The equation of state of the $n$-vector model: collective variables method

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Received 2 June 2010, in final form 1 October 2010
Published 11 November 2010
Online at stacks.iop.org/JPhysA/43/495001

Abstract

The critical behavior of the three-dimensional $n$-vector model in the presence of an external field is investigated. The mathematical description is performed with the collective variables method in the framework of the $\rho^4$ model approximation at the microscopic level without any adjustable parameters. The recurrence relations of the renormalization group as functions of the external field and temperature were found. The analytical expression for the free energy of the system for the temperatures $T > T_c$ and different $n$ was obtained. The equation of state of the $n$-vector model for the general case of small and large external fields was written. The explicit form of the correspondent scaling function for different values of the order parameter was derived. The obtained results are in qualitative agreement with the data of Monte Carlo simulations.

PACS numbers: 05.50.+q, 05.70.Ce, 64.60.Fr, 75.10.Hk

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The investigation of the critical behavior of the real three-dimensional (3D) magnets is one of the most important problems of condensed matter physics. This work is connected with investigation of the classical $n$-vector model on the simple 3D cubic lattice in the presence of an external magnetic field by the collective variables (CV) method. Originally this method was introduced by Bom [1], then used by Zubarev for systems of charged particles [2] and later developed for calculation of the thermodynamic and structural characteristics of the 3D systems near the phase transition (PT) point [3]. The above-mentioned model is well known as the classical $O(n)$-vector model or, in field-theoretic language, as the $O(n)$-invariant nonlinear $\sigma$-model. Depending on components of an order parameter this model can describe a number of physical systems such as polymers, ferromagnets, antiferromagnets, the critical point of the liquid–vapor transition, the Bose-condensation, PTs in binary alloys, etc.
The investigations of the critical properties of the $O(n)$-vector models and their partial cases were carried out by various methods such as: high- and low-temperature expansions, the field theory, the semi-microscopic scaling field theory and Monte Carlo (MC) simulations. In general, much attention was devoted to investigation of the universal characteristics of the system such as critical exponents and relations of the critical amplitudes of the thermodynamic functions.

The CV method as well as Wilson’s approach [4] is based on use of the hypothesis of scaling invariance and the renormalization group (RG) method for the PT theory suggested by Patashynskii, Pokrovskii [5] and Kadonoff [6].

The RG method was used to obtain the equation of state of the Ising system up to the order $\epsilon^2$ by Avdeiva and Migdal [7] and by Bresin et al [8]. The obtained results were generalized for the case of the $n$-vector model [9].

Besides, the positive results were achieved by calculation of the thermodynamic functions near the critical point. In Wegner’s work [10] an expression was obtained for the free energy by taking into account the so-called irrelevant operators in Wilson’s approach. Riedel and Wegner [11] suggested the method of scaling fields for obtaining the crossover scaling functions of the free energy and the susceptibility. The works of Fisher and Aharony [12], Nicoll and Albright [13] and also Nelson [14] are dedicated to the crossover scaling functions for $T > T_c$ in the zero magnetic field near four dimensions. In the framework of the massive field theory by Bagnuls and Bervillier [15] the explicit results for the correlation length, the susceptibility and the heat capacity as functions of the temperature in the disordered phase along the critical isochore for one-, two- and three-component systems were obtained. The nonasymptotic behavior was described as crossover between Wilson–Fisher’s (near the critical temperature $T_c$) and the mean field’s (far from $T_c$) behaviors using three adjustable parameters. But this crossover cannot realistically describe the situation in the system, because there are some physical restrictions of the model. Thus, in the works of Dohm and co-workers [16, 17] the calculation of the thermodynamical characteristics of the system without $\epsilon$-expansion was performed in the framework of some minimal subtraction scheme based on the high-ordered perturbation theory and Borel’s resummation. This minimizing scheme is related to the use of the general relations between the heat capacity coefficients for approximation of the temperature dependence of the coefficient $u(t)$ near the fourth term in the Ginsburg–Landau Hamiltonian. This method allows us to obtain the nonuniversal critical behavior of the thermodynamic functions below and above the critical temperature, such as the heat capacity and the susceptibility as functions of $u(t)$ without any adjustable parameters. But it does not provide the possibility of analyzing the dependence of the thermodynamic variables on the microscopic parameters of the interaction potential.

Besides, the essential success was achieved in calculation of the universal relations of the critical amplitudes. Okabe and Ohno [18], and Okabe and Ideura [19] investigated the relations of the critical amplitudes of the susceptibility by high-temperature, $1/n$- and $\epsilon$-expansion up to the order $O(\epsilon^2)$. Bresin, Le Guillou and Zinn-Justin [20] calculated the universal relations of the critical amplitudes for the heat capacity, the susceptibility and the correlation length by Wilson–Fisher’s $\epsilon$-expansion.

It should be mentioned that PT is actively investigated by the MC method. Thus, Ferrenberg and Landau [21, 22] found the critical temperature and critical exponents for the Ising and classical Heisenberg models using the high-resolution MC method. Besides, the universal relations of the critical amplitudes and the equation of state were obtained by Engels for the $O(1)$, $O(2)$, $O(4)$ models [23–25] and by Campostrini et al for the $O(3)$ model [26].

A number of new results were obtained using for the description of the PT the CV method. The specificity of the CV method is a successive microscopic approach and the
method of integration of the partition function by short-wave fluctuations without applying the perturbation theory. In the framework of this method the general recurrence relations (RR) which correspond to the RG equations, the critical exponents and the relation of the critical amplitudes of the Ising model were obtained.

The investigation of the $O(n)$ model allows us to obtain, in the unified form, results for the critical behavior of whole class of systems such as polymers in $n \to 0$ limit, the Ising model for $n = 1$, the XY-model for $n = 2$, the Heisenberg model for $n = 3$, the model with $n = 4$ is important for quantum chromodynamics with two degenerate light-quark flavors at finite temperature and the spherical model in the case $n \to \infty$ which has the exact solution.

The quantity $n$ is related to the dimensionality of the order parameter of the system. The investigation of the $n$-vector model was carried out by the CV method in [27] using the Stratanovich–Hubbard representation. The CV method was used for the investigation of the properties of the pre-transition behavior and description of the structural PT in the system with the $n$-component order parameter [28]. The thermodynamical characteristics of the $n$-vector model in the zero magnetic field were found in [29, 30] using the CV method.

In general, the real physical systems are characterized by the presence of the external fields. The description of systems with the $n$-component order parameter in the presence of the external fields is a complicated task and needs detailed study. Thus, taking into account the results obtained in [29, 30], we investigate the influence of the external field on the critical behavior of the $n$-vector model.

2. The model

The Hamiltonian $H$ of the $n$-vector model in the presence of the external field has the form

$$H = -\frac{1}{2} \sum_i \sum_j \Phi(|i-j|)S_i S_j - \sum_i H_i S_i,$$

(2.1)

where $S_i = (S_i^{(1)}, \ldots, S_i^{(n)})$ is the classical $n$-component spin of length $m$ localized at the $N$ sites of $d$-dimensional cubic lattice with coordinates $i$, $\Phi(|i-j|)$ is the interaction potential.

The partition function of the model (2.1) is the functional integral over all possible orientations of the spin vector and can be written in the form

$$Z = \int \prod_i dS_i \delta(S_i - m) e^{-\beta H}, \quad m > 0,$$

(2.2)

where we take into account the condition that length of the spin is $m$. We will integrate the partition function in the space of the CV. Let us introduce the variables

$$\hat{\rho}_k^c = \frac{1}{\sqrt{N}} \sum_i \cos(k_i) S_i,$$

(2.3)

$$\hat{\rho}_k^s = \frac{1}{\sqrt{N}} \sum_i \sin(k_i) S_i,$$

(2.4)

$$\hat{\rho}_0 = \frac{1}{\sqrt{N}} \sum_i S_i,$$

(2.5)

which are the $n$-component vectors. The CV $\rho_k$ are introduced as a functional representation for the operators of the fluctuation of the spin density:

$$\hat{\rho}_k = \int \rho_k J(\rho - \hat{\rho})(d\rho_k)^N.$$

(2.6)
In the CV representation the partition function of the model [3] is

$$ Z = \int \exp \left[ \frac{1}{2} \sum_k \beta \Phi(k) \rho_k \rho_{-k} + h \rho_0 \right] J[\rho](d\rho_k)^N, \tag{2.7} $$

where

$$ h = \beta H. $$

The Jacobian of transition from the spin variables to the CV has the form

$$ J[\rho] = \int \prod_i dS_i \delta(S_i - m) \delta(\rho_{i0} - \hat{\rho}_{i0}) \prod_k \delta(\rho^c_k - \hat{\rho}^c_k) \delta(\rho^s_k - \hat{\rho}^s_k). \tag{2.8} $$

Calculation of the partition function is performed in the general framework [29, 30]. The main idea is that the phase space is divided into the intervals (layers) to depend on the value \( k \) and the interaction potential is averaged on each of these intervals. The Fourier transform of the interaction potential is replaced by the following approximation [29–31]:

$$ \Phi(k) = \begin{cases} \Phi(0)(1 - 2b^2 k^2), & k \in B' \\ \Phi = \text{const}, & k \in B/B'. \end{cases} \tag{2.9} $$

Here \( B \) is the Brillouin zone of a simple cubic lattice with the spacing \( c \):

$$ B = \left\{ k = (k_x, k_y, k_z) | k_i = \frac{\pi}{c} \left( \frac{n_i}{N_i} - 1 \right); \quad n_i = 1, 2, \ldots, N_i; \quad i = x, y, z \right\}, \tag{2.10} $$

where \( N = N_xN_yN_z \) is a number of cells. And \( B' \) defines the new Brillouin zone with the spacing \( c' = cs_0 \), and number of cells \( N' = N's_0^{-d} \). The parameter \( s_0 \) characterizes the parabolic approximation. We assume \( \Phi = 0 \). Such cutting of the potential do not affect the general picture of the critical behavior but is appreciable when we want to estimate the critical temperature. We use the method suggested in [32] for integration of the partition function in the presence of the external field. It should be mentioned that in our work we use the quartic measure density that allows us to describe the PT on qualitative good level [33]. After integration by \( l \) layers we obtain the partition function \( Z \) in the form

$$ Z = 2^{\frac{4}{2}(N_{N-t-1})} Q_0 Q_1 \ldots Q_l Q^{N_i+1}(P_l) Z_{l+1}, \tag{2.11} $$

where \( Q_i \) is the partial partition function of the \( i \)'s layer

$$ Q_0 = Q^N(u) Q^{N_t}(d_0), $$
$$ Q^N(u) = J'[0] \exp(\alpha'_0 N'), $$
$$ Q_l = Q^{N_l}(P_{l-1}) Q^{N_l}(d_l). \tag{2.12} $$

The number of variables on the \( i \)'s layer is

$$ N_l = N's^{-di}, \tag{2.13} $$

and the following definitions for the values \( Q(d_l) \) and \( Q(P_l) \) were introduced:

$$ Q(d_l) = (2\pi)^\frac{3}{2} \left( \frac{3}{a_4^{(l)}} \right)^{\frac{3}{2}} U \left( \frac{n - 1}{2}, x_i \right) \exp \left( \frac{x_i^2}{4} \right), \tag{2.14} $$

$$ Q(P_l) = (2\pi)^{-\frac{3}{2}} \left[ s^d n + 2 \frac{a_4^{(l)}}{3} \phi(x_i) \right]^{\frac{3}{2}} U \left( \frac{n - 1}{2}, y_l \right) \exp \left( \frac{y_l^2}{4} \right). \tag{2.14} $$
Here $U(a, x)$ is Weber’s parabolic cylinder function, the function $\varphi(x_l)$ is defined in the appendix. The nonintegrated part of $Z$ has the form

$$Z_l+1 = \int (d\rho_k)^N \exp \left\{ \sqrt{Nh}\rho_0 - \frac{1}{2} \sum_{k > B_l} d^{(l+1)}(k)\rho_k\rho_{-k} - \frac{a^{(l+1)}}{4!N^{l+1}} \sum_{k_1, \ldots, k_4 < B_l+1} \rho_{(k_1 \cdots k_4)} \delta_{k_1 \cdots k_4} \right\}.$$  

(2.15)

The presence of the external field results in appearance of the linear term in the exponent. Let us assume that the external field is oriented along one of the coordinate axes (e.g. $x$ axes). Thus, we receive

$$Z_l+1 = \int (d\rho_k)^N \exp \left\{ \sqrt{N^{l+1}}a^{(l+1)} \rho_0 + \frac{1}{2} \sum_{k < B_l+1} d^{(l+1)}(k)\rho_k\rho_{-k} - \frac{a^{(l+1)}}{4!N^{l+1}} \sum_{k_1, \ldots, k_4 < B_l+1} \rho_{(k_1 \cdots k_4)} \delta_{k_1 \cdots k_4} \right\}.$$  

(2.16)

For the coefficients near different powers of $\rho_k$ we have the following RR:

$$a^{(l+1)}_1 = a^{(l)}_1 s^\frac{2}{d},$$

$$a^{(l+1)}_2 = a^{(l)}_2 + d^{(l)}(B_l+1, B_l)M(x_l),$$

$$a^{(l+1)}_4 = a^{(l)}_4 s^{-d}E(x_l),$$  

(2.17)

where

$$M(x_l) = N(x_l) - 1, \quad N(x_l) = \frac{y_l U_n(y_l)}{x_l U_n(x_l)}, \quad E(x_l) = s^{2d}\frac{\varphi(y_l)}{\varphi(x_l)},$$  

(2.18)

and the arguments $x_l$ and $y_l$ are

$$x_l = \sqrt{\frac{3}{a^{(l)}_4}}(B_l+1, B_l), \quad y_l = s^\frac{2}{d} U_n(x_l) \sqrt{n + 2} \frac{n + 2}{\varphi(x_l)}.$$  

(2.19)

For convenience the following designation were introduced:

$$d^{(l)}(B_l+1, B_l) = d^{(l)}(0) + q s^{-2j}, \quad q = \beta \Phi(0)\tilde{q},$$

$$a^{(l)}_1 = s^{-d} \omega_l, \quad d^{(l)}(0) = s^{-d} r_l, \quad a^{(l)}_4 = s^{-d} u_l.$$  

(2.20)

Thus, the RR (2.17) can be written in the form

$$\omega_{l+1} = s^{-d} \omega_l,$$

$$r_{l+1} = s^{-d}[r_l + q]N(x_l) - q],$$

$$u_{l+1} = s^{-d} u_l E(x_l).$$  

(2.21)

The initial values of $\omega_l, r_l, u_l$ are (for $l = 0$):

$$\omega_0 = s^\frac{d}{2} h^\prime, \quad r_0 = a_2 - \beta \Phi(0), \quad u_0 = a_4.$$  

(2.22)

In that way we passed to the parametric space of the RG transformation. The PT point is represented by the fixed point with coordinates

$$\omega^* = 0, \quad r^* = -f_a\beta \Phi(0), \quad u^* = \phi_0[\beta \Phi(0)]^2.$$  

(2.23)
where
\[ f_n = \frac{\hat{q} s^2 [N(x^*) - 1]}{s^2 N(x^*) - 1}, \quad \phi_n = \frac{\hat{q}^2 3}{x^2} \left[ \frac{1 - s^{-2}}{N(x^*) - s^{-2}} \right]^2. \] (2.24)

Here \( x^* \) is the solution of equation [29]
\[ s^4 \psi(x^*) = \psi(x^*). \] (2.25)

So, when \( \tau = 0, h = 0 \) and \( l \to \infty \) the system is in the fixed point. It is obvious that near the critical point when \( \tau \to 0, h \to 0 \) and for large \( l \) in the parametric space the system will be near the fixed point. This case is called the critical regime (CR). In the CR the RR may be expanded by the deviation from the fixed point
\[
\begin{pmatrix}
\omega_{l+1} - \omega^* \\
\tau_{l+1} - \tau^* \\
u_{l+1} - u^*
\end{pmatrix}
= \mathcal{R}
\begin{pmatrix}
\omega_l - \omega^* \\
\tau_l - \tau^* \\
u_l - u^*
\end{pmatrix}.
\] (2.26)

The elements of matrix \( \mathcal{R} \) in a linear by the \((x_l - x^*)\) approximation have the form
\[
\begin{align*}
R_{11} &= s^{\frac{2}{3}} U_n(y^*), \\
R_{12} &= R_{21} = R_{13} = R_{31}, \\
R_{22} &= \sqrt{3} s^2 \mu_1, \\
R_{23} &= \frac{s^2}{2} \sqrt{u^*} (\mu_0 - \mu_1 x^*), \\
R_{32} &= \sqrt{3} u^* s^d \omega_1, \\
R_{33} &= s^d \left( \frac{\omega_0 - \omega_1 x^*}{2} \right).
\end{align*}
\] (2.27)

where the coefficients are
\[
\begin{align*}
\mu_0 &= \sqrt{\frac{n + 2}{3 \psi(x^*)}} s^\frac{2}{3} U_n(y^*), \\
\mu_1 &= \mu_0 \left( a_1 - \frac{q_1}{2} \right), \\
\omega_0 &= s^2 \frac{\psi(x^*)}{\psi(x^*)}, \\
\omega_1 &= \omega_0 (b_1 - q_1).
\end{align*}
\] (2.28)

Here we made the designations
\[
a_1 = \tilde{p}_1 y^* r_1, \quad r_1 = \tilde{\alpha}_1 - \frac{q_1}{2}, \quad b_1 = \tilde{q}_1 y^* r_1. \] (2.29)

For the derivatives \( \tilde{p}_m, \tilde{q}_l, r_1, q_1 \) which appear in equation (2.29) we have
\[
\begin{align*}
\tilde{p}_m &= \frac{1}{U_n(y^*)} \left[ \frac{d^n U_n(y)}{dy^n} \right]_{y^*}, \\
\tilde{q}_m &= \frac{1}{\psi(y^*)} \left[ \frac{d^n \psi(y)}{dy^n} \right]_{y^*}, \\
\partial_m &= \frac{1}{U_n(x^*)} \left[ \frac{d^n U_n(x)}{dx^n} \right]_{x^*}, \\
q_m &= \frac{1}{\psi(x^*)} \left[ \frac{d^n \psi(x)}{dx^n} \right]_{x^*}.
\end{align*}
\] (2.30)

An action of the matrix \( \mathcal{R} \) allows us to receive the coefficients of the partition function of the next layer. In order to receive the coefficient of the \( l \)'s layer we need to act by \( \mathcal{R} \) \( l \) times on the coefficients of the zero layer:
\[
\begin{pmatrix}
\omega_l - \omega^* \\
\tau_l - \tau^* \\
u_l - u^*
\end{pmatrix}
= \mathcal{R}^l
\begin{pmatrix}
\omega_0 - \omega^* \\
\tau_0 - \tau^* \\
u_0 - u^*
\end{pmatrix}.
\] (2.31)

It is easy to obtain the form of the matrix \( \mathcal{R}^l \) when the matrix \( \mathcal{R} \) is reduced to the diagonal form. In order to do it, we must pass to the base from the eigenvectors of \( \mathcal{R} \). The eigenvalues of \( \mathcal{R} \) are universal quantities:
\[
E_1 = R_{11}, \quad E_{2,3} = \frac{1}{2} \left[ R_{22} + R_{33} \pm \sqrt{(R_{22} - R_{33})^2 + 4 R_{23} R_{32}} \right].
\] (2.32)
The eigenvectors have the form
\[ \omega_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \omega_2 = \begin{pmatrix} 0 \\ 1 \\ R_1 \end{pmatrix}, \quad \omega_3 = \begin{pmatrix} 0 \\ R \\ 1 \end{pmatrix}. \] (2.33)

The inverse vectors are written as
\[ v_1 = (1 \ 0 \ 0), \quad v_2 = \frac{1}{D}(0 \ 1 - R), \quad v_3 = \frac{1}{D}(0 - R_1 \ 1), \] (2.34)

\[ R = \frac{R_{23}}{E_3 - R_{22}}, \quad R_1 = \frac{E_2 - R_{22}}{R_{23}}. \]

The determinant of the inverse matrix is
\[ D = \frac{E_3 - E_2}{E_3 - R_{22}}. \] (2.35)

After expanding the coefficients in (2.21) by eigenvectors we obtain
\[ \omega_l = s \, d^2 \, h E^l_1, \]
\[ r_l = r^* + c_1 E^l_2 + c_2 R E^l_3, \] (2.36)
\[ u_l = u^* + c_1 R E^l_2 + c_2 E^l_3. \]

The coefficients \( c_1, c_2 \) can be found from the initial conditions at \( l = 0 \).
\[ c_1 = \frac{1}{D} \left[ r_0 - r^* - R(u_0 - u^*) \right], \]
\[ c_2 = \frac{1}{D} \left[ (u_0 - u^*) - R_1 (r_0 - r^*) \right]. \] (2.37)

The eigenvalue \( E_2 > 1 \) is responsible for the deviation from the fixed point, the \( E_3 < 1 \) is much more smaller than \( E_2 \) and we can neglect it. This approximation neglects the confluent corrections. Taking into account that at the PT point \( r_1 = r^* \), we obtain the equation for the critical temperature in the form [29]
\[ \frac{\beta c}{\Phi_1(0)} \left( 1 - f_n - R^* \sqrt{\phi_n} \right) - a_2 \beta c(0) + a_4 R^* / \sqrt{\phi_n} = 0, \]
\[ R^* = R \sqrt{u^*}. \] (2.38)

This equation allows us to write the solutions of the RR as a function of the temperature and the external field for the CR:
\[ \omega_l = s \, d^{2} \, h E^l_1, \]
\[ r_l = \beta \Phi(0) \left( -f_n + c_1 \tau E^l_2 + R^* c_2 T E^l_3 / \sqrt{\phi_n} \right), \] (2.40)
\[ u_l = \left[ \beta \Phi(0) \right] \left( \sqrt{\phi_n} \, c_1 \tau E^l_2 + c_2 T E^l_3 \right). \]

The obtained coefficients are exponential functions of \( l \). For small \( l \) their values are small and then increase rapidly. For big \( l \), the value of \( r_l \) (the coefficient near the square term in the partition function) is bigger than \( u_l \) (the coefficient near the quartic term in the partition function). Thus, we can integrate the partition function in this region using the Gaussian approximation. But in the CR we must use the distributions of fluctuations higher than Gaussian’s one and take into account the quartic term in the partition function. So let us find the number \( l \) after what we can pass from accounting quartic to accounting only quadratic terms. We call this number as the exit point from the CR. In zero magnetic field this point has
been already studied \[31\]. Let us designate it as \(m_τ\) and find it from the condition of deviation from the fixed point:

\[
rm_{τ,1} - r^* = -δr^*, \quad δ = \frac{τ}{|τ|}.
\] (2.41)

As a result we obtain

\[
m_τ = -\ln |\tilde{τ}| - 1,
\] (2.42)

where

\[
\tilde{τ} = τ \frac{c_{1k}}{f_0}
\] (2.43)

is the renormalized reduced temperature. In the presence of the external field the exit point from the CR is found from the condition

\[
o_{n_τ,1} - ω^* = h_0.
\] (2.44)

From this we found \[34, 35\]

\[
n_{n_τ} = -\ln \tilde{h} - 1, \quad \tilde{h} = s_0^\frac{g}{h_0} h',
\] (2.45)

The quantity \(h_0\) is found from the normalization condition for the scaling function.

If there are both the temperature and field the exit point depends on the relation between \(τ\) and \(h\). Some boundary temperature field \(h_c\) which divides the values of fields on strong and weak was found in \[33, 36\]. The condition of this division on strong and week fields has the form

\[
m_τ = n_{n_τ}.
\] (2.46)

After substituting the equations for the exit points from the CR we obtain

\[
h_c = |\tilde{τ}|^{p_0},
\] (2.47)

where the critical exponent \(p_0\) has the form

\[
p_0 = \frac{\ln E_1}{\ln E_2} = \frac{ν}{μ}, \quad μ = \frac{2}{d+2}.
\] (2.48)

The critical exponent of the correlation length \(ν\) for \(h = 0\) is

\[
ν = \frac{\ln s}{\ln E_2}.
\] (2.49)

The critical exponent \(μ\) describes the dependence of the correlation length on the field for \(T = T_c\). Therefore we can rewrite (2.42) in the form

\[
m_τ = -\ln h_c - 1.
\] (2.50)

In the general case deviations by the temperature and by the field from the fixed point should be united. This united point \(n_p\) can be found from the equation \[36\]

\[
\left(\delta_0^{d/2} E_1^{n_τ+1}\right)^2 + \left(c_{17} τ β(0) E_2^{n_τ+1}\right)^2 = r^{*2}.
\] (2.51)

The value of \(n_p\) can be found numerically. But numerical solution does not allow us to take into account the influence of the temperature and the field on the critical behavior analytically. The formula for united exit point from the CR was introduced in \[34\]. The above-mentioned
equation for united exit point from the CR depends on the field and temperature and in the limit of zero field or zero temperature it passes to the equation (2.45) or (2.50), respectively

\[ n_p = -\frac{\ln (\hbar^2 + h_c^2)}{2 \ln E_1} - 1. \]  

Information about the exit point from the CR allows us to divide the integration of the partition function on two stages: integration by quartic distribution in the CR, where values of \( r_l \) and \( u_l \) are commensurable and integration by the Gaussian distribution (the Gaussian regime) for the phase space layers with \( l > n_p \). But deviation from the fixed point occurs not so sharp to exactly distinguish the critical and the Gaussian regimes. Therefore, we should take into account the transition regime (TR) in which \( r_l \) exceeds \( u_l \) but we still cannot use the Gaussian distribution. In order to integrate the partition function in the TR one must use the quartic measure density. Fortunately, there is only one layer in the phase space for which \( r_l \) and \( u_l \) behave like described for the TR. The number of this layer is next after the CR (\( n_p + 1 \)), so from the layer with \( n_p + 2 \) the Gaussian region is present. Thus, the partition function has the form

\[ Z = \underbrace{O_0 O_1 \cdots O_{n_p}}_{\text{CR}} \underbrace{Q_{n_p+1} Z_{n_p+2}}_{\text{TR}} \underbrace{2^{1/4(N_{n_p+1}-1)} Q_{N_{n_p+1}}^N (P_{n_p+1}) Z_{n_p+2}}_{\text{LGR}}, \]  

where CR designates the critical region, TR is the transition region and LGR is the limiting Gaussian region.

The coefficients near the CV change their behavior for \( l > n_p \). It simplifies calculations. Let us take \( l = n_p + 1 \) in (2.14). Then in order to integrate \( Z_{n_p+2} \) is important to know below or above \( T_c \) is the system. The coefficients

\[ r_{n_p+2} = \beta \Phi (0) f_n (-1 + E_2 H_c), \]
\[ u_{n_p+2} = [\beta \Phi (0)]^2 \phi_n (1 + \Phi E_2 H_c), \]
\[ \Phi = \frac{f_n}{\sqrt{\phi_n}} R^+_{n_p}, \quad H_c = \tilde{t} E_2^{n_p+1} \]

depend on the temperature and field. The values of \( u_{n_p+2} \) are always positive that provide convergence of (2.53). The coefficient \( r_{n_p+2} \) is positive and exceeds \( u_{n_p+2} \) for large \( \tau (h_c \gg \hbar) \). In this case the partition function can be integrated in the Gaussian approximation. But for small \( \tau (h_c \ll \hbar) \), \( r_{n_p+2} \) decreases and becomes negative. In this case the Gaussian approximation is useless. This problem can be solved by introduction of the substitution

\[ \rho^\alpha_k = \eta^\alpha_k + \sqrt{\alpha} \delta_k, \quad \bar{\sigma} = (\sigma, \ldots, 0). \]

Thus, \( Z_{n_p+2} \) can be written in the form

\[ Z_{n_p+2} = e^{N E_0 (\sigma)} \int (d\eta)^{N_{n_p+2}} \exp \left[ -\frac{1}{2} \sum_{k \in B_{n_p+2}} d^{(n_p+2)} (k) \eta_k \eta_{-k} \right. \]
\[ - \frac{a_4^{(n_p+2)}}{12} \delta_{0,3} \delta_{3(n_p+2)} \sigma^2 \left( \sum_{k \in B_{n_p+2}} \eta_k \eta_{-k} + 2 \sum_{k_1 \in B_{n_p+2}} \eta_{k_1}^{(1)} \eta_{k_1}^{(-1)} \right) \]
\[ - \frac{a_4^{(n_p+2)}}{6 \sqrt{N_{n_p+2}}} \sum_{k_1 \in B_{n_p+2}} \left[ \frac{1}{2} \right] d_k \delta_{k_1; k_2; k_3; \ldots} \]
\[ - \frac{a_4^{(n_p+2)}}{24 N_{n_p+2}} \sum_{k_1 \ldots k_{n_p+2} \in B_{n_p+2}} \eta_{k_1} \ldots \eta_{k_{n_p+2}} \delta_{k_1; k_2; k_3; \ldots} \right]. \]
where
\[ E_0(\sigma) = h' \sigma - \frac{1}{2} d^{n_p+2} (0) \sigma^2 - \frac{d_4}{24} S_0^3 (n_p+2) \sigma^4. \] (2.57)

The shift \( \sigma_+ \) is found from the condition
\[ \frac{\partial E_0(\sigma_+)}{\partial \sigma_+} = 0. \] (2.58)

This condition causes the coefficient near the first power of \( \eta_0^{(1)} \) equal to zero and results to a cubic equation for \( \sigma_+ \). The solution of this equation can be found in the form
\[ \sigma_+ = \sigma_0 (n_p+2)/2. \] (2.59)

Finally one obtains
\[ \sigma_0^3 + p \sigma_0 + q = 0, \] (2.60)

where the following designations were introduced:
\[ p = \frac{6r_{n_p+2}}{u_{n_p+2} S_0}, \quad q = -\frac{6h_0 s}{u_{n_p+2} S_0} \sqrt{\tilde{h}/h_c^2 + h_c^2}. \] (2.61)

Solutions of a cubic equation depend on the sign of the discriminant
\[ Q = \left( \frac{p}{3} \right)^3 + \left( \frac{q}{2} \right)^2. \] (2.62)

For \( T > T_c \) the value of \( Q \) is always positive. So equation (2.60) has one real and two complex roots. We select the real one:
\[ \sigma_0 = A + B, \]
\[ A = \left( \frac{q}{2} + \sqrt{Q} \right)^{\frac{1}{3}}, \quad B = \left( \frac{q}{2} - \sqrt{Q} \right)^{\frac{1}{3}}. \] (2.63)

Integral (2.56) is calculated in the Gaussian approximation. This integration terminates the calculation of the partition function:
\[ Z_{n_p+2} = e^{-N E_0(\sigma_+)} \left( \frac{\pi}{2} \right)^{n(N_p+2)} \sqrt{\frac{\pi}{d_1(0)}} \sqrt{\frac{\pi}{d_2(0)}} \prod_{k>0} \frac{1}{d_1(k)} \left( \frac{1}{d_2(k)} \right)^{(n-1)}, \] (2.64)

where
\[ d_1(k) = r_R^{(1)} + \beta \Phi(0) h_2^2 k^2, \]
\[ r_R^{(1)} = s^{-2(n_p+2)} r_R^{(1)}, \]
\[ r_R^{(2)} = s^{-2(n_p+2)} r_R^{(2)}, \]
\[ r_R^{(1)} = r_{n_p+2} + \frac{1}{2} \sigma_0^2 u_{n_p+2}, \]
\[ r_R^{(2)} = r_{n_p+2} + \frac{1}{6} \sigma_0^2 u_{n_p+2}. \] (2.65)

Thus, dividing the phase space of the CV on layers depending on the values of the wave vector, we distinguished two main states of the system to refer to the critical behavior: the critical region which corresponds to short-wave fluctuations and the Gaussian region which corresponds to long-wave fluctuations. Short-wave fluctuations are connected with the microscopic parameters of the model and long-wave fluctuations determine the critical behavior. In contrast to earlier approaches we pay attention to both irrelevant short-wave and long-wave fluctuations.
3. The free energy

After calculation of the partition function we can find the free energy of the system:
\[ F = -kT \ln Z. \]  
(3.1)

Described above structure of the partition function allows us to present the free energy as a sum of terms which correspond to different regimes of fluctuations:
\[ F = F_0 + F_{\text{CR}} + F_{\text{TR}} + F_{\text{LGR}}. \]  
(3.2)

Here
\[ F_0 = -kTN \ln \left[ \frac{(2\pi)^{\frac{n}{2}}}{\Gamma(n/2)} \right] \]  
(3.3)
is the free energy of noninteracting spins,
\[ F_{\text{CR}} = -kT \sum_{l=0}^{n_p} \ln Q_l \]  
(3.4)
is the energy to refer to the critical region,
\[ F_{\text{TR}} = -kT Q_{n_p+1} \]  
(3.5)
is the contribution which corresponds to the transition region and, respectively,
\[ F_{\text{LGR}} = -kT \ln \left[ 2^{\frac{n}{2}} (N_{n_p+1} - N_{n_p}) Q_{n_p+1} (P_{n_p+1}) Z_{n_p+2} \right] \]  
(3.6)
is the contribution which comes from the Gaussian region.

Equation (3.4) depends on the exit point from the CR. In order to know this dependence explicitly we need to sum up elements \( Q_l \). For this purpose let us extract dependence on index \( l \) in \( Q_l \). The quantity \( Q_l \) is a function of \( y_l \). The variable \( y \) is bigger than 1 (\( y_l \gg 1 \)) for any temperature. Thus, we can use the expansion for Weber’s parabolic cylinder function \( U(a, x) \) in \( Q_l \) by inverse powers of \( y_l \).

Using appropriate expansions we have
\[ F_{\text{CR}} = -kTN' f_{\text{CR}}^0 - kT \sum_{l=1}^{n_p} N_l f_l, \]  
(3.7)
where
\[ f_{\text{CR}}^0 = u_0' + \frac{x_0^2}{4} + \frac{3u_0^2}{4u_4'} + \ln U\left( \frac{n-1}{2}, x_0 \right) + \frac{n}{4} \left[ \ln \left( \frac{3}{u_4} \right) + \ln \left( \frac{3}{a_4} \right) \right], \]  
(3.8)
\[ f_l = \ln U\left( \frac{n-1}{2}, x_l \right) + \frac{x_l^2}{4} + \frac{n}{2} \ln y_l + \frac{n}{4y_l^{n-1}}(2n + 7). \]

To extract the dependence on \( l \) from \( f_l \) we expand it by powers of \( x_l - x^* \) and substitute in obtained formula the solutions of the RR. After summing up we obtain
\[ F_{\text{CR}} = -kTN' \left[ \gamma_0' + \gamma_1' + \gamma_2' \tau^2 - \gamma' \left( h \tau^2 + h_c \right) \right], \]  
(3.9)
where
\[ \gamma' = \gamma_1 + \gamma_2 H_c + \gamma_3 H_c^2, \]  
(3.10)
and the coefficients near powers of \( H_c \) have the form
\[ \gamma_1 = \frac{f_{\text{CR}}}{1 - s^2 \tau}, \quad \gamma_2 = \frac{f_{\text{CR}}}{1 - s^3 E_2}, \quad \gamma_3 = \frac{f_{\text{CR}}}{1 - s^3 E_2^2}, \]  
(3.11)
For the free energy of the TR we obtain

$$F_{TR} = -kT N' f_{np+1} \left( \tilde{h}^2 + h_c^2 \right)^{\frac{\sigma}{s}},$$

with

$$f_{np+1} = \ln U \left( \frac{n-1}{2}, x_{np+1} \right) + \frac{n^2}{4} \ln y_{np} + \frac{n}{4y_{np}^2} (2n + 7).$$

For the LGR we have

$$\ln Z_{np+2} = NE_0(\sigma_{+}) + \frac{n}{2}(N_{np+2} - 1) \ln \frac{\pi}{2} + \frac{n}{2} \ln \pi - \frac{1}{2} \ln d_1(0)$$

$$- \frac{n-1}{2} \ln d_2(0) - \sum_{k=0}^{\infty} \ln d_1(k) - (n-1) \sum_{k=0}^{\infty} \ln d_2(k).$$

In order to sum up by $k$ we change the summation by integration that results in

$$F_{LGR} = F_0^{(+)} - kTN_{np+2} \left[ n \left[ -\frac{1}{2} \ln 2 + \ln s - \frac{1}{4} \ln 3 + \frac{1}{4} \ln u_{np+1} - \frac{1}{2} \ln U(x_{np+1}) - \frac{n+2}{8y_{np+1}^2} \right] \right.$$

$$- \frac{1}{2} \left[ \ln \hat{R}_R^{(1)} + f_{G_1} + (n-1) \left( \ln \hat{R}_R^{(2)} + f_{G_2} \right) \right].$$

where

$$f_{G_i} = \ln \left( a_i^2 + 1 \right) - \frac{2}{3} + \frac{2}{a_i^2} - \frac{2}{a_i} \arctan a_i,$$

$$a_i = \frac{\pi b \sqrt{\beta \Phi(0)}}{\hat{R}_R^{(i)}}.$$  
(3.16)

For the convenience $F_{LGR}$ were split into the two parts:

$$F_{LGR} = F_0^{(+)} + F_G,$$

where

$$F_0^{(+)} = -kTNE_0(\sigma_{+}), \quad F_G = -kTN_{np+2}f_G,$$  
(3.17)

and

$$f_G = n \left[ -\frac{1}{2} \ln 2 + \ln s - \frac{1}{4} \ln 3 + \frac{1}{4} \ln u_{np+1} - \frac{1}{2} \ln U(x_{np+1}) - \frac{n+2}{8y_{np+1}^2} \right]$$

$$- \frac{1}{2} \left[ \ln \hat{R}_R^{(1)} + f_{G_1} + (n-1) \left( \ln \hat{R}_R^{(2)} + f_{G_2} \right) \right].$$  
(3.19)

Finally, we obtain the free energy which is dependent on the temperature and the external field:

$$F = -kTN \left[ \ln \left( \frac{(2\pi)^{\frac{1}{2}}m^{n-1}}{\Gamma \left( \frac{n}{2} \right)} \right) - \frac{1}{s_0} (\gamma_0' + \gamma_1 + \gamma_2 \Gamma) \right.$$

$$- e_0 h'(\tilde{h}^2 + h_c^2)^{\frac{\sigma}{s_0}} - \gamma_0^+ \left( f_{np+1} - \gamma' + f_G \right) \right].$$

where

$$e_0 = \frac{\sigma_0}{\sqrt{3}}, \quad e_2 = \frac{\sigma_0}{2s_0^3} \left( r_{np+2} + \frac{1}{12} u_{np+2} \sigma_0^2 \right)$$

$$\gamma_0' = \frac{1}{s_0} \left( f_{np+1} - \gamma' + f_G \right).$$  
(3.20)

$$\gamma_0^+ = \frac{1}{s_0} \left( f_{np+1} - \gamma' + f_G \right).$$

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4. The order parameter

From the formula for the free energy we obtain the order parameter of the system by direct differentiation by field:

\[ M = -\frac{1}{N} \left( \frac{dF}{dh} \right)_T. \]

The structure of the free energy allows us to separately differentiate parts connected with different fluctuation processes. The result reduces to the form

\[ M = \sigma_0^+ (\tilde{h}^2 + h_c^2)^{\frac{1}{2}}. \] (4.1)

The quantity \( \sigma_0^+ \) depends on the variable \( \alpha \) which represents the ratio between the field and the temperature:

\[ \sigma_0^+ = e_0 \left( 1 + \frac{1}{2} \frac{\alpha^2}{1 + \alpha^2} \right) + e_0 \frac{\alpha}{\sqrt{1 + \alpha^2}} + e_0^2, \]

\[ \alpha = \tilde{h}/h_c. \] (4.2)

Below, there are equations for the coefficients that depend on \( \alpha \), \( n \) and other parameters of the model. The method of calculation of the order parameter for the \( n \)-vector model is analogous to the method for the Ising model [32]. For convenience we use the same designations, but in \( n \)-vector model there appears dependence on \( n \). Thus, we obtain

\[ e_{00} = \frac{6s_0^{3/2}}{5h_0} (\gamma_s^+ - e_2), \]

\[ e_{02} = \frac{s_0^{3/2}}{5h_0} \left( f_{\gamma_1} + \sigma_0^2 q_s \left[ 1 + \frac{1}{12} q_s \sigma_0^2 \right] \right), \] (4.3)

where the following designations were introduced:

\[ q_s = \frac{\beta \Phi(0)}{2s^3} \Phi_1 H_{cd} E_2 f_n, \quad q_1 = \frac{\beta \Phi(0)}{\Phi_1 s^3} \frac{S_0}{f_n}. \] (4.4)

The coefficient \( f_{\gamma_1} \) appears as a result of differentiation of the corresponding parts of equation (3.21) by field. According to equation (3.21) the derivation of \( \gamma_s^+ \) is

\[ f_{\gamma_1} = \frac{1}{8s_0} \left( \gamma_p + f_p + f_{\gamma_1} \right), \] (4.5)

where \( \gamma_p \) is the derivation of \( \gamma' \) (see equation (3.10)):

\[ \gamma_p = H_{cd} (\tilde{g}_2 + 2g_1 H_c). \] (4.6)

The part corresponding to the LGR is

\[ f_{g_{uv}} = \frac{n}{4 + \Phi H_{cd}} + \left[ \frac{n(n + 2)}{4} \frac{r_{p+1}}{\gamma_{n+1}^2} - \frac{nU'(x_{n+1})}{2U(x_{n+1})} \right] g_{p+1} \]

\[ -\frac{1}{2} \left[ \frac{g_k^{(1)}}{f_k^{(1)}} + a_k^{(1)} g_{a}^{(1)} + (n - 1) \left( \frac{g_k^{(2)}}{f_k^{(2)}} + a_k^{(2)} g_{a}^{(2)} \right) \right], \] (4.7)

and the part from the TR is

\[ f_p = \frac{n}{2} \left[ r_p g_p \left( 1 - \frac{2n + 7}{\gamma_{n+1}^2} \right) - g_{p+1} U_n(x_{n+1}) \right]. \] (4.8)

The rest of coefficients can be found in the appendix.
Figure 1. The dependence of the order parameter on the field for $\tau = 0$ and $n = 1$.

Figure 2. The dependence of the order parameter on the field for $\tau = 0$ and $n = 2$.

Thus, we obtained explicitly the equation of state of the $n$-vector model in the presence of the external field. Its form allows easily to pass to boundary cases of dependence only on the temperature or on the field. So this equation is called the crossover equation. The quantity $\sigma_0^+$ is the scaling function of the crossover equation of state. It depends on the ratio of the field to the temperature $\alpha$. Equation (4.1) allows us to obtain a graph of dependence of the order parameter on the field for $T = T_c$ and compare it with the results of MC simulations for analogous models. Graphs of such dependences for different $n$ and different parameters of the interaction potential are presented in figures 1–4. As we can see from these figures the order parameter $M$ decreases as the number of components $n$ of the model increases.

There are different forms of the equation of state. Some discussion about convenience of the correspondent forms of the equation of state is presented in [32]. The equation of state
Figure 3. The dependence of the order parameter on the field for $\tau = 0$ and $n = 3$.

Figure 4. The dependence of the order parameter on the field for $\tau = 0$ and $n = 4$.

(4.1) can be reduced to the form [23–25]

$$M = h^{1/\delta} f_G(z),$$

(4.9)

where

$$h = H / H_0, \quad z = \tilde{t} / h^{\beta \delta}, \quad \tilde{t} = \tau T_c / T_0,$$

(4.10)

and $f_G$ is the scaling function. The explicit form of $f_G$ can be found from extrapolation of the MC data obtained in [23–26]. $H_0$ and $T_0$ are the normalization constants. Such form is equivalent to the Widom–Griffiths equation of state [37]:

$$y = f(x),$$

(4.11)

where

$$y \equiv h / M \delta, \quad x \equiv t / M^{1/\beta}.$$
Figure 5. The scaling function for \( n = 1 \) and \( b/c = 0.5 \), solid curve—our results, dashed curve—Monte Carlo data [23].

Figure 6. The scaling function for \( n = 2 \) and \( b/c = 0.5 \), solid curve—our results, dashed curve—Monte Carlo data [24].

The scaling function obtained from equation (4.1) has the form
\[
f_G = (\frac{s_0^{3/2}}{h_o})^{1/2} \sigma_{00}(1 + \alpha^{-2})^{1/2}.
\] (4.13)

It depends on \( \alpha \)
\[
\alpha = \frac{\tilde{\tau}}{\tilde{\tau}_{00}}.
\] (4.14)

The variables \( \alpha \) and \( z \) are connected with the ratio:
\[
\alpha = \frac{s_0^{3/2}}{h_o} \left( \frac{f_n}{\epsilon_{1k}} \right)^{p_0} z^{-p_0},
\] (4.15)
that allows us to compare our results with the MC data. Figures 5–8 present graphs of the scaling functions for different $n$, where the dashed curves are the results of MC simulations.

The comparison of the obtained results shows good agreement between the MC data [23–26] and our results for small and big $z$. But there is some distinction for intermediate values of the scaling variable, where values of the field and temperature are commensurable. We believe the deviation is caused by two reasons. The first one is that we put the value of critical exponent $\eta$ equal to zero in our calculation. The second is that we neglect the eigenvalue $E_3$ of the matrix $R$ (2.31) when use solutions of RR (2.40). It corresponds to neglecting corrections to the scaling.
5. Conclusions

We obtained the partition function of the \( n \)-vector model in the presence of the external field above the critical temperature by the CV method. The method of calculation corresponds to the general scheme of the RG approach. Taking into account the explicit form of the interaction potential allows us to obtain the explicit dependence of the coefficients of the linearized RR on the temperature and the microscopic parameters of the model.

The explicit form of the exit point from the CR allows us to obtain the equations for the RR in the CR suitable for any ratios of the temperature and the field. The structure of the partition function as a product of the partial partition functions that present different fluctuation processes allows us to obtain the explicit form for the free energy of the system. The order parameter of the model was found by direct differentiation by the field.

The formulas to describe the field dependences of the order parameter of the \( n \)-vector model with exponentially decreasing interaction potential for different ratios \( b/c \) (\( b \) is range of the interaction potential, \( c \) is period of the simple cubic lattice) were obtained. It was found that for each value of \( n \) there is an appropriate value of \( b \) for which our dependences are close to the MC data (see figures 5–8).

The explicit form of the scaling function (4.13) was found. The comparison with the MC data shows some difference for the behavior of \( f_G(z) \) for intermediate values of \( z \). It may be caused by used approximation in which the critical exponent \( \eta = 0 \) and corrections to scaling were neglected. But further specification of calculations is a subject of a separate investigation.

Appendix

Here we present the designations made in the second section:

\[
a_4 = -3a_0^2 \frac{n^2}{m^2} \left(1 - z' U_n(z') - U_0^2\right),
\]

\[
U_0 = \left(\frac{n}{2} + 2\right) U_n(z'), \quad z' = \frac{3}{a_4} u_2,
\]

where

\[
U_n(x) = \frac{U \left(\frac{n+1}{2}, x\right)}{U \left(\frac{n-1}{2}, x\right)}, \quad x = \frac{3}{a_4} d(B_1, B'),
\]

and for the function \( \varphi(x) \) we have

\[
\varphi(x) = (n + 2) U_n^2(x) + 2x U_n(x) - 2.
\]

The coefficients that appear in equation (4.8) are

\[
r_{p+m} = \frac{U'_n(x_{n,p+m})}{U_n(x_{n,p+m})} - \frac{1}{2} \frac{\varphi(x_{n,p+m})}{\varphi(x_{n,p+m})},
\]

\[
g_{p+m} = \frac{-\bar{x} E_n^{m-1} H_{c0}}{\sqrt{1 + \Phi E_n^{m-1} H_{c}}} \left(1 - \frac{H_c \Phi E_n^{m-1}}{2 \left[1 + \Phi E_n^{m-1} H_{c}\right]}\right),
\]

\[
\bar{x} = f_a \frac{3}{\phi_n}.
\]
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