terms of universality is determined by the relations

$$\begin{aligned} &u_3^{(l)-} = c_\nu^3 c_{\Delta_1}^l \bar{u}_3^{(l)-} \qquad l = 0, 1 \\ &\bar{u}_3^{(0)-} = 3\nu\bar{\gamma}_3^{(0)-} \qquad \bar{u}_3^{(1)-} = (3\nu + \Delta_1)\bar{\gamma}_3^{(1)-} \\ &c_3^{(l)-} = c_\nu^3 c_{\Delta_1}^l \bar{c}_3^{(l)-} \\ &\bar{c}_3^{(0)-} = 3\nu(3\nu - 1)\bar{\gamma}_3^{(0)-} \\ &\bar{c}_3^{(1)-} = (3\nu + \Delta_1)(3\nu + \Delta_1 - 1)\bar{\gamma}_3^{(1)-}. \end{aligned} \tag{29}$$

Representing the specific heat from (28) by the dependence

$$\begin{aligned} &\frac{C}{kN'} = \frac{A^-}{\alpha}|\tau|^{-\alpha}(1 + \alpha a_c^-|\tau|^{\Delta_1}) + B^- \\ &A^- = c_\nu^3 \alpha \bar{c}_3^{(0)-} \\ &a_c^- = \frac{c_{\Delta_1}}{\alpha}\frac{\bar{c}_3^{(1)-}}{\bar{c}_3^{(0)-}} \qquad B^- = c_0 \end{aligned} \tag{30}$$

(similar to the $T > T_c$ case), we obtain the following expressions for ratios of the leading critical amplitudes and the amplitudes of corrections to scaling at temperatures above and below the phase transition temperature:

$$\frac{A^+}{A^-} = \frac{\bar{c}_3^{(0)+}}{\bar{c}_3^{(0)-}} \qquad \frac{a_c^+}{a_c^-} = \frac{\bar{c}_3^{(1)+}}{\bar{c}_3^{(1)-}}\frac{\bar{c}_3^{(0)-}}{\bar{c}_3^{(0)+}}. \tag{31}$$

It should be noted that B^- is equal to B^+ calculated for $T > T_c$. The amplitudes A^- and a_c^- are given in table 6.

Equation (21) makes it possible to calculate the susceptibility of the system per particle, i.e., $\chi = \mu_B(\partial\langle\sigma\rangle/\partial\mathcal{H})$:

$$\chi = \Gamma^-|\tau|^{-\gamma}(1 + a_\chi^-|\tau|^{\Delta_1})\frac{\mu_B^2}{\tilde{\Phi}(0)}. \tag{32}$$

Here $\gamma = 2\nu$ is the critical exponent of the susceptibility. The values of the amplitudes Γ^- and a_χ^- [19] are given in table 6. Our estimates for the leading critical amplitude Γ^- (see table 6; $b = b_1$) agree closely with the low-temperature susceptibility amplitude $\Gamma^- = 0.220 \pm 0.004$ calculated by Liu and Fisher [20].

Using the results of calculations for $T > T_c$ [8] as well as the results obtained here, we can plot graphs of the temperature dependences of the entropy S/kN, specific heat C/kN, and susceptibility χ (in units of μ_B^2/A, $A = \tilde{\Phi}(0)/[8\pi(b/c)^3]$ being the interaction potential constant) near T_c for various values of the effective radius b of the potential (see figures 2–4). The method of calculation developed here allows us to trace the evolution of thermodynamic characteristics with increasing ratio of the effective radius b of the potential to the lattice constant c. Such an evolution of the free energy F/N of the system (in units of A) at the phase transition point ($\tau = 0$) as well as those of the average spin moment $\langle\sigma\rangle$ for $\tau = -10^{-3}$ and the specific heat C/kN of the system for $|\tau| = 10^{-3}$ are presented in figures 5–7.

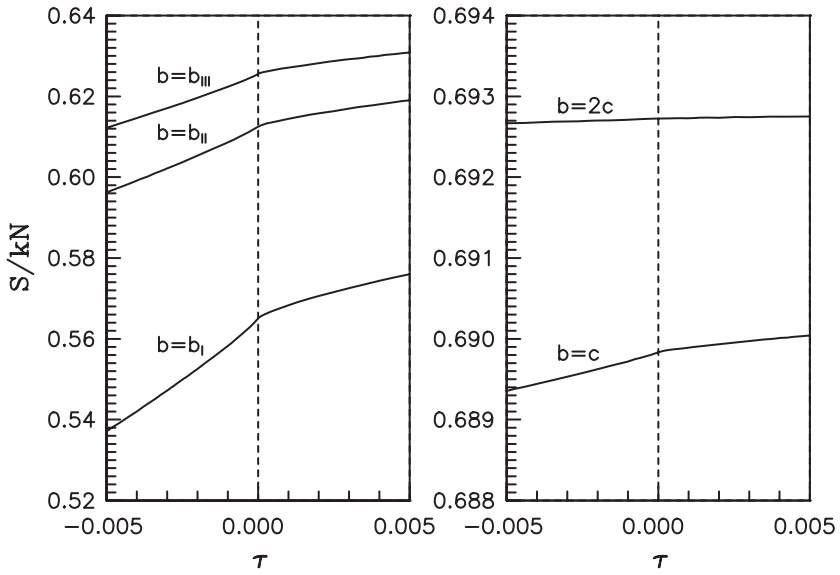

Figure 2. The dependence of the entropy of the system on τ. The notation is the same as in figure 1.

Table 6. Numerical values of the amplitudes A^-, a_c^-, Γ^-, and a_χ^-.

b	b_{I}	b_{II}	b_{III}	c	$2c$
			$s = 2.0000$		
A^-	1.9734	1.8071	1.7436	1.2012	1.1741
a_c^-	7.2567	10.5104	11.7347	21.7395	22.2353
Γ^-	0.2133	0.2262	0.2317	0.2970	0.3015
a_χ^-	0.1872	0.2711	0.3027	0.5608	0.5736
			$s = 2.7349$		
A^-	1.2026	1.1027	1.0648	0.7486	0.7328
a_c^-	8.1288	9.3588	9.8206	13.5975	13.7882
Γ^-	0.2341	0.2480	0.2539	0.3211	0.3257
a_χ^-	0.3536	0.4071	0.4272	0.5915	0.5998
			$s = 3.0000$		
A^-	1.0331	0.9484	0.9164	0.6506	0.6373
a_c^-	7.9599	8.9081	9.2633	12.1558	12.3022
Γ^-	0.2437	0.2580	0.2640	0.3318	0.3364
a_χ^-	0.3884	0.4346	0.4519	0.5931	0.6002

7. Conclusions

Thus, the critical behaviour of a one-component spin system is described on the basis of sextic density of measure (ρ^6 model). As compared with the quartic approximation (ρ^4 model), the ρ^6 model ensures a more correct quantitative pattern for this description. This follows from the results of our previous calculations (see, for example, [8, 14, 15]) as well as from the temperature dependences of the average spin moment $\langle\sigma\rangle$ (figure 8) and the specific heat C/kN (figure 9) of the 3D Ising model. The calculations were made for a simple cubic lattice in zero external field with the interaction between nearest neighbours. In our calculations, we put $b = b_{\mathrm{I}} = c/(2\sqrt{3})$. The ρ^6 model approximation includes the first confluent correction,

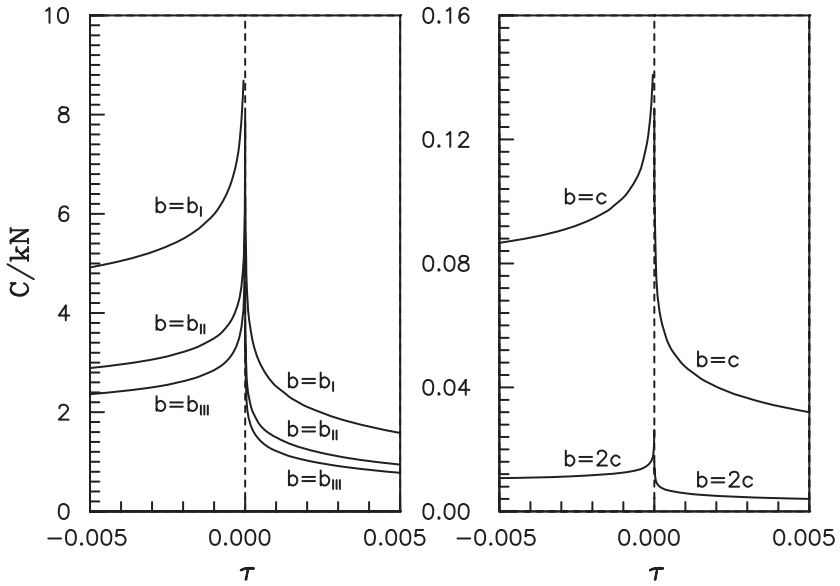

Figure 3. The specific heat of the spin system for various values of b. The notation is the same as in figure 1.

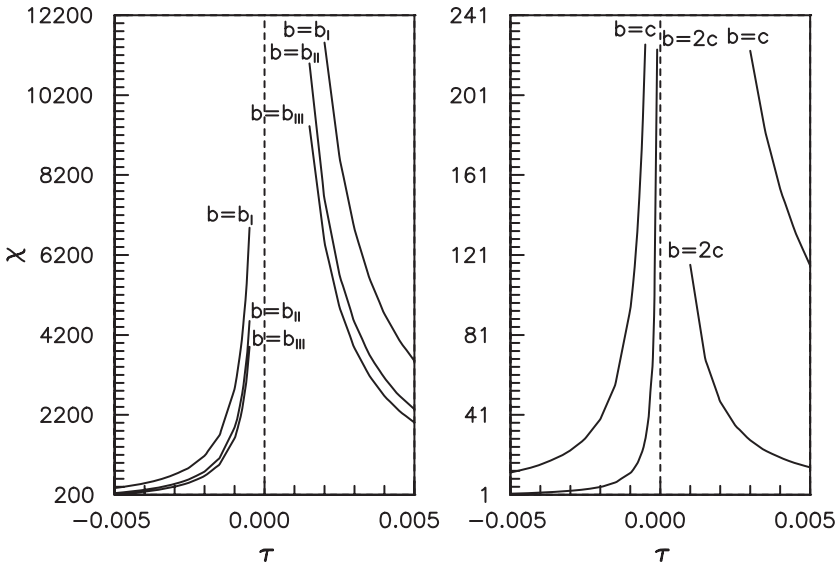

Figure 4. The temperature dependence of the susceptibility of the system for various values of b. The notation is the same as in figure 1.

while the approximation on the basis of the ρ^4 model takes into account the first and second confluent corrections (see [11–13]). The straight line 1 in figure 8 for the average spin moment corresponds to the ρ^4 model, line 2 to the ρ^6 model, and line 3 to the results obtained by Liu and Fisher [20] for $\tau = |T - T_c|/T_c$. The high-temperature region in figure 9 is represented by the curves 1, 2, and 3, while the low-temperature region is represented by the curves 1′,

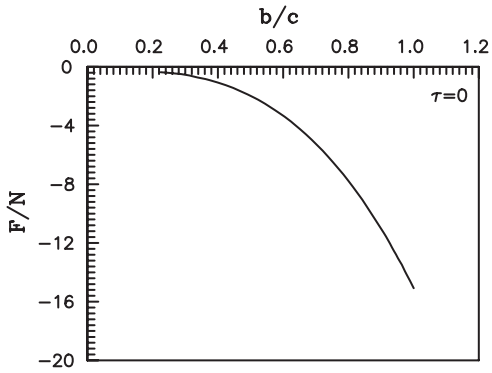

Figure 5. The dependence of the free energy of the system at the phase transition point ($\tau = 0$) on the ratio of the effective radius b of the exponentially decreasing interaction potential to the simple cubic lattice constant c.

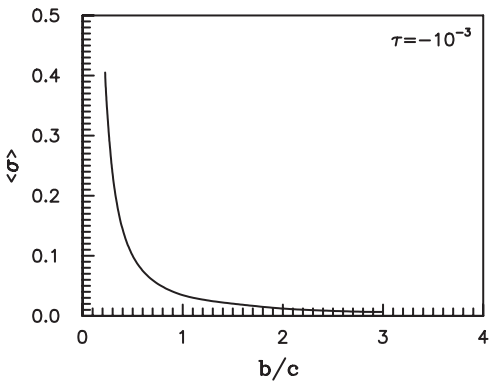

Figure 6. The behaviour of the average spin moment for $\tau = -10^{-3}$ with increasing ratio b/c.

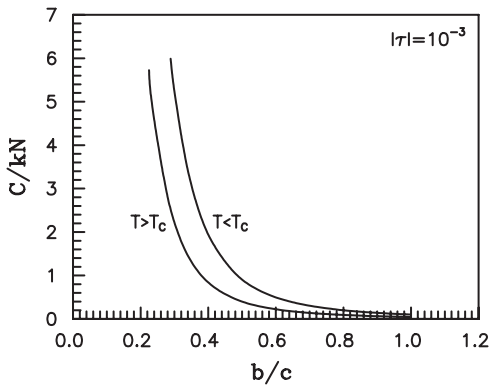

Figure 7. The evolution of the specific heat of the system for $|\tau| = 10^{-3}$ with increasing ratio b/c.

$2'$, and $3'$. The curves 1 and $1'$were obtained on the basis of the ρ^4 model, curves 2 and $2'$ in the ρ^6 model approximation, and curves 3 and $3'$correspond to the results obtained by Liu and Fisher [20]. It should be noted that the latter carried out a new numerical analysis of leading

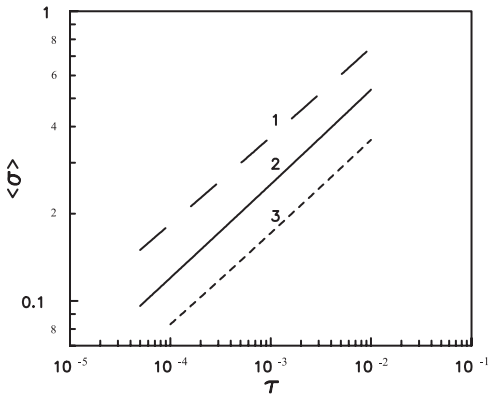

Figure 8. The temperature dependence of the order parameter of the 3D Ising model for a simple cubic lattice. Straight line 1 corresponds to the ρ^4 model, line 2 to the ρ^6 model, and line 3 to the results obtained in [20].

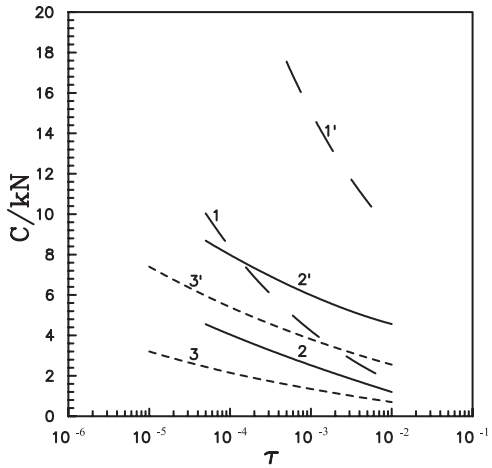

Figure 9. The dependence of the specific heat of the system on $\tau = |T - T_c|/T_c$. Curves 1, 2, and 3 correspond to $T > T_c$; curves $1'$, $2'$, and $3'$correspond to $T < T_c$. Curves 1 and $1'$correspond to the ρ^4 model, curves 2 and $2'$correspond to the ρ^6 model, and curves 3 and $3'$correspond to the results obtained in [20].

critical amplitudes of the susceptibility, correlation length, specific heat, and spontaneous magnetization of 3D nearest-neighbour sc (simple cubic), bcc (body-centred cubic), and fcc (face-centred cubic) Ising models, as well as universal relations between these amplitudes. Modern estimates of the critical temperature and exponents in [20] are used in conjunction with biased inhomogeneous differential approximants to extrapolate the longest available series expansions to find the critical amplitudes. As is clearly seen from figures 8 and 9, the plots for the ρ^6 model agree more closely with the Liu and Fisher's results than the estimates in the ρ^4 model approximation.

The CV method makes it possible to carry out the approximate calculation of the partition function of the system and to obtain universal (critical exponents) and nonuniversal quantities (expressions for leading critical amplitudes and the amplitudes of confluent corrections to thermodynamic characteristics) by using a unified approach. The results of calculations for a

3D Ising system on the basis of the ρ^4 and ρ^6 models are in accord with the results obtained by other authors. For example [14, 15], we found the critical exponents of the correlation length $\nu = 0.637$, the specific heat $\alpha = 0.088$, the average spin moment $\beta = 0.319$, the susceptibility $\gamma = 1.275$, and the exponent of the first correction to scaling $\Delta_1 = 0.525$ (ρ^6 model, $s = s^*$), as well as universal ratios of critical amplitudes of the specific heat $A^+/A^- = 0.435$, the susceptibility $\Gamma^+/\Gamma^- = 6.967$, and their combinations $\mathcal{P} = [1 - A^+/A^-]/\alpha = 3.054$, $R_c^+ = A^+\Gamma^+/[s_0^3(\langle\sigma\rangle^{(0)})^2] = 0.098$ (ρ^4 model, $s = s^*$), where $s_0 = \pi\sqrt{2}b/c$, $\langle\sigma\rangle^{(0)}$ is the critical amplitude of the average spin moment (see (25)). These estimates agree with the values $\nu = 0.630$, $\alpha = 0.110$, $\beta = 0.325$, $\gamma = 1.241$, $\Delta_1 = 0.498$, $A^+/A^- = 0.465$, $\Gamma^+/\Gamma^- = 5.12$, $\mathcal{P} = 3.90$, $R_c^+ = 0.052$ obtained by using the field-theory approach [21–23] as well as with the values $\nu = 0.638$, $\alpha = 0.125$, $\beta = 0.312$, $\gamma = 1.250$, $\Delta_1 = 0.50$, $A^+/A^- = 0.51$, $\Gamma^+/\Gamma^- = 5.07$, $R_c^+ = 0.059$ calculated with the help of high-temperature expansions [24–28]. The methods existing at present make it possible to calculate universal quantities to a quite high degree of accuracy (see, for example, [3, 5, 20, 29]). The advantage of the method under investigation lies in the possibility of obtaining and analysing expressions for thermodynamic characteristics as functions of microscopic parameters of the system.

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