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METASTABLE STATES IN MODIFIED ISING MODEL

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INTRODUCTION

The problem of theoretical investigation of metastable states attracts a great interest in recent years. These states may be treated in the kinetical theory as nonequilibrium states having very long lifetimes[1-4]. The statistical equilibrium treatment is permissible too, as far as it is applicable to all kinds of equilibrium states, whether stable, metastable or unstable[5,6]. The renormalization-group approach for describing the metastability has been formulated in ref.[7]. A detailed review dedicated to mathematical problems concerning the metastability has been given by Sewell[8]. As has been cleared up, thermodynamic functions of metastable states might be considered as analytical continuations of the corresponding functions for absolutely stable states[8,9]. This idea has been efficiently analysed by Schulman and colleagues[10,11]. One of the main problems when dealing with metastable states is the behaviour of their probabilities or lifetimes in the thermodynamic limit. This has been investigated for some classical models in ref.[12] and for the two-dimensional Ising model with nearest-neighbour interactions in refs.[13,14]. As has been discovered[13,14], the lifetimes of metastable states and their probabilities as well tend to zero when $N \to \infty$. That is, the thermodynamic limit destroys metastable states. The same result has been obtained[15] for the droplet model[16,17]. However, there exists a class of the so-called heterophase models[18-20] that can possess metastable states even in the thermodynamic limit. In these models heterophase fluctuations are stabilized by the existence of a disordering interaction[21]. For example, a modification of the long-range ferromagnetic Heisenberg model, taking into account coexisting ferro- and paramagnetic states has been analysed in refs.[22,23]. And it has been shown that this heterophase system in the thermodynamic limit does have metastable states whose presence depends on the relation between the values of ordering (exchange) and disordering (direct) interactions.

In the present paper we generalize the Ising model with the nearest-neighbour interactions so that it could include heterophase states. This case is of special interest, since Ising model proponents claim it to be a paradigm for all phase transitions (well may be not all, but many). We find exact solutions for the two-dimensional heterophase Ising model. Analysing these solutions we come to the conclusion that heterophase states in our model are either metastable or unstable.

Such a result is in agreement with inferences of the investigation of heterophase fluctuations in the Ising model when limited Gibbs distributions /24/ have been used.

The structure of the paper is as follows. In Section 1 the heterophase modification of the Ising model is formulated. Section 2 is devoted to the Bragg-Williams approximation for a two-dimensional model. Exact solutions for the nearest-neighbour interaction are obtained in Section 3. A brief discussion of results is given in the Conclusion.

1. HETEROPHASE MODIFICATION OF THE ISING MODEL

When constructing theory of pure thermodynamic phases of macroscopically degenerated systems one should invoke the Bogolubov /25,26/ concept of quasi-averages. And phase mixtures can be considered by using the concept of the spontaneous restoration of a broken symmetry /27/.

The Hamiltonian of a two-phase mixture is of the form

$$H = \bigoplus_{p=1,2} H_p , \tag{1.1}$$

where H_p are defined on the spaces of states $\mathcal{F}_p$,

$$H_p \mathcal{F}_p = \mathcal{F}_p \qquad (p=1,2). \tag{1.2}$$

The total space of states of a mixture is

$$\mathcal{F} = \bigotimes_{p=1,2} \mathcal{F}_p . \tag{1.3}$$

The probability of a fixed phase is defined as

$$w_p = N_p/N \qquad (N = N_1 + N_2), \tag{1.4}$$

where N_p is the mean number of particles in the corresponding phase, N is the total number of particles. Taking into account a natural normalization condition

$$w_1 + w_2 = 1, \tag{1.5}$$

we put $w \equiv w_1$, $w_2 = 1 - w$.

One can obtain the equation for the phase probability w from the condition of the heterophase equilibrium

$$\frac{\partial g}{\partial w} = 0, \quad g = -\frac{\Theta}{N}\cdot \ln \mathrm{Tr}\, e^{-\beta H} \qquad (\beta\cdot\Theta = 1). \tag{1.6}$$

From (1.1) and (1.3) we obtain for the free energy of the two-phase mixture

$$g = \sum_{p=1,2} g_p . \tag{1.7}$$

The Ising model can be considered as a limiting case of a strong anisotropy in the Heisenberg model. So, in analogy with the model of a heterophase ferromagnet /22,23/, we have

$$H_p = N\cdot\frac{U}{2}\cdot w_p^2 - \frac{I}{2}\cdot w_p^2 \cdot \sum_{<i,j>} \sigma_i \cdot \sigma_j - h\cdot w_p \cdot \sum_i \sigma_i , \tag{1.8}$$

where $\sum_{<i,j>}$ denotes the summation over nearest neighbours; $\sigma_i = \pm 1$; the constant U is expressed through the matrix elements of the two-particle interaction over Wannier functions /22/:

$$U = \sum_{i,j} (<i,j|\Phi|j,i> - \frac{1}{2} <i,j|\Phi|i,j>).$$

Here the first term corresponds to the direct interaction; and the second one,to the exchange interaction /22/; h is the external magnetic field. The usual periodic conditions are assumed. The first phase is interpreted as an ordered phase. The space of states $\mathcal{F}_1$ has the vacuum state described by the completely ordered configuration of parallel spins. The spontaneous magnetization of this phase

$$M_1 = -\lim_{h\to 0} \frac{\partial g_1}{\partial h} = w_1 \cdot \frac{1}{N}\cdot \sum_i <\sigma_i>_1 \tag{1.9}$$

should be nonzero below the Curie point. The second phase is completely disordered, so that when $h=0$, then the space of physical states $\mathcal{F}_2$ has the vacuum corresponding to the spin configuration, in which each cluster of neighbours has zero magnetization /29/. Thus, the total magnetization of this phase M_2 satisfies the condition

$$\lim_{h\to 0} M_2 = 0. \tag{1.10}$$

2. BRAGG-WILLIAMS APPROXIMATION

Let us first try the Bragg-Williams approximation for the model defined. This approximation is a version of the mean-field theory, which, as is known, gives exact results for the infinitely long-range interaction.

In the Bragg-Williams approximation one gets for the magnetization

$$M_p = w_p \cdot \tanh(z_0 \cdot \beta \cdot I \cdot w_p \cdot M_p/2), \tag{2.1}$$

where z_0 is the number of the nearest neighbours. The non-trivial solution of this equation corresponds to the ordered phase; and the trivial one, to the disordered phase. So, the total spontaneous magnetization is

$$M = \sum_{p=1,2} M_p = M_1 = wL, \qquad L = \tanh(z_0 \cdot \beta I w^2 L/2). \tag{2.2}$$

The free energy takes the form

$$g = \frac{U}{2} \cdot [\, w^2 + (1-w)^2 \,] + \frac{1}{4} \cdot z_0 \cdot I \cdot w^2 L^2 - \frac{1}{2\beta} \cdot \ln(\frac{1-L^2}{4}). \tag{2.3}$$

For simplicity we use the following notations:

$$A = \frac{U}{z_0 \cdot I}, \qquad T = \frac{\Theta}{z_0 \cdot I}.$$

The equation (1.6) allows us to obtain the probability of the ordered (ferromagnetic) phase

$$w = \frac{2A}{(4A - L^2)}, \qquad (A \neq 0). \tag{2.4}$$

The correct solution for w is to be selected in the following manner. By definition (1.4) we have $0 \leq w \leq 1$. Besides that the heterophase system is stable, when the second derivative

$$\frac{\partial^2 g}{\partial w^2} = \frac{1}{2} z_0 I \cdot \{\, 4A - L^2 \cdot [\, \frac{2T + 3w^2(1-L^2)}{2T - w^2(1-L^2)} \,] \,\} \tag{2.5}$$

is positive.

In accordance with (2.4) the heterophase states exist above the nucleation temperature

$$T_h = \frac{\sqrt{2A}}{2 \cdot \mathrm{artanh}(\sqrt{2A})}.$$

For $A=0$ the nucleation point coincides with the critical one, and in this case one returns to the standard Ising model.

At low temperatures ($T \ll 1$) we have

$$L \simeq 1 - 2 \cdot \exp[-\frac{4A^2}{T \cdot (4A-1)^2}], \quad w \simeq \frac{2A}{(4A-1)}\{1 - \frac{4}{(4A-1)} \cdot \exp[-\frac{4A^2}{T(4A-1)^2}]\},$$

if $A \leq 0$ or $A \geq 1/2$. Substituting this into (2.5), we see that the system with heterophase fluctuations is stable for $A > 1/2$. In other cases, when the solution (2.4) does not minimize the free energy $g\{w\}$ we must compare two possibilities: $w = 1$ and $w = 0$. It is easy to obtain that

$$g\{w=1\} \leq g\{w=0\} \qquad (0 \leq A \leq 1/2, \; T=0).$$

The specific heat may be written as

$$C_v = \frac{A \cdot w^4 \cdot L^2 \cdot (1-L^2)}{2T \cdot [\, 2AT - w^2(1-L^2)(A + 2wL^2)\,]};$$

in the low temperature region $C_v > 0$ and $C_v \to 0$ when $T \to 0$ for all values of the parameter A. The specific entropy of the heterophase system at zero temperature is equal to $\ln 2$.

The critical temperature obtained from the condition $L=0$ is $T_c = 1/8$, $w(T_c) = 1/2$.

So, the critical temperature for the heterophase model is four times as less as that for the pure model.

The expression (2.5) at the critical point $T_c = 1/8$ is positive for $A > 1.5$. In addition $g\{w=1/2\} < g\{w=0\}$ $(A > 0, \; T = T_c)$. Expanding (2.2) in powers of $\epsilon \equiv T/T_c - 1$ we have

$$L \simeq \begin{cases} (\frac{6A}{2A-3})^{1/2} \cdot (-\epsilon)^{1/2}, & A \neq 1.5 \\ 1.712 \cdot (-\epsilon)^{1/4}, & A = 1.5. \end{cases} \tag{2.6}$$

For the phase concentration w in the critical region we obtain

$$w \simeq \begin{cases} \frac{1}{2} + \frac{3}{4(2A-3)} \cdot (-\epsilon), & A \neq 1.5 \\ \frac{1}{2} + 0.244\,(-\epsilon)^{1/2}, & A = 1.5. \end{cases} \tag{2.7}$$

The specific heat at the critical point is equal to

$$C_v = \frac{3A}{(2A-3)}. \tag{2.8}$$

This expression coincides with the specific-heat leap for the pure model in the limit $A \to \pm\infty$.

Equations (2.6)-(2.8) show that the phase transition in the heterophase system is the second-order one for $A < 0$ and $A > 1.5$. Negative values of A corresponds to metastable states. If $0 < A \leq 1.5$, the phase transition is of first order, and all expansions in powers of ϵ become invalid.

3. EXACT SOLUTION

Let us find exact solutions for the modified Ising model with heterophase fluctuations in zero field. For doing this we use eigenvalues of the transfer-matrix calculated by Onsager [30]. The maximum eigenvalue corresponds to completely ordered phase; while minimum eigenvalue, to disordered phase. So, we have

$$g_p = \frac{U}{2} \cdot w_p^2 - \frac{\Theta}{2} \cdot \ln(2\sinh \alpha_p) - \Theta \cdot \Lambda_p , \tag{3.1}$$

where $\alpha_p = \beta \cdot w_p^2 \cdot I$, $\Lambda_p = \frac{1}{2\pi} \int_0^{\pi} \gamma_p(\nu)\, d\nu$, and the functions $\gamma_p(\nu)$ are defined by the equation $\cosh \gamma_p(\nu) = \cosh \alpha_p \cdot \coth \alpha_p - \cos\nu$. Here the positive solution is denoted as $\gamma_1(\nu)$; and the negative one, as $\gamma_2(\nu)$. The latter equation can be transformed to the form

$$\gamma_p(\nu) = (-1)^{p+1} \cdot \{ \ln 2 - \ln(\sinh \alpha_p) + \frac{1}{\pi} \int_0^{\pi} d\nu' \cdot \ln[\cosh^2\alpha_p - (\cos\nu + \cos\nu') \cdot \sinh \alpha_p]\}.$$

Therefore, we have for the free energy

$$g = \frac{U}{2} \cdot [w^2 + (1-w)^2] - \Theta \cdot (Q_1 - Q_2) - \Theta \cdot \ln(2\sinh \alpha_2), \tag{3.2}$$

where $Q_p = \frac{1}{2\pi^2} \cdot \int_0^{\pi} d\nu \int_0^{\pi} d\nu' \cdot \ln[\cosh^2\alpha_p - (\cos\nu - \cos\nu') \cdot \sinh \alpha_p]$.

In accordance with the condition (1.6) we obtain the equation for the definition of the phase concentration w:

$$w = \left(\frac{2A - B_2}{4A - B_1 - B_2} \right), \tag{3.3}$$

where $B_p = \frac{2}{z_0 N} \cdot \sum_{\langle i,j \rangle} \langle \sigma_i \sigma_j \rangle_p$.

Differentiating (3.2), we find

$$B_p = [\frac{1}{2} + (-1)^{p+1} \cdot \frac{1}{\pi} \cdot \left(\frac{\sinh \alpha_p - 1}{\sinh \alpha_p + 1} \right) K(\phi_p)] \cdot \coth \alpha_p ;$$

here $K(\phi) = \int_0^{\pi} \frac{d\nu}{(1 - \phi \cdot \sin^2\nu)^{1/2}}$ is the full elliptic integral of the first kind [31] and $\phi_p \equiv \frac{8 \sinh \alpha_p \cdot \cosh^2 \alpha_p}{(1 + \sinh \alpha_p)^4}$.

The spontaneous magnetization in the pure Ising model on the square lattice was calculated by Yang [32]. Using this result

for our model we obtain

$$M = wL, \quad L = \left(1 - \frac{1}{\sinh^4 \alpha_1}\right)^{1/8}. \tag{3.4}$$

The specific heat has the form

$$C_v = -2\beta^2 \cdot I^2 \cdot \left\{ \frac{2A(X_2 - X_1) + X_1 \cdot Y_2 - X_2 \cdot Y_1}{4A - (Y_1 + Y_2)} \right\}, \tag{3.5}$$

where

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

To check the stability of the system, we need to verify the positiveness of the derivative

$$\frac{\partial^2 g}{\partial w^2} = 2I \cdot [4A - (Y_1 + Y_2)], \tag{3.6}$$

and also the sign of the function $\Delta g = g\{w\} - g\{w=1\}$, for which we have

$$\Delta g = U \cdot w(w-1) - \Theta \cdot [Q_1 - Q_2 - Q + \ln(2\sinh \alpha_2)], \tag{3.7}$$

where $Q = \frac{1}{2\pi^2} \cdot \int_0^{\pi} d\nu \int_0^{\pi} d\nu' \ln[\cosh^2\alpha - (\cos\nu + \cos\nu') \sinh \alpha]$; $\alpha \equiv \beta I$.

Finally, the specific entropy of the hybrid system is equal to

$$S = Q_1 - Q_2 + \ln(2\sinh \alpha_2) - \beta I \cdot [w B_1 - 4A(1-w)(w - \frac{1}{2})]. \tag{3.8}$$

The critical temperature T_c defined by the condition L=0

$$T_c = \frac{1}{16a}, \quad a = \operatorname{arsinh} 1. \tag{3.9}$$

This is four times as less as the critical temperature for the corresponding pure model.

The expansion of the order parameter L in powers ϵ differs from the corresponding expansion for the usual Ising model where $L \sim (-\epsilon)^{1/8}$. In the model with heterophase fluctuations we have

$$L \simeq \xi^{1/8} \cdot (-\epsilon)^{1/8} \cdot [\ln(-\epsilon)]^{1/8}, \quad \xi = \frac{4\sqrt{2}\cdot a^2}{\pi\cdot(A+0.087)}. \tag{3.10}$$

For the phase concentration w in the critical region we obtain

$$w \simeq \frac{1}{2} + \frac{a}{4\pi(A+0.087)} \cdot (-\epsilon)\ln(-\epsilon). \tag{3.11}$$

When approaching the critical point the specific heat diverges stronger than in the pure model:

$$C_v \simeq \frac{8a^3}{\pi^2 (A+0.087)} \cdot [\ln(-\epsilon)]^2. \tag{3.12}$$

Let us remind that in the usual case $C_v \sim \ln(-\epsilon)$.

In the low-temperature region the phase concentration has two branches of solutions, whose asymptotic forms (see fig.1) are

$$w \simeq \frac{2A}{(4A-1)} \cdot \left\{1 - \frac{(2A-1)}{A(4A-1)} \cdot e^{-\frac{1}{2T}\left(\frac{2A-1}{4A-1}\right)^2} - \frac{4}{(4A-1)} \cdot e^{-\frac{1}{T}\left(\frac{2A}{4A-1}\right)^2}\right\},$$

$$w \simeq 1 + \frac{1}{2(2A-1)} \cdot T \qquad (T \ll 1). \tag{3.13}$$

The numerical solution of (3.3) at all temperatures for various values of the parameter A is depicted in fig.1, the behaviour of the specific heat is shown in fig.2. The unphysical solutions (for which either the specific heat is negative, or the specific entropy diverges in the low-temperature region) are depicted by dotted lines. The continuous line describes the solutions for which $C_v > 0$. These solutions exist only for $A \geq 0.5$.

The numerical analysis of expressions (3-6) and (3.7) shows that the free energy of the heterophase system is always higher than that of the pure Ising model. Consequently, the states labelled in pictures by continuous lines are metastable. The transition from a metastable heterophase branch to the stable pure state is the nucleation which is here the first-order phase transition. Note that some metastable heterophase states can have a negative entropy. This is analogous to the case of the low-temperature Sherrington-Kirckpatrick spin glass [33,34].

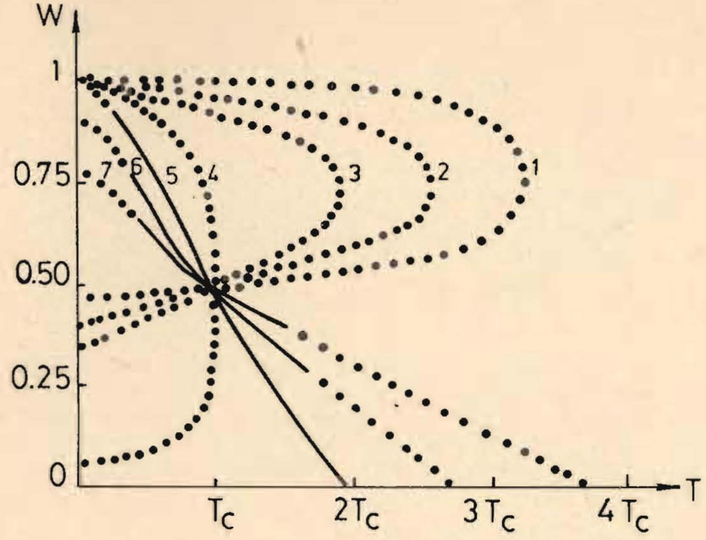

Fig.1. Temperature dependence of the phase concentration for the values of A = − 3 *(curve 1);* A = −1.5 *(curve 2);* A = −1 *(curve 3);* A = −0.087 *(curve 4);* A = 0.5 *(curve 5);* A = 1.5 *(curve 6);* A = 3 *(curve 7).*

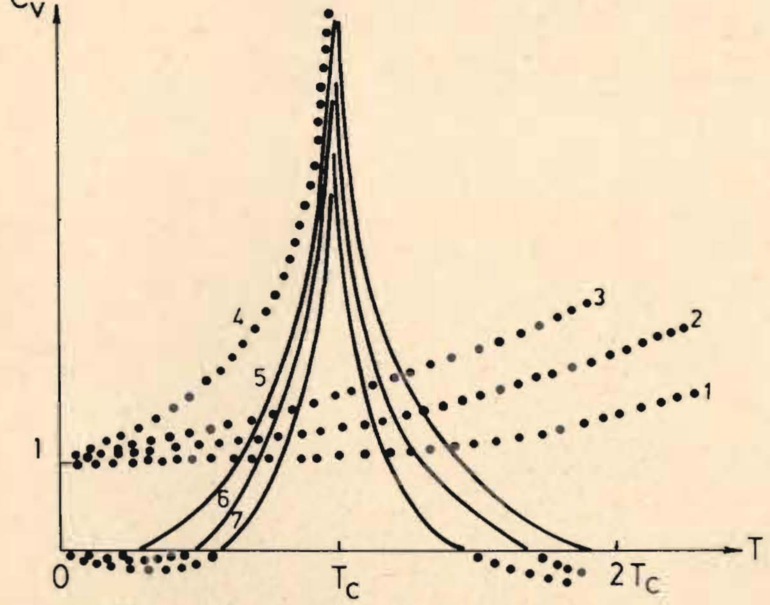

Fig.2. Specific heat as a function of temperature; the values of A *are the same as in fig.1.*

CONCLUSION

The two-dimensional Ising model with heterophase states is an example of the system in which metastable states survive after the thermodynamic limit. This is due to the presence of the direct interaction besides the exchange one. The comparison of the results of Section 3 (the short-range model) and the results of Section 2 (the long-range approximation) shows that the thermodynamic behaviour of heterophase systems strongly depends on the kind of interaction, the long- or short-range one. The increasing range of the interaction stabilizes heterophase states.

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E17-85-237

Метастабильные состояния
в модифицированной модели Изинга

Предлагается модификация модели Изинга, в которой возможны гетерофазные состояния. Дано ее точное в термодинамическом пределе решение для двумерной решетки в нулевом поле с взаимодействием ближайших соседей. Показано, что такая система всегда является либо метастабильной, либо нестабильной. Рассмотрены изменения в термодинамическом поведении при переходе к дальнодействующему взаимодействию.

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Metastable States
in Modified Ising Model

A modification of the Ising model is proposed when heterophase states are possible. An exact solution in the thermodynamic limit for the two-dimensional zero-field lattice with the nearest-neighbour interaction is given. It is shown that this system is either metastable or unstable. The change in the thermodynamic behaviour due to the transition to the long-range interaction is considered.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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