Condensed Matter Physics, 2012, Vol. 15, No 4, 43006: 1–10
DOI: 10.5488/CMP.15.43006
http://www.icmp.lviv.ua/journal

CONDENSED MATTER PHYSICS

Critical behaviour of a 3D Ising-like system in the ρ^6 model approximation: Role of the correction for the potential averaging

I.V. Pylyuk[1]*, M.V. Ulyak[2]

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

[2] Chervonograd State College of Mining Technologies and Economics, 17 Stus St., 80100 Chervonograd, Ukraine

Received July 3, 2012, in final form September 12, 2012

The critical behaviour of systems belonging to the three-dimensional Ising universality class is studied theoretically using the collective variables (CV) method. The partition function of a one-component spin system is calculated by the integration over the layers of the CV phase space in the approximation of the non-Gaussian sextic distribution of order-parameter fluctuations (the ρ^6 model). A specific feature of the proposed calculation consists in making allowance for the dependence of the Fourier transform of the interaction potential on the wave vector. The inclusion of the correction for the potential averaging leads to a nonzero critical exponent of the correlation function η and the renormalization of the values of other critical exponents. The contributions from this correction to the recurrence relations for the ρ^6 model, fixed-point coordinates and elements of the renormalization-group linear transformation matrix are singled out. The expression for a small critical exponent η is obtained in a higher non-Gaussian approximation.

Key words: *three-dimensional Ising-like system, critical behaviour, sextic distribution, potential averaging, small critical exponent*

PACS: *05.50.+q, 64.60.F-, 75.10.Hk*

1. Method

We shall use the approach of collective variables (CV) [1, 2], which allows us to calculate the expression for the partition function of a system and to obtain complete expressions for thermodynamic functions near the phase-transition temperature T_c in addition to universal quantities (i.e., critical exponents). The CV approach is non-perturbative and similar to the Wilson non-perturbative renormalization-group (RG) approach (integration on fast modes and construction of an effective theory for slow modes) [3–5].

The term collective variables is a common name for a special class of variables that are specific for each individual physical system. The CV set contains variables associated with order parameters. Consequently, the phase space of CV is most natural in describing a phase transition. For magnetic systems, the CV $\rho_{\mathbf{k}}$ are the variables associated with the modes of spin-moment density oscillations, while the order parameter is related to the variable ρ_0, in which the subscript "0" corresponds to the peak of the Fourier transform of the interaction potential. The methods available at present, make it possible to calculate universal quantities to a quite high degree of accuracy (see, for example, [6]). The advantage of the CV method lies in the possibility to obtain and analyse thermodynamic characteristics as functions of microscopic parameters of the original system. The use of the non-Gaussian basis distributions of fluctuations in calculating the partition function of a system does not bring about a problem of summing various classes of divergent (with respect to the Gaussian distribution) diagrams at the critical point. A considera-

* E-mail: piv@icmp.lviv.ua

tion of the increasing number of terms in the exponent of the non-Gaussian distribution is an alternative to the use of a higher-order perturbation theory based on the Gaussian distribution.

The integration of partition function begins with the variables $\rho_{\mathbf{k}}$ having a large value of the wave vector k (of the order of the Brillouin half-zone boundary) and terminates at $\rho_{\mathbf{k}}$ with $k \to 0$. For this purpose, we divide the phase space of the CV $\rho_{\mathbf{k}}$ into layers with the division parameter s. In each nth layer (corresponding to the region of wave vectors $B_{n+1} < k \leqslant B_n$, $B_{n+1} = B_n/s$, $s > 1$), the Fourier transform of the interaction potential is replaced by its average value. This simplified procedure leads to a zero value of the critical exponent η characterizing the behaviour of the pair-correlation function at the critical temperature T_{c}.

2. The setup

The object of investigation is a three-dimensional (3D) Ising-like system. The Ising model, despite its simplicity, has, on the one hand, a wide scope of realistic applications, and, on the other hand, it can be considered as a model, which serves as a standard in studying other models possessing a much more complicated construction.

In our previous calculations (for example, [7–10]), we assumed that the correction for the potential averaging is zero. As a result, we lost some information in the process of calculating the partition function of the system. In particular, the critical exponent η was equal to zero.

In [11], the correction for the averaging of the Fourier transform of the potential is taken into account in the simplest non-Gaussian approximation (the ρ^4 model based on the quartic fluctuation distribution). The inclusion of this correction gives rise to a nonzero value of the critical exponent η. Recurrence relations (RR) between the coefficients of the effective distributions take another form as compared with the case when $\eta = 0$. A fixed point is shifted. Critical exponents of the correlation length ν, susceptibility γ and specific heat α are renormalized. Critical amplitudes are also modified. As is seen from table 1, the inclusion of a nonzero exponent η within the CV method reduces the critical exponent ν (like in the non-perturbative RG approach [12]). In order to obtain better quantitative estimates of ν and other critical exponents, it is necessary to use the distributions of fluctuations more complicated than the quartic distribution. In the case of $\eta = 0$, the critical exponent of the correlation length for these distributions takes on larger values than ν for the ρ^4 model (figure 1) [2, 8]. The results of calculations and their comparison with the other authors' data show that the sextic distribution (the ρ^6 model) provides a more adequate

Table 1. Estimates of the critical exponents for the ρ^4 model and the RG parameter $s = 4$ in the case of the correction for the potential averaging not taken into account ($\Delta\tilde{\Phi}(k) = 0$) and in the case of the correction for the potential averaging taken into account ($\Delta\tilde{\Phi}(k) \neq 0$).

Condition	η	ν	γ	α
$\Delta\tilde{\Phi}(k) = 0$	0	0.612	1.225	0.163
$\Delta\tilde{\Phi}(k) \neq 0$	0.024	0.577	1.141	0.268

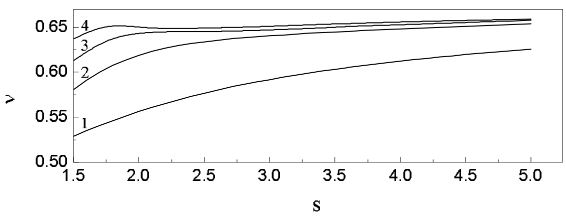

Figure 1. Evolution of the critical exponent of the correlation length ν with an increasing parameter of division of the CV phase space into layers s. Curves 1, 2, 3 and 4 correspond to the ρ^4, ρ^6, ρ^8 and ρ^{10} models, respectively.

quantitative description of the critical behaviour of a 3D Ising ferromagnet than the quartic distribution [2, 13]. The sextic distribution for the modes of spin-moment density oscillations is presented as an exponential function of the CV whose argument includes the sixth power of the variable in addition to the second and the fourth powers.

In the present publication, our aim is to investigate the effect of the above-mentioned correction for the potential averaging on the critical properties of a 3D Ising-like system and to elaborate a technique for calculating the small critical exponent η in the ρ^6 model approximation. The analytic results, obtained in this higher non-Gaussian approximation, provide the basis for accurate analysis of the behaviour of the system near T_{c} with allowance for the exponent η.

The developed approach permits to perform the calculations for a one-component spin system in real 3D space on the microscopic level without any adjustable parameters. The calculation technique for η is similar to that proposed in the case of the quartic distribution [11]. New special functions appearing in the construction of the phase-transition theory using the sextic distribution were considered in [2, 14]. In the case of the ρ^6 model, we exploit the special functions with two arguments more complicated than the parabolic cylinder functions with one argument for the ρ^4 model.

3. Basic relations

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

$$H = -\frac{1}{2}\sum_{\mathbf{i},\mathbf{j}} \Phi\left(r_{\mathbf{ij}}\right) s_{\mathbf{i}} s_{\mathbf{j}} - h \sum_{\mathbf{i}} s_{\mathbf{i}}\,, \tag{3.1}$$

where $s_{\mathbf{i}}$ is the operator of the z-component of spin at the $\mathbf{i}$th site, having two eigenvalues $+1$ and -1. The interaction potential is an exponentially decreasing function

$$\Phi\left(r_{\mathbf{ij}}\right) = A \exp\left(-r_{\mathbf{ij}}/b\right). \tag{3.2}$$

Here, A is a constant, $r_{\mathbf{ij}}$ is the interparticle distance, and b is the radius of effective interaction. In the representation of the CV $\rho_{\mathbf{k}}$, the partition function of the system in the absence of an external field $\mathscr{H}$ ($h = \mu_{\mathrm{B}}\mathscr{H} = 0$, μ_{B} is the Bohr magneton) can be written in the form

$$\begin{aligned} Z \;=\; & 2^N 2^{(N_1-1)/2} Q_0 [Q(P)]^{N_1} \int \exp\left\{-\frac{1}{2}\sum_{k\leqslant B_1}\left[d'(k) - d'\left(B_1, B'\right)\right]\rho_{\mathbf{k}}\rho_{-\mathbf{k}}\right\} \\ & \times \left(1 + \hat{\Delta}_g + \cdots\right) \exp\left[-\frac{1}{2} R_2 \sum_{k\leqslant B_1} \rho_{\mathbf{k}}\rho_{-\mathbf{k}} \right. \\ & \left. - \sum_{l=2}^{3} \frac{R_{2l}}{(2l)! N_1^{l-1}} \sum_{k_1,\ldots,k_{2l}\leqslant B_1} \rho_{\mathbf{k}_1}\cdots\rho_{\mathbf{k}_{2l}} \delta_{\mathbf{k}_1+\cdots+\mathbf{k}_{2l}} \right] (\mathrm{d}\rho)^{N_1}\,, \end{aligned} \tag{3.3}$$

where $B_1 = B'/s$, $N_1 = N' s^{-3}$, $B' = \left(b\sqrt{2}\right)^{-1}$, $N' = N s_0^{-3}$, $s_0 = B/B'$, $B = \pi/c$ is the boundary of Brillouin half-zone, and $\delta_{\mathbf{k}_1+\cdots+\mathbf{k}_4}$ is the Kronecker symbol. For the coefficient $d'(k)$, we have

$$d'(k) = a_2' - \beta\tilde{\Phi}(k). \tag{3.4}$$

Here, $\beta = 1/(kT)$ is the inverse temperature. For the Fourier transform of the interaction potential, we use the following approximation [8, 15]:

$$\tilde{\Phi}(k) = \begin{cases} \tilde{\Phi}(0)\left(1 - 2b^2k^2\right), & k \leqslant B', \\ 0, & B' < k \leqslant B. \end{cases} \tag{3.5}$$

The quantities Q_0, $Q(P)$ and R_{2l} are ultimate functions of the initial coefficients a_{2l}' ($l = 0, 1, 2, 3$) [2, 16]. The coefficients a_{2l}' are determined by special functions of two arguments and are dependent on the ratio of the effective interaction radius b to the lattice constant c, i.e., on the microscopic parameters of the system (see, for example, [17]).

The correction, which is introduced by the operator $\hat{\Delta}_g$, is considered in the linear approximation in

$$\Delta\tilde{\Phi}(k) = q - 2b^2\beta\tilde{\Phi}(0)k^2. \tag{3.6}$$

The quantity $\Delta\tilde{\Phi}(k)$ corresponds to the deviation $\beta\tilde{\Phi}(k)$ from the average value $\beta\tilde{\Phi}(B_1, B')$. Here, $q = \bar{q}\beta\tilde{\Phi}(0)$, $\bar{q}$ defines the geometric mean value of k^2 on the interval $(1/s, 1]$. In the above-mentioned approximation, we arrive at the expression

$$\begin{aligned}\hat{\Delta}_g^{(1)} \;=\; & \frac{1}{2}\sum_{k_1,\ldots,k_6\leqslant B_1}\left[\frac{4C(h,\alpha)}{a_4'}\right]^2\frac{\partial^6}{\partial\rho_{\mathbf{k}_1}\cdots\partial\rho_{\mathbf{k}_6}}(N')^{-4}\sum_{B_1<k\leqslant B'}\Delta g(k)\\ & \times\sum_{\mathbf{l}_1,\mathbf{l}_2}\exp\left[-\mathrm{i}\left(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3+\mathbf{k}\right)\mathbf{l}_1-\mathrm{i}\left(\mathbf{k}_4+\mathbf{k}_5+\mathbf{k}_6-\mathbf{k}\right)\mathbf{l}_2\right],\end{aligned} \tag{3.7}$$

which defines the operator $\hat{\Delta}_g$ accurate to within the term proportional to $\frac{\partial^6}{\partial\rho_{\mathbf{k}_1}\cdots\partial\rho_{\mathbf{k}_6}}$ (the terms proportional to the higher orders of operators $\partial/\partial\rho_{\mathbf{k}}$ are not taken into account). The summation over the sites $\mathbf{l}_1, \mathbf{l}_2$ in (3.7) is carried out for the lattice with period $c' = \pi b\sqrt{2}$. The role of $\Delta g(k)$ is played by the quantity

$$\Delta g(k) = \frac{\Delta\tilde{\Phi}(k)}{1 - S_2(2\pi)^{-2}\Delta\tilde{\Phi}(k)}, \tag{3.8}$$

where $S_2 = (2\pi)^2\left(24/a_4'\right)^{1/2}F_2(h,\alpha)$. The forms of the functions $C(h,\alpha)$ and $F_2(h,\alpha)$ as well as of their arguments h and α are presented in the next section. We assume that $\hat{\Delta}_g^{(1)}$ operates only on $\exp\left(-\frac{1}{2}R_2\sum_{k\leqslant B_1}\rho_{\mathbf{k}}\rho_{-\mathbf{k}}\right)$ in (3.3). This assumption is associated with small contributions from R_4 and R_6 in comparison with the contribution from R_2 (in particular, $R_4/\left(6R_2^2\right) \sim 10^{-4}$ [11]).

4. Partition function of the system with allowance for the correction for the potential averaging

The integration over the zeroth, first, second, …, nth layers of the CV phase space leads to the representation of the partition function in the form of a product of the partial partition functions $\tilde{Q}_n$ of individual layers and the integral of the "smoothed" effective distribution of fluctuations. We have

$$Z = 2^N 2^{(N_{n+1}-1)/2}\tilde{Q}_0\tilde{Q}_1\cdots\tilde{Q}_n[Q(P_n)]^{N_{n+1}}\int\tilde{\mathscr{W}}_6^{(n+1)}(\rho)(\mathrm{d}\rho)^{N_{n+1}}. \tag{4.1}$$

The effective sextic distribution of fluctuations in the $(n+1)$th block structure is written as follows:

$$\tilde{\mathscr{W}}_6^{(n+1)}(\rho) = \exp\left[-\frac{1}{2}\sum_{k\leqslant B_{n+1}}\tilde{d}_{n+1}(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}} - \sum_{l=2}^{3}\frac{\tilde{a}_{2l}^{(n+1)}}{(2l)!N_{n+1}^{l-1}}\sum_{k_1,\ldots,k_{2l}\leqslant B_{n+1}}\rho_{\mathbf{k}_1}\cdots\rho_{\mathbf{k}_{2l}}\delta_{\mathbf{k}_1+\cdots+\mathbf{k}_{2l}}\right]. \tag{4.2}$$

Here, $B_{n+1} = B's^{-(n+1)}$, $N_{n+1} = N's^{-3(n+1)}$, and $\tilde{d}_{n+1}(k)$, $\tilde{a}_4^{(n+1)}$, $\tilde{a}_6^{(n+1)}$ are the renormalized values of coefficients $d'(k)$, a_4', a_6' after integration over $n+1$ layers of the phase space of CV.

In comparison with the results obtained earlier without taking into account the correction for the potential averaging (see, for example, [2, 8, 16, 17]), the expression (4.1) includes new quantities. In particular, the function

$$f(h_n,\alpha_n) = -48s^{9/2}C^{1/2}(h_n,\alpha_n)F_2^3(\eta_n,\xi_n)\frac{q_n t_n}{\sqrt{\tilde{a}_4^{(n)}}}\mathscr{F}_0 \tag{4.3}$$

appearing in $\tilde{Q}_n$ characterizes the correction to the partial partition functions. The basic arguments $h_n = \tilde{d}_n(B_{n+1},B_n)\left(6/\tilde{a}_4^{(n)}\right)^{1/2}$ and $\alpha_n = \sqrt{6}\tilde{a}_6^{(n)}/\left[15\left(\tilde{a}_4^{(n)}\right)^{3/2}\right]$ are expressed in terms of the coefficients $\tilde{d}_n(B_{n+1},B_n)$ (the average value of $\tilde{d}_n(k)$ in the nth layer of the CV phase space), $\tilde{a}_4^{(n)}$ and $\tilde{a}_6^{(n)}$. The intermediate variables $\eta_n = \left(6s^3\right)^{1/2}F_2(h_n,\alpha_n)/C^{1/2}(h_n,\alpha_n)$ and $\xi_n = \sqrt{6}s^{-3/2}N(h_n,\alpha_n)/\left[15C^{3/2}(h_n,\alpha_n)\right]$

are functions of h_n and α_n. The special functions $C(h_n,\alpha_n) = -F_4(h_n,\alpha_n) + 3F_2^2(h_n,\alpha_n)$ and $N(h_n,\alpha_n) = F_6(h_n,\alpha_n) - 15F_4(h_n,\alpha_n)F_2(h_n,\alpha_n) + 30F_2^3(h_n,\alpha_n)$ are combinations of the functions $F_{2l}(h_n,\alpha_n) = I_{2l}(h_n,\alpha_n)/I_0(h_n,\alpha_n)$, where $I_{2l}(h_n,\alpha_n) = \int_0^\infty t^{2l}\exp\left(-h_n t^2 - t^4 - \alpha_n t^6\right)\mathrm{d}t$. The relation (4.3) for $f(h_n,\alpha_n)$, except

$$q_n = q\frac{1+\alpha_0'}{s^2}\frac{1+\alpha_1'}{s^2}\cdots\frac{1+\alpha_{n-1}'}{s^2}, \tag{4.4}$$

contains the factor

$$t_n = \sqrt{\frac{\tilde{a}_4^{(n)}}{24}}\frac{1}{F_2(h_n,\alpha_n)}\frac{s^2}{1+\alpha_0'}\frac{s^2}{1+\alpha_1'}\cdots\frac{s^2}{1+\alpha_{n-1}'}t_0^{(n)}\frac{1}{\beta\tilde{\Phi}(0)}. \tag{4.5}$$

For the quantity α_n', which defines the correction for the averaging of the Fourier transform of the potential in the nth layer of the phase space of CV, we obtain

$$\alpha_n' = 144\pi^2 s^6 F_2^4(\eta_n,\xi_n)\bar{q}\,t_n\mathscr{B}_0. \tag{4.6}$$

The expressions for $\mathscr{F}_0$ (appearing in $f(h_n,\alpha_n)$), $t_0^{(n)}$ (appearing in t_n) and $\mathscr{B}_0$ (appearing in α_n') are presented in [2, 11]. At large values of the RG parameter s, there emerge large intervals of wave vectors, in which $\tilde{\Phi}(k)$ is averaged. In this case ($s > 5$), the correction $\beta\tilde{\Phi}(k) - \beta\tilde{\Phi}(B_{n+1},B_n)$ is substantial, so that its accounting in the linear approximation is incorrect.

5. Analysis of recurrence relations for the ρ^6 model. Critical exponent η

The coefficients $\tilde{d}_{n+1}(k)$, $\tilde{a}_4^{(n+1)}$ and $\tilde{a}_6^{(n+1)}$ in (4.2) satisfy the following RR:

$$\begin{aligned}
\tilde{d}_{n+1}(B_{n+2},B_{n+1}) &= (\tilde{a}_4^{(n)})^{1/2}\tilde{Y}(h_n,\alpha_n) - q\frac{1+\alpha_0'}{s^2}\frac{1+\alpha_1'}{s^2}\cdots\frac{1+\alpha_{n-1}'}{s^2}\left(1-\frac{1+\alpha_n'}{s^2}\right),\\
\tilde{a}_4^{(n+1)} &= \tilde{a}_4^{(n)}s^{-3}\tilde{B}(h_n,\alpha_n),\\
\tilde{a}_6^{(n+1)} &= \left(\tilde{a}_4^{(n)}\right)^{3/2}s^{-6}\tilde{D}(h_n,\alpha_n).
\end{aligned} \tag{5.1}$$

The contributions to the functions

$$\begin{aligned}
\tilde{Y}(h_n,\alpha_n) &= Y(h_n,\alpha_n)\left[1 - G(h_n,\alpha_n)\mathscr{A}_0\right],\\
\tilde{B}(h_n,\alpha_n) &= B(h_n,\alpha_n)\left[1 + \mathscr{K}(h_n,\alpha_n)\mathscr{C}_0\right],\\
\tilde{D}(h_n,\alpha_n) &= D(h_n,\alpha_n)\left[1 - \mathscr{L}(h_n,\alpha_n)\mathscr{D}_0\right]
\end{aligned} \tag{5.2}$$

from the potential averaging are given by the terms $G(h_n,\alpha_n)\mathscr{A}_0$, $\mathscr{K}(h_n,\alpha_n)\mathscr{C}_0$ and $\mathscr{L}(h_n,\alpha_n)\mathscr{D}_0$. Here,

$$\begin{aligned}
Y(h_n,\alpha_n) &= s^{3/2}F_2(\eta_n,\xi_n)C^{-1/2}(h_n,\alpha_n),\\
B(h_n,\alpha_n) &= s^6 C(\eta_n,\xi_n)C^{-1}(h_n,\alpha_n),\\
D(h_n,\alpha_n) &= s^{21/2}N(\eta_n,\xi_n)C^{-3/2}(h_n,\alpha_n),
\end{aligned} \tag{5.3}$$

and

$$\begin{aligned}
G(h_n,\alpha_n) &= 288 s^{9/2}F_2^3(\eta_n,\xi_n)C^{1/2}(h_n,\alpha_n)\frac{q\,t_n}{\sqrt{\bar{u}_n}},\\
\mathscr{K}(h_n,\alpha_n) &= 1728 s^{3/2}\frac{F_2^5(\eta_n,\xi_n)}{C(\eta_n,\xi_n)}C^{1/2}(h_n,\alpha_n)\frac{q\,t_n}{\sqrt{\bar{u}_n}},\\
\mathscr{L}(h_n,\alpha_n) &= 17280 s^{-3/2}\frac{F_2^6(\eta_n,\xi_n)}{N(\eta_n,\xi_n)}C^{1/2}(h_n,\alpha_n)\frac{q\,t_n}{\sqrt{\bar{u}_n}}.
\end{aligned} \tag{5.4}$$

The quantities $\mathscr{A}_0$, $\mathscr{C}_0$ and $\mathscr{D}_0$ as well as the quantities $\mathscr{F}_0$ and $\mathscr{B}_0$ mentioned above appear due to the inclusion of the averaging correction. They are calculated with the help of the summation over the distances to the particles located at the lattice sites (see [2, 11]). In terms of the variables

$$\begin{aligned}
\tilde{r}_n &= \frac{s^2}{1+\alpha'_0}\frac{s^2}{1+\alpha'_1}\cdots\frac{s^2}{1+\alpha'_{n-1}}\tilde{d}_n(0),\\
\tilde{u}_n &= \frac{s^4}{\left(1+\alpha'_0\right)^2}\frac{s^4}{\left(1+\alpha'_1\right)^2}\cdots\frac{s^4}{\left(1+\alpha'_{n-1}\right)^2}\tilde{a}_4^{(n)},\\
\tilde{w}_n &= \frac{s^6}{\left(1+\alpha'_0\right)^3}\frac{s^6}{\left(1+\alpha'_1\right)^3}\cdots\frac{s^6}{\left(1+\alpha'_{n-1}\right)^3}\tilde{a}_6^{(n)},
\end{aligned}\tag{5.5}$$

the RR (5.1) assume the forms

$$\begin{aligned}
\tilde{r}_{n+1} &= \frac{s^2}{1+\alpha'_n}\left[-q+(\tilde{u}_n)^{1/2}\,\tilde{Y}(h_n,\alpha_n)\right],\\
\tilde{u}_{n+1} &= \frac{s}{\left(1+\alpha'_n\right)^2}\tilde{u}_n\tilde{B}(h_n,\alpha_n),\\
\tilde{w}_{n+1} &= \frac{1}{\left(1+\alpha'_n\right)^3}(\tilde{u}_n)^{3/2}\tilde{D}(h_n,\alpha_n).
\end{aligned}\tag{5.6}$$

There are two essential distinctions between the RR (5.6) and those obtained without involving the correction for $\Delta\tilde{\Phi}(k)$ [2, 14, 18]. The first of them consists in the specific substitution of variables (5.5), which differs from the corresponding substitution without the correction by including the factors $\left(1+\alpha'_0\right)\left(1+\alpha'_1\right)\cdots\left(1+\alpha'_{n-1}\right)$. The second distinction concerns the transformation of special functions $Y(h_n,\alpha_n)$, $B(h_n,\alpha_n)$ and $D(h_n,\alpha_n)$ (5.3) into the functions $\tilde{Y}(h_n,\alpha_n)$, $\tilde{B}(h_n,\alpha_n)$ and $\tilde{D}(h_n,\alpha_n)$ (5.2). This distinction is associated with a shift of the fixed-point coordinates and with corrections to the critical exponents of thermodynamic functions.

A particular solution of RR (5.6) is a new fixed point $(\tilde{r},\tilde{u},\tilde{w})$, which differs at $\Delta\tilde{\Phi}(k)\neq 0$ from the fixed point $(r^{(0)},u^{(0)},w^{(0)})$ for the case of $\Delta\tilde{\Phi}(k)=0$ [2, 14, 18]. The coordinates of the fixed point of RR (5.6) can be expressed as follows:

$$\tilde{r}=-\tilde{f}\beta\tilde{\Phi}(0),\qquad \tilde{u}=\tilde{\varphi}[\beta\Phi(0)]^2,\qquad \tilde{w}=\tilde{\psi}[\beta\Phi(0)]^3.\tag{5.7}$$

Here,

$$\begin{aligned}
\tilde{f} &= \bar{q}\left[\tilde{Y}\left(\tilde{h},\tilde{\alpha}\right)-\tilde{h}/\sqrt{6}\right]\left[\tilde{Y}\left(\tilde{h},\tilde{\alpha}\right)-\left(1+\alpha'^{(0)}\right)\tilde{h}\Big/\left(s^2\sqrt{6}\right)\right]^{-1},\\
\tilde{\varphi} &= \bar{q}^2\left[1-\left(1+\alpha'^{(0)}\right)s^{-2}\right]^2\left[\tilde{Y}\left(\tilde{h},\tilde{\alpha}\right)-\left(1+\alpha'^{(0)}\right)\tilde{h}\Big/\left(s^2\sqrt{6}\right)\right]^{-2},\\
\tilde{\psi} &= \left(1+\alpha'^{(0)}\right)^{-3}\left(\tilde{\varphi}\right)^{3/2}\tilde{D}\left(\tilde{h},\tilde{\alpha}\right),
\end{aligned}\tag{5.8}$$

and

$$\begin{aligned}
\tilde{h} &= \sqrt{6}\frac{\tilde{r}+q}{(\tilde{u})^{1/2}},\\
\tilde{\alpha} &= \frac{\sqrt{6}}{15}\frac{\tilde{w}}{(\tilde{u})^{3/2}},\\
\alpha'^{(0)} &= 144\pi^2 s^6 F_2^4\left(\eta^{(0)},\xi^{(0)}\right)\bar{q}\,t^{(0)}\mathscr{B}_0,\\
t^{(0)} &= t_n(u^{(0)},h^{(0)},\alpha^{(0)}).
\end{aligned}\tag{5.9}$$

The quantities $h^{(0)}$, $\alpha^{(0)}$ and $\eta^{(0)}$, $\xi^{(0)}$ describe, respectively, the basic (h_n, α_n) and intermediate (η_n, ξ_n) arguments at the fixed point obtained without involving the correction for the potential averaging. In the linear approximation in $\Delta\tilde{\Phi}(k)$, we have

$$\begin{aligned}
\tilde{f} &= f_0\Big(1+\Big\{\Big[Y_h'\big(h^{(0)},\alpha^{(0)}\big)h^{(0)}/\sqrt{6}-Y\big(h^{(0)},\alpha^{(0)}\big)/\sqrt{6}\Big]\Delta h+Y_\alpha'\big(h^{(0)},\alpha^{(0)}\big)h^{(0)}/\sqrt{6}\Delta\alpha\\
&-Y\big(h^{(0)},\alpha^{(0)}\big)G\big(h^{(0)},\alpha^{(0)}\big)\mathscr{A}_0h^{(0)}/\sqrt{6}\Big\}\big(1-s^{-2}\big)\Big\{\Big[Y\big(h^{(0)},\alpha^{(0)}\big)-h^{(0)}/\sqrt{6}\Big]\\
&\times\Big[Y\big(h^{(0)},\alpha^{(0)}\big)-h^{(0)}/\big(s^2\sqrt{6}\big)\Big]\Big\}^{-1}+\alpha'^{(0)}h^{(0)}/\big(s^2\sqrt{6}\big)\Big[Y\big(h^{(0)},\alpha^{(0)}\big)-h^{(0)}/\big(s^2\sqrt{6}\big)\Big]^{-1}\Big),\\
\tilde{\varphi} &= \varphi_0\Big(1+2\Big\{-\Big[Y_h'\big(h^{(0)},\alpha^{(0)}\big)-1/\big(s^2\sqrt{6}\big)\Big]\Delta h-Y_\alpha'\big(h^{(0)},\alpha^{(0)}\big)\Delta\alpha+Y\big(h^{(0)},\alpha^{(0)}\big)G(h^{(0)},\alpha^{(0)})\mathscr{A}_0\\
&+\alpha'^{(0)}h^{(0)}/\big(s^2\sqrt{6}\big)\Big\}\Big[Y\big(h^{(0)},\alpha^{(0)}\big)-h^{(0)}/\big(s^2\sqrt{6}\big)\Big]^{-1}-2\alpha'^{(0)}s^{-2}/\big(1-s^{-2}\big)\Big),\\
\tilde{\psi} &= \psi_0\Big[1+3\Big(\Big\{\Big[Y\big(h^{(0)},\alpha^{(0)}\big)-h^{(0)}/\big(s^2\sqrt{6}\big)\Big]D_h'\big(h^{(0)},\alpha^{(0)}\big)/3-\Big[Y_h'\big(h^{(0)},\alpha^{(0)}\big)-1/\big(s^2\sqrt{6}\big)\Big]\\
&\times D\big(h^{(0)},\alpha^{(0)}\big)\Big\}\Delta h+\Big\{\Big[Y\big(h^{(0)},\alpha^{(0)}\big)-h^{(0)}/\big(s^2\sqrt{6}\big)\Big]D_\alpha'\big(h^{(0)},\alpha^{(0)}\big)/3\\
&-Y_\alpha'\big(h^{(0)},\alpha^{(0)}\big)D\big(h^{(0)},\alpha^{(0)}\big)\Big\}\Delta\alpha+Y\big(h^{(0)},\alpha^{(0)}\big)D\big(h^{(0)},\alpha^{(0)}\big)G\big(h^{(0)},\alpha^{(0)}\big)\mathscr{A}_0\\
&+\alpha'^{(0)}h^{(0)}D(h^{(0)},\alpha^{(0)})/\big(s^2\sqrt{6}\big)\Big)\Big\{\Big[Y\big(h^{(0)},\alpha^{(0)}\big)-h^{(0)}/\big(s^2\sqrt{6}\big)\Big]D\big(h^{(0)},\alpha^{(0)}\big)\Big\}^{-1}\\
&-3\alpha'^{(0)}/\big(1-s^{-2}\big)-\mathscr{L}\big(h^{(0)},\alpha^{(0)}\big)\mathscr{D}_0\Big]. \qquad (5.10)
\end{aligned}$$

The quantities f_0, φ_0 and ψ_0 characterize the fixed-point coordinates in the case when $\eta=0$. Formulas for the derivatives $Y_h'\big(h^{(0)},\alpha^{(0)}\big)$, $Y_\alpha'\big(h^{(0)},\alpha^{(0)}\big)$, $D_h'\big(h^{(0)},\alpha^{(0)}\big)$ and $D_\alpha'(h^{(0)},\alpha^{(0)})$ can be written using series expansions of the corresponding functions in the vicinity of the fixed point [14]. The differences $\Delta h=\tilde{h}-h^{(0)}$ and $\Delta\alpha=\tilde{\alpha}-\alpha^{(0)}$ determine the displacements of the basic arguments h_n and α_n at the fixed points $(\tilde{r},\tilde{u},\tilde{w})$ and $\big(r^{(0)},u^{(0)},w^{(0)}\big)$.

The RR (5.6) make it possible to find the elements of the RG linear transformation matrix. These matrix elements $\tilde{R}_{ij}$ $(i=1,2,3;\ j=1,2,3)$ can be presented in the following forms (the linear approximation in $\Delta\tilde{\Phi}(k)$):

$$\begin{aligned}
\tilde{R}_{11} &= R_{11}\big(1-\alpha'^{(0)}\big)+R_{11}^{(1h)}\Delta h+R_{11}^{(1\alpha)}\Delta\alpha+R_{11}^{(2)}\mathscr{A}_0,\\
\tilde{R}_{22} &= R_{22}\big(1-2\alpha'^{(0)}\big)+R_{22}^{(1h)}\Delta h+R_{22}^{(1\alpha)}\Delta\alpha+R_{22}^{(2)}\mathscr{C}_0,\\
\tilde{R}_{33} &= R_{33}\big(1-3\alpha'^{(0)}\big)+R_{33}^{(1h)}\Delta h+R_{33}^{(1\alpha)}\Delta\alpha+R_{33}^{(2)}\mathscr{D}_0,\\
\tilde{R}_{ij} &= \tilde{R}_{ij}^{(0)}(\tilde{u})^{(i-j)/2}, \qquad i\neq j,\\
\tilde{R}_{1k_1}^{(0)} &= R_{1k_1}^{(0)}\big(1-\alpha'^{(0)}\big)+R_{1k_1}^{(1h)}\Delta h+R_{1k_1}^{(1\alpha)}\Delta\alpha+R_{1k_1}^{(2)}\mathscr{A}_0, \qquad k_1=2,3,\\
\tilde{R}_{2k_2}^{(0)} &= R_{2k_2}^{(0)}\big(1-2\alpha'^{(0)}\big)+R_{2k_2}^{(1h)}\Delta h+R_{2k_2}^{(1\alpha)}\Delta\alpha+R_{2k_2}^{(2)}\mathscr{C}_0, \qquad k_2=1,3,\\
\tilde{R}_{3k_3}^{(0)} &= R_{3k_3}^{(0)}\big(1-3\alpha'^{(0)}\big)+R_{3k_3}^{(1h)}\Delta h+R_{3k_3}^{(1\alpha)}\Delta\alpha+R_{3k_3}^{(2)}\mathscr{D}_0, \qquad k_3=1,2. \qquad (5.11)
\end{aligned}$$

It should be noted that formulas for the quantities R_{ii} and $R_{ij}^{(0)}$ $(i\neq j)$ from (5.11) coincide with the corresponding expressions for the matrix elements obtained without taking into account the correction for the potential averaging [2]. The contributions to the matrix elements $\tilde{R}_{ij}$ from terms $R_{ij}^{(1h)}\Delta h$ and $R_{ij}^{(1\alpha)}\Delta\alpha$ correspond to a fixed-point shift due to the inclusion of the dependence of the Fourier transform of the interaction potential on the wave vector. The terms like $R_{ij}^{(2)}\mathscr{A}_0$, $R_{ij}^{(2)}\mathscr{C}_0$ and $R_{ij}^{(2)}\mathscr{D}_0$ describe a direct contribution to $\tilde{R}_{ij}$ from the correction for averaging.

The explicit solutions of RR

$$\begin{aligned}
\tilde{r}_n &= \tilde{r}+\tilde{c}_1\tilde{E}_1^n+\tilde{c}_2\tilde{w}_{12}^{(0)}(\tilde{u})^{-1/2}\tilde{E}_2^n+\tilde{c}_3\tilde{w}_{13}^{(0)}(\tilde{u})^{-1}\tilde{E}_3^n,\\
\tilde{u}_n &= \tilde{u}+\tilde{c}_1\tilde{w}_{21}^{(0)}(\tilde{u})^{1/2}\tilde{E}_1^n+\tilde{c}_2\tilde{E}_2^n+\tilde{c}_3\tilde{w}_{23}^{(0)}(\tilde{u})^{-1/2}\tilde{E}_3^n,\\
\tilde{w}_n &= \tilde{w}+\tilde{c}_1\tilde{w}_{31}^{(0)}\tilde{u}\tilde{E}_1^n+\tilde{c}_2\tilde{w}_{32}^{(0)}(\tilde{u})^{1/2}\tilde{E}_2^n+\tilde{c}_3\tilde{E}_3^n \qquad (5.12)
\end{aligned}$$

in terms of (5.5) read

$$\begin{aligned}
\tilde{d}_n(B_{n+1},B_n) &= s^{-2n}\left[\prod_{m=0}^{n-1}\left(1+\alpha'_m\right)\right]\left[\tilde{r}+q+\tilde{c}_1\tilde{E}_1^n+\tilde{c}_2\tilde{w}_{12}^{(0)}(\tilde{u})^{-1/2}\tilde{E}_2^n+\tilde{c}_3\tilde{w}_{13}^{(0)}(\tilde{u})^{-1}\tilde{E}_3^n\right],\\
\tilde{a}_4^{(n)} &= s^{-4n}\left[\prod_{m=0}^{n-1}\left(1+\alpha'_m\right)^2\right]\left[\tilde{u}+\tilde{c}_1\tilde{w}_{21}^{(0)}(\tilde{u})^{1/2}\tilde{E}_1^n+\tilde{c}_2\tilde{E}_2^n+\tilde{c}_3\tilde{w}_{23}^{(0)}(\tilde{u})^{-1/2}\tilde{E}_3^n\right],\\
\tilde{a}_6^{(n)} &= s^{-6n}\left[\prod_{m=0}^{n-1}\left(1+\alpha'_m\right)^3\right]\left[\tilde{w}+\tilde{c}_1\tilde{w}_{31}^{(0)}\tilde{u}\tilde{E}_1^n+\tilde{c}_2\tilde{w}_{32}^{(0)}(\tilde{u})^{1/2}\tilde{E}_2^n+\tilde{c}_3\tilde{E}_3^n\right].
\end{aligned} \tag{5.13}$$

Here, $\tilde{r}$, $\tilde{u}$ and $\tilde{w}$ are given in (5.7) and (5.10). The coefficients $\tilde{c}_l$ are obtained from the initial conditions at $n=0$. The temperature-independent quantities $\tilde{w}_{il}^{(0)}$ determine the eigenvectors of the RG linear transformation matrix, and $\tilde{E}_l$ are the eigenvalues of this matrix.

The main distinction between the solutions (5.13) and the solutions of RR in the absence of the correction for the potential averaging [2, 8] lies in the availability of factors of the type $\left(1+\alpha'_m\right)$. Taking into account the fact that $\lim_{m\to\infty}\alpha'_m(T_c)=\alpha'^{(0)}$ at $T=T_c$, we obtain the following asymptotics in n for the quantities $\tilde{d}_n$, $\tilde{a}_4^{(n)}$ and $\tilde{a}_6^{(n)}$ from (5.13):

$$\begin{aligned}
\tilde{d}_n(B_{n+1},B_n) &= (\tilde{r}+q)s^{-n(2-\eta)},\\
\tilde{a}_4^{(n)} &= \tilde{u}s^{-2n(2-\eta)},\\
\tilde{a}_6^{(n)} &= \tilde{w}s^{-3n(2-\eta)}.
\end{aligned} \tag{5.14}$$

The quantity η is given by the formula

$$\eta=\frac{\alpha'^{(0)}}{\ln s} \tag{5.15}$$

and corresponds to the critical exponent of the correlation function. Thus, the correction for the potential averaging being involved in calculating the partition function of the system, leads to a change of the asymptotics for the coefficients $\tilde{d}_n$, $\tilde{a}_4^{(n)}$ and $\tilde{a}_6^{(n)}$ at $T=T_c$ (in contrast to the case of $\Delta\tilde{\Phi}(k)=0$, the exponents of these coefficients contain the quantity η).

The renormalization of the critical exponent of the correlation length $\nu=\ln s/\ln\tilde{E}_1$, compared to the case of $\eta=0$, is associated with a change of the larger eigenvalue ($\tilde{E}_1>1$) of the RG linear transformation matrix. In contrast to ν, the critical exponent of the susceptibility $\gamma=(2-\eta)\nu$ explicitly depends on η. The specific heat of the system is characterized by the exponent $\alpha=2-3\nu$, the expression for which contains a renormalized critical exponent of the correlation length ν.

6. Discussion and conclusions

Within the CV approach, an analytic method for calculating the free energy of a 3D Ising-like system near the critical point was elaborated in [11] with the allowance for the simplest non-Gaussian fluctuation distribution (the ρ^4 model) and the critical exponent η. The critical exponent of the correlation function $\eta=0.024$ was found in [11] by including the correction for the potential averaging in the course of calculating the partition function of the system. This value of η is in accord with the other authors' data. For comparison, the exponents $\eta=0.0335(25)$, $\eta=0.0362(8)$ and $\eta=0.033$ were obtained within the framework of the field-theory approach (7-loop calculations) [19], Monte Carlo simulations [20] and non-perturbative RG approach (the order ∂^4 of the derivative expansion) [12], respectively. Some difference between the value of $\eta=0.024$ and other authors' data can be connected with the approximations in calculations, in particular, with the approximations which are made within the CV method (the simplest non-Gaussian distribution is used for obtaining $\eta=0.024$; the correction inserted by the operator $\hat{\Delta}_g$ is considered in the linear approximation in $\Delta\tilde{\Phi}(k)$; the terms proportional to the higher orders of operators $\partial/\partial\rho_{\mathbf{k}}$ are not taken into account in the expression for $\hat{\Delta}_g$; the operator $\hat{\Delta}_g$ in (3.3) acts only on the first term in the exponent). As is established in [11], the inclusion of a nonzero exponent η within the CV method leads to a reduction of the value of the critical exponent for the correlation length, ν (in comparison with the case of $\eta = 0$). For better quantitative estimates of ν and other renormalized critical exponents, it is necessary to use the non-Gaussian approximations higher than the quartic distribution (e.g., the sextic one).

This paper supplements the previous study [11] based on the ρ^4 model. In the present publication, the correction for the averaging of the Fourier transform of the interaction potential is taken into account using the sextic fluctuation distribution (the ρ^6 model). The effect of the mentioned correction on the critical behaviour of a 3D uniaxial magnet is investigated in the linear approximation.

Extending the method for the layer-by-layer integration of the partition function of the system to the case of the ρ^6 model, the RR for the coefficients of the effective distributions are written and analysed. It is shown that the inclusion of the correction for the potential averaging gives rise to a change of the asymptotics for the RR solutions at $T = T_c$.

The critical exponents of the correlation length, susceptibility and specific heat are renormalized due to the above-mentioned correction.

Our analytic representations acquire a more general and complete character as compared with the case when $\eta = 0$. An explicit expression (4.1) for the partition function allows us to calculate the free energy and other thermodynamic characteristics of the system near T_c taking into account the non-Gaussian sextic distribution and the small critical exponent η.

An analytic procedure for the calculation of the critical exponent of the correlation function developed in this paper on the basis of the ρ^6 model for a one-component spin system may be generalized to the case of a system with an n-component order parameter.

References

1. Yukhnovskii I.R., Phase Transitions of the Second Order. Collective Variables Method, World Scientific, Singapore, 1987.
2. Yukhnovskii I.R., Kozlovskii M.P., Pylyuk I.V., Microscopic Theory of Phase Transitions in the Three-Dimensional Systems, Eurosvit, Lviv, 2001 (in Ukrainian).
3. Berges J., Tetradis N., Wetterich C., Phys. Rep., 2002, **363**, No. 4–6, 223; doi:10.1016/S0370-1573(01)00098-9.
4. Tetradis N., Wetterich C., Nucl. Phys. B, 1994, **422**, No. 3, 541; doi:10.1016/0550-3213(94)90446-4.
5. Bagnuls C., Bervillier C., Phys. Rep., 2001, **348**, No. 1–2, 91; doi:10.1016/S0370-1573(00)00137-X.
6. Pelissetto A., Vicari E., Phys. Rep., 2002, **368**, No. 6, 549; doi:10.1016/S0370-1573(02)00219-3.
7. Pylyuk I.V., Kozlovskii M.P., Izv. Akad. Nauk SSSR, Ser. Fiz., 1991, **55**, 597 (in Russian).
8. Yukhnovskii I.R., Kozlovskii M.P., Pylyuk I.V., Phys. Rev. B, 2002, **66**, No. 13, 134410; doi:10.1103/PhysRevB.66.134410.
9. Kozlovskii M.P., Pylyuk I.V., Prytula O.O., Nucl. Phys. B, 2006, **753**, No. 3, 242; doi:10.1016/j.nuclphysb.2006.07.006.
10. Pylyuk I.V., Kozlovskii M.P., Physica A, 2010, **389**, No. 23, 5390; doi:10.1016/j.physa.2010.08.022.
11. Yukhnovskii I.R., Kozlovskii M.P., Pylyuk I.V., Ukr. J. Phys., 2012, **57**, No. 1, 80 [Ukr. Fiz. Zh., 2012, **57**, No. 1, 83 (in Ukrainian)].
12. Canet L., Delamotte B., Mouhanna D., Vidal J., Phys. Rev. B, 2003, **68**, No. 6, 064421; doi:10.1103/PhysRevB.68.064421.
13. Pylyuk I.V., Low Temp. Phys., 1999, **25**, No. 12, 953; doi:10.1063/1.593847 [Fiz. Nizk. Temp., 1999, **25**, No. 12, 1271 (in Russian)].
14. Pylyuk I.V., Ukr. Fiz. Zh., 1996, **41**, No. 9, 885 (in Ukrainian).
15. Yukhnovs'kii I.R., Riv. Nuovo Cimento, 1989, **12**, No. 1, 1; doi:10.1007/BF02740597.
16. Pylyuk I.V., Theor. Math. Phys., 1998, **117**, No. 3, 1459; doi:10.1007/BF02557185 [Teor. Mat. Fiz., 1998, **117**, No. 3, 442 (in Russian)].
17. Kozlovskii M.P., Pylyuk I.V., Dukhovii V.V., Condens. Matter Phys., 1997, **11**, 17.
18. Kozlovskii M.P., Theor. Math. Phys., 1989, **78**, No. 3, 300; doi:10.1007/BF01017668 [Teor. Mat. Fiz., 1989, **78**, No. 3, 422 (in Russian)].
19. Guida R., Zinn-Justin J., J. Phys. A, 1998, **31**, No. 40, 8103; doi:10.1088/0305-4470/31/40/006.
20. Hasenbusch M., Int. J. Mod. Phys. C, 2001, **12**, No. 7, 911; doi:10.1142/S0129183101002383.

Критична поведінка тривимірної ізингоподібної системи в наближенні моделі ρ^6: Роль поправки на усереднення потенціалу

І.В. Пилюк[1], М.В. Уляк[2]

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

[2] Державний вищий навчальний заклад "Гірничо-економічний коледж", вул. Стуса, 17, 80100 Червоноград, Україна

З використанням методу колективних змінних (КЗ) вивчається критична поведінка систем, які належать до класу універсальності тривимірної моделі Ізинга. Статистична сума однокомпонентної спінової системи обчислюється шляхом інтегрування за шарами фазового простору КЗ в наближенні негаусового шестирного розподілу флуктуацій параметра порядку (модель ρ^6). Особливістю запропонованого розрахунку є прийняття до уваги залежності фур'є-образу потенціалу взаємодії від хвильового вектора. Врахування поправки на усереднення потенціалу приводить до відмінного від нуля критичного показника кореляційної функції η і перенормування значень інших критичних показників. Виділено внески від цієї поправки в рекурентні співвідношення для моделі ρ^6, координати фіксованої точки та елементи матриці лінійного перетворення ренормалізаційної групи. Вираз для малого критичного показника η отримано у вищому негаусовому наближенні.

Ключові слова: *тривимірна ізингоподібна система, критична поведінка, шестирний розподіл, усереднення потенціалу, малий критичний показник*