Condensed Matter Physics 2009, Vol. 12, No 2, pp. 151–166

CONDENSED MATTER PHYSICS

Free energy of $3D$ Ising-like system near the phase transition point

M.P.Kozlovskii*

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

Received February 20, 2009, in final form March 31, 2009

A generalized representation for the scaling form of free energy of the system near the phase transition point is proposed. Explicit expressions for coefficients as functions of the reduced temperature and external field in the case of $T > T_{\rm c}$ are obtained at the microscopic level.

Key words: *phase transition, external field, free energy*

PACS: *05.50.+q, 64.60.Fr, 75.10.Hk*

1. Introduction

An urgent problem in describing critical phenomena lies in the development of a generalized theory which allows one to obtain (except the calculation of critical exponents and some other universal characteristics) explicit expressions for physical quantities like in the case of classic theories [1,2]. The scaling theory turns out to be the most developed with respect to this problem. It is based on the similarity hypothesis proposed in [3–6] and on the scheme of constructing effective Kadanoff spin blocks [5]. We consider the system based on the Ising model on a simple cubic lattice having a lattice constant c. The initial lattice is split into blocks with linear sizes $s \cdot c$, where s is an arbitrary number ($s > 1$). Then, instead of N initial sites with period c we get N_1 sites ($N_1 = Ns^{-d}$) with period $c_1(c_1 = cs)$ each of which contains s^d spins. When the system is near the phase transition point (PTP), the correlation length ξ is large and greatly exceeds C_1. The free energy of such a system with effective spins F_s is related to the free energy of initial spins F by the known relation

$$F_s(\tilde{\tau}, \tilde{h}) = s^d F(\tau, h). \tag{1}$$

Here $\tau = (T - T_{\rm c})/T_{\rm c}$ is a reduced temperature, h is external field. The variables $\tilde{\tau}$ and $\tilde{h}$ related to τ and h by means of relations

$$\tilde{\tau} = s^{y_\tau}\tau, \quad \tilde{h} = s^{y_h}h, \tag{2}$$

where y_τ and y_h are some numbers defined by critical exponents

$$y_t = \frac{1}{\nu}, \quad y_h = \frac{1}{\mu}. \tag{3}$$

Here ν is the critical exponent of the correlation length at the absence of the external field $\xi_\tau = \xi^{\pm}|\tau|^{-\nu}$, and μ is the critical exponent of the same quantity at $T = T_{\rm c}$: $\xi_h = \xi^{(c)}h^{-\mu}$. It is known that $\mu = \nu/\beta\delta$, where β and δ are critical exponents (temperature and field ones) of the order parameter.

The above expressions enable one to write down the scaling form of the singular part for free energy near PTP as

$$F(\tau, h) = s^{-d}F_s\left(s^{y_t}\tau, s^{y_h}h\right). \tag{4}$$

*E-mail: mpk@ph.icmp.lviv.ua

The theory parameter s is arbitrary but it cannot exceed the system correlation length since near the PTP there are two typical values which could be considered for the quantity s. The first one predicts the fulfillment of condition $|s^{y_t}\tau| = 1$ that is equivalent to the parameter value $s = s_\tau$:

$$s_\tau = |\tau|^{-1/y_t} = |\tau|^{-\nu}. \tag{5}$$

In this case the equality (4) takes on the form

$$F(\tau, h) = |\tau|^{\mathrm{d}\nu} f_s\left(1, \frac{h}{|\tau|^{\beta\delta}}\right). \tag{6}$$

The first multiplier describes the temperature behaviour of free energy of the system in the case of small values of the field or rather the quantity

$$\alpha_0 = \frac{h}{|\tau|^{\beta\delta}}\,. \tag{7}$$

The second one f_s is the so-called scaling function of the free energy. It depends on the ratio of the reduced external field h to the temperature field

$$h'_{\mathrm{c}} = |\tau|^{\beta\delta}\,. \tag{8}$$

The function f_s does not contain any explicit dependence on τ and h.

The second typical value of the parameter s related to the condition $|s^{y_h}h| = 1$, which corresponds to the relation

$$s_h = h^{-\frac{1}{y_h}} = h^{-\mu}. \tag{9}$$

At this value of the parameter we get an expression for the free energy (4) in the form

$$F(\tau, h) = h^{\frac{\mathrm{d}\nu}{\beta\delta}} f_s\left(\frac{\tau}{h^{1/\beta\delta}}, 1\right). \tag{10}$$

It is evident that such a representation is valid for large values of the field or in other words for small values of the variable

$$z = \frac{\tau}{h^{1/\delta\beta}}\,. \tag{11}$$

Note that quantities z and α_0 are mutually inverse $z = \alpha_0^{-1/\delta\beta}$.

The free energy presentations (6) and (10) are basic in the scaling theory. Depending on the ratio between quantities τ and h one could use the first one or another. In particular, in the case of the absence of an external field, the dependence (6) should be used. At the presence of the external field ($h \neq 0$) with the temperature T tending to the critical point T_{c}, the presentation (10) is more appropriate since an arbitrary small field becomes essential (the quantity z tends to zero).

In both cases of the RG transformation, this parameter (s_τ or s_h) exceeds the value of the correlation length. One could find these results in papers [7,8] where an explicit dependence of the correlation length on the temperature and field is presented. Therefore, the above expressions for free energy (6) and (10) are formal. They are valid only in some limiting cases. The formula (6) could be used at $h = 0$ and the relation (10) is valid at $T = T_{\mathrm{c}}$ only. As a consequence, the choice of the parameter s via conditions (5) and (9) does not enable one to describe the dependence of the free energy on both the field and the temperature parameters.

Thus, the problem of the free energy calculation with the possibility of unifying the dependences (6) and (10) appears to be actual. Considering the relation (4) it is easy to see that there is no such a value of s which could make it possible to unify the expressions (6) and (10). They are obtained via considering diametrically opposite limiting cases. It turned out that it is possible to find an explicit form for the free energy using the results presented in [7–11]. Such a calculation employs the collective variables (CV) set [12] and it is valid for arbitrary values of the field and temperature. This is some combination of the expressions (6) and (10) and it is derived based on the mathematically rigorous microscopic approach. Using this method one could obtain an explicit form for the scaling function f_{s}.

2. Method for calculation of the partition function near the second order phase transition point

Let us use the results of papers [7,9], where the method for calculating the partition function of the Ising-like model near the T_{c} is proposed for the cases of small and large values of the external field. As was shown in these works, the distinction between small and large fields is related to the introduction of some temperature field $h_{\mathrm{c}} = |\tilde{\tau}|^{p_0}$, where $\tilde{\tau} = \tau c_{k_1}^{(0)}/f_0$, $p_0 = (d+2)\nu/2$. The constants $c_{k_1}^{(0)}$, f_0 are defined in [7]. We also present some normalized field $\tilde{h}$ where some constants are presented in [8]. In the case of $\tilde{h} \gg h_{\mathrm{c}}$, the free energy is defined by the field dependence (10) and at $\tilde{h} \ll h_{\mathrm{c}}$ the formula for free energy contains the temperature dependence only and is similar to (6). For free energy description the most problematic is the case of intermediate values of the field $\tilde{h} \approx h_{\mathrm{c}}$. Therefore, the corresponding expressions obtained in [7] should be generalized.

As a result of step-by-step calculation for partition function for the Ising model in the external field we have the expression

$$Z = Z_0[Q(d)]^{N_0} \left(\prod_{n=1}^{n_p} Q_n \right) Z_{\mathrm{LGR}}\,, \tag{2.1}$$

where in correspondence with [12,13] we have

$$Q(d) = (2\pi)^{1/2}\,(3/a_4)^{1/4} \exp\left(\frac{x^2}{4}\right) U(0,x). \tag{2.2}$$

The variable x of the Weber's parabolic cylinder function $U(0,x)$ has the form

$$x = d(B_1,B_0)\,(3/a_4)^{1/2}\,, \tag{2.3}$$

and for these functions the integral presentation could be written down as follows

$$U(a,x) = \frac{2}{\Gamma\left(a+\frac{1}{2}\right)} \exp\left(-\frac{x^2}{4}\right) \int_0^\infty t^{2a} \exp\left(-xt^2 - \frac{1}{2}t^4\right) \mathrm{d}t. \tag{2.4}$$

The quantities Q_n are partial partition functions of the n-th level

$$Q_n = [Q(P_{n-1})Q(d_n)]^{N_n}\,, \tag{2.5}$$

where $N_n = N_0 s^{-3n}$, s is the parameter of splitting the set of CV into subsets ($s \geqslant 1$),

$$\begin{aligned}
Q(d_n) &= (2\pi)^{1/2} \left(3/a_4^{(n)}\right)^{1/4} \exp\left(\frac{x_n^2}{4}\right) U(0,x_n), \\
Q(P_n) &= (2\pi)^{-1/2} \left(\frac{a_4^{(n)}}{\varphi(x_n)}\right)^{1/4} s^{3/4} \exp\left(\frac{y_n^2}{4}\right) U(0,y_n).
\end{aligned} \tag{2.6}$$

For variables x_n and y_n we have the expressions

$$\begin{aligned}
x_n &= d_n(B_{n+1},B_n) \left(\frac{3}{a_4^{(n)}}\right)^{1/2}, \\
y_n &= s^{3/2} U(x_n) \left(\frac{3}{\varphi(x_n)}\right)^{1/2},
\end{aligned} \tag{2.7}$$

where

$$d_n(B_{n+1},B_n) = a_2^{(n)} - \beta\Phi(B_{n+1},B_n). \tag{2.8}$$

The quantity $\Phi(B_{n+1}, B_n)$ is the averaged value of the Fourier transform for interaction potential [8] in the region of wave vectors $\vec{k} \in \mathcal{B}_n \backslash \mathcal{B}_{n+1}$. Here

$$\mathcal{B}_n = \left\{ \vec{k} = (k_x, k_y, k_z) | k_i = -\frac{\pi}{c_n} + \frac{\pi}{c_n}\frac{n_i}{N_{ni}}\, ; \, n_i = 1, 2, \ldots, 2N_{ni}; \, i = x, y, z \right\}, \tag{2.9}$$

where $c_n = c_0 s^n$, $N_n = N_{nx}N_{ny}N_{nz}$ is the sites number of n-th effective block structure, and $N_n = N_0 s^{-3n}$. For special functions $U(t)$ and $\varphi(t)$ we have

$$U(t) = U(1,t)/U(0,t); \qquad \varphi(t) = 3U^2(t) + 2tU(t) - 2. \tag{2.10}$$

For quantity $d_n(B_{n+1}, B_n)$ and $a_4^{(n)}$ the reccurance relations (RR) take place. Their explicit form was obtained in [14]. By introducing notations

$$d_n(B_{n+1}, B_n) = d_n(0) + qs^{-2n}, \qquad q = \beta\Phi(0)\bar{q},$$

$$a_1^{(n)} = s^{-n} w_n\,, \qquad d_n(0) = s^{-2n} r_n\,, \qquad a_4^{(n)} = s^{-4n} u_n\,,$$

we obtain RR

$$\begin{aligned} w_{n+1} &= s^{\frac{d+2}{2}} w_n\,, \\ r_{n+1} &= s^2 \left[-q + (r_n + q) N(x_n) \right], \\ u_{n+1} &= s u_n E(x_n), \end{aligned} \tag{2.11}$$

where

$$N(x_n) = \frac{y_n U(y_n)}{x_n U(x_n)}\,, \qquad E(x_n) = s^{2d}\frac{\varphi(y_n)}{\varphi(x_n)}\,.$$

For initial values of quantities w_n, r_n and u_n (at $n = 0$) we have

$$w_0 = s_0^{d/2} h, \qquad r_0 = a_2 - \beta\Phi(0)(1 - \bar{\Phi}), \qquad u_0 = a_4\,. \tag{2.12}$$

Here, the values of quantities a_2, a_4 and $\bar{\Phi}$ are presented in [8,9].

The RR (2.11) differ from the ones obtained in [12] by the appearance of the additional equation for the quantity w_n, which represents the existing external field.

In the expression (2.1) the quantity Z_{LGR} is still undefined. It has the form

$$Z_{\mathrm{LGR}} = 2^{(N_{n_p}-1)/2} Q(P_{n_p})^{N_{n_p+1}} Z_{n_p+1}\,, \tag{2.13}$$

where

$$\begin{aligned} Z_{n_p+1} \quad = \quad & \int (\mathrm{d}\eta)^{N_{n_p+1}} \exp\left(a_1^{(n_p+1)} N_{n_p+1}^{1/2} \eta_0 - \frac{1}{2} \sum_{k \in \mathcal{B}_{n_p+1}} d_{n_p+1}(k) \eta_{\vec{k}} \eta_{-\vec{k}} \right. \\ & \left. - \frac{a_4^{(n_p+1)}}{4!} N_{n_p+1}^{-1} \sum_{\substack{\vec{k}_1, \ldots, \vec{k}_4 \\ \vec{k}_i \in \mathcal{B}_{n_p+1}}} \eta_{\vec{k}_1} \ldots \eta_{\vec{k}_4} \delta_{\vec{k}_1 + \ldots \vec{k}_4} \right). \end{aligned} \tag{2.14}$$

The number n_p characterizes the effective block structure of spins with corresponding period c_{n_p}, where

$$c_{n_p} = c_0 s^{n_p}. \tag{2.15}$$

The representation of the partition function in the form (2.1) is related to the presence of the new distance scale near PTP. When the system is far from this point, the lattice constant c plays the role of such a distance. However, in the vicinity of the critical point the characteristic distance is equal to the correlation length $\xi = c_{n_p}$ of the system.

As far as the value of the effective lattice period c_n is less than c_{n_p}, the renormalization group (RG) symmetry takes place in the system [12] and for all $n < n_{n_p}$, the general RR (2.11) could be substituted by approximated RR which corresponds to the linear deviations from the fixed point. In the case of $c_n > c_{n_p}$, the RG symmetry breaks down and for the following calculations of the contribution to the free energy one should use general RR.

The quantity n_p is an important characteristic for a description of phase transitions. It defines the number of iterations at which the system is still in the scaling region. Note that the result of calculation (2.1) does not depend on the choice of n_p. Indeed, the quantity n_p splits the set of CV into two parts. The first one takes into account the contributions from CV $\eta_{\vec{k}}$ with $\vec{k} \in \mathcal{B}\backslash\mathcal{B}_{n_p+1}$. The second part corresponds to the contributions of CV $\eta_{\vec{k}}$ with $\vec{k} \in \mathcal{B}_{n_p+1}$, including the contribution from the "macroscopic" variable η_0. A decrease or an increase of the quantity n_p should not effect the total result of partition function calculation. The purpose of introducing this quantity is to optimize the mathematical evaluations near PTP. In the case of exact calculations, the choice of quantity n_p would be arbitrary. However, linearization of the RR (2.11) near the fixed point predicts some restrictions to this quantity.

The general expression for the system exit point from the order parameter critical fluctuation regime at $T > T_{\mathrm{c}}$ was found in [8,15]. It is as follows:

$$n_p = -\frac{\ln(\tilde{h}^2 + h_{\mathrm{c}}^2)}{2\ln E_1} - 1, \tag{2.16}$$

where

$$\tilde{h} = h s_0^{d/2}/h_0\,, \qquad h_{\mathrm{c}} = |\tilde{\tau}|^{p_0}\,, \qquad \tilde{\tau} = \tau c_{k_1}^{(0)}/f_0\,. \tag{2.17}$$

Quantities h_0, f_0 and $c_{k_1}^{(0)}$ are presented in [7,16,17]. We will use this expression in (2.1) for the following calculations of the partition function near PTP at $T > T_{\mathrm{c}}$.

Note that the calculations performed below concern the region of the temperatures $|\tau| < \tau^*$, where $\tau^* \sim 10^{-2}$. We shall not apply any restrictions to the values of the field h as well.

3. Free energy calculation scheme near T_{c} ($T > T_{\mathrm{c}}$)

The calculation of the one-component spin system free energy is performed near the PTP based on the expression for the partition function (2.1). In the case of the external field presence, the main difference of such an approach is that it is necessary to determine a generalized exit point from the critical regime of the order parameter fluctuations. In the case of $T > T_{\mathrm{c}}$ coordinates of this point (on the plane filed-reduced temperature) are defined using the expression (2.16). Let us present the system free energy in the form of several terms

$$F = F_0 + F_{\mathrm{CR}}^{(+)} + F_{\mathrm{LGR}}\,. \tag{3.1}$$

Each of these terms is the contribution of a certain multiplier from expression (2.1). Particularly,

$$F_0 = -kTN[\ln 2 + \ln ch h] - \frac{1}{2}N\Phi(0)\bar{\Phi} \tag{3.2}$$

corresponds to the expression for Z_0 and describes the free energy of noninteractive spins. The term $F_{\mathrm{CR}}^{(+)}$ is responsible for the contribution to the free energy from the critical regime of fluctuations. According to (2.1) it has the form

$$F_{\mathrm{CR}}^{(+)} = -kT\sum_{n=1}^{n_p} N_n f_n\,, \tag{3.3}$$

where $N_n = N_0 \cdot s^{-3n}$, and for function $f_n(x_n, y_{n-1})$ the expression

$$f_n = \frac{1}{4}\ln\left(3/\varphi(y_{n-1})\right) + \frac{1}{4}\left(x_n^2 + y_{n-1}^2\right) + \ln U(0, x_n) + \ln U(0, y_{n-1}) \tag{3.4}$$

is valid. In comparison with the similar expression used in the case of the absence of the field [16] the difference of (3.3) is that we employ a more generalized expression for the exit point n_p from the critical fluctuations regime. Quantities x_n and y_n, which belong to the (3.4), are presented in (2.7).

The term F_{LGR} has the form

$$F_{\mathrm{LGR}} = -kT \ln Z_{\mathrm{LGR}}\,, \tag{3.5}$$

where the expression for Z_{LGR} is defined in (2.13). Note that Z_{n_p+1} from (2.14) can be presented in the form which is similar to the contribution from the critical regime of fluctuations, in other words, via the product of partial partition functions. Then for (3.5) we get

$$F_{\mathrm{LGR}} = F_{\mathrm{TR}}^{(+)} + F'. \tag{3.6}$$

Here

$$F_{\mathrm{TR}}^{(+)} = -kTN_0 s^{-3(n_p+1)} \sum_{m=1}^{m_0} s^{-3(m-1)} f_{n_p+m}\,, \tag{3.7}$$

where for f_{n_p+m} we have (3.4) at $n = n_p + m$, and for F' we obtain

$$F' = -kTN \ln Z'. \tag{3.8}$$

Here

$$Z' = 2^{(N_{n'+1}-1)/2}[Q(P_{n'})]^{N_{n'+1}} Z_{n'+1}\,. \tag{3.9}$$

The quantity $n' = n_p + m_0$ is the number of the spin blocks structure, and $n' > n_p$. The quantity $Q(P_{n'})$ coincides with (2.6) at $n = n'$. For $Z_{n'+1}$ we have expression (2.14), where n_p should be substituted by n'.

Note the distinction in the type of the expressions for $F_{\mathrm{CR}}^{(+)}$ from (3.3) and $F_{\mathrm{TR}}^{(+)}$ from(3.7). Despite the same functional form of these expressions, the values of variables x_n and y_n are different in magnitude. Partially, for $F_{\mathrm{CR}}^{(+)}$ (region $n < n_p$) these quantities are close to their values near the fixed point ($x_n \approx x^*$, $y_n \approx y^*$). Nevertheless performing the calculations for $F_{\mathrm{TR}}^{(+)}$ (region $n_p < n \leqslant n_p + m_0$) one should take into account their deviation from the fixed point.

Let us find the quantity $F_{\mathrm{CR}}^{(+)}$ from (3.3). In order to do that one should extract the explicit dependence of the quantity f_n on n. Such calculations have been performed in [12]. It was established that the variable y_n takes on large values for arbitrary values of the temperature. Therefore, the asymptotic series expansions are used for Weber's parabolic cylinder functions $U(0, y_n)$ and their combinations as well as for $\varphi(y_n)$ from (2.10)

$$\begin{aligned}
U(0, y_n) &= y_n^{-1/2} e^{-y_n^2/4}\left(1 - \frac{3}{8}y_n^{-2} + \frac{105}{108}y_n^{-4}\right), \\
U(y_n) &= y_n^{-1}\left(1 - \frac{3}{2}y_n^{-2} + 6y_n^{-4}\right), \\
\varphi(y_n) &= 3y_n^{-4}\left(1 - \frac{21}{2}y_n^{-2} + \frac{447}{4}y_n^{-4}\right).
\end{aligned} \tag{3.10}$$

We have a simplified expression for f_n from (3.4)

$$f_n = \frac{1}{2}\ln y_{n-1} + \frac{9}{4}y_{n-1}^{-2} + \frac{x_n^2}{4} + \ln U(0, x_n) + 0(y_{n-1})^{-4}\,. \tag{3.11}$$

We restrict ourselves to the consideration of the case when the value of quantity x_n in the fixed point reduces to zero ($x^* = 0$). It is fulfilled at some value of the RG parameter $s = s^*$, where

$s^* = 3.5977$. In this case for all $n \leqslant n_p$ we have $x_n \ll 1$. The quantity (3.11) is represented in the form

$$f_n = f_{\rm CR}^{(0)} + A_1 x_{n-1} + A_3 x_n\,, \tag{3.12}$$

where

$$f_{\rm CR}^{(0)} = \frac{1}{2}\ln y_0 + \frac{9}{4} y_0^{-2} + \ln U(0,0),$$
$$y_0 = s^{3/2} y_0^{(0)}, \qquad y_0^{(0)} = U(0)\,(3/\varphi(0))^{1/2}\,. \tag{3.13}$$

For coefficients A_l we have

$$A_1 = \frac{1}{2} r_1 \left(1 - 9(y_0^{(0)})^{-2}\right), \qquad A_3 = -\frac{1}{2}U(0), \tag{3.14}$$

where the quantity r_1 is expressed via parabolic cylinder functions $U(0)$, $\varphi(0)$ and their derivatives. In (3.12) we take into account the linear terms with respect to the x_n only. The quadratic approximation is described in [12]. In accordance with the results of work [17], we find

$$f_{\rm CR}^{(0)} = 1.496, \quad A_1 = 0.115, \quad A_3 = -0.478. \tag{3.15}$$

Using an explicit solution of RR in the region $n \leqslant n_p$ we obtain the expression for x_n:

$$x_n = c_{1T} B_3 \tau E_2^n + c_{1T}^2 B_6 \tau^2 E_3^{2n}. \tag{3.16}$$

Here, the terms which are proportional to E_3^n are not taken into account. ($E_3 < 1$). For coefficients B_l we have

$$B_3 = \sqrt{3}\varphi_0^{-1/2}, \qquad B_6 = -\frac{\sqrt{3}}{2} R_1^{(0)} \varphi_0^{-1}.$$

Taking into account (3.16) from (3.11) we obtain

$$f_n = f_{\rm CR}^{(0)} + d_1 c_{1T} \tau E_2^n + d_3 c_{1T}^2 \tau^2 E_2^{2n}, \tag{3.17}$$

where

$$d_1 = B_3(A_3 + A_1/E_2), \qquad d_3 = B_6(A_3 + A_1/E_2^2).$$

Let us use (3.17) to calculate (3.3). Note that due to (2.16) equalities

$$\begin{aligned}
s^{-(n_p+1)} &= \left(\tilde{h}^2 + h_{\rm c}^2\right)^{\frac{1}{d+2}}, & E_1^{n_p+1} &= \left(\tilde{h}^2 + h_{\rm c}^2\right)^{-1/2},\\
\tilde{\tau} E_2^{n_p+1} &= H_{\rm c}, & H_{\rm c} &= \tilde{\tau}\left(\tilde{h}^2 + h_{\rm c}^2\right)^{-1/2p_0},\\
E_3^{n_p+1} &= H_3, & H_3 &= \left(\tilde{h}^2 + h_{\rm c}^2\right)^{\Delta/2p_0}
\end{aligned} \tag{3.18}$$

are valid. Here notations

$$\nu = \frac{\ln s^*}{\ln E_2}, \qquad \Delta = -\frac{\ln E_3}{\ln E_2}, \qquad p_0 = \frac{\ln E_1}{\ln E_2} = \frac{d+2}{2}\nu, \tag{3.19}$$

are used. The quantity Δ is the critical exponent for scaling correction , p_0 is the crossover critical exponent. For the model ρ^4 at $s = s^*$ they take on values [1]

$$\nu = 0.605, \qquad \Delta = 0.465, \qquad p_0 = 1.512.$$

The result of calculating (3.3) is as follows:

$$F_{\rm CR}^{(+)} = -kTN_0\left(\gamma_{01} + \gamma_{02}\tau + \gamma_{03}\tau^2\right) + F_{\rm CR}^{(s)}, \tag{3.20}$$

[1] The conservative value ν in comparison with the data obtained in MC method [18] is related to the use of a too simple approximation for the Jacobian of transition from spins to CV. The use of higher approximations [16] leads the values close to these ones.

where for coefficients γ_{0l} one found expressions [17]

$$
\begin{aligned}
\gamma_{01} &= s^{-3} f_{\mathrm{CR}}^{(0)} \left(1 - s^{-3}\right)^{-1}, \\
\gamma_{02} &= s^{-3} d_1 c_{1k} E_2 (1 - E_2 s^{-3})^{-1}, \\
\gamma_{03} &= s^{-3} d_3 c_{1k}^2 E_2^2 (1 - s^{-3} E_2^2)^{-1} + s^{-3} c_{1k1} d_1 E_2 (1 - E_2 s^{-3})^{-1},
\end{aligned} \tag{3.21}
$$

which coincide with the result of the same calculations in the case of the absence of the field [12]. The singular part $F_{\mathrm{CR}}^{(s)}$ of expression (3.20) has the form

$$
F_{\mathrm{CR}}^{(s)} = kTN_0 \bar{\gamma}^+ s^{-3(n_p+1)}. \tag{3.22}
$$

The coefficient $\bar{\gamma}^+$ is the function of H_{c}. It is presented in the form

$$
\bar{\gamma}^+ = \bar{\gamma}_1 + \bar{\gamma}_2 H_{\mathrm{c}} + \bar{\gamma}_3 H_{\mathrm{c}}^2. \tag{3.23}
$$

Here $\bar{\gamma}_l$ are constants

$$
\begin{aligned}
\bar{\gamma}_1 &= f_{\mathrm{CR}}^{(0)} (1 - s^{-3})^{-1}, \\
\bar{\gamma}_2 &= d_1 f_0 (1 - E_2 s^{-3})^{-1}, \\
\bar{\gamma}_3 &= d_3 f_0^2 (1 - E_2^2 s^{-3})^{-1},
\end{aligned} \tag{3.24}
$$

which at $s = s^*$ take on the values: $\bar{\gamma}_1 = 1.529$, $\bar{\gamma}_2 = -0.635$, $\bar{\gamma}_3 = -0.058$. The singular part of the contribution $F_{\mathrm{CR}}^{(s)}$ essentially differs from the same quantity at $h = 0$. Note that at the absence of the field we have $H_{\mathrm{c}} = 1$, thus

$$
\bar{\gamma}^+(h = 0) = \gamma^+ = \bar{\gamma}_1 + \bar{\gamma}_2 + \bar{\gamma}_3\,. \tag{3.25}
$$

At $h \neq 0$, the quantity $H_{\mathrm{c}} < 1$. For $\tilde{h} \gg h_{\mathrm{c}}$ we have $H_{\mathrm{c}} \to 0$. The main contribution to $\bar{\gamma}^+$ is formed by quantity $\bar{\gamma}_1$. One should note that similar calculations have been performed in [10]. The exit point from CR was determined in [10] as a solution of some equation. Therefore, the results of calculations were presented in the form of figures. In this work the explicit expressions for the system free energy are obtained as functions of the temperature and field.

The contribution to the free energy F_{LGR} in accordance with (3.6) contains two terms. In order to calculate the first one $F_{\mathrm{TR}}^{(+)}$ from (3.7) it is necessary to find an explicit dependence of the quantity f_{n_p+m} on m. Let us use the solutions of RR. Taking into account (3.18) they take on the form

$$
\begin{aligned}
w_{n_p+m} &= h_0 E_1^{m-1} \tilde{h} \left(\tilde{h}^2 + h_{\mathrm{c}}^2\right)^{-1/2}, \\
r_{n_p+m} &= \beta\Phi(0) f_0 \left[-1 + H_{\mathrm{c}} E_2^{m-1} + R^{(0)} f_0^{-1} \varphi_0^{-1/2} c_{2T} E_3^{m-1} H_3\right], \\
u_{n_p+m} &= (\beta\Phi_f(0))^2 \varphi_0 \left[1 + \Phi_f H_{\mathrm{c}} E_2^{m-1} + c_{2T} E_3^{m-1} H_3\right].
\end{aligned} \tag{3.26}
$$

Here $\Phi_f = f_0 \varphi_0^{-1/2} R_1^{(0)}$. The terms which are proportional to $H_3 E_3^{m-1}$ are neglected since near PTP the quantity H_3 from (3.18) is small, and E_3^{m-1} at $m \gg 1$ tends to zero ($E_3 < 1$). Such an approximation corresponds to scaling corrections being neglected. If necessary, such corrections could be taken into account by using the method suggested in [12].

Taking into account (3.26) from (2.7) we find

$$
x_{n_p+m} = \bar{x} E_2^{m-1} H_{\mathrm{c}} (1 + \Phi_f E_2^{m-1} H_{\mathrm{c}})^{-1/2}, \tag{3.27}
$$

where the notation is presented

$$
\bar{x} = f_0 \varphi_0^{-1/2} \sqrt{3}. \tag{3.28}
$$

The variable x_{n_p+m} increases with m increasing and depends on the value of $H_{\rm c}$. The quantity $H_{\rm c}$ is unambiguously defined by parameter

$$\alpha = \tilde{h}/h_{\rm c} \tag{3.29}$$

for every value of $\tilde{h}$. For small values of the fields the quantity $H_{\rm c}$ tends to unity but with α increasing it reduces to zero. Such a behaviour of $H_{\rm c}$ causes a different character of the dependence of the quantity x_{n_p+m} from (3.27) on m at small and large values of the filed.

Taking into consideration the solutions (3.26) one could claim that the value of the quantity $m_0 = 1$ causes the quitting of the large values of the variable $x_{n_p+m_0+1}$. It is a sufficient condition for using Gauss distribution of fluctuations for arbitrary $\rho_{\vec{k}}$ with $|\vec{k}| \in \mathcal{B}_{n_p+2}$. Thus, the contribution to the system free energy (3.7) from the transition region contains just one term, which has the form

$$F_{\rm TR}^{(+)} = -kTN_0 f_{n_p+1}\left(\tilde{h}^2 + h_{\rm c}^2\right)^{\frac{d}{d+2}}. \tag{3.30}$$

The coefficient f_{n_p+1} is presented as

$$f_{n_p+1} = \frac{1}{2}\ln y_{n_p} + \frac{9}{4}y_{n_p}^{-2} + \frac{1}{4}x_{n_p+1}^2 + \ln U(o, x_{n_p+1}). \tag{3.31}$$

To evaluate the last contribution F' to the system free energy from (3.6) we calculate the expression for Z' from (3.8). At $m_0 = 1$ we have

$$Z' = 2^{(N_{n_p+2}-1)/2}\left[Q(P_{n_p+1})\right]^{N_{n_p+2}} Z_{n_p+2}\,, \tag{3.32}$$

where

$$\begin{aligned} Z_{n_p+2} \;=\; & \int (\mathrm{d}\rho)^{N_{n_p+2}} \exp\Bigg(h\sqrt{N}\rho_0 - \frac{1}{2}\sum_{k\in\mathcal{B}_{n_p+2}} d_{n_p+2}(k)\rho_{\vec{k}}\rho_{-\vec{k}} \\ & -\frac{a_4^{(n_p+2)}}{24}N_{n_p+2}^{-1}\sum_{\substack{k_1,\ldots,k_4\\ k_i\in\mathcal{B}_{n_p+2}}} \rho_{\vec{k}_1}\ldots\rho_{\vec{k}_4}\delta_{k_1+\cdots+k_4}\Bigg). \end{aligned} \tag{3.33}$$

For coefficients d_{n_p+2} and $a_4^{(n_p+2)}$ we get

$$\begin{aligned} d_{n_p+2}(k) &= d_{n_p+2}(0) + 2\beta\Phi(0)b^2k^2, \\ d_{n_p+2}(0) &= s^{-2(n_p+2)}r_{n_p+2}\,, \\ a_4^{(n_p+2)} &= s^{-4(n_p+2)}u_{n_p+2}\,. \end{aligned} \tag{3.34}$$

Note that the method for calculation of (3.33) in the case of $h = 0$ is developed in [12]. It is based on the condition that the quantity $r_{n_p+2}(h=0) \gg u_{n_p+2}(h=0)$, since it permits to use the Gauss approximation in calculating the (3.33). However, at the presence of the field, the coefficient r_{n_p+2} decreases with the field increasing and takes on the negative values at strong fields. Therefore, improvements are required to the method developed earlier.

4. Extracting the macroscopic part of the order parameter

The calculation of the explicit expression for quantity Z_{n_p+2} from (3.33) depends both on the presence of the field and on the system state above or bellow critical temperature. Such a situation is conditioned by the behaviour of the coefficients r_{n_p+2} and u_{n_p+2}, for which we have the expressions

$$\begin{aligned} r_{n_p+2} &= \beta\Phi(0)f_0\left(-1 + E_2H_{\rm c}\right), \\ u_{n_p+2} &= (\beta\Phi(0))^2\varphi_0\left(1 + \Phi_f E_2 H_{\rm c}\right). \end{aligned} \tag{4.1}$$

The coefficient u_{n_p+2} is always positive for arbitrary values of the field h and temperature τ h. It provides a convergence of the integration in (3.33). The coefficient r_{n_p+2} is positive and greatly exceeds u_{n_p+2} at small values of the field. ($h_{\rm c} \gg \tilde{h}$). To calculate (3.33) at these temperatures one can use Gauss approximation which is discussed in detail in [12]. However, for large values of the field ($h_{\rm c} \ll \tilde{h}$) the coefficient r_{n_p+2} is small and takes on negative values with the temperature decreasing. In this temperature region the use of the Gauss approximation is groundless. It can be improved by performing the substitution of variables in (3.33)

$$\rho_{\vec{k}} = \eta_{\vec{k}} + \sqrt{N}\delta_{\vec{k}}\sigma_+ \,, \tag{4.2}$$

where σ_+ is some constant. In the case of $T < T_{\rm c}$, the presence of the spontaneous order parameter in the system is the reason for substitution of variable ρ_0 (average value of which is related to the order parameter). A similar situation takes place for temperatures above $T_{\rm c}$ at the presence of the external field. In this case the order parameter induced by the field exists. As a result of substitution of variables (4.2) the expression (3.33) takes on the form

$$\begin{aligned} Z_{n_p+2} \;=\; & {\rm e}^{NE_0(\sigma_+)} \int ({\rm d}\eta)^{N_{n_p+2}} \exp\Bigg[A_0\sqrt{N}\eta_0 - \frac{1}{2}\sum_{\vec{k}\in\mathcal{B}_{n_p+2}} \bar{d}(k)\eta_{\vec{k}}\eta_{-\vec{k}} \\ & -\frac{1}{6}\bar{b}N_{n_p+2}^{-1/2}\sum_{\vec{k}_1,\ldots,\vec{k}_3}\eta_{\vec{k}_1}\ldots\eta_{\vec{k}_3}\delta_{\vec{k}_1+\cdots+\vec{k}_3} - \frac{1}{24}\bar{a}_4 N_{n_p+2}^{-1}\sum_{\vec{k}_1,\ldots,\vec{k}_4}\eta_{\vec{k}_1}\ldots\eta_{\vec{k}_4}\delta_{\vec{k}_1+\cdots+\vec{k}_4}\Bigg]. \end{aligned} \tag{4.3}$$

Here

$$E_0(\sigma_+) = h\sigma_+ - \frac{1}{2}d_{n_p+2}(0)\sigma_+^2 - \frac{1}{24}a_4^{(n_p+2)}\frac{N}{N_{n_p+2}}\sigma_+^4 \,. \tag{4.4}$$

For the coefficients A_0, $\bar{d}(k)$, $\bar{b}$ and $\bar{a}_4$ we have expressions

$$\begin{aligned} A_0 &= h - d_{n_p+2}(0)\sigma_+ - \frac{1}{6}a_4^{(n_p+2)}s_0^3 s^{3(n_p+2)}\sigma_+^3 \,, \\ \bar{d}(k) &= \bar{d}(0) + 2\beta\Phi(0)b^2k^2 \,, \\ \bar{d}(0) &= d_{n_p+2}(0) + \frac{1}{2}a_4^{(n_p+2)}s_0^3 s^{3(n_p+2)}\sigma_+^2 \,, \\ \bar{b} &= a_4^{(n_p+2)}s_0^{3/2}s^{3/2(n_p+2)}\sigma_+ \,, \qquad \bar{a}_4 = a_4^{(n_p+2)}. \end{aligned} \tag{4.5}$$

In order to carry out the following calculations one should define the quantity σ_+. Since the expressions (4.3)–(4.5) are valid for arbitrary values of σ_+, we find this quantity via using the condition

$$\frac{\partial E_0(\sigma_+)}{\partial\sigma_+} = 0.$$

Taking into account (4.4), we get the equation

$$A_0 = 0, \tag{4.6}$$

the solution of which will be found in the form

$$\sigma_+ = \sigma_0 s^{-(n_p+2)/2}. \tag{4.7}$$

For quantity σ_0 we obtain the cubic equation

$$\sigma_0^3 + p\sigma_0 + q = 0, \tag{4.8}$$

where for coefficients p and q we have expressions

$$\begin{aligned} p &= 6s_0^{-3}\frac{r_{n_p+2}}{u_{n_p+2}}\,, \\ q &= -6s_0^{-9/2}s^{5/2}\frac{h_0}{u_{n_p+2}}\frac{\tilde{h}}{(\tilde{h}^2+h_c^2)^{1/2}}\,. \end{aligned} \tag{4.9}$$

In a general case, the quantities p and q are functions of temperature and field. The form of the solutions (4.8) depends on the discriminant sign

$$Q = (p/3)^3 + (q/2)^2.$$

It is known that for positive Q we have one real solution and in the case of $Q < 0$ the equation (4.8) has three real solutions. It is evident that at $T > T_c$ the quantity Q is positive at arbitrary values of the field.

We consider some partial cases for solutions of (4.8). When $h = 0$, then $q = 0$ for arbitrary $\tau \neq 0$ and corresponding solutions (4.8) have the form

$$\sigma_0^{(1)} = 0; \qquad \sigma^{(2,3)} = \pm\sqrt{-p}. \tag{4.10}$$

The sign of the quantity p depends on the localization of the system above or below T_c. Taking into account equalities (3.18) and (4.1), in the case of $T > T_c$ we obtain

$$\begin{aligned} r^{(+)}_{n_p+2} &= \beta\Phi(0)f_0(E_2-1), \\ u^{(+)}_{n_p+2} &= (\beta\Phi(0))^2\varphi_0(1+\Phi_f E_2). \end{aligned} \tag{4.11}$$

Using equalities (4.11), from (4.9) we find that the value of the quantity

$$p^{(+)} = 6s_0^{-3}\frac{f_0}{\varphi_0}\frac{1}{\beta\Phi(0)}\frac{E_2-1}{1+\Phi_f E_2} \tag{4.12}$$

is positive. In this case ($h = 0, T > T_c$) the equation (4.8) has no real solutions.

The condition $T = T_c$ is another partial case for solutions of equation (4.8). Corresponding quantities p and q from (4.9) become independent of the field. Indeed at $T = T_c$ we have $H_c = 0$, and

$$\begin{aligned} r^{(c)}_{n_p+2} &= -\beta\Phi(0)f_0\,, \\ u^{(c)}_{n_p+2} &= (\beta\Phi(0))^2\varphi_0\,. \end{aligned} \tag{4.13}$$

Then, from (4.9) we get

$$\begin{aligned} p^{(c)} &= -6s_0^{-3}\,(f_0/\varphi_0)\,(\beta_c\Phi(0))^{-1}\,, \\ q^{(c)} &= -6s_0^{-9/2}s^{5/2}\frac{h_0}{\varphi_0}\,(\beta_c\Phi(0))^{-2}\,. \end{aligned} \tag{4.14}$$

The quantity $Q^{(c)} = Q(\tau = 0)$ has the form

$$Q^{(c)} = Q^{(0)}\left[1 - \frac{8}{9}\frac{f_0^3}{\varphi_0 h_0^2}s^{-5}\beta_c\Phi(0)\right], \tag{4.15}$$

where

$$Q^{(0)} = 9s_0^{-9}s^5\,(h_0/\varphi_0)^2\,(\beta_c\Phi(0))^{-4}\,. \tag{4.16}$$

The sign $Q^{(c)}$ is defined by square brackets of expression (4.15). The quantity $Q^{(c)}$ takes on positive values only due the existence of the small multiplier s^{-5}. Note that $Q^{(c)}$ does not depend on the magnitude of the field and is defined by microscopic parameters of the system. For their following values [17]

$$s_0 = 2, \qquad b/c = 0.3, \qquad h_0 = 0.760 \tag{4.17}$$

we find

$$p^{(c)} = -0.389, \quad q^{(c)} = -2.790, \quad Q^{(c)} = 1.944. \tag{4.18}$$

One can prove that for other values of the system parameters s_0 and b/c the quantity $Q^{(c)}$ is positive only. At $T = T_{\rm c}$ the solutions of equation (4.8) have the form

$$\sigma_{\rm c} = A_{\rm c} + B_{\rm c}\,, \tag{4.19}$$

where

$$A_{\rm c} = \left(-q^{(c)}/2 + (Q^{(c)})^{1/2}\right)^{1/3},$$
$$B_{\rm c} = -\left(q^{(c)}/2 + (Q^{(c)})^{1/2}\right)^{1/3}.$$

In the case of (4.17) we find

$$A_{\rm c} = 1.408, \qquad B_{\rm c} = 0.092, \qquad \sigma_{\rm c} = 1.500. \tag{4.20}$$

At $T = T_{\rm c}$ the magnitude of the displacement σ_+ from (4.2) is described by the expression:

$$\sigma_+ = \tilde{h}^{1/5}\sigma_{\rm c}\,. \tag{4.21}$$

In general case the solution of the equation (4.8) depends both on the field and on the temperature. For arbitrary $\tau > 0$ at $h \neq 0$ we find the solution for equation (4.8) using the Cardano's method $\sigma_0 = A + B$, where

$$A = \left(-q/2 + Q^{1/2}\right)^{1/3}, \qquad B = -\left(q/2 + Q^{1/2}\right)^{1/3}.$$

The dependence $\sigma_0(\tau)$ is presented in figure 1 for different values of the field.

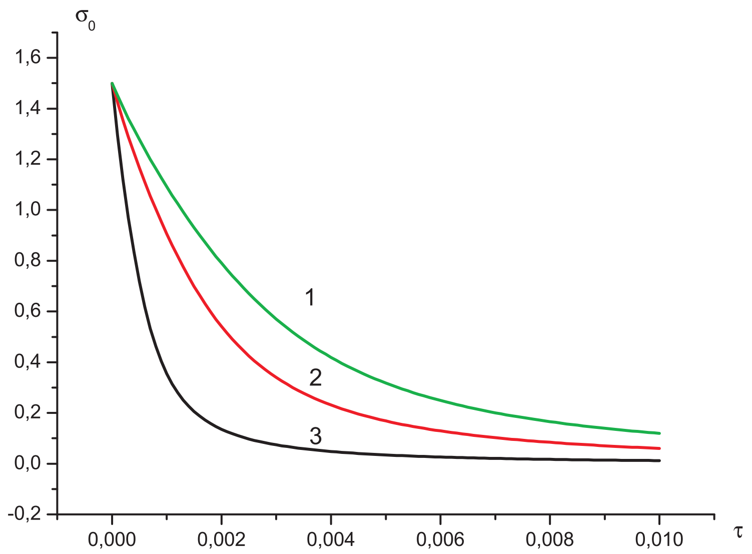

Figure 1. Dependence of the solution σ_0 for equation (4.8) on the temperature. The curve 1 corresponds to the value $h = 0.0001$, the curve 2 presents the case of $h = 0.00005$, and curve 3 describes the case of $h = 0.00001$.

Note that the value $\sigma_0 = 1.500$ at $\tau = 0$ does not depend on the field magnitude.

We write down expressions for renormalized coefficients (4.5) in the form

$$\begin{aligned}\bar{d}(0) &= s^{-2(n_p+2)} r_R\,,\\ \bar{b} &= s^{-3(n_p+2)} v_R\,,\\ \bar{a} &= s^{-4(n_p+2)} u_R\,.\end{aligned} \tag{4.22}$$

Here

$$\begin{aligned}r_R &= r_{n_p+2} + \frac{1}{2} u_{n_p+2} s_0^3 \sigma_0^2\,,\\ v_R &= u_{n_p+2} s_0^{3/2} \sigma_0, \qquad u_R = u_{n_p+2}\,.\end{aligned} \tag{4.23}$$

For calculation of expression (4.3) we use the Gauss approximation. It is related to the small values of coefficients v_r and u_r in comparison with r_R. Performing the substitution of variables in (4.3)

$$\eta_{\vec{k}} = \rho_{\vec{k}} s^{(n_p+2)} \sqrt{2/r_R}$$

we obtain

$$Z_{n_p+2} = \mathrm{e}^{NE_0(\sigma)} s^{(n_p+2)N_{n_p+2}} (2/r_R)^{N_{n_p+2}/2} Z_{\mathrm{G}}\,, \tag{4.24}$$

where

$$\begin{aligned}Z_{\mathrm{G}} &= \int (\mathrm{d}\rho)^{N_{n_p+2}} \exp\Bigg[- \sum_{\vec{k}\in\mathcal{B}_{n_p+2}} \left(1 + 2\beta\Phi(0) b^2 k^2 s^{2(n_p+2)}/r_R\right) \rho_{\vec{k}}\rho_{-\vec{k}}\\ &\quad - x_3 N_{n_p+2}^{-1/2} \sum_{\vec{k}_1,\ldots,\vec{k}_3} \rho_{\vec{k}_1}\ldots\rho_{\vec{k}_3}\delta_{\vec{k}_1+\cdots+\vec{k}_3} - x_4 N_{n_p+2}^{-1} \sum_{\vec{k}_1,\ldots,\vec{k}_4} \rho_{\vec{k}_1}\ldots\rho_{\vec{k}_4}\delta_{\vec{k}_1+\cdots+\vec{k}_4}\Bigg]\,.\end{aligned} \tag{4.25}$$

The quantities x_n

$$x_3 = \frac{\sqrt{2}}{3} v_r/(r_R)^{3/2}, \qquad x_4 = \frac{1}{6} u_r/r_R^2 \tag{4.26}$$

are small in comparison with the unity and decrease at $T \to T_{\mathrm{c}}$. Therefore, the expression (4.25) is reduced to the product of the simple integrals

$$Z_{\mathrm{G}} \approx \prod_{\vec{k}\in\mathcal{B}_{n_p+2}} \int \mathrm{d}\rho_{\vec{k}} \exp\left(-\left(1 + 2\beta\Phi(0)\frac{b^2}{r_R} k^2 s^{2(n_p+2)}\right)\rho_{\vec{k}}\rho_{-\vec{k}}\right)\,. \tag{4.27}$$

The contribution to the system free energy from (4.24) has the form

$$\begin{aligned}F_{n_p+2} &= -kTNE_0(\sigma) - \frac{1}{2}kTN_{n_p+2}\ln\pi - kTN_{n_p+2}(n_p+2)\ln s + \frac{1}{2}kTN_{n_p+2}\ln r_R\\ &\quad + \frac{1}{2}kT \sum_{\vec{k}\in\mathcal{B}_{n_p+2}} \ln\left(1 + 2\beta\Phi(0)b^2k^2 s^{2(n_p+2)}/r_R\right)\,.\end{aligned} \tag{4.28}$$

Here

$$E_0(\sigma_+) = e_0 h \left(\tilde{h}^2 + h_{\mathrm{c}}^2\right)^{\frac{1}{2(d+2)}} - e_2\left(\tilde{h}^2 + h_{\mathrm{c}}^2\right)^{\frac{d}{(d+2)}}\,, \tag{4.29}$$

where the following notation is introduced:

$$\begin{aligned}e_0 &= \sigma_0 s^{-1/2},\\ e_2 &= \frac{1}{2}\sigma_0^2 s^{-3}\left(r_{n_p+2} + \frac{1}{12}u_{n_p+2}s_0^3\sigma_0^2\right)\,.\end{aligned} \tag{4.30}$$

In (4.28) the sum with respect to the $\vec{k} \in \mathcal{B}_{n_p+2}$ can be calculated using the transition to the integral which could be calculated via method [19].

Taking into account the expressions (3.32) and (4.24), we write down the corresponding part of the free energy (3.32) as the sum of two contributions

$$F' = F_0^{(+)} + F'_{\mathrm{G}}\,.$$

The term

$$F_0^{(+)} = -kTNE_0(\sigma_+) \tag{4.31}$$

corresponds to extracting the macroscopic part of the order parameter. For F'_{G} we have

$$F'_{\mathrm{G}} = -kTN_{n_p+2} f_{\mathrm{G}}\,. \tag{4.32}$$

The coefficient f_{G} has the form

$$f_{\mathrm{G}} = \ln s - \frac{1}{4}\ln 3 + \frac{1}{4}\ln u_{n_p+1} - \frac{1}{2}\ln r_R - \frac{1}{2}\ln U(x_{n_p+1}) - \frac{3}{8} y_{n_p+1}^{-2} - \frac{1}{2} f''_{\mathrm{G}}\,. \tag{4.33}$$

Here

$$\begin{aligned} u_{n_p+1} &= (\beta\Phi(0))^2 \varphi_0 (1 + \Phi_f H_{\mathrm{c}}), \\ x_{n_p+1} &= \bar{x} H_{\mathrm{c}} (1 + \Phi_f H_{\mathrm{c}})^{-1/2}, \end{aligned} \tag{4.34}$$

the quantities r_R and y_{n_p+2} are defined in (4.23) and (2.7) respectively, and for f''_{G} we have the expression

$$f''_{\mathrm{G}} = \ln(1 + a^2) - \frac{2}{3} + \frac{2}{a^2} - \frac{2}{a^3}\mathrm{arctg} a, \tag{4.35}$$

where

$$a = \frac{\pi}{s_0}\frac{b}{c}\left(\frac{2\beta\Phi(0)}{r_R}\right)^{1/2}. \tag{4.36}$$

5. System free energy in the external field near the phase transition point at $T > T_{\mathrm{c}}$

Let us collect the contributions to the system free energy from different fluctuation processes which are present near the second order PTP. In accordance with the free energy representation, we have a few types of contributions. Taking into account (3.2) one can see that the expression for F_0 contains the analytic dependence on the field h only. The term F_{CR} exhibits the same type of dependence in expression (3.20). Unifying these contributions we present the notes

$$F_a = F_0 + \left(F_{\mathrm{CR}}^{(+)} - F_{\mathrm{CR}}^{s}\right). \tag{5.1}$$

This is the analytic part of the free energy. It has the form

$$F_a = -kTN \ln \mathrm{ch} h - \frac{1}{2} N\Phi(0)\bar{\Phi} - kTN\left(\gamma_0 + \gamma_1\tau + \gamma_2\tau^2\right), \tag{5.2}$$

where

$$\gamma_0 = \ln 2 + \gamma_{01} s_0^{-3}, \qquad \gamma_1 = \gamma_{02} s_0^{-3}, \qquad \gamma_2 = \gamma_{03} s^{-3}. \tag{5.3}$$

The free energy contributions $F_{\mathrm{CR}}^{(s)}$ (3.22), $F_{\mathrm{TR}}^{(+)}$ (3.30) and F' (4.31) and (4.32) contain the nonanalytic dependence on the temperature τ and field h. We write down their sum in the form of the two types of terms. The first one $F_0^{(+)}$ is related to the displacement of the variable ρ_0 and has the form presented in (4.31). The second type $F_s^{(+)}$ is presented by the sum of the other nonanalytic contributions (the region $T > T_{\mathrm{c}}$)

$$F_s^{(+)} = F_{\mathrm{CR}}^{(s)} + F_{\mathrm{TR}}^{(+)} + F'_{\mathrm{G}} \tag{5.4}$$

and can be represented in the form

$$F_s^{(+)} = -kTN\gamma_s^{(+)} \left(\tilde{h}^2 + h_{\rm c}^2\right)^{\frac{d}{d+2}} , \tag{5.5}$$

where

$$\gamma_s^{(+)} = s_0^{-3} \left(f_{n_p+1} - \bar{\gamma}^+ + f_{\rm G}/s^3\right) . \tag{5.6}$$

Thus, instead of presenting the free energy in the form of (5.1) we have an equivalent expression

$$F = F_a + F_s^{(+)} + F_0^{(+)}, \tag{5.7}$$

where the analytic part F_a is written down as (5.2), and for $F_s^{(+)}$ we have (5.5), The term $F_0^{(+)}$ from (4.31) is described by the expression

$$F_0^{(+)} = -kTN \left[e_0 h(\tilde{h}^2 + h_{\rm c}^2)^{\frac{1}{2(d+2)}} - e_2(\tilde{h}^2 + h_{\rm c}^2)^{\frac{d}{d+2}}\right] . \tag{5.8}$$

The formulas for coefficients e_0 and e_2 are presented in (4.30). The last term of expression (5.8) is the same as the for quantity F_s. Therefore, the free energy can be written down in a more simple form

$$F = F_a + F_h \, , \tag{5.9}$$

where F_a given in (5.2),

$$F_h = -kTN \left(e_0 h(\tilde{h}^2 + h_{\rm c}^2)^{\frac{1}{2(d+2)}} + \gamma_N \left(\tilde{h}^2 + h_{\rm c}^2\right)\right)^{\frac{d}{d+2}} ,$$

and

$$\gamma_N = \gamma_s^{(+)} - e_2 \, . \tag{5.10}$$

The free energy contribution F_h plays the main role in describing the effect of the external field on the system behaviour near the critical point.

6. Conclusions

In this work the method for free energy calculation near the second order phase transition point is suggested. The explicit analytical expression for free energy of the Ising-like system as a function of the temperature and field is found. It could be reduced to the well-known formulas [20,21] represented by (6) and (10) via proceeding to limits $T \to T_{\rm c}$ or $h \to 0$ correspondingly.

It is demonstrated that for such an evaluation one should take into account the presence of two different fluctuation regions. One of them (region CR) is formed by the order parameter fluctuation modes, the wavelength of which does not exceed the system correlation length at a given temperature and external field. In this fluctuation region the RG symmetry takes place. It is responsible for forming the nonclassic values of critical exponents. The second fluctuation region (LGR) is formed by the order parameter fluctuations the wavelength of which exceeds the system correlation length. It is characterized by the Gauss fluctuation distribution and does not effect the values of the critical exponents. Each of these fluctuation regions gives the corresponding contribution to the system free energy.

The evaluation of the expression for free energy also includes the presence of the contribution $F_{\rm TR}$ from the transition region (between regions CR and LGR) as well as the contribution F_0 from the macroscopic part of the average value related to the order parameter. The contribution $F_{\rm TR}$ is formed by the order parameter fluctuations with wavelengths which are measurable with the system correlation length. The contribution F_0^+ is one of the crucial in describing the critical behaviour of the system. It represents some microscopic analogue of Landau free energy and allows one to qualitatively describe all characteristics of the system near the phase transition point. This is some variant of the series expansion for the system free energy in the order parameter. Corresponding coefficients of this expansion are defined as functions of the field and temperature.

References

1. Brout R., Phase Transitions, Benjamin, 1965.
2. Fisher M. Critical Phenomena. ed. M.S. Green and I.V. Sengers, NBS Miscellaneous Publication 273, Washington, 1965.
3. Widom B., J. Chem. Phys., 1965, **43**, 3898–3905.
4. Domb C., Hunter D.L., Proc. Phys. Soc., 1965, **86**, 1147–1151.
5. Kadanoff L.P., Physics, 1966, **2**, 263–273.
6. Patashinskii G.V., Pokrovskii V.L. Fluctuation Theory of Phase Transitions. Nauka, Moscow, 1975 (in Russian).
7. Kozlovskii M.P., Pylyuk I.V., Prytula O.O., Phys. Rev. B, 2006, **73**, 174406.
8. Kozlovskii M.P., Phase Transitions, 2007, **80**, 3–9.
9. Kozlovskii M.P., Pylyuk I.V., Prytula O.O., Physica A, 2006, **369**, 562–576.
10. Kozlovskii M.P. , Pylyuk I.V., Prytula O.O., Nucl. Phys. B, 2006, **753**, 242–251.
11. Kozlovskii M.P., Pylyuk I.V., Prytula O.O., Ferroelectrics, 2005, **317**, 43–47.
12. Yukhnovskii I.R., Kozlovskii M.P., Pylyuk I.V. Microscopic Theory of Phase Transition in the three dimensional systems. Eurosvit, Lviv, 592 p., 2001 (in Russian).
13. Usatenko Z.E., Kozlovskii M.P., Phys.Rev.B. **62**, 9599–9615 (2000).
14. Kozlovskii M.P., Condens. Matter Phys., 2005, **8**, 473–506.
15. Kozlovskii M.P., Condens. Matter Phys., 2007, **10**, 173–178.
16. Yukhnovskii I.R., Kozlovskii M.P., Pylyuk I.V., Phys. Rev. B, 2002, **66**, 134410.
17. Kozlovskii M.P., Analytical method for description of the critical behaviour of 3D Ising-like model in an external field. Preprint of the Institute for Condensed Matter Physics, ICMP–08–10U, Lviv, 2008, 85 p. (in Ukrainian).
18. Ferrenberg A.M., Landau D.P., Phys. Rev. B, 1991, **44**, 5081–5091.
19. Yukhnovskii I.R. Phase Transitions of the Second Order. Collective Variables Method. World Scientific, 1987.
20. Zinn-Justin J., Phys. Rept., 2001, **344**, 159–178.
21. Engels J., Fromme L., Seniuch M., Nucl. Phys. B, 2003, **655**, 277–299.

Вільна енергія $3D$ ізингоподібної системи поблизу точки фазового переходу

М.П.Козловський

Інститут фізики конденсованих систем НАН України, 79011 Львів, вул. Свєнціцького, 1

Отримано 20 лютого 2009 р., в остаточному вигляді – 31 березня 2009 р.

Запропонована узагальнена форма запису скейлінгової форми вільної енергії системи поблизу точки фазового переходу. На мікроскопічному рівні строгості отримані явні вирази для коефіцієнтів як функцій відносної температури та зовнішнього поля для випадку $T > T_{\mathrm{c}}$.

Ключові слова: *фазовий перехід, зовнішнє поле, вільна енергія*

PACS: *05.50.+q, 64.60.Fr, 75.10.Hk*