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METASTABLE HETEROPHASE SYSTEM OF THE ISING TYPE

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The role of grain-course fluctuations is known to be extremely important near phase-transition points. There are two kinds of such fluctuations: homophase (or homogeneous) and heterophase (or heterogeneous). The first kind can be investigated by several methods, for instance, by means of the renormalization-group technique [1] or the transfer-matrix approach.

The heterophase fluctuations can be described by the microscopic statistical method suggested in refs. [2-4] (see also [5]). This approach is based on the Bogolubov concept of quasiaverages [6], which being introduced by one of various manners [7], breaks the symmetry of a system and allows us to separate pure phases. Having recourse to the concept of partial spontaneous restoration of a broken symmetry [8] one can consider phase mixtures.

The description of possible states of a heterophase system, as it has been shown in [9], includes the description of metastable states too, when the free energy of a phase mixture is higher than, e.g., that of a pure state. The whole set of solutions corresponding to stable as well as to metastable states has been analyzed for the model of heterophase ferromagnet with long-range forces [10]. In this model, however, homophase fluctuations are absent at all, while it would be interesting to consider the case when they exist in the neighbourhood of heterophase ones. And it would be fine, of course, if an exact solution can be found in such a case.

The Ising model with a nearest-neighbour interaction, being generalized in order to include heterophase fluctuations and considered in two dimensions, satisfies the conditions mentioned. The heterophase generalization of the Ising model can be done by the known recipe [2-4]. The main question is either such a system is stable or becomes metastable; or, maybe, both the situations are possible depending on model parameters. The answer obtained in the present paper is as follows:

the heterophase two-dimensional Ising model with nearest-neighbour interactions can have only metastable states which occur in a wide region around the critical point.

We should mention that an attempt to describe metastable states for the two-dimensional Ising model has been undertaken by Schulman [11]. However, he has examined only pure states in finite volume, while the corresponding metastable states have disappeared in the thermodynamic limit. On the other hand, as

we know [9], metastable states in a heterophase system are able to survive when the thermodynamic limit is taken.

The Hamiltonian of a two-phase mixed system should be defined in the usual way [2-4], $H = \bigoplus_{p=1,2} H_p$, where p is the phase index, H_p acts on the space $\mathcal{F}_p$, and the total space of physical states is $\mathcal{F} = \bigotimes_{p=1,2} \mathcal{F}_p$. The probability of the system to be in a fixed-phase state is $w_p = N_p/N$, $N = N_1 + N_2$, where N_p is the average number of particles in the corresponding phase, N is the total number of particles. We use the notation $w \equiv w_1$, $w_2 \equiv 1 - w$. An equation for w can be derived from the condition of the heterophase equilibrium

$$\frac{\partial g}{\partial w} = 0, \quad g = -\frac{\Theta}{N} \ln \mathrm{Tr}\, e^{-\beta H}, \quad \beta\Theta \equiv 1. \tag{1}$$

The Ising model may be regarded as a limiting anisotropic case of the Heisenberg model. Thus, using the model of the heterophase ferromagnet [10], we have

$$H_p = N \frac{U}{2} w_p^2 - \frac{I}{2} w_p^2 \sum_{\langle ij \rangle} S_i S_j, \tag{2}$$

where the sum $\sum_{\langle ij \rangle}$ means the summation only over different nearest neighbours; $S_i = \pm 1$; U is a constant containing a combination of the direct interaction and the exchange one. The usual periodic conditions are assumed. We define the first phase as an ordered phase, whose vacuum corresponds to the configuration of spins all having the same sign. The second phase is interpreted as an absolutely disordered phase whose vacuum corresponds to the spin configuration for which each pair of neighbour sites have opposite spins [7]. Thus, the spontaneous magnetizations of the phases, M_p, are

$$M_1 \neq 0, \quad M_2 = 0. \tag{3}$$

The free energy of the mixture in the thermodynamic limit can be obtained by means of the transfer-matrix eigenvalues [12], since the maximum eigenvalue corresponds to the completely ordered phase, while the minimum eigenvalue to the disordered phase. For the square lattice we obtain

$$g = \frac{U}{2}\left[w^2 + (1-w)^2 \right] - \Theta(\Lambda_1 - \Lambda_2) - \Theta \ln(2 \sinh a_2),$$

where

$$\Lambda_p = \frac{1}{2\pi^2} \int_0^\pi d\nu \int_0^\pi d\nu' \ln\left[\cosh^2 a_p - (\cos\nu + \cos\nu') \sinh a_p \right], \quad a_p = \beta w_p^2 I.$$

Define $A \equiv \frac{U}{4I}$, $T \equiv \frac{\Theta}{4I}$. By means of (1) we get the equation for the phase probability $w = \frac{2A - B_2}{4A - B_1 - B_2}$, where

$$B_p \equiv [\frac{1}{2} + (-1)^{p+1} (\frac{\sinh \alpha_p - 1}{\sinh \alpha_p + 1}) K(\phi_p) \coth \alpha_p ,$$

$$K(\phi_p) \equiv \int_0^{\pi} \frac{d\nu}{(1 - \phi_p \sin^2 \nu)^{1/2}} , \qquad \phi_p \equiv \frac{8 \sinh \alpha_p \cdot \cosh^2 \alpha_p}{(1 + \sinh \alpha_p)^4} .$$

The spontaneous magnetization of the mixed system is

$$M = wL , \quad L = (1 - \frac{1}{\sinh^4 \alpha_1})^{1/8} . \qquad (4)$$

The specific heat per one lattice site is of the form

$$C_V = -2\beta^2 I [2A (X_2 - X_1) + X_1 Y_2 - X_2 Y_1]/[4A - (Y_1 + Y_2)] ,$$

where

$$X_p \equiv w_p^3 \{(-1)^p \frac{B_p}{\sinh 2\alpha_p} + \frac{\cosh^2 \alpha_p}{\sinh \alpha_p} [(-1)^{p+1} \frac{B_p \tanh \alpha_p - \frac{1}{2}}{\sinh^2 \alpha_p - 1} - \frac{4}{\pi} \cdot \frac{(\sinh \alpha_p - 1)^4}{(\sinh \alpha_p + 1)^6} \cdot \frac{dK(\phi_p)}{d\phi_p}]\} , \qquad Y_p \equiv B_p + \frac{\beta}{w_p} X_p (-1)^{p+1} .$$

To analyze the stability of the mixed system we must check the signs of two functions: $\frac{\partial^2 g}{\partial w^2}$ and $\Delta g = g(w) - g(1)$. We have

$$\frac{\partial^2 g}{\partial w^2} = 2I [4A - (Y_1 + Y_2)] ,$$

$$\Delta g = Aw (w - 1) - \Theta [\Lambda_2 - \Lambda_1 - \Lambda + \ln (2 \sinh \alpha_2)] ,$$

where

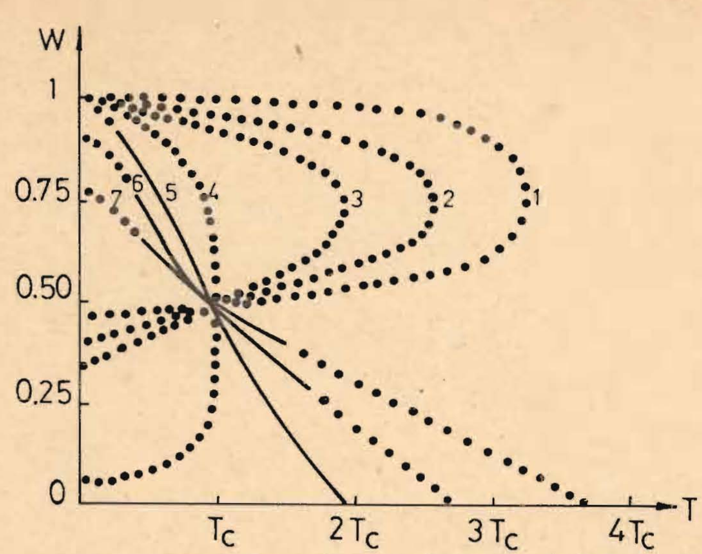
$$\Lambda \equiv \frac{1}{2\pi^2} \int_0^{\pi} d\nu \int_0^{\pi} d\nu' \ln [\cosh^2 (\beta I) - (\cos\nu + \cos\nu') \sinh (\beta I)] .$$

The specific entropy is

$$S = \Lambda_1 - \Lambda_2 + \ln (2 \sinh \alpha_2) - \frac{I}{\Theta} [wB_1 - 4A (1 - w)(w - \frac{1}{2})] .$$

The critical temperature is defined from (4) and is equal to

$$T_C = \frac{1}{16 \operatorname{arccosh} 1} . \qquad (5)$$



The temperature dependence of the probability of the ordered (ferromagnetic) phase in the heterophase system for $A = -3$ *(curve 1);* $A = -1.5$ *(curve 2);* $A = -1$ *(curve 3);* $A = -0.087$ *(curve 4);* $A = 0.5$ *(curve 5);* $A = 1.5$ *(curve 6);* $A = 3$ *(curve 7). Dotted lines correspond to unstable solutions; continuous ones, to metastable states.*

So, the critical temperature is four times as small as that in a pure Ising model. An expansion of L in powers of $\epsilon \equiv \frac{\beta_C}{\beta} - 1$ yields

$$L \simeq Q^{1/8} (-\epsilon)^{1/8} |\ln (-\epsilon)|^{1/8} , \qquad Q \equiv \frac{4\sqrt{2} (\operatorname{arcsinh} 1)^2}{\pi (A + 0.087)} .$$

The specific heat diverges for $T \to T_C$ as

$$C_V \simeq \frac{8 (\operatorname{arcsinh} 1)^3}{\pi (A + 0.087)} \ln^2 (-\epsilon) .$$

The behaviour of the phase probability w obtained by numerical calculations at all temperatures is presented in the Figure. The unphysical solutions, for which either the specific heat is negative or the specific entropy diverges at low temperatures, are depucted by dotted lines. The continuous lines describe the metastable states for which $C_V > 0$. These solutions exist only if $A > 0.5$. The absolutely stable solution corresponds to the pure phase with $w \equiv 1$. This is because the free energy of the heterophase system is always higher than that one of the pure system. The transition from a metastable branch to the stable one (or the inverse procedure) occurs at the nucleation point. The nucleation here is the first-order phase transition. Note also that some of metastable heterophase states can have a negative entropy in analogy with the property of metastable states in the replica-symmetric Sherrington-Kirkpatrick spin-glass model /13,14/.

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Метастабильная гетерофазная система изинговского типа

Предложена модифицированная модель Изинга, которая позволяет рассматривать метастабильные состояния, соответствующие частично упорядоченной и частично разупорядоченной системе. Термодинамика такой системы для случая квадратной решетки исследована точно, что удается сделать, используя метод трансфер-матрицы.

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