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ANALYTICAL DESCRIPTION OF THE CRITICAL BEHAVIOR OF A THREE-DIMENSIONAL UNIAXIAL MAGNET IN AN EXTERNAL FIELD BY SINGLING OUT A REFERENCE SYSTEM

The critical behavior of systems belonging to the universality class of the three-dimensional Ising model has been studied theoretically. A three-dimensional Ising-like system with exponentially decreasing interaction potential and in the presence of a homogeneous external field was considered in the framework of the collective variables method. A specific feature in the calculation of the partition function and the free energy of a uniaxial magnet consists in singling out a reference system. The role of the latter is played by the molecular-field Hamiltonian. A method to describe the critical behavior with the use of a singled out reference system is developed on the basis of a non-Gaussian (quartic) distribution of order-parameter fluctuations (the ρ^4 model).

Keywords: Ising model, critical behavior, reference system, non-Gaussian distributions, free energy.

1. Introduction

In this paper, we study the behavior of a three-dimensional Ising-like system in a vicinity of its critical point. Similarly to what is done while studying the critical behavior of fluid systems [1], we select a reference system in calculations of the partition function of the Ising model. This reference system is a somewhat idealized physical one describing the most common features of the analyzed system, being rather simple at the same time. It does not pretend to give a complete description of the phenomenon, but makes it possible to obtain an exact or sufficiently general solution of the problem. An example of such systems for fluids is an ensemble of hard spheres. In the case of the Ising model, a model system with the mean-field Hamiltonian is proposed to be used as a reference one. The idea of this approach was proposed in [2], where a complicated equation for the self-consistent field was obtained up to the fourth virial coefficient. However, in the critical region, each of the virial coefficients contains diverging integrals resulting from the application of a Gaussian basis distribution.

This work aims at constructing a method to describe the critical behavior, in which the Hamiltonian of a self-consistent field is used as a reference system, whereas the partition function is calculated with the use of the non-Gaussian distributions of fluctuations of the order parameter. The microscopic description of the critical behavior of Ising-like systems built in this work can be applied to develop the theory of critical phenomena in various three-dimensional systems. The theoretical description of the critical behavior of real systems at a certain stage of calculations is reduced to the description of a phase transition in the framework of a definite model [3]. The development of the method for the calculation of main thermodynamic and structural characteristics for one of the basic phase transition models, namely, the three-dimensional Ising model, opens a way to the description of more complicated physical systems. Therefore, the solution, as complete as possible, obtained for the three-dimensional Ising-like system is a key to the description of the critical behavior of many physical objects.

The research procedure proposed in this work can be applied, e.g., while studying crystals with strongly anisotropic interactions, in which the magnetic moments of molecules can be considered as directed only “upward” or “downward”; for example, $FeCl_2$ and $FeCO_3$ [4]. Other examples of Ising (anisotropic) ferromagnets include some rare-earth hydroxides $R(OH)_3$ – e.g., $Tb(OH)_3$, $Dy(OH)_3$, and $Ho(OH)_3$ – and rare-earth lithium fluorides $LiRF_4$ ($LiTbF_4$ and $LiHoF_4$) [5]. Rare-earth ortho-aluminates $DyAlO_3$ and $TbAlO_3$, as well as rare-earth aluminate garnets $Dy_3Al_5O_{12}$ and $Tb_3Al_5O_{12}$, are also the examples of Ising antiferromagnets. The Ising model and real magnetic materials provide a convenient opportunity for the theory and the experiment to profitably interact with each other [6].

2. Reference System

Let us calculate the partition function of a system with the Hamiltonian

$$H = -\frac{1}{2}\sum_{\mathbf{i},\mathbf{j}} \Phi(r_{\mathbf{ij}})\sigma_{\mathbf{i}}\sigma_{\mathbf{j}} - \mathcal{H}\sum_{\mathbf{l}}\sigma_{\mathbf{l}}. \quad (1)$$

Here, $\sigma_{\mathbf{i}} = \pm 1$ is the spin variable, $\Phi(r_{\mathbf{ij}}) = A\exp(-r_{\mathbf{ij}}/b)$ is the exponentially decreasing interaction potential characterized by the constants A and b, $r_{\mathbf{ij}}$ is the distance between the particles, and $\mathcal{H}$ is the external field. The summation in Eq. (1) is performed over the sites of a simple cubic lattice with period c. The task consists in calculating the partition function

$$Z = \mathrm{Sp}\, e^{-\beta H} \quad (2)$$

and the free energy

$$F(T, \mathcal{H}) = -kT \ln Z(T, \mathcal{H}). \quad (3)$$

Here, $\beta = (kT)^{-1}$ is the inverse temperature. Formula (2) will be calculated in the space of collective variables (CVs) constructed on the operators

$$\hat{\rho}_{\mathbf{k}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{l}} \sigma_{\mathbf{l}} e^{-i\mathbf{kl}}, \quad \hat{\rho}_0 = \frac{1}{\sqrt{N}}\sum_{\mathbf{l}} \sigma_{\mathbf{l}},$$

$$(\hat{\rho}_0)^2 = \frac{1}{N}\left(\sum_{\mathbf{l}}\sigma_{\mathbf{l}}\right)^2,$$

where N is the number of particles in the system. In the CV representation, expression (2) is written in the form

$$Z = \mathrm{Sp}\left\{\int (d\rho)^N e^{\frac{1}{2}\sum\limits_{\mathbf{k}\in\mathcal{B}} \beta\Phi(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}} + h\sum\limits_{\mathbf{l}}\sigma_{\mathbf{l}}} \times \right.$$
$$\left. \times \prod_{\mathbf{k}\in\mathcal{B}} \delta(\rho_{\mathbf{k}} - \hat{\rho}_{\mathbf{k}})\right\}. \quad (4)$$

Here, $h = \beta\mathcal{H}$, $\rho_{\mathbf{k}}$ is a collective variable defined in work [2], $\Phi(k)$ is the Fourier transform of the interaction potential, and the product contains delta-functions. The summation is carried out over the wave vectors belonging to the first Brillouin zone,

$$\mathcal{B}\left\{\mathbf{k} = (k_x, k_y, k_z) | k_i = -\frac{\pi}{c} + \frac{\pi}{c}\frac{n_i}{N_i};\right.$$
$$\left. n_i = 1, 2, ..., 2N_i, \quad i = x, y, z\right\}, \quad (5)$$

where the quantities N_i determine the total number of particles, $N = N_x N_y N_z$.

Let us substitute the term $\frac{1}{2}\beta\Phi(0)\rho_0^2$ in Eq. (4) by the expression

$$\frac{1}{2}\beta\Phi(0)\frac{1}{N}\left(\sum_{\mathbf{l}}\sigma_{\mathbf{l}}\right)^2.$$

This operation is valid, because the integrand in Eq. (4) contains the delta-function $\delta(\rho_0 - \hat{\rho}_0)$ enabling the mutual exchange of the variable ρ_0 and the operator $\hat{\rho}_0$ to be done. As a result, expression (4) reads

$$Z = \int (d\rho)^N e^{\frac{1}{2}\sum\limits_{k\neq 0} \beta\Phi(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}}} J_{RS}(\rho), \quad (6)$$

where

$$J_{RS}(\rho) = \mathrm{Sp}\left\{ e^{\frac{\beta\Phi(0)}{2N}\left(\sum\limits_{\mathbf{l}}\sigma_{\mathbf{l}}\right)^2 + h\sum\limits_{\mathbf{l}}\sigma_{\mathbf{l}}} \prod_{\mathbf{k}\in\mathcal{B}} \delta(\rho_{\mathbf{k}} - \hat{\rho}_{\mathbf{k}})\right\}. \quad (7)$$

In order to calculate the explicit form of expression (7), let us take advantage of the integral representation

$$\prod_{\mathbf{k}\in\mathcal{B}} \delta(\rho_{\mathbf{k}} - \hat{\rho}_{\mathbf{k}}) = \int (d\omega)^N \exp\left[2\pi i \sum_{\mathbf{k}\in\mathcal{B}} (\rho_{\mathbf{k}} - \hat{\rho}_{\mathbf{k}})\omega_{\mathbf{k}}\right], \quad (8)$$

where the variables $\omega_{\mathbf{k}}$ are conjugate to the CVs $\rho_{\mathbf{k}}$. Substituting Eq. (8) into Eq. (7), we obtain

$$J_{RS}(\rho) = \int (d\omega)^N e^{2\pi i \sum\limits_{\mathbf{k}\in\mathcal{B}} \omega_{\mathbf{k}}\rho_{\mathbf{k}}} \times$$
$$\times \operatorname{Sp}\left\{ e^{\frac{\beta\Phi(0)}{2N}\left(\sum\limits_{\mathbf{l}}\sigma_{\mathbf{l}}\right)^2 + h\sum\limits_{\mathbf{l}}\sigma_{\mathbf{l}}} e^{-2\pi i \sum\limits_{\mathbf{k}\in\mathcal{B}} \omega_{\mathbf{k}}\hat{\rho}_{\mathbf{k}}} \right\}. \quad (9)$$

Now, let us put $\Phi(k) = 0$ for $k \neq 0$ in expression (6) and let us designate the partition function corresponding to this condition as Z_{RS}. We come to the known relation for the partition function in the molecular field approximation,

$$Z_{RS} = \operatorname{Sp}\left\{ \exp\left[\frac{\beta\Phi(0)}{2N} \sum_{\mathbf{l},\mathbf{l}'} \sigma_{\mathbf{l}}\sigma_{\mathbf{l}'} + h\sum_{\mathbf{l}}\sigma_{\mathbf{l}} \right] \right\}. \quad (10)$$

The free energy corresponding to formula (10) looks like [4]

$$F = -kTN\left\{ \frac{1}{2}\ln\frac{4}{1-M^2} \right\} + \frac{1}{2}\Phi(0)M^2. \quad (11)$$

In this approximation, the magnetization M per one site is given by the expression

$$M = \tanh\left[(\Phi(0)M + \mathcal{H})\,\beta \right], \quad (12)$$

which was obtained in work [7] for the first time. It is easy to see that, for $\mathcal{H} = 0$, we obtain different solutions for M at $T > T_{\rm CM}$ and $T < T_{\rm CM}$, where $T_{\rm CM}$ is the phase transition temperature in the molecular field approximation, $T_{\rm CM} = \Phi(0)/k$. The non-zero order parameter exists only at $T < T_{\rm CM}$. According to Eq. (12), the known relation can be written down as

$$\mathcal{H} = -\Phi(0)M + kT\,\operatorname{arctanh} M. \quad (13)$$

Let us return to expression (6), where the reference system is singled out, but no approximations are made. We intend to use the known identity

$$e^{\frac{1}{2}\beta\Phi(0)\frac{1}{N}\left(\sum\limits_{\mathbf{l}}\sigma_{\mathbf{l}}\right)^2} = \left(\frac{N}{2\pi\beta\Phi(0)}\right)^{1/2} \times$$
$$\times \int\limits_{-\infty}^{\infty} \exp\left(-\frac{N\varphi^2}{2\beta\Phi(0)} + \varphi\sum_{\mathbf{l}}\sigma_{\mathbf{l}} \right) d\varphi, \quad (14)$$

which is valid at $\Phi(0) > 0$. Then the partition function of the system can be expressed in the form

$$Z = \left(\frac{N}{2\pi\beta\Phi(0)}\right)^{1/2} \int\limits_{-\infty}^{\infty} d\varphi\, e^{-\frac{N\varphi^2}{2\beta\Phi(0)}} \int (d\rho)^N (d\omega)^N \times$$
$$\times \exp\left(\frac{1}{2}\sum_{k\neq 0}\beta\Phi(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}} + 2\pi i \sum_{\mathbf{k}\in\mathcal{B}} \omega_{\mathbf{k}}\rho_{\mathbf{k}} \right) \times$$
$$\times \operatorname{Sp}\left\{ e^{(h+\varphi)\sum\limits_{\mathbf{l}}\sigma_{\mathbf{l}} - 2\pi i \sum\limits_{\mathbf{k}\in\mathcal{B}} \omega_{\mathbf{k}} \frac{1}{\sqrt{N}} \sum\limits_{\mathbf{l}=1}^{N} \sigma_{\mathbf{l}} e^{-i\mathbf{k}\mathbf{l}}} \right\}. \quad (15)$$

Executing the Sp operation, we obtain the sought expression for the partition function in the CV representation with the singled out reference system,

$$Z = \left(\frac{N}{2\pi\beta\Phi(0)}\right)^{1/2} 2^N \int\limits_{-\infty}^{\infty} d\varphi\, e^{-\frac{N\varphi^2}{2\beta\Phi(0)}} \times$$
$$\times \int (d\rho)^N (d\omega)^N e^{\frac{1}{2}\sum\limits_{k\neq 0}\beta\Phi(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}}} e^{2\pi i \sum\limits_{\mathbf{k}\in\mathcal{B}} \omega_{\mathbf{k}}\rho_{\mathbf{k}}} J_{\rm CM}(\omega). \quad (16)$$

Here, we introduced the notation

$$J_{\rm CM}(\omega) = \exp\left[\sum_{\mathbf{l}} \ln\cosh\left(\varphi + h - 2\pi i \omega_{\mathbf{l}} \right) \right], \quad (17)$$

where

$$\omega_{\mathbf{l}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\in\mathcal{B}} \omega_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{l}}. \quad (18)$$

Expression (17) can be written in the form of a cumulant series expansion

$$J_{\rm CM}(\omega) = \exp\left(\sum_{n\geq 0} D(\omega) \right), \quad (19)$$

where

$$D_n(\omega) = \frac{(-2\pi i)^n}{n!} \frac{\mathcal{M}_n(h,\varphi)}{N^{n/2-1}} \times$$
$$\times \sum_{\substack{\mathbf{k}_1,\ldots,\mathbf{k}_n \\ \mathbf{k}_i\in\mathcal{B}}} \omega_{\mathbf{k}_1}\ldots\omega_{\mathbf{k}_n} \delta_{\mathbf{k}_1+\ldots+\mathbf{k}_n}, \quad (20)$$

and $\delta_{\mathbf{k}_1+\ldots+\mathbf{k}_n}$ is the Kronecker symbol. For the cumulants $\mathcal{M}_n(h,\varphi)$, the following expressions are applicable:

$$\begin{aligned}
&\mathcal{M}_0 = \ln\cosh(\varphi + h), \quad \mathcal{M}_1 = \tanh(\varphi + h), \\
&\mathcal{M}_2 = 1 - \mathcal{M}_1^2, \quad \mathcal{M}_3 = -2\mathcal{M}_1\mathcal{M}_2, \\
&\mathcal{M}_4 = -2\mathcal{M}_2 + 4\mathcal{M}_1^2\mathcal{M}_2, \\
&\mathcal{M}_5 = 16\mathcal{M}_1\mathcal{M}_2^2 - 8\mathcal{M}_1^3\mathcal{M}_2, \\
&\mathcal{M}_6 = 16\mathcal{M}_2^2 - 88\mathcal{M}_1^2\mathcal{M}_2^2 + 16\mathcal{M}_1^4\mathcal{M}_2, \quad \ldots .
\end{aligned} \quad (21)$$

Expression (16), in which $J_{\rm CM}$ is given by formulas (19)–(21), forms a basis for further calculations. The cumulants $\mathcal{M}_n$ in Eqs. (21) depend on the external field magnitude $\mathcal{H}$ and a certain internal field φ. To elucidate the nature of the latter, let us put $\beta\Phi(k) = 0$ for all $k \neq 0$, which takes place, when we neglect the contributions of many-particle interactions. Then, with the use of Eq. (16) and

$$J_{\rm CM}(\omega) = J_{\rm CM}(0) = e^{N \ln\cosh(h+\varphi)}, \quad (22)$$

we find the corresponding expression for the partition function,

$$Z_0 = \left(\frac{N}{2\pi\beta\Phi(0)}\right)^{1/2} 2^N \int\limits_{-\infty}^{\infty} e^{-\frac{N\varphi^2}{2\beta\Phi(0)} + N\ln\cosh(h+\varphi)} d\varphi. \quad (23)$$

Applying the saddle-point method, we obtain the free energy

$$F_0 = -kTN\left[-\frac{\bar\varphi^2}{2\beta\Phi(0)} + \ln\cosh(h+\bar\varphi)\right], \quad (24)$$

where the quantity $\bar\varphi$ is determined from the equation

$$\bar\varphi = \beta\Phi(0)\tanh(h+\bar\varphi). \quad (25)$$

Comparing Eqs. (25) and (12) with each other, we find

$$\bar\varphi = \beta\Phi(0)M. \quad (26)$$

Hence, the average value of internal field $\bar\varphi$ is connected with the order parameter. However, unlike the "introduction" of an internal field in the molecular field method, the proposed approach gives rise to expression (23), which implies the integration over all possible fields φ with a certain distribution function.

In the general case, the quantity $\beta\Phi(k)$ differs from zero, and just this circumstance is responsible for the influence of many-particle interactions on the formation of physical quantities near the second-order phase transition point. For the partition function, we have representation (16), where the quantity $J_{\rm CM}(\omega)$ is given by expression (19) containing both even and odd cumulants, which, in turn, are functions of the external, h, and internal, φ, fields.

3. Particular Representations of the Partition Function with the Singled Out Reference System

The functional representation of the partition function (16) is rather complicated from the viewpoint of its further integration over the variable φ and the determination of the dependence on the external field h, because each of those quantities governs the cumulants, i.e. $\mathcal{M}_n(h,\varphi)$. Therefore, let us return to expression (15) and write it in the form

$$Z = \left(\frac{N}{2\pi\beta\Phi(0)}\right)^{1/2} \int\limits_{-\infty}^{\infty} d\varphi e^{-\frac{N\varphi^2}{2\beta\Phi(0)}} \int (d\rho)^N (d\omega)^N \times$$
$$\times e^{\frac{1}{2}\sum\limits_{k\neq 0}\beta\Phi(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}}} e^{h\sqrt{N}\rho_0 + 2\pi i\sum\limits_{\mathbf{k}\in\mathcal{B}}\omega_{\mathbf{k}}\rho_{\mathbf{k}}} \times$$
$$\times \mathrm{Sp}\left\{e^{\varphi\sum\limits_{\mathbf{l}}\sigma_{\mathbf{l}}} \exp\left(-2\pi i\sum_{\mathbf{k}\in\mathcal{B}}\omega_{\mathbf{k}}\frac{1}{\sqrt{N}}\sum_{l=1}^{N}\sigma_{\mathbf{l}}e^{-i\mathbf{kl}}\right)\right\}. \quad (27)$$

In comparison with Eq. (15), the exponential function $\exp\left(h\sum_{\mathbf{l}}\sigma_{\mathbf{l}}\right)$ is removed here from the expression under the Sp sign, because of the multiplier $\delta(\rho_0 - \hat\rho_0)$ is present in the integrand, which allows the operator $\hat\rho_0$ to be substituted by the variable ρ_0. As a result of this operation, we obtain the following expression for the partition function:

$$Z = \left(\frac{N}{2\pi\beta\Phi(0)}\right)^{1/2} 2^N \int\limits_{-\infty}^{\infty} d\varphi e^{-\frac{N\varphi^2}{2\beta\Phi(0)}} \times$$
$$\times \int (d\rho)^N (d\omega)^N e^{\frac{1}{2}\sum\limits_{k\neq 0}\beta\Phi(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}}} \times$$
$$\times \exp\left(h\sqrt{N}\rho_0 + 2\pi i\sum_{\mathbf{k}\in\mathcal{B}}\omega_{\mathbf{k}}\rho_{\mathbf{k}}\right) J_\varphi(\omega), \quad (28)$$

where

$$J_\varphi(\omega) = \exp\left[\sum_{n\geq 0}\frac{(-2\pi i)^n}{n!}\frac{\mathcal{M}_n(\varphi)}{N^{n/2-1}} \times\right.$$
$$\left.\times \sum_{\substack{\mathbf{k}_1,\ldots,\mathbf{k}_n \\ \mathbf{k}_i\in\mathcal{B}}} \omega_{\mathbf{k}_1}\ldots\omega_{\mathbf{k}_n}\delta_{\mathbf{k}_1+\ldots+\mathbf{k}_n}\right]. \quad (29)$$

Here, in contrast to Eqs. (21), the cumulants $\mathcal{M}_n(\varphi)$ depend only on the internal field φ, whereas the dependence on the external field is contained only in the term $h\sqrt{N}\rho_0$ entering the argument of the exponential function in the integrand of expression (28). Now,

$$\begin{aligned}
\mathcal{M}_0(\varphi) &= \ln\cosh\varphi, \quad \mathcal{M}_1(\varphi) = \tanh\varphi \equiv x_\varphi, \\
\mathcal{M}_2(\varphi) &= 1 - x_\varphi^2 \equiv y_\varphi, \quad \mathcal{M}_3(\varphi) = -2x_\varphi y_\varphi, \\
\mathcal{M}_4(\varphi) &= -2y_\varphi + 4x_\varphi^2 y_\varphi, \\
\mathcal{M}_5(\varphi) &= 16x_\varphi y_\varphi^2 - 8x_\varphi^3 y_\varphi, \\
\mathcal{M}_6(\varphi) &= 16y_\varphi^2 - 88x_\varphi^2 y_\varphi^2 + 16x_\varphi^4 y_\varphi, \quad \ldots .
\end{aligned} \quad (30)$$

Representation (28) substantially simplifies further calculations aimed at finding the dependence on the external field. However, the dependence of cumulants on the internal field survives.

Expression (15) enables us to write another representation for the partition function,

$$Z=\left(\frac{N}{2\pi\beta\Phi(0)}\right)^{1/2} 2^N \int\limits_{-\infty}^{\infty} d\varphi e^{-\frac{N\varphi^2}{2\beta\Phi(0)}} \times$$
$$\times \int (d\rho)^N (d\omega)^N e^{\frac{1}{2}\sum\limits_{k\neq 0}\beta\Phi(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}}} \times$$
$$\times \exp\left(\varphi\sqrt{N}\rho_0 + 2\pi i \sum_{\mathbf{k}\in\mathcal{B}} \omega_{\mathbf{k}}\rho_{\mathbf{k}}\right) J_h(\omega), \tag{31}$$

where

$$J_h(\omega) = \exp\Bigg[\sum_{n\geq 0} \frac{(-2\pi i)^n}{n!}\frac{\mathcal{M}_n(h)}{N^{n/2-1}} \times$$
$$\times \sum_{\substack{\mathbf{k}_1,\ldots,\mathbf{k}_n\\ \mathbf{k}_i\in\mathcal{B}}} \omega_{\mathbf{k}_1}\ldots\omega_{\mathbf{k}_n}\delta_{\mathbf{k}_1+\ldots+\mathbf{k}_n}\Bigg]. \tag{32}$$

Here, the cumulants $\mathcal{M}_n(h)$ look like expressions (30), but depend on h rather than φ.

The simplest form for a representation of the partition function with the singled out reference system is given by the formula

$$Z=\left(\frac{N}{2\pi\beta\Phi(0)}\right)^{1/2} 2^N \int\limits_{-\infty}^{\infty} d\varphi e^{-\frac{N\varphi^2}{2\beta\Phi(0)}} \times$$
$$\times \int (d\rho)^N (d\omega)^N e^{\frac{1}{2}\sum\limits_{k\neq 0}\beta\Phi(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}}} \times$$
$$\times \exp\left[(\varphi+h)\sqrt{N}\rho_0 + 2\pi i \sum_{\mathbf{k}\in\mathcal{B}} \omega_{\mathbf{k}}\rho_{\mathbf{k}}\right] J(\omega), \tag{33}$$

where the transition Jacobian $J(\omega)$ looks like

$$J(\omega)= \exp\Bigg[\sum_{n\geq 1} \frac{(-2\pi i)^{2n}}{(2n)!}\mathcal{M}_{2n}N^{1-n} \times$$
$$\times \sum_{\mathbf{k}_1,\ldots,\mathbf{k}_{2n}} \omega_{\mathbf{k}_1}\ldots\omega_{\mathbf{k}_{2n}}\delta_{\mathbf{k}_1+\ldots+\mathbf{k}_{2n}}\Bigg]. \tag{34}$$

Note that all odd cumulants and the cumulant $\mathcal{M}_0$ in Eq. (33) equal zero, and the even cumulants have the following specific numerical values [2]:

$$\mathcal{M}_2 = 1, \quad \mathcal{M}_4 = -2, \quad \mathcal{M}_6 = 16, \quad \ldots . \tag{35}$$

By comparing the expressions obtained above, we arrive at the following important conclusion. The functional representation of the partition function for the Ising model in the presence of an external field in a singled out reference system (the molecular-field Hamiltonian) can include only even cumulants, as in formula (33), or both even and odd cumulants, as in formulas (16), (28) and (31). Each of the representations given above is exact and can be used in further calculations. Certainly, in specific calculations, the number of terms in the argument of the exponential function in the integrand has to be finite. While describing the phenomena in a vicinity of the second-order phase transition point, all the terms up to the fourth order in the variable inclusive have to be taken into consideration [2]. This makes possible to obtain a qualitative picture of a phase transition in the presence of an external field [8]. Taking the sixth-order terms into consideration allows one to say about the quantitative results of the theory [9]. Therefore, the accuracy of a calculation technique should be related only to the number of terms (cumulants) that were taken into account, while calculating the partition function rather than the form of a distribution containing only even (or odd) power exponents of the variable in the exponential function argument.

4. ρ^4 Model

For further calculations, let us take expression (33) as a basis. In the corresponding expression for $J(\omega)$, only the terms of the second and fourth orders in $\omega_{\mathbf{k}}$ will be taken into account. In this case, the partition function of the system reads

$$Z=\left(\frac{N}{2\pi\beta\Phi(0)}\right)^{1/2} 2^N \int\limits_{-\infty}^{\infty} d\varphi e^{-\frac{N\varphi^2}{2\beta\Phi(0)}} \times$$
$$\times \int (d\rho)^N (d\omega)^N e^{\frac{1}{2}\sum\limits_{k\neq 0}\beta\Phi(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}}} e^{(h+\varphi)\sqrt{N}\rho_0} \times$$
$$\times \exp\Bigg[2\pi i \sum_{\mathbf{k}\in\mathcal{B}} \omega_{\mathbf{k}}\rho_{\mathbf{k}} - \frac{(2\pi)^2}{2}\sum_{\mathbf{k}\in\mathcal{B}}\omega_{\mathbf{k}}\omega_{-\mathbf{k}} -$$
$$- \frac{(2\pi)^4}{12}\frac{1}{N}\sum_{\substack{\mathbf{k}_1,\ldots,\mathbf{k}_4\\ \mathbf{k}_i\in\mathcal{B}}} \omega_{\mathbf{k}_1}\ldots\omega_{\mathbf{k}_4}\delta_{\mathbf{k}_1+\ldots+\mathbf{k}_4}\Bigg]. \tag{36}$$

Integrating over the variables $\omega_{\mathbf{k}}$ and using the calculation procedure described in work [10], we obtain the following explicit form for the partition function in the ρ^4-model approximation:

$$Z=\left(\frac{N}{2\pi\beta\Phi(0)}\right)^{1/2} 2^N e^{a_0 N}\int\limits_{-\infty}^{\infty} d\varphi e^{-\frac{N\varphi^2}{2\beta\Phi(0)}}\times$$
$$\times\int (d\rho)^N e^{\frac{1}{2}\sum\limits_{k\neq 0}\beta\Phi(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}}}\times$$
$$\times\exp\Bigg[(h+\varphi)\sqrt{N}\rho_0-\frac{1}{2}a_2\sum_{\mathbf{k}\in\mathcal{B}}\rho_{\mathbf{k}}\rho_{-\mathbf{k}}-$$
$$-\frac{1}{4!}\frac{a_4}{N}\sum_{\substack{\mathbf{k}_1,\ldots,\mathbf{k}_4\\ \mathbf{k}_i\in\mathcal{B}}}\rho_{\mathbf{k}_1}\cdots\rho_{\mathbf{k}_4}\delta_{\mathbf{k}_1+\cdots+\mathbf{k}_4}\Bigg]. \qquad (37)$$

The coefficients a_{2l} are calculated according to the formulas

$$\begin{aligned} a_0 &= \ln\left[(2\pi)^{-1/2}(3/2)^{1/4}e^{y^2/4}U(0,y)\right],\\ a_2 &= (3/2)^{1/2}U(y), \quad a_4=(3/2)\varphi(y), \end{aligned} \qquad (38)$$

where $U(y)$ and $\varphi(y)$ are the combinations of parabolic cylinder functions $U(a,y)$ [10], with the argument y accepting the value $y=(3/2)^{1/2}$. Then, $a_0=-1.0557$, $a_2=0.6449$, and $a_4=0.1826$. By its functional form, the part of the integrand dependent on CVs is similar to the corresponding expression obtained in work [8]. There are only two differences. One of them consists in the substitution of the dimensionless field h by the quantity

$$h_\varphi = h+\varphi. \qquad (39)$$

The other is associated with the absence of a term with $k=0$ in Eq. (37). This circumstance is not essential from the viewpoint of the step-by-step calculation of the partition function in the framework of the Yukhnovskii method [2, 10]. The variable ρ_0 is used in this process only at the final calculation stage, i.e. after the point of exit of the system from the critical fluctuation regime. Therefore, according to the results of work [8], the partition function of the model with Hamiltonian ((1) takes the form

$$Z=2^N\int\limits_{-\infty}^{\infty} d\varphi e^{-\frac{N\varphi^2}{2\beta\Phi(0)}}e^{-\beta F_a-\beta F_{\rm CR}^{(+)}-\beta F_{\rm TR}}Z'(\varphi), \qquad (40)$$

where the analytical part of the free energy, F_a, being a function of the relative temperature $\tau=(T-T_c)/T$, looks like

$$F_a=-kTN(\gamma_0+\gamma_1\tau+\gamma_2\tau^2)-\frac{1}{2}N\Phi(0)\bar{\Phi}. \qquad (41)$$

The expressions for the coefficients γ_l and the quantity $\bar{\Phi}$ can be found in work [8].

The contribution to the free energy from the critical regime of fluctuations equals

$$F_{\rm CR}^{(+)}=kTN_0\bar{\gamma}^+ s^{-3(n_p+1)}. \qquad (42)$$

Here, $N_0=Ns_0^{-d}$, and $d=3$ is the space dimensionality. The parameter s_0 determines the interval of wave vectors, where the Fourier transform of the potential $\Phi(k)$ is well approximated by a parabola. The coefficient $\bar{\gamma}^+$ was determined in work [8], and s is the parameter of division of the CV phase space into layers. For n_p, we have the relation

$$n_p+1=-\frac{\ln(\tilde{h}_\varphi+h_c)}{\ln E_1}, \qquad (43)$$

where the notations

$$\tilde{h}_\varphi=s_0^{d/2}(h+|\varphi|)/h_0, \quad h_c=|\tilde{\tau}|^{p_0} \qquad (44)$$

are introduced, and

$$\tilde{\tau}=\tau\,(c_{1k}/f_0), \quad p_0=\frac{\ln E_1}{\ln E_2}. \qquad (45)$$

Here, E_1 and E_2 are the larger and smaller, respectively, eigenvalues of the matrix for the linear renormalization-group transformation. The quantities c_{1k} and f_0 characterize one of the coefficients in the solutions of the recurrence relations and one of the fixed point coordinates, respectively, whereas the parameter h_0 determines the normalization condition for the critical amplitude of the correlation length (at the critical temperature T_c).

The contribution to the free energy from the transition region (from non-Gaussian to Gaussian order-parameter fluctuations) is given by the formula (see work [8])

$$F_{\rm TR}=-kTN_0 f_{n_p+1}s^{-3(n_p+1)}. \qquad (46)$$

For $Z'(\varphi)$ in Eq. (40), we have

$$Z'=2^{(N_{n_p+2}-1)/2}\left[Q\left(P_{n_p+1}\right)\right]^{N_{n_p+2}}Z_{n_p+2}, \qquad (47)$$

where

$$Z_{n_p+2}=\int (d\rho)^{N_{n_p+2}}\exp\Bigg[h_\varphi\sqrt{N}\rho_0-$$
$$-\frac{1}{2}\sum_{\mathbf{k}\in\mathcal{B}_{n_p+2}}{}' d_{n_p+2}(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}}-$$

$$- \frac{a_4^{(n_p+2)}}{4!} N_{n_p+2}^{-1} \sum_{\substack{\mathbf{k}_1,\dots,\mathbf{k}_4 \\ \mathbf{k}_i \in \mathcal{B}_{n_p+2}}} \rho_{\mathbf{k}_1} \dots \rho_{\mathbf{k}_4} \delta_{\mathbf{k}_1+\dots+\mathbf{k}_4} \Bigg]. \quad (48)$$

The primed sum sign means that, for $k = 0$, the equality

$$d_{n_p+2}(0) = a_2^{(n_p+2)} \quad (49)$$

is obeyed. For all $k \neq 0$, the expression

$$d_{n_p+2}(k) = a_2^{(n_p+2)} - \beta\Phi(0)(1 - 2b^2k^2) \quad (50)$$

is valid. Let us use the notations

$$\begin{aligned} r_{n_p+2} &= (a_2^{(n_p+2)} - \beta\Phi(0)) s^{2(n_p+2)}, \\ u_{n_p+2} &= a_4^{(n_p+2)} s^{4(n_p+2)}, \end{aligned} \quad (51)$$

where the quantities

$$\begin{aligned} r_{n_p+2} &= \beta\Phi(0) f_0 \, (-1 + E_2 H_c), \\ u_{n_p+2} &= (\beta\Phi(0))^2 \, \varphi_0 \, (1 + \Phi_f E_2 H_c) \end{aligned} \quad (52)$$

were calculated in work [8]. Carrying out the change of variables,

$$\rho_{\mathbf{k}} = \eta_{\mathbf{k}} + \sqrt{N} \sigma \delta_{\mathbf{k}},$$

in Eq. (48), we obtain

$$\begin{aligned} Z_{n_p+2} &= e^{NE_0(\sigma,\varphi)} \int (d\eta)^{N_{n_p+2}} \times \\ &\times \exp\Bigg[A_0 \sqrt{N} \eta_0 - \frac{1}{2} \sum_{\mathbf{k} \in \mathcal{B}_{n_p+2}} \bar{d}(k) \eta_{\mathbf{k}} \eta_{-\mathbf{k}} - \\ &- \frac{\bar{b}}{6} \frac{1}{\sqrt{N_{n_p+2}}} \sum_{\mathbf{k}_i \in \mathcal{B}_{n_p+2}} \eta_{\mathbf{k}_1} \dots \eta_{\mathbf{k}_3} \delta_{\mathbf{k}_1+\dots+\mathbf{k}_3} - \\ &- \frac{a_4^{(n_p+2)}}{24} \frac{1}{N_{n_p+2}} \sum_{\mathbf{k}_i \in \mathcal{B}_{n_p+2}} \eta_{\mathbf{k}_1} \dots \eta_{\mathbf{k}_4} \delta_{\mathbf{k}_1+\dots+\mathbf{k}_4} \Bigg]. \end{aligned} \quad (53)$$

Here,

$$\begin{aligned} E_0(\sigma, \varphi) &= (\varphi + h)\sigma - \frac{1}{2}\sigma^2 a_2^{(n_p+2)} - \\ &- \frac{u_{n_p+2}}{24} s_0^3 s^{-(n_p+2)} \sigma^4, \\ A_0 &= (\varphi + h) - \sigma a_2^{(n_p+2)} - \frac{u_{n_p+2}}{6} s_0^3 s^{-(n_p+2)} \sigma^3, \\ \bar{b} &= u_{n_p+2} s_0^{3/2} s^{-5/2(n_p+2)} \sigma. \end{aligned} \quad (54)$$

As was done in work [8], the shift σ is determined from the condition

$$\frac{\partial E_0(\sigma, \varphi)}{\partial \sigma} \equiv A_0 = 0. \quad (55)$$

It is easy to see that, for large n_p values (the region of critical fluctuations), Eq. (55) has a solution

$$\sigma = \frac{\varphi + h}{a_2^{(n_p+2)}}. \quad (56)$$

Comparing the shift value given by formula (56) with the corresponding expression obtained in work [8] (where the reference system was not singled out), we reveal a principal difference. It consists in the absence of the term $\beta\Phi(0)\rho_0^2$ in the argument of the exponential function in expression (48).

Substituting Eq. (56) into the formula for $E_0(\sigma, \varphi)$ in Eqs. (54), we obtain

$$E_0(\varphi) = \frac{1}{2} \frac{h_\varphi^2}{\bar{a}_2} - \frac{u_{n_p+2} s_0^3}{24 \bar{a}_2^4} s^{-(n_p+2)} h_\varphi^4. \quad (57)$$

Here, the notation $\bar{a}_2 = a_2^{(n_p+2)}$ is introduced. For $k = 0$, the coefficient $\bar{d}(k)$ in expression (53) satisfies the relation

$$\bar{d}(0) = \bar{a}_2 + \frac{1}{2} u_{n_p+2} s_0^3 s^{-(n_p+2)} \frac{h_\varphi^2}{\bar{a}_2^2}, \quad (58)$$

whereas, for all $k \neq 0$,

$$\begin{aligned} \bar{d}(k) &= r_{n_p+2} s^{-2(n_p+2)} + \frac{1}{2} u_{n_p+2} s_0^3 s^{-(n_p+2)} \frac{h_\varphi^2}{\bar{a}_2^2} + \\ &+ 2\beta\Phi(0) b^2 k^2. \end{aligned} \quad (59)$$

In the case where $T > T_c$ and the field is low, the coefficient $r_{n_p+2} > 0$. Therefore, while calculating Eq. (53), the Gaussian distribution of fluctuations can be used, as was proposed in work [8]. Then, the contribution to the free energy from Eq. (47) reads

$$F'(\varphi) = -kTN \left[E_0(\varphi) + s_0^{-3} s^{-3} f_G s^{-3(n_p+1)} \right]. \quad (60)$$

Here,

$$\begin{aligned} f_G &= \frac{1}{2}\ln 2 - \frac{1}{4}\ln 3 + \ln s + \frac{1}{4}\ln u_{n_p+1} - \frac{1}{2}\ln r_R - \\ &- \frac{1}{2}\ln U(x_{n_p+1}) - \frac{3}{8} y_{n_p+1}^{-2} - \frac{1}{2} f_G'', \end{aligned} \quad (61)$$

and

$$r_R = r_{n_p+2} + \frac{1}{2}\frac{u_{n_p+2}}{\bar{a}_2^2} s_0^3 s^{n_p+2} h_\varphi^2,$$

$$x_{n_p+1} = d_{n_p+1}(B_{n_p+2}, B_{n_p+1})\left(\frac{3}{a_4^{(n_p+1)}}\right)^{1/2},$$

$$y_{n_p+1} = s^{3/2} U(x_{n_p+1})\left(\frac{3}{\varphi(x_{n_p+1})}\right)^{1/2},$$

$$d_{n_p+1}(B_{n_p+2}, B_{n_p+1}) = a_2^{(n_p+1)} - \beta\Phi(B_{n_p+2}, B_{n_p+1}). \tag{62}$$

The quantity $\Phi(B_{n_p+2}, B_{n_p+1})$ is the average value of the Fourier transform for the potential $\Phi(k)$ in the wave vector interval $\mathbf{k} \in \mathcal{B}_{n_p+1} \backslash \mathcal{B}_{n_p+2}$. For f_G'', we obtain

$$f_G'' = \ln\left(1 + a^2\right) - \frac{2}{3} + \frac{2}{a^2} - \frac{2}{a^3}\arctan a, \tag{63}$$

where

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

Taking the expressions obtained above into account, we write the partition function for the Ising model with the singled out reference system in the following form:

$$Z = \int\limits_{-\infty}^{\infty} d\varphi \exp\left[-\frac{\varphi^2 N}{2\beta\Phi(0)} - \beta F_a - \beta F_{\mathrm{CR}}^{(+)} - \right.$$
$$\left. - \beta F_{\mathrm{TR}} - \beta F'(\varphi)\right]. \tag{64}$$

Here, F_a describes the analytical part of the free energy, which does not depend on φ (see Eq. (41)), and $F_{\mathrm{CR}}^{(+)}$ is the contribution from the critical regime of fluctuations. The latter is given by formula (42), where the dependence on φ is contained in the quantity n_p from Eq. (43). Formula (64) is calculated using the saddle-point method. The equation for the extreme point of the integrand in Eq. (64) looks like

$$\left\{\frac{\varphi + h}{\bar{a}_2} - \frac{\varphi}{\beta\Phi(0)} + \frac{\partial\gamma_s^{(+)}}{\partial\varphi} s^{-3(n_p+1)} - \right.$$
$$- \frac{u_{n_p+2} s_0^3}{6\bar{a}_2^4} s^{-(n_p+2)} h_\varphi^3 - \ln s \frac{\partial n_p}{\partial\varphi} \times$$
$$\left.\left. \times \left[3\gamma_s^{(+)} s^{-3(n_p+1)} - \frac{u_{n_p+2} s_0^3}{24\bar{a}_2^4} s^{-(n_p+2)} h_\varphi^4\right]\right\}\right|_{\varphi=\bar{\varphi}} = 0. \tag{65}$$

In Eq. (65), all terms proportional to h_φ^4 are taken into account, and $\gamma_s^{(+)} = s_0^{-3}(f_{n_p+1} - \bar{\gamma}^{(+)} + f_G/s^3)$.

The total contribution from all fluctuation regimes to the free energy of the system at temperatures $T > T_c$ equals

$$F = F_a + F_s(\bar{\varphi}) + F_0^{(+)}. \tag{66}$$

Here,

$$F_s(\bar{\varphi}) = -kTN\gamma_s^{(+)}\left(\tilde{h}_{\bar{\varphi}} + h_c\right)^{\frac{2d}{d+2}}, \tag{67}$$

and

$$F_0^{(+)} = -kTNE_0(\bar{\varphi}). \tag{68}$$

The value of $\bar{\varphi}$ is determined from Eq. (65). In the case $\tau > \tau^*$, the quantity n_p is constant (close to unity) and does not depend on h_φ and, hence, φ. Therefore, its derivative with respect to φ vanishes. The same is valid for the quantity $\gamma_s^{(+)}$. Equation (65) reproduces the result of the molecular field theory for $\bar{\varphi}$. For all $\tau < \tau^*$, the dependence of $\bar{\varphi}$ on the variables τ and h is not analytical, and, consequently, we have expression (66) for the free energy in the critical region.

5. Conclusions

A technique for the description of the critical behavior of a three-dimensional uniaxial magnet in an external field has been developed. In its framework, the Hamiltonian of the self-consistent field is used as a reference system, and the partition function is calculated in the quartic approximation for the distribution of order-parameter fluctuations. Various forms of a functional representation for the partition function with the singled out reference system are obtained and discussed. Each of them is exact and can be used for further calculations. The choice of the simplest representation form for the partition function, which includes only even power exponents of the variable (up to the fourth order inclusive), allowed us to apply the results of previous researches, which were obtained without singling out the reference system. Proceeding from this simplest form of a representation, the free energy of a one-component spin system in the critical region is calculated.

The performed researches make our knowledge concerning the critical properties of the systems belonging to the Ising class of universality more comprehensive, being also a certain methodological contribution to the theoretical description of critical phenomena. The results of this work obtained for the three-dimensional Ising-like system in an external field may be found useful for the description of fluid-gas critical points in both a one-component fluid [11–13] and a binary fluid mixture (see, e.g., work [14]). The functional of the partition function for those systems corresponds to the partition function of the Ising model in an external field. A new result in the description of the fluid-gas critical point in comparison with the Ising model is the dependence of the grand partition function on the temperature and the chemical potential. The latter is equivalent to the inclusion of a constant external field into the Ising model.

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АНАЛІТИЧНИЙ ОПИС КРИТИЧНОЇ ПОВЕДІНКИ ТРИВИМІРНОГО ОДНОВІСНОГО МАГНЕТИКА В ЗОВНІШНЬОМУ ПОЛІ З ВИДІЛЕННЯМ СИСТЕМИ ВІДЛІКУ

Р е з ю м е

Роботу присвячено теоретичному вивченню критичної поведінки систем класу універсальності тривимірної моделі Ізинга. Тривимірна ізингоподібна система з експоненційно спадним потенціалом взаємодії досліджується в методі колективних змінних за наявності однорідного зовнішнього поля. Характерною особливістю розрахунку статистичної суми та вільної енергії одновісного магнетика є виділення системи відліку. Роль останньої відіграє гамільтоніан молекулярного поля. Метод опису критичної поведінки з виділеною системою відліку розвинуто на основі негаусового (четвірного) розподілу флуктуацій параметра порядку (моделі ρ^4).