A Method for the Calculation of Thermodynamic Functions for the 3D Model Systems in the Critical Region

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Dedicated to Dr. Karl Heinzinger on the occasion of his 60th birthday

A method for the calculation of the thermodynamic functions in the three-dimensional Ising model near the phase transition is proposed. In the frame of a uniform approach, the critical exponents and the critical amplitudes of the main characteristics of the model (i.e. free energy, enthropy, specific heat, etc.) are obtained as functions of microscopic Hamiltonian parameters.

It is shown that the correct sign and temperature behaviour of the entropy are provided due to the contribution of the long-wave spin moment modes. The short-wave ones are responsible for the values of the critical exponents.

Investigations of thermodynamic and structural functions near phase transitions have shown that there exist characteristics which depend on the universality class of the system only. First of all, this refers to the critical exponents and the ratio of the critical amplitudes below and above the phase transition temperature T_c, including confluent corrections [1–3]. However, the main problem of phase transition theory, i.e. the calculation of explicit expressions for the thermodynamic and correlation functions near the phase transition as functions of temperature and macroscopic parameters of the system is still unsolved. An essential progress in the solution of this problem was achieved by the collective variables (CV) method [4, 5] for the calculation of the partition function of the 3D Ising model. Using this method, it was found that the microscopic calculations of the explicit expressions for the free energy, specific heat, and other characteristics of the system near T_c can be performed by separating the contributions of the short-wave and long-wave fluctuations of the spin moment density.

In the present paper, expressions for the main thermodynamic functions near T_c, including corrections to scaling, are obtained and discussed in the frame of the CV method. These expressions contain an universal part and a part which depends on the microscopic parameters of the system. The correct description of the liquid-gas transition is necessary for the construction of a comprehensive liquid state theory. The order parameter, which arises in the liquid phase, should be introduced into the calculation of the thermodynamic and distribution functions of the liquid. There are several stages in the description of the phase tranition, and the main one can be reduced to the solution of the Ising problem. Therefore, in the liquid-gas problem the Ising model is of special importance. In this connection we suggest a complete solution of the Ising model, which can be used for a comprehensive description of the properties of equilibrium liquids. We hope that the present paper may be considered as complementary to some extent to the investigations of liquids by Dr. Heinzinger and his co-workers.

1. Main Statements

Let us consider the simplest nontrivial model for a phase transition, that is the 3D Ising model. The Hamiltonian is

$$H = -\tfrac{1}{2} \sum_{i,j} \Phi(r_{ij})\, \sigma_i\, \sigma_j\,,$$

where $\Phi(r_{ij})$ is the potential of the interaction between particles located at the sites i and j of a simple cubic lattice with the lattice constant c, and σ_i is the operator of the z-component of the spin belonging to the site i and possessing the two eigenvalues ± 1. The interaction potential can be represented in the form

$$\Phi(r_{ij}) = A \exp(-r_{ij}/b)$$

with A being a constant and b standing for the distance of the effective interaction.

The application of the CV method is connected with the existence of the Fourier transform $\tilde{\Phi}$ of Φ. In the

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present consideration we use the parabolic approximation $\tilde{\Phi}(\varkappa)=\tilde{\Phi}(0)(1-2b^2\varkappa^2)$, where $\tilde{\Phi}(0)=8\pi A(b/c)^3$. The wavevector $\varkappa$ varies in the range $[0, B']$, where $B'=1/(b\sqrt{2})$. In the following consideration we take into account that the general expression for the Fourier transform takes small values in the range $\varkappa\in(B', B]$, where $B=\pi/c$ is the boundary of the first Brillouin semizone. In this range we put $\tilde{\Phi}(\varkappa)=0$ [5].

The transition from spin variables to collective variables $\varrho_{\varkappa}$ is performed using the functional representation for the operators of spin density vibration modes:

$$\begin{aligned}
\hat{\varrho}^c_{\varkappa} &= \int \varrho^c_{\varkappa}\, J(\varrho-\hat{\varrho})(\mathrm{d}\varrho)^N, \\
\hat{\varrho}^s_{\varkappa} &= \int \varrho^s_{\varkappa}\, J(\varrho-\hat{\varrho})(\mathrm{d}\varrho)^N, \qquad (1.1)\\
\hat{\varrho}_0 &= \int \varrho_0\, J(\varrho-\hat{\varrho})(\mathrm{d}\varrho)^N,
\end{aligned}$$

where

$$\hat{\varrho}^c_{\varkappa} = \frac{1}{\sqrt{N}}\sum_e \sigma_e \cos(\varkappa\, \boldsymbol{l}),$$

$$\hat{\varrho}^s_{\varkappa} = \frac{1}{\sqrt{N}}\sum_e \sigma_e \sin(\varkappa\, \boldsymbol{l}),$$

$$\hat{\varrho}_0 = \frac{1}{\sqrt{N}}\sum_e \sigma_e\,.$$

The transition operator $J(\varrho-\hat{\varrho})$ has the form

$$J(\varrho-\hat{\varrho}) = \delta(\varrho_0-\hat{\varrho}_0)\prod_{\varkappa}{}'\,[\delta(\varrho^c_{\varkappa}-\hat{\varrho}^c_{\varkappa})\,\delta(\varrho^s_{\varkappa}-\hat{\varrho}^s_{\varkappa})].$$

The validity of (1.1) is easily verified when replacing the δ functions by their integral representations:

$$J(\varrho-\hat{\varrho}) = \int(\mathrm{d}\omega)^N \exp\Big\{2\pi i\,[\omega_0(\varrho_0-\hat{\varrho}_0) + \sum_{\varkappa}{}'\,\omega^c_{\varkappa}(\varrho^c_{\varkappa}-\hat{\varrho}^c_{\varkappa})+\omega^s_{\varkappa}(\varrho^s_{\varkappa}-\hat{\varrho}^s_{\varkappa})]\Big\},$$

where

$$(\mathrm{d}\omega)^N = \mathrm{d}\omega_0\prod_{\varkappa}{}'\,\mathrm{d}\omega^c_{\varkappa}\,\mathrm{d}\omega^s_{\varkappa}\,.$$

The prime at the product sign means that the subscripts $\varkappa$ take the values from the upper semicube of the Brillouin zone, except $|\varkappa|\,[/]=0$.

$$(\mathrm{d}\varrho)^N = \mathrm{d}\varrho_0\prod_{\varkappa}{}'\,\mathrm{d}\varrho^c_{\varkappa}\,\mathrm{d}\varrho^s_{\varkappa}\,.$$

N is the number of sites. For convenience the complex variables $\varrho_{\varkappa}=\varrho^c_{\varkappa}-i\varrho^s_{\varkappa}$ are introduced, as well as the conjugated ones $\omega_{\varkappa}=\frac{1}{2}(\omega^c_{\varkappa}+i\omega^s_{\varkappa})$.

The partition function of the system $Z=\mathrm{Sp}\, e^{-\beta H}$ takes the following form in the CV space [5, 7]:

$$Z = \int\exp\Big(\tfrac{1}{2}\sum_{\varkappa\leqq B}\beta\tilde{\Phi}(\varkappa)\,\varrho_{\varkappa}\varrho_{-\varkappa}\Big) J(\varrho)(\mathrm{d}\varrho)^N. \qquad (1.2)$$

Here $\beta=(kT)^{-1}$ and $J(\varrho)$ is the transition Jacobian from the spin variables to the CVs:

$$J(\varrho) = \exp\sum_{p>m}\hat{\mathscr{D}}_{2p}\left(\frac{\partial}{\partial\varrho_{\varkappa}}\right)J^{(0)}_m(\varrho)\,,$$

where the basic transition Jacobian of the ϱ^{2m} model has the form

$$J^{(0)}_m(\varrho) = 2^N\int\exp\left[2\pi i\sum_{\varkappa\leqq B}\omega_{\varkappa}\varrho_{\varkappa}+\sum_{n=1}^{m}D_{2n}(\omega)\right](\mathrm{d}\omega)^N, \qquad (1.3)$$

where

$$\begin{aligned}
&\hat{\mathscr{D}}_{2p}\left(\frac{\partial}{\partial\varrho_{\varkappa}}\right)\\
&\quad = \frac{\mathscr{M}_{2p}}{(2p)!}\sum_{\varkappa_1,\dots,\varkappa_{2p}}N^{1-p}\frac{\partial}{\partial\varrho_{\varkappa_2}}\cdots\frac{\partial}{\partial\varrho_{\varkappa_{2p}}}\delta_{\varkappa_1+\dots+\varkappa_{2p}}\,,
\end{aligned}$$

$$D_{2n}(\omega) = \frac{(2\pi i)^{2n}}{(2n)!}\frac{\mathscr{M}_{2n}}{N^{n-1}}\sum_{\varkappa_1,\dots,\varkappa_{2n}}\omega_{\varkappa_1}\dots\omega_{\varkappa_{2n}}\delta_{\varkappa_1+\dots+\varkappa_{2n}}\,,$$

$$\mathscr{M}_{2n} = \frac{\partial^{2n}}{\partial h^{2n}}\ln\mathrm{ch}\, h\Big|_{h\to 0}\,.$$

The choice of the ϱ^{2m} model implies a certain approximation of the integrand in (1.3) (ϱ^4 model for $m=2$, ϱ^6 model for $m=3$, etc.). The simplest nontrivial model allowing to exceed the frame of the "classical" description of the system near the phase transition is the ϱ^4 model. The latter one is the subject of the following considerations, where we put $J(\varrho)=J^{(0)}_m(\varrho)$.

The explicit expression for the partition function of the model is obtained from (1.2) by performing the integration over the variables $\omega_{\varkappa}$ in (1.3): (1.4)

$$\begin{aligned}
Z = {}&2^N\,2^{\frac{1}{2}(N'-1)}\,e^{a_0' N'}\int\exp\Bigg[-\frac{1}{2}\sum_{\varkappa\leqq B'}d'(\varkappa)\,\varrho_{\varkappa}\varrho_{-\varkappa}\\
&-\frac{1}{4!}(N')^{-1}\sum_{\varkappa_1,\dots,\varkappa_4\leqq B'}a_4'\,\varrho_{\varkappa_1}\dots\varrho_{\varkappa_4}\delta_{\varkappa_1+\dots+\varkappa_4}\Bigg](\mathrm{d}\varrho)^{N'}.
\end{aligned}$$

Here

$$e^{a_0'} = (2\pi)^{-\frac{1}{2}}\left(\frac{3}{\mathscr{M}_4'}\right)^{\frac{1}{4}}\exp[(y')^2/4]\,U(0, y'),$$

$$d'(\varkappa) = \mathrm{a}_2' - \beta\tilde{\Phi}(\varkappa),\quad \alpha_2' = \left(\frac{3}{\mathscr{M}_4'}\right)^{\frac{1}{2}}U(y'), \qquad (1.5)$$

$$a_4' = \frac{3}{\mathscr{M}_4'}\varphi(y'),\quad \mathscr{M}_4' = 2^{-\frac{1}{2}}\pi^{-3}\left(\frac{c}{b}\right)^3,$$

$$N' = N s_0^{-3}\quad\left(s_0=\pi\sqrt{2}\,\frac{b}{c}\right).$$

The functions $U(y')$, $\varphi(y')$ are combinations of the Weber parabolic cylinder function $U(a, y')$ [9]:

$$U(y') = U(1, y')/U(0, y'),$$
$$\varphi(y') = 3\,U^2(y') + 2\,y'\,U(y') - 2\,,$$

where

$$y' = 2\sqrt{3}\,\pi^{\frac{3}{2}}\left(\frac{b}{c}\right)^{\frac{3}{2}}.$$

The coefficients a'_{2l} are functions of the microscopic parameters of the model. In the considered case they depend on the ratio of the effective interaction radius b and the lattice constant c. In the case $b=c$ we have $a'_0 = -0.9217$, $a'_2 = 0.9889$, $a'_4 = 0.0211$.

The calculation of (1.4) is performed by using the layer integration technique described in [5] and [6]. For this purpose, the phase space is divided into layers which involve $\varrho_{\varkappa}$ with certain values of the wave vector. In every layer of CVs (corresponding to the wave vector region (B_{n+1}, B_n), $B_{n+1} = \dfrac{B_n}{s}$, $s>1$), $\tilde{\Phi}(\varkappa)$ is replaced by its mean value. In the result of n consecutive integrations performed for relatively great wave vectors, the partition function is represented in the form of the product of the partial partition functions up to Q_n and the remaining integral:

$$Z = 2^N\,Q_0 Q_1 \ldots Q_n \int \mathscr{W}_{n+1}(\varrho)(\mathrm{d}\varrho)^{N_{n+1}}\,. \qquad (1.6)$$

The measure density of the $(n+1)$-th block structure $\mathscr{W}_{n+1}(\varrho)$ is of the form

$$\mathscr{W}_{n+1}(\varrho) = \exp\Bigg[-\frac{1}{2}\sum_{\varkappa \leqq B_{n+1}} d_{n+1}(\varkappa)\,\varrho_{\varkappa}\,\varrho_{-\varkappa} \qquad (1.7)$$
$$-\frac{1}{4!}\,N_{n+1}^{-1}\sum_{\varkappa_1,\ldots,\varkappa_4 \leqq B_{n+1}} a_4^{(n+1)}\,\varrho_{\varkappa_1}\ldots\varrho_{\varkappa_4}\,\delta_{\varkappa_1+\cdots+\varkappa_4}\Bigg].$$

Here $d_{n+1}(\varkappa) = a_2^{(n+1)} - \beta\tilde{\Phi}(\varkappa)$, $N_{n+1} = N's^{-3(n+1)}$, and $a_{2l}^{(n+1)}$ are the transformed a'_{2l} coefficients after integration over the $(n+1)$-th layer of CVs. For Q_n we have

$$Q_n^{1/N_n} = \left(\frac{3}{\varphi(y_{n-1})}\right)^{\frac{1}{4}} \exp\left(\frac{x_n^2}{4} + \frac{y_{n-1}^2}{4}\right) U(0, x_n)\,U(0, y_{n-1}). \qquad (1.8)$$

For $n=0$:

$$Q_0^{1/N'} = e^{a'_0}\,Q(d), \quad \text{where} \quad N' = N s_0^{-3}\left(s_0 = \frac{B}{B'}\right),$$

$$Q(d) = (2\pi)^{\frac{1}{2}}\left(\frac{3}{a'_4}\right)^{\frac{1}{4}} \exp\left(\frac{x_0^2}{4}\right) U(0, x_0)\,.$$

We use the following integral representation for the parabolic cylinder function $U(a, t)$ of the a-th order with argument t [9]:

$$U(a, t) = \frac{2}{\Gamma(a+\frac{1}{2})}\,e^{-\frac{t^2}{4}}\int_0^\infty x^{2a}\exp\{-t x^2 - \tfrac{1}{2}x^4\}\,\mathrm{d}x\,.$$

The argument t may be the main variable

$$x_n = d_n(B_{n+1}, B_n)(3/a_4^{(n)})^{\frac{1}{2}} \qquad (1.9)$$

with $d_n(B_{n+1}, B_n)$ corresponds to the mean value of $d_n(\varkappa)$ over the segment (B_{n+1}, B_n), or the intermediate variable

$$y_n = s^{\frac{3}{2}}\,U(x_n)(3/\varphi(x_n))^{\frac{1}{2}}\,. \qquad (1.10)$$

2. Free Energy in the Critical Region

The peculiarity of the microscopic calculation of the explicit expression for the free energy of the system near T_c consists in the separation of the contributions from short-wave (CR) and long-wave (LGR) phases of the spin moment density:

$$F = -kT\,N\ln 2 + F_{\mathrm{CR}} + F_{\mathrm{LGR}}\,.$$

Here the correlation length

$$\xi = \xi_0\,|\tau|^{-\nu}(1 + a_{\xi}\,|\tau|^{\Delta}), \qquad (2.1)$$

where ν and Δ are critical exponents and ξ_0 and a_{ξ} are critical amplitudes, is the characteristic length scale. Because ξ contains an essential dependence on $\tau = (T-T_c)/T_c$, the short-wave fluctuations region increases as temperature tends to T_c, and in the limit $\tau \to 0$ the distances between the arbitrary particles in the system become relatively small as compared with the correlation length. The calculation of (2.1), especially of the quantities ξ_0 and a_{ξ}, is connected with the investigation of the contributions of short- and long-wave fluctuations in the formation of the special kind of symmetry arising in the critical region, that is, the renormalization group (RG) symmetry. Therefore it is necessary to perform a self-consistent calculation of all quantities which characterize the system in the critical region.

Further consideration refers to the temperature region $\tau < \tau^*$ ($\tau^* < 10^{-2}$). Numerical calculations have shown that two main fluctuation processes appear in

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[*] For $T < T_c$ the LGR is replaced by inverse Gaussian regime (IGR) [5].

this temperature region, namely the critical regime (CR) process and the limiting Gaussian region (LGR) process*. The nature of these regimes can be followed considering the change of the main variable x_n (1.9), with increase of n (see Figure 1). The region of the CR process corresponds to the short-wave fluctuations, which are described by a non-Gaussian measure density. Here the renormalization group symmetry takes place and, therefore, the renormalization group approach can be applied. It is connected with the application of the fixed point method for the solution of recursion relations (RR) arising at the layer integration of the partition function. The RRs for the ϱ^4 model have the form [5, 6, 8]:

$$r_{n+1}=s^2\left[(r_n+q)\,N(x_n)-q\right],$$
$$u_{n+1}=s^{4-d}u_n E(x_n)\,. \tag{2.2}$$

Here s denotes the RG parameter, d is the spatial dimensionality of the problem, and the quantities x_n, y_n are given by (1.9), (1.10). The quantities r_n and u_n are connected with the coefficients $d_n(B_{n+1}, B_n)$, $a_4^{(n)}$ of the effective measure density of (1.7) type by the relations

$$d_n(B_{n+1}, B_n)=s^{-2n}(r_n+q), \quad a_4^{(n)}=s^{-4n}u_n\,. \tag{2.3}$$

The quantity $q=\bar{q}\,\beta\,\tilde{\Phi}(0)$ determines the mean value of $\tilde{\Phi}$ in the n-th layer $\beta\tilde{\Phi}(B_{n+1}, B_n)=\beta\tilde{\Phi}(0)+s^{-2n}q$ [5, 10]. In the following results $\bar{q}=(1+s^{-2})/2$, which corresponds to the arithmetical average of the square of the wave vector $\varkappa$ over the segment $(s^{-1}, 1)$. The functions $N(x_n)$ and $E(x_n)$ have the form

$$N(x_n)=\frac{y_n u(y_n)}{x_n u(x_n)}, \quad E(x_n)=s^6\,\frac{\varphi(y_n)}{\varphi(x_n)}\,.$$

The recursion relations (2.2) possess the fixed point (r^*, u^*) as partial solution. Equations (2.2) are easily extended to cases of more complicated measure densities than the quartic one [11, 12].

The expression for the short-wave part of the free energy is calculated using the summation of the partial free energies over the layers of the CV phase space:

$$F_{\mathrm{CR}}=-\,kT\sum_{n=0}^{m_\tau}\ln Q_n\,. \tag{2.4}$$

The above expression corresponds to the contribution of variable $\varrho_\varkappa$ with $\varkappa > B_{m_\tau}$, where $B_{m_\tau}=B's^{-m_\tau}$, to the free energy of the system. The quantity m_τ determines the number of the CV phase layer which corresponds to the point of the system's exit from the CR (see Figure 1). m_τ is determined by the condition

$$d_{m_\tau+1}(0)=0\,. \tag{2.5}$$

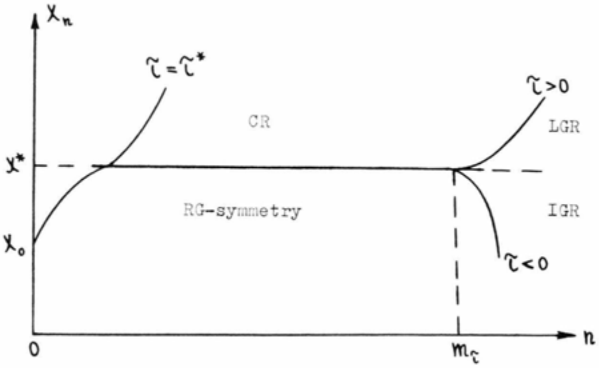

Fig. 1. Evolution of the main variable x_n (1.9) versus the phase layer number n in the critical region $(0, \tau^*)$, where $\tau=(T-T_c)/T_c$ and $\tau^*\approx 10^{-2}$. The values $n\in(0, m_\tau)$ characterize the critical regime arrising in the system for $\tau<\tau^*$ only. In case $n>m_\tau$ the system is described by the Gaussian measure density.

The physical sense of this equality consists in the quantity $d_n(\varkappa)$ for $n>m_\tau+1$ becoming positive for all wave vectors. This makes it possible to use the Gaussian measure density as the basic one for the calculations to the free energy from the integrals over the variables $\varrho_\varkappa$ with $\varkappa<B_{m_\tau+1}$. Taking (2.3) and the solutions of the RG equations [8, 13] into account, we find for m_τ

$$m_\tau=-\frac{\ln\tau}{\ln E_1}+m_0-1+m_\Delta\tau^\Delta\,. \tag{2.6}$$

Here E_1 is the greatest eigenvalue of the RG transformation matrix linearized in the vicinity of the fixed point, and the coefficients m_0, m_Δ depend on the microscopic parameters of the Hamiltonian [14]. In the case $b=c$ and for $s=s^*$ ($s^*=3.5862$ for the ϱ^4 model (see [5, 8])) we obtain

$$E_1=8.2551, \quad m_0=-0.2105, \quad m_\Delta=-0.4639\,.$$

The summation in (2.4) over m_τ CV phase space layers according to the technique proposed in [5, 14, 15] yields

$$F_{\mathrm{CR}}=-kTN'\left[\gamma'_{01}+\gamma_1\tau+\gamma_2\tau^2-\gamma_{10}^{\pm}|\tau|^{3\nu}-\gamma_{11}^{\pm}|\tau|^{3\nu+\Delta}\right], \tag{2.7}$$

where $\nu=0.605$, $\Delta=0.463$. The coefficients at integer powers of τ are the same for temperature lower and higher than T_c, and in case $b=c$ take the value

$$\gamma'_{01}=0.3892, \quad \gamma_1=-0.6793, \quad \gamma_2=-0.0939\,. \tag{2.8}$$

The quantities $\gamma_{1l}^{\pm}$ correspond to temperatures above and below T_c and are

$$\gamma_{10}^{+}=1.0582, \quad \gamma_{11}^{+}=5.9604\,,$$
$$\gamma_{10}^{-}=3.9055, \quad \gamma_{11}^{-}=-6.8812\,. \tag{2.9}$$

The region of the LGR (for $T > T_c$) or IGR (for $T < T_c$) corresponds to long-wave fluctuations. Here the renormalization group method can not be applied, and the variables $\varrho_\varkappa$ with $\varkappa < B_{m_\tau}$ are described by the distribution

$$\mathscr{W}_G(\varrho) = \exp\left[-\frac{1}{2}\sum_{\varkappa < B_{m_\tau}} \tilde{d}_{m_\tau}(\varkappa)\,\varrho_\varkappa\,\varrho_{-\varkappa}\right]. \tag{2.10}$$

The quantity $\tilde{d}_{m_\tau}(\varkappa)$ depends on temperature as follows:

$$\tilde{d}_{m_\tau}(\varkappa) = \beta\tilde{\Phi}(0)\,g_0\,|\tau|^{2\nu}(1+g_1|\tau|^{\Delta}) + 2\beta\tilde{\Phi}(0)\,b^2\varkappa^2, \tag{2.11}$$

where g_0, g_1 are constants connected with microscopic Hamiltonian parameters (these relations are given in [14]). The contribution to the free energy from the long-wave fluctuations is represented in the form

$$F_{\mathrm{LGR}} = -kTN'[f_0^\pm|\tau|^{3\nu} + f_1^\pm|\tau|^{3\nu+\Delta}]. \tag{2.12}$$

The "+" and "−" signs in the above expression refer to the cases $T > T_c$ and $T < T_c$, respectively. In case $b = c$: the coefficients $f_l^\pm$ are

$$f_0^+ = 2.5263, \quad f_1^+ = 4.8960,$$
$$f_0^- = 7.2791, \quad f_1^- = -3.9803. \tag{2.13}$$

Taking (2.7) and (2.12) for the free energy of the three-dimensional Ising model into account, we obtain

$$F = -kTN'[\gamma_0 + \gamma_1\tau + \gamma_2\tau^2 + \gamma_{30}^\pm|\tau|^{3\nu} + \gamma_{31}^\pm|\tau|^{3\nu+\Delta}]. \tag{2.14}$$

Here $\gamma_0 = \gamma'_{01} + s_0^3 \ln 2$ and the coefficients

$$\gamma_{30}^\pm = f_0^\pm - \gamma_{10}^\pm, \quad \gamma_{31}^\pm = f_1^\pm - \gamma_{11}^\pm \tag{2.15}$$

consist of contributions from short- and long-wave fluctuations, the main contribution arising from variables $\varrho_\varkappa$ with small values of wave vectors as compared with B_{m_τ}. Each coefficient γ_{3l} can be represented in the form of a product of the universal part and a non-universal factor:

$$\gamma_{30}^\pm = c_\nu^3\,\bar{\gamma}_{30}^\pm, \qquad c_\nu = c_{1\varkappa}/f_0,$$
$$\gamma_{31}^\pm = c_\Delta c_\nu^3\,\bar{\gamma}_{31}^\pm, \quad c_\Delta = c_{2\varkappa}\left(\frac{c_{1\varkappa}}{f_0}\right)^{\Delta}, \tag{2.16}$$

where $\bar{\gamma}_{30}^\pm$ and $\bar{\gamma}_{31}^\pm$ do not depend on microscopic parameters of the sytem and take the values

$$\bar{\gamma}_{30}^+ = 0.6554, \quad \bar{\gamma}_{31}^+ = 0.5758,$$
$$\bar{\gamma}_{30}^- = 1.5061, \quad \bar{\gamma}_{31}^- = -1.5692. \tag{2.17}$$

For the $c_{l\varkappa}$ coefficients we obtain

$$c_{1\varkappa} = [1 - f_0 - R^{(0)}\varphi_0^2 - a'_4 R^{(0)}\varphi_0^{-1/2}(\beta_c\tilde{\Phi}(0))^{-2}]\,\mathscr{D}^{-1},$$

$$R^{(0)} = \frac{R_{12}^{(0)}}{E_2 - R_{11}}, \quad R_1^{(0)} = \frac{E_1 - R_{11}}{R_{12}^{(0)}}, \quad \mathscr{D} = \frac{E_1 - E_2}{R_{11} - E_2},$$

$$c_{2\varkappa} = \left[R_1^{(0)}\varphi_0^{\frac{1}{2}} - \varphi_0 - R_1^{(0)}\varphi_0^{\frac{1}{2}} - \frac{a'_2 R_1^{(0)}\varphi_0^{\frac{1}{2}}}{\beta_c\tilde{\Phi}(0)} + \frac{a'_4}{(\beta_c\tilde{\Phi}(0))^2}\right]\mathscr{D}^{-1}. \tag{2.18}$$

Here R_{ij} and E_l are the matrix elements and eigenvalues of the RRs (2.2), linearized in the vicinity of the fixed point, $r^* = -f_0\beta\tilde{\Phi}(0)$, $u^* = \varphi_0(\beta_c\tilde{\Phi}(0))^2$ ($f_0 = 0.5389$, $\varphi_0 = 0.6889$). The temperature dependence of the free energy F/N for the case $b = c$ is plotted in Figure 2. In the same figure the dependence on τ of the leading contribution to the nonanalytical part of the free energy, which is proportional to $|\tau|^{3\nu}$, is shown.

The proposed method for the calculation of the free energy of the 3D Ising model is valid for temperatures both above and below the critical point. It is successfully applied also for the description of phase transitions in other systems. In the papers [16, 17] the important problem of the statistical physics concerning the difference in the description of liquid and gas states is being solved. For this purpose the statistical problem of the liquid-gas phase transition is investigated in the vicinity of the critical point, and explicit expressions for the coefficients determining the functional measure density defined over the CV set are given. The application of the method described above makes is possible to obtain the explicit expression for the free energy and other thermodynamic functions for the liquid-gas system at the critical point [17].

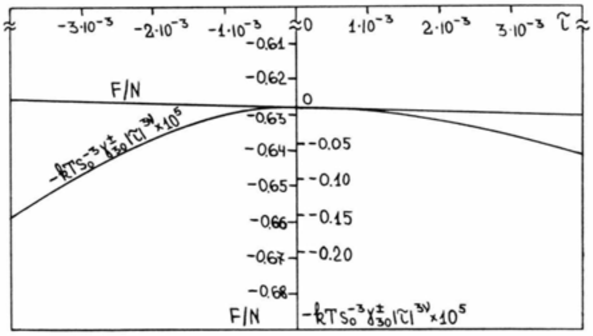

Fig. 2. Temperature dependence of the free energy F/N (left hand scale of ordinate axis) and the non-analytical contribution to the free energy (cf. (2.14)) $-kTs_0^{-3}\gamma_{30}^\pm|\tau|^{3\nu}$ (right hand scale of ordinate axis) for $s = s^*$ and $b = c$. $s_0 = \pi\sqrt{2}$, $\nu = 0.605$.

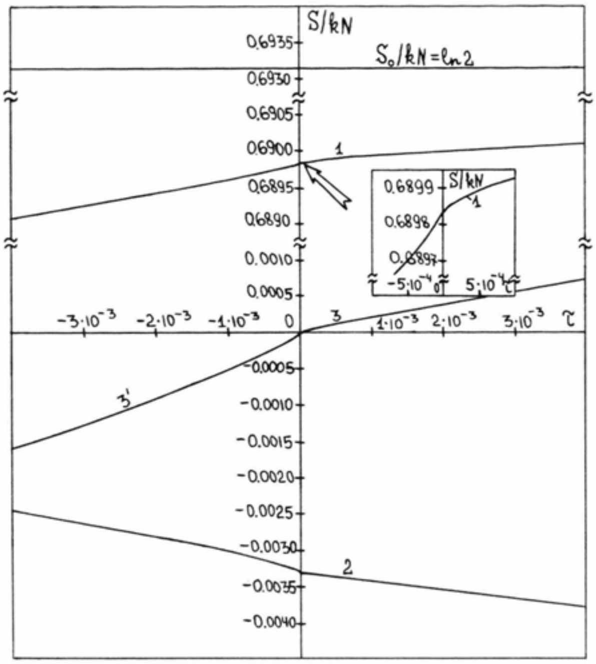

Fig. 3. Entropy of the system in the critical region. Designations are explained in the text.

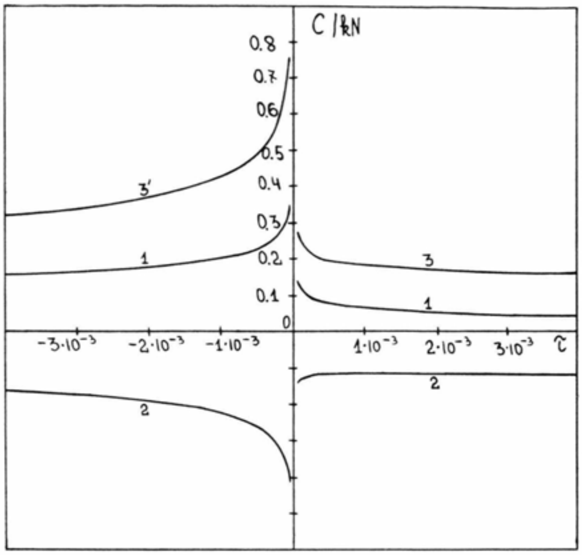

Fig. 4. Full specific heat of the system vs. temperature and the behaviour of different contributions. Curves are denoted in the same way as in Figure 3.

3. Other Thermodynamic Functions

The obtained expression (2.14) for the free energy of the system in the critical region provides the possibility to calculate other thermodynamic functions. Taking the derivative of the free energy with respect to temperature, one obtains the entropy $S = -\partial F/\partial T$:

$$S = k N' [S_0 + S_1 \tau + S_3^{\pm} |\tau|^{1-\alpha} + S_4^{\pm} |\tau|^{1-\alpha-\Delta}] . \quad (3.1)$$

Here $\alpha = 2 - 3\nu$,

$$S_0 = \gamma_0 + \gamma_1 , \quad S_1 = 2(\gamma_1 + \gamma_2) ,$$
$$S_3^{\pm} = 3\nu\, \gamma_{30}^{\pm} , \quad S_4 = (3\nu + \Delta)\, \gamma_{31}^{\pm} . \quad (3.2)$$

The universality of the $S_{3,4}^{\pm}$ coefficients is determined by the universality of the quantities $\gamma_{3l}^{\pm}$. The dependence of the entropy for $b = c$ is given in Fig. 3 (curve 1). For comparison the contributions corresponding to the CR region (curve 2), the LGR region (curve 3) and the IGR region (curve 3′) are displayed in the same plot. It should be emphasized that the contribution to the general expression for the entropy from the CR region leads to an increase of entropy with decreasing temperature. This could be explained by the RG symmetry in the system near T_c. The contribution of the entropy the LGR ($T > T_c$) or IGR ($T < T_c$) region is dominating and leads to the decrease of the entropy with decreasing temperature. If we were restricting ourselves to the RG method for the calculation of the entropy, then the obtained entropy of the system would increase with decreasing temperature.

The specific heat near the second-order phase transition point is represented in the form

$$C = k N' [C_0 + C_3^{\pm} |\tau|^{-\alpha} + C_4 |\tau|^{\Delta - \alpha}] , \quad (3.3)$$

where

$$C_0 = 2(\gamma_1 + \gamma_2) , \quad (3.4)$$
$$C_3^{\pm} = 3\nu(3\nu - 1)\, \gamma_{30}^{\pm} , \quad C_4^{\pm} = (3\nu + \Delta)(3\nu + \Delta - 1)\, \gamma_{31}^{\pm} .$$

Its temperature behaviour for $b = c$ is given in Figure 4. The designations are the same as for Figure 3. The positiveness of the specific heat is provided by the contributions from the long-range spin moment density fluctuations.

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