The order parameter and susceptibility of a 3D Ising-like system in an external field

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Abstract

The present poster is based on the work [1] which is dedicated to the investigation of the 3D Ising-like model in the presence of an external field in the vicinity of the critical point. The method of the collective variables is used. General expressions for the order parameter and susceptibility is calculated as functions of temperature and the external field as well as scaling functions of that are explicitly obtained. The results are compared with ones obtained within the framework of the parametric representation of the equation of state and Monte Carlo simulations.

Partition function of the model

Properties of spin systems are known to be described by the Ising model very well. The Hamiltonian of this model in the external field is written in the form

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

Here $\Phi(r_{\mathbf{i},\mathbf{j}})$ is a short-range interaction potential between spins located at the i-th and j-th sites of a simple cubic lattice with a lattice constant c. The spin variables $\sigma_{\mathbf{i}}$ take on two values ± 1, and $\mathcal{H}$ is an external field.

The partition function of the three-dimensional (3D) Ising model can be expressed in terms of the collective variables (CV) [2]

$$Z = \int \exp\Big(\frac{1}{2}\sum_{\mathbf{k}\in\mathcal{B}} \beta\tilde{\Phi}(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}}\Big) J_h(\rho)(d\rho)^N \qquad (2)$$

where $J_h(\rho)$ is the transition Jacobian from the spin variables $\sigma_{\mathbf{i}}$ to the CV $\rho_{\mathbf{k}}$.

In the expression for the partition function (2) the Fourier transform of an interaction potential arises. In the case of the exponentially decreasing potential

$$\Phi(r_{\mathbf{i},\mathbf{j}}) = A\exp(-r_{\mathbf{i},\mathbf{j}}/b) \qquad (3)$$

its Fourier transform has the form

$$\tilde{\Phi}_G(k) = \frac{\tilde{\Phi}(0)}{(1+b^2k^2)^2}, \qquad \tilde{\Phi}(0) = 8\pi A(b/c)^3. \qquad (4)$$

Here b is the effective interaction range.

In our investigation we will use the so-called parabolic approximation for $\tilde{\Phi}_G(k)$ with "small" values of wave vector $\mathbf{k}$ and an averaged estimation in the short-wave region

$$\tilde{\Phi}(k) = \begin{cases} \Phi(0)(1-2b^2k^2), & \mathbf{k}\in\mathcal{B}_0 \\ \Phi_0 = \Phi(0)\bar{\Phi}, & \mathbf{k}\in\mathcal{B}\backslash\mathcal{B}_0. \end{cases} \qquad (5)$$

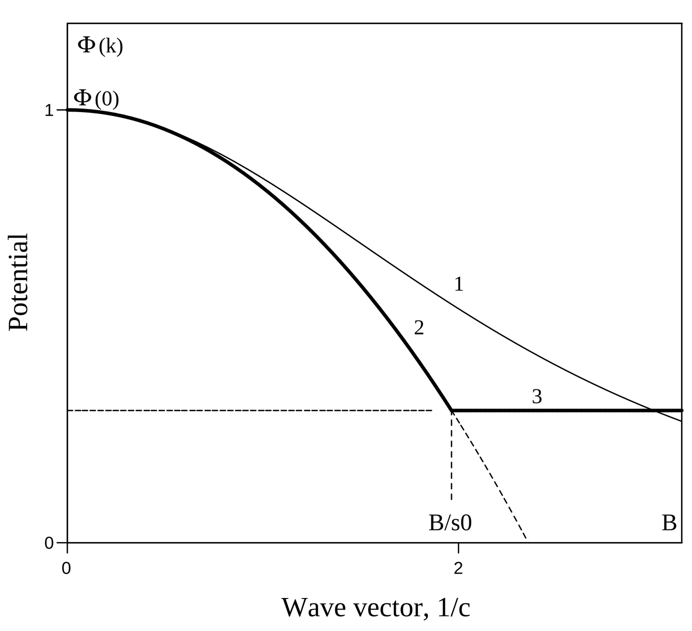

Figure 1: A sketch for the Fourier transform (4) **of the interaction potential** (3)**(Curve 1) and its parabolic approximation** (5) **(Curve 2). The curve 3 corresponds to** $\Phi_0 = \Phi(0)\bar{\Phi}$ **.**

In our calculations we will use the "ρ^4-model" approximation. The functional representation for the partition function in this approximation is as follows [2]

$$Z = Z_0\int (d\rho)^{N_0}\exp\Big[a_1\sqrt{N_0}\rho_0 - \frac{1}{2}\sum_{\mathbf{k}\in\mathcal{B}_0} d(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}} - \frac{a_4}{4!}N_0^{-1}\sum_{\mathbf{k}_i\in\mathcal{B}_0}\rho_{\mathbf{k}_1}\ldots\rho_{\mathbf{k}_4}\delta_{\mathbf{k}_1+\ldots+\mathbf{k}_4}\Big]. \qquad (6)$$

Computation of (6) is performed by using the Kadanoff's idea of constructing block lattices [3]. First, this calculations were realized by K.Wilson [4]. In our work we will use the CV method proposed by I.Yuchnovskii [2] and generalized to the case of an external field presence in [5]. Based on it, the step-by-step integration of the partition function over the layers of the CV phase space leads to the following expression

$$Z = Z_0\big[Q(d)\big]^{N_0}\Big(\prod_{n=1}^{n_p} Q_n\Big) Z_{LGR}. \qquad (7)$$

Here Z_0 is the partition function of non-interacting spins in external field, the quantity $Q(d)$ represents contribution of large values of the wave vector to the statistical sum, Q_n corresponds with the partial partition function of the n-th layer (or, in other words, the n-th block structure). Each Q_n is characterized by its own set of coefficients $d_n(k)$, $a_1^{(n)}$ and $a_4^{(n)}$. For them, recurrence relations take place with initial values from (6). One of solutions for the recurrence relations is the fixed point. In terms of variables

$$\omega_n = s^n a_1^{(n)}, \quad r_n = s^{2n}d_n(0), \quad u_n = s^{4n}a_4^{(n)} \qquad (8)$$

it takes the form

$$\omega^* = 0, \quad r^* = -f_0\beta\Phi(0), \quad u^* = \phi_0(\beta\Phi(0))^2 \qquad (9)$$

Last factor in (7) corresponds to the limit Gaussian regime (LGR) of the order parameter fluctuations in the case of $T > T_c$ (T_c is the critical temperature) or to the inverse Gaussian regime (IGR) when $T < T_c$. The explicit expression for Z_{LGR} is presented in [6] and for Z_{IGR} in [7] respectively.

The quantity n_p determines the number of iterations, which separates two regimes of the order parameter fluctuations: critical regime, where renormalization group symmetry held, and Gaussian regime. Therefore, the quantity n_p is referred to as the exit point.

When $n \le n_p$ the system possesses renormalization group (RG) symmetry and the solutions of RR can be written in the form of eigenvalue expansions

$$\begin{aligned} w_n &= s_0^{3/2}hE_1^n, \\ r_n &= r^* + c_1E_2^n + c_2RE_3^n, \\ u_n &= u^* + c_1R_1E_2^n + c_2E_3^n \end{aligned} \qquad (10)$$

where E_l are the eigen values of a matrix of RG transformation for the RR linearized near the fixed point (9) [5].

The free energy

The scheme for calculating the free energy of the system near T_c according to (7) is presented in [6] ($T > T_c$) and [7]($T < T_c$) in detail. Thus, here we present the final expressions.

$$F = F_a + F_s + F_0 \qquad (11)$$

The first term contains the analytical dependence on temperature and an external field. The next term in (11) represents non-analytical dependence of free energy on temperature and field

$$F_s = -k_BTN\gamma_s\left(\tilde{h}+h_c\right)^{\frac{d\nu}{\beta\delta}} \qquad (12)$$

The quantity γ_s includes contributions from the critical regime, from the so-called transition region and from limit (inverse) Gaussian regime. The quantities $\tilde{h}$ and h_c are the renormalized field ($\tilde{h} \sim |h|$) and temperature ($h_c \sim |\tau|^{\beta\delta}$ respectively. And β, ν and δ are the common notations for critical exponents. In our approach, they take on the following numerical values as $\beta = \nu/2 = 0.3025$, $\delta = d+2 = 5$, and $d = 3$ is the space dimension.

Finally, the last contribution to the free energy (11) comes from the final step of integrating the partition function. It corresponds to the system free energy contribution from the collective variable ρ_0, mean value of which is known to connect with the order parameter [2]. It has the form

$$F_0^{(\pm)} = -k_BTN\Big[e_0^{(\pm)}h(\tilde{h}+h_c)^{\frac{1}{\delta}} - e_2^{(\pm)}(\tilde{h}+h_c)^{\frac{d\nu}{\beta\delta}}\Big]. \qquad (13)$$

The order parameter

Expression for the model's magnetization as a function of temperature and field is derived by direct differentiation of F with respect to external field

$$M = -\frac{1}{N}\left(\frac{dF}{d\mathcal{H}}\right)_T. \qquad (14)$$

The result of calculation is reduced to the equation of state in the form

$$M = \sigma_{00}^{(\pm)}\left(\tilde{h}+h_c\right)^{\frac{1}{\delta}} \qquad (15)$$

Here the quantity σ_{00} is the explicit function of scaling variable $\alpha = h/\tau^{\beta\delta}$ [1]. This expression can be easily rewritten in more familiar form

$$M = h^{1/\delta}f_G(z). \qquad (16)$$

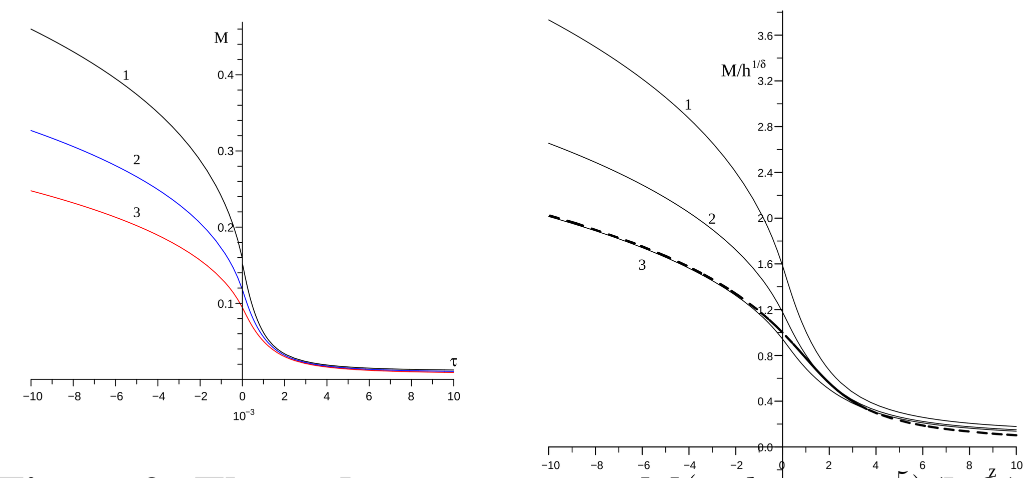

Figure 2: The order parameter $M(\tau, h = 10^{-5})$**(left) and its scaling function** $f_G(z)$**(right). 1 –** $b/c = 0.3$**, 2 –** $b/c = 0.4$**, 3 –** $b/c = 0.5$

Susceptibility

The system susceptibility are found by means of direct differentiation of the equation of state with respect to the external field h. The result one arrives at is

$$\frac{\chi}{\beta} = \chi_{00}^{(\pm)}(\tilde{h}+h_c)^{\frac{1}{\delta}-1} \qquad (17)$$

or, rewritten in more usual form

$$\frac{\chi}{\beta} = h^{1/\delta-1}f_\chi(z) \qquad (18)$$

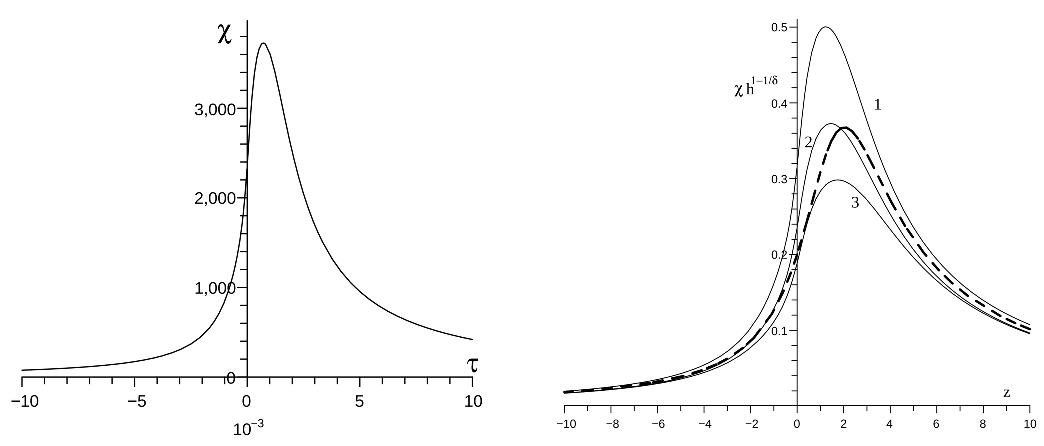

Figure 3: Susceptibility $\chi(\tau)$ **in constant external field** $h = 10^{-5}$ **at** $b/c = 0.4$**(left) and its scaling function** $f_\chi(z)$**(right) 1 –** $b/c = 0.3$**, 2 –** $b/c = 0.4$**, 3 –** $b/c = 0.5$

Summary

In the present work we investigate the 3D Ising-like model on a simple cubic lattice. The research is carried out using formalism of collective variables and in the framework of "ρ^4 – model" approximation. The critical exponent η is considered to be equal to zero. This approach also neglects corrections to scaling but main critical exponents take on non-classical values. However, we have obtained explicit expressions for physics quantities as functions of reduced temperature τ, external field h and microscopic parameters of model (the ratio of the effective range of interaction b to the lattice constant c). Namely, we have calculated free energy as well as the order parameter and susceptibility.

References

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