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MODEL OF ANTIFERROMAGNET WITH HETEROPHASE FLUCTUATIONS

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The model of an antiferromagnet with paramagnetic nuclei is considered. The behaviour of phase probabilities is analysed especially near zero temperature and Neel temperature. Stability conditions show when such an antiferromagnet with paramagnetic fluctuational nuclei is stable, metastable or unstable. The specific heat in the vicinity of the critical point is also analyzed. The presence of heterophase fluctuations can lead to the change of phase transition order from second to first; the criteria for this change are found and discussed.

1. Introduction

A number of recent experiments have shown that many magnetic materials should be regarded as mixtures of competing phases. For example, polarization-analysis measurements of the intermetallic compound $Pd_{1.4}Cu_{0.6}MnIn$ have proved that this compound is largely ferromagnetic with the remainder of antiferromagnetic type$^{1)}$. Nuclear magnetic resonance methods$^{2)}$ and Mössbauer methods$^{3)}$ are especially fruitful for distinguishing different phases in magnetic materials. So, the NMR study of $CoTi_{1-x}Al_x$ and $CoTi_{1-x}Ga_x$ has clearly demonstrated that

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in these materials there exists Co with ferromagnetic and paramagnetic properties; the concentration of the so-called ferromagnetic Co changing under variations of the temperature and applied magnetic field[4]. The Mössbauer study has been used to define the content of paramagnetic phase as a function of the temperature in $KFeS_2$[5], that is an amorphous antiferromagnet[6]. Neutron-scattering methods[7,8] are also quite useful for determining magnetic structures of polyphase substances. For instance, neutron-diffraction measurements of polycrystals of $NiS_{2-x}Se_x$ and NiS_2 have argued that in these materials there coexist weak ferromagnetism and antiferromagnetism[9]. A list of other examples of magnetic phase mixtures can be continued[10].

A general approach for describing heterophase systems has been constructed in Refs. 11—15. This approach has been applied to mixtures of several types: crystal — liquid[16–18], superconductor — normal conductor[19] and ferromagnet — paramagnet[20–22].

In this paper we consider the mixture of antiferromagnetic and paramagnetic states, which can coexist in some materials. A simplified model for such a mixture was suggested earlier[23], where only the interaction between sublattices was taken into account, and the interaction of particles inside each sublattice was neglected. Here we investigate in detail a more general case, taking into consideration all interactions.

2. *General model*

The Hamiltonian of the model can be written as follows:

$$H = \bigoplus_{i=1}^{2} \Big\{ N \left[\frac{A_1}{2} w_1^{(i)2} + \frac{A_2}{2} w_2^{(i)2} + A w_1^{(i)} w_2^{(i)} \right] -$$

$$- w_1^{(i)2} \sum_{f,f'} J_1 (f - f') \vec{S}_f^{(i)} \vec{S}_{f'}^{(i)} - w_2^{(i)2} \sum_{g,g'} J_2 (g - g') \vec{S}_g^{(i)} \vec{S}_{g'}^{(i)} +$$

$$+ 2 w_1^{(i)} w_2^{(i)} \sum_{f,g} J (f - g) \vec{S}_f^{(i)} \vec{S}_g^{(i)} \Big\}, \tag{1}$$

where $i = 1$ corresponds to the ordered phase ($\langle \vec{S}_h^{(1)} \rangle \neq 0$, $h = f, g$ for the values of temperature below the critical point), $i = 2$ — to the nonordered phase ($\langle \vec{S}_h^{(2)} \rangle = 0$ for all temperatures); $w_j^{(i)}$ are the phase probabilities (i. e. concentrations), index j numbers the sublattices, the sites in the first sublattice are denoted by f, in the second by g; $\vec{S}_f$ is the vector of spin localized in the site f of the 1-st sublattice (analogously $\vec{S}_g$ is the vector of spin localized in the site g of the 2-nd sublattice), the values of spin are equal to S_1 and S_2, respectively and not obligatory to each other; $J_1 (f - f')$, $J_2 (g - g')$, $J (f - g)$ are exchange interactions in the sublattices and between them, all $J(\cdot)$ are positive for all values of arguments; A_1, A_2, A are constants corresponding to each sublattice and to the interaction between sublattices and connected with the effective direct and exchange interactions in the usual way:

$$A_j = \Phi_j - \frac{J_j}{2}; \; \Phi_j = \frac{1}{N} \sum_{h,h'} \langle h, h' | \Phi(\cdot) | h', h \rangle; \; J_j = \frac{1}{N} \sum_{h,h'} \langle h, h' | \Phi(\cdot) | h, h' \rangle;$$

$|h, h'\rangle$ is the product of Wannier functions $|h\rangle|h'\rangle$ and $h, h' = f, f'$; g, g'; or f, g; $\Phi(\cdot)$ is the potential of a two-particle interaction; N is the number of sites in each sublattice (in this way the sublattices are equivalent).

Let us consider now the thermodynamical properties of the system described by the Hamiltonian (1) in the molecular field approximation. This consideration gives us the possibility to see the main characteristic features of the system. The free energy per site of the system in this approximation can be written as follows:

$$\begin{aligned} f = \frac{F}{2N} = {} & \frac{A_1}{2}\left(w_1^2 - w_1 + \frac{1}{2}\right) + \frac{A_2}{2}\left(w_2^2 - w_2 + \frac{1}{2}\right) + \\ & + A\left(w_1 w_2 - \frac{w_1}{2} - \frac{w_2}{2} + \frac{1}{2}\right) + \frac{1}{2}(J_1 w_1^2 + J w_1 w_2) C_1^2 + \\ & + \frac{1}{2}(J_2 w_2^2 + J w_1 w_2) C_2^2 - \frac{1}{2} J w_1 w_2 C^2 - \\ & - \frac{1}{2}\Theta \ln\left(\frac{\operatorname{sh} \frac{2S_1 + 1}{2S_1} x_1}{\operatorname{sh} \frac{1}{2S_2} x_1}\right) - \frac{1}{2}\Theta \ln\left(\frac{\operatorname{sh} \frac{2S_2 + 1}{2S_2} x_2}{\operatorname{sh} \frac{1}{2S_2} x_2}\right) - \\ & - \frac{1}{2}\Theta \ln(2S_1 + 1) - \frac{1}{2}\Theta \ln(2S_2 + 1), \end{aligned} \tag{2}$$

where

$$w_j = w_j^{(1)} \; (w_j^{(2)} = 1 - w_j^{(1)}),$$

$$J_1 = \frac{1}{N} \sum_{f,f'} J_1(f - f'), \; J_2 = \frac{1}{N} \sum_{g,g'} J_2(g - g'), \; J = \frac{1}{N} \sum_{f,g} J(f - g),$$

$$x_k = \frac{2}{\Theta} S_k \left| J_k w_k^2 \vec{C}_k + J w_1 w_2 \vec{C}_k - J w_1 w_2 \vec{C} \right|,$$

C_1, C_2, C are variational parameters.

To obtain self-consistent equations, defining C_1, C_2, C and the phase probabilities w_1, w_2, we must minimize the free energy (2) using the minimax principle[24]. As a result, we obtain for the order parameters the following equations

$$\begin{aligned} \vec{C} &= \vec{C}_1 + \vec{C}_2, \\ C_1 &= S_1 B_{S_1}(x_1), \quad C_1 = |\vec{C}_1|, \\ C_2 &= S_2 B_{S_2}(x_2), \quad C_2 = |\vec{C}_2|, \end{aligned} \tag{3}$$

where $B_S(x)$ is the Brillouin function for the spin S

$$B_S(x) = \frac{2S+1}{2S} \operatorname{cth} \frac{2S+1}{2S} x - \frac{1}{2S} \operatorname{cth} \frac{1}{2S} x;$$

vectors $\vec{C}_1$ and $\vec{C}_2$ are antiparallel; to underline this fact, we change in (3) C_2 by $-C_2$, thus meaning later on that C_2 is negative. Ultimately we have:

$$f = \frac{A_1}{2}\left(w_1^2 - w_1 + \frac{1}{2}\right) + \frac{A_2}{2}\left(w_2^2 - w_2 + \frac{1}{2}\right) + A\left(w_1 w_2 - \frac{w_1}{2} - \frac{w_2}{2} + \right.$$
$$\left. + \frac{1}{2}\right) + \frac{1}{2} J_1 w_1^2 C_1^2 + \frac{1}{2} J_2 w_2^2 C_2^2 - J w_1 w_2 C_1 C_2 -$$
$$- \frac{1}{2} \Theta \ln \left(\frac{\operatorname{sh} \frac{2S_1+1}{2S_1} x_1}{\operatorname{sh} \frac{1}{2S_1} x_1} \right) - \frac{1}{2} \Theta \ln \left(\frac{\operatorname{sh} \frac{2S_2+1}{2S_2} x_2}{\operatorname{sh} \frac{1}{2S_2} x_2} \right) - \tag{4}$$
$$- \frac{1}{2} \Theta \ln (2S_1 + 1) - \frac{1}{2} \Theta \ln (2S_2 + 1),$$

$$C_1 = S_1 B_{s_1}(x_1), \quad x_1 = \frac{2}{\Theta} S_1 (J_1 w_1^2 C_1 - J w_1 w_2 C_2),$$
$$C_2 = S_2 B_{s_2}(x_2), \quad x_2 = \frac{2}{\Theta} S_2 (J_2 w_2^2 C_2 - J w_1 w_2 C_1). \tag{5}$$

The order parameters C_1 and C_2 are the mean values of spin in the sites of corresponding sublattices and are connected with the corresponding magnetizations by the relations

$$\vec{M}_j = w_j \vec{C}_j \quad (j = 1, 2). \tag{6}$$

The orientation of the antiferromagnetism vector $\vec{M} = \vec{M}_1 - \vec{M}_2$ in the absence of an external magnetic field is arbitrary.

For the phase probabilities in the approximation considered the following equations can be obtained:

$$w_1 = \frac{1}{2} \frac{(A_1 A_2 - A^2) - J_2 (A_1 + A) C_2^2 - J (A_2 + A) C_1 C_2}{(A_1 A_2 - A^2) - (J_1 A_2 C_1^2 + 2JAC_1 C_2 + J_2 A_1 C_2^2) + (J_1 J_2 - J^2) C_1^2 C_2^2},$$
$$w_2 = \frac{1}{2} \frac{(A_1 A_2 - A^2) - J_1 (A_2 + A) C_1^2 - J (A_1 + A) C_1 C_2}{(A_1 A_2 - A^2) - (J_1 A_2 C_1^2 + 2JAC_1 C_2 + J_2 A_1 C_2^2) + (J_1 J_2 - J^2) C_1^2 C_2^2}. \tag{7}$$

As the temperature approaches the Neel point ($\Theta \to \Theta_N$), for the case of the 2-nd order phase transition $C_1 \to 0$, $C_2 \to 0$ and, correspondingly, $w_1 \to \frac{1}{2}$, $w_2 \to \to \frac{1}{2}$. Using the expansion series of the Brillouin function at the point $x = 0$, we have

$$C_1 = S_1 B_{S_1}(x_1) \approx \frac{S_1(S_1+1)}{6\Theta_N}(J_1 C_1 - J C_2),$$

$$C_2 = S_2 B_{S_2}(x_2) \approx \frac{S_2(S_2+1)}{6\Theta_N}(J_2 C_2 - J C_1).$$

As was underlined above, $C_1 > 0$, $C_2 < 0$. Let us introduce the notation

$$\tau_j = \frac{S_j(S_j+1)}{12} \qquad (j = 1, 2),$$

$$\varrho = \lim_{\Theta \to \Theta_N} \frac{C_2}{C_1}.$$

Then for the determination of Θ_N, ϱ we have the following system of equations:

$$\Theta_N - 2\tau_1 J_1 + 2\varrho\tau_1 J = 0,$$

$$\varrho\Theta_N - 2\varrho\tau_2 J_2 + 2\tau_2 J = 0,$$

and consequently the equation for ϱ

$$\tau_1 J \varrho^2 - (\tau_1 J_1 - \tau_2 J_2)\varrho - \tau_2 J = 0.$$

Of the two roots of this equation we should choose, naturally, only the negative one, since vectors $\vec{C}_1$ and $\vec{C}_2$ are antiparallel (the positive root corresponds to the maximum of the free energy). So, we have

$$\varrho = \frac{\tau_1 J_1 - \tau_2 J_2 - [(\tau_1 J_1 - \tau_2 J_2)^2 + 4\tau_1\tau_2 J^2]^{\frac{1}{2}}}{2\tau_1 J},$$

and, correspondingly, the expression for the critical point

$$\Theta_N = \tau_1 J_1 + \tau_2 J_2 + [(\tau_1 J_1 - \tau_2 J_2)^2 + 4\tau_1\tau_2 J^2]^{\frac{1}{2}} > 0. \tag{8}$$

Let us now consider the properties of transitions which are realized in the system. For this purpose, expressing from Eq. (5) the temperature as a function of C_1 and C_2, we can obtain the expansion series of this expression near the critical point:

$$\Theta \cong \Theta_N \left[1 + K C_1^2 + O(C_1^4)\right] \cong \Theta_N \left[1 + \frac{1}{\varrho^2} K C_2^2 + O(C_2^4)\right]; \tag{9}$$

we use here the following notation

$$K = \tau_1 \left[\varrho^2 G_2 - G_1 - \frac{3}{10}(\varrho^2 L_2 - L_1)\right]\left(\tau_1 + \frac{\tau_2}{\varrho^2}\right)^{-1} - \frac{3}{10} L_1,$$

$$G_2 = \left(2A_1 J_2 - A_1 \frac{J}{\varrho} + 2A \frac{J}{\varrho} - AJ_1 \frac{1}{\varrho^2} - AJ_2 \frac{\tau_2}{\tau_1 \varrho^2} - A_2 J \frac{\tau_2}{\tau_1 \varrho^3}\right) \times$$
$$\times (A_1 A_2 - A^2)^{-1},$$

$$G_1 = \left(2A_2 J_1 - A_2 J\varrho + 2AJ\varrho - AJ_2 \varrho^2 - AJ_1 \varrho^2 \frac{\tau_1}{\tau_2} - A_1 J \varrho^3 \frac{\tau_1}{\tau_2}\right) \times$$
$$\times (A_1 A_2 - A^2)^{-1},$$

$$L_j = \frac{2S_j^2 + 2S_j + 1}{S_j^2 (S_j + 1)^2}, \quad j = 1, 2.$$

It can be easily seen that, depending on the value of K, the following cases can be realized in the system:

1) $K < 0$, the phase transition is of the 2-nd order with the magnetization critical index $\beta = \frac{1}{2}$;
2) $K > 0$, the phase transition is of the 1-st order;
3) $K = 0$, the type of transition is determined by the coefficient of C_j^4; if it is negative, the transition is of 2-nd order with $\beta = \frac{1}{4}$, if it is positive, the transition is of 1-st order.

So the value $K = 0$ is the value separating different orders of transition. The analysis of the condition 3) in the general case is complicated, so we limit ourselves to the case $S_1 = S_2 = S$ (correspondingly, $\tau_1 = \tau_2 = \tau$, $L_1 = L_2 = L$). Then we have

$$2(A_2 J_1 - A_2 J\varrho + AJ\varrho - AJ_2\varrho^2 - AJ_1\varrho^2 - A_1 J\varrho^3 + AJ\varrho^3 + A_1 J_2 \varrho^4) \times$$
$$\times (A_1 A_2 - A^2)^{-1} - \frac{3}{10} L (\varrho^4 + 1) = 0. \tag{10}$$

Let us furthermore simplify our task, for which we shall fix J_1, J_2, J, changing only the direct interactions. Then (10) determines the 2-nd order surface in the

A_1, A_2, A axes (since ϱ is a rather complicated function of J_1, J_2, J, we shall not consider this case in the J_1, J_2, J axes). Let us change the variables:

$$A = A' + A^{\circ}, \quad A^{\circ} = \frac{\varrho}{\frac{3}{10} L (\varrho^4 + 1)} (J_2\varrho + J_1\varrho - J - J\varrho^2),$$

$$A_1 = A_1' + A_1^{\circ}, \quad A_1^{\circ} = \frac{2\varrho^3}{\frac{3}{10} L (\varrho^4 + 1)} (J_2\varrho - J),$$

$$A_2 = A_2' + A_2^{\circ}, \quad A_2^{\circ} = \frac{2}{\frac{3}{10} L (\varrho^4 + 1)} (J_1 - J\varrho).$$

Then under the condition $A_1A_2 - A^2 \neq 0$ in new variables we have the equation of the cone

$$(A')^2 - A_1'A_2' = 0. \tag{11}$$

In the old variables its centre is at the point $P = \{A_1^{\circ}, A_2^{\circ}, A^{\circ}\}$ of the surface of another cone

$$A_1A_2 - A^2 = 0. \tag{12}$$

It is obvious that the phase transition realized in the system has to be of 1-st order when both the numerator and denominator in the expression for K are of the same sign, i. e. when

i) $A_1A_2 - A^2 > 0, \quad (A - A^{\circ})^2 - (A_1 - A_1^{\circ})(A_2 - A_2^{\circ}) > 0,$

ii) $A_1A_2 - A^2 < 0, \quad (A - A^{\circ})^2 - (A_1 - A_1^{\circ})(A_2 - A_2^{\circ}) < 0.$

Let R_1 and R_2 be the regions inside the cones defined by equations (11), (12), respectively. Then the phase transition of 1-st order occurs in the region R determined as follows

$$R = R_1 \cup R_2 / R_1 \cap R_2.$$

Otherwise, the phase transition is of the 2-nd order (see Fig. 1).

With the expression for the free energy per site (4), we can obtain the expression for the internal energy per site

$$u = \frac{A_1}{2}\left(w_1^2 - w_1 + \frac{1}{2}\right) + \frac{A_2}{2}\left(w_2^2 - w_2 + \frac{1}{2}\right) + A\left(w_1w_2 - \frac{w_1}{2} - \frac{w_2}{2} + \right.$$
$$\left. + \frac{1}{2}\right) - \frac{1}{2} J_1 w_1^2 C_1^2 - \frac{1}{2} J_2 w_2^2 C_2^2 + J w_1 w_2 C_1 C_2,$$

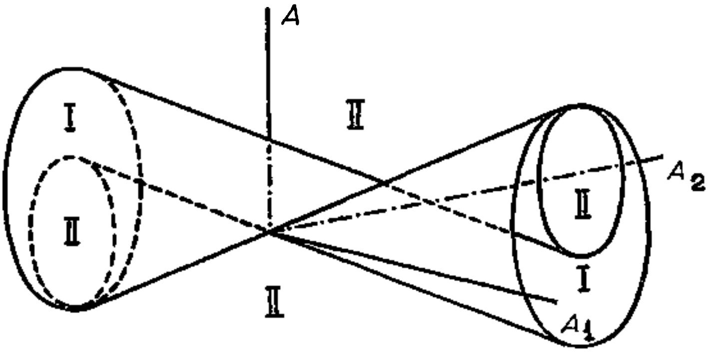

Fig. 1. The phase diagram of a general model: region I corresponds to the phase transition of 1-st order; region II corresponds to the phase transition of 2-nd order.

the entropy per site

$$s = \frac{1}{2}\ln\left(\frac{\operatorname{sh}\frac{2S_1+1}{2S_1}x_1}{\operatorname{sh}\frac{1}{2S_1}x_1}\right) + \frac{1}{2}\ln\left(\frac{\operatorname{sh}\frac{2S_2+1}{2S_2}x_2}{\operatorname{sh}\frac{1}{2S_2}x_2}\right) + \frac{1}{2}\ln(2S_1+1) +$$

$$+\frac{1}{2}\ln(2S_2+1) - \frac{1}{\Theta}(J_1 w_1^2 C_1^2 + J_2 w_2^2 C_2^2 - 2Jw_1 w_2 C_1 C_2);$$

and therefore the following expression for the specific heat of the system in the zero magnetic field

$$c_H = \Theta\frac{\mathrm{d}s}{\mathrm{d}\Theta} = (Jw_1w_2C_2 - J_1w_1^2C_1)\frac{\mathrm{d}C_1}{\mathrm{d}\Theta} + (Jw_1w_2C_1 - J_2w_2^2C_2)\frac{\mathrm{d}C_2}{\mathrm{d}\Theta}.$$

Now it is seen that the heat instability ($c_H < 0$) results from the 1-st order phase transition and vice versa. On the contrary, the specific heat is positive, and the system is stable at any temperature if the 2-nd order phase transition occurs. Using the expansion series (9), it is easy to define the behaviour of the specific heat near the critical point. If $K < 0$, then

$$c_H = \frac{1}{8\Theta_N K}(2J\varrho - J_1 - J_2\varrho^2) + 0(t), \quad t = \frac{\Theta - \Theta_N}{\Theta_N},$$

and the specific heat critical index $a = 0$ (finite jump). If $K = 0$, as on the surface of the cone (11) (see Fig. 1), and if the coefficient of C_1^4 in (9) is negative, the specific heat diverges with the critical index $a = \frac{1}{2}$:

$$c_H \sim (-t)^{-\frac{1}{2}}.$$

Here it is necessary to make the following remark. Obviously, the expansion series (9) and all the consequences are valid when $A_1A_2 - A^2 \neq 0$. If this condition is not valid, then, as follows from (7), in this case the phase probabilities do not tend to $\frac{1}{2}$ when C_1, $C_2 \to 0$, but have the limit values:

$$w_1 \to \frac{1}{2} \cdot \frac{J_2 (A_1 + A) \varrho^2 + J (A + A_2) \varrho}{J_1 A_2 + 2AJ\varrho + J_2 A_1 \varrho^2},$$

$$w_2 \to \frac{1}{2} \frac{J_1 (A_2 + A) \varrho^2 + J (A + A_1) \varrho}{J_1 A_2 + 2AJ\varrho + J_2 A_1 \varrho^2}.$$

Thus, Θ_N will be determined not by the formula (8), but by a more complicated expression which depends now on A_1, A_2, A (the expression for ϱ will also be more complicated). So, when we go from the $A_1A_2 - A^2 \neq 0$ to $A_1A_2 - A^2 = 0$, the phase probabilities and the transition temperature will have jumps. Therefore, all characteristics of the system will have jump as well. Such an abrupt change of properties of the model under an infinitesimally small change of parameters of the Hamiltonian corresponds to an instability of the system. In the framework of the model considered this instability is to all appearance an artifact, that can be easily avoided after defining the corresponding limits on the both sides of the surface (12). Such an instability could be connected with a lattice instability; however, for a detailed investigation of this question it is necessary to analyse the Hamiltonian with a soft lattice, adding phonon terms. But the consideration of spin-phonon interactions in a heterophase antiferromagnet is a separate and quite complicated problem which should be analysed in a separate paper.

Let us now consider the limitations imposed by the conditions of stability and normalization of phase probabilities. That is, we must take into account that it may be thermodynamically more preferable for the system to stay in the »usual«, »nonhybrid« state, i. e. when $w_1 = w_2 = 1$ and heterophase fluctuations are absent (in that case we have the »usual« Heisenberg antiferromagnet considered in the molecular field approximation). In order to decide which case is realized, we must compare the free energies per site for the following cases:

1) hybrid system, antiferromagnetic phase — the free energy per site $f_1(\Theta) = f(\Theta)$ is given by the expression (4);
2) usual system, antiferromagnetic phase,

$$f_2(\Theta) = \frac{A_1 + A_2 + 2A}{4} + \frac{1}{2}(J_1 C_1^2 + J_2 C_2^2 - 2JC_1C_2) - \frac{1}{2}\Theta \ln (2S_1 + 1) -$$

$$- \frac{1}{2}\Theta \ln (2S_2 + 1) - \frac{1}{2}\Theta \ln \left(\frac{\operatorname{sh} \frac{2S_1 + 1}{2S_1} x_1}{\operatorname{sh} \frac{1}{2S_1} x_1} \right) - \frac{1}{2}\Theta \ln \left(\frac{\operatorname{sh} \frac{2S_2 + 1}{2S_2} x_2}{\operatorname{sh} \frac{1}{2S_2} x_2} \right),$$

$$x_1 = \frac{2}{\Theta} S_1 (J_1 C_1 - JC_2), \qquad x_2 = \frac{2}{\Theta} S_2 (JC_1 - J_2 C_2);$$

3) hybrid system, paramagnetic phase,

$$f_3(\Theta) = \frac{A_1 + A_2 + 2A}{8} - \Theta \ln(2S_1 + 1) - \Theta \ln(2S_2 + 1);$$

4) usual system, paramagnetic phase:

$$f_4(\Theta) = \frac{A_1 + A_2 + 2A}{4} - \Theta \ln(2S_1 + 1) - \Theta \ln(2S_2 + 1).$$

Let us underline that the temperature of the 1-st order phase transition Θ_{tr} in the hybrid system is determined from the condition

$$f_1(\Theta_{tr}) = f_3(\Theta_{tr}).$$

Since the comparison of different free energies at arbitrary temperatures is rather complicated, for the simplicity we do this at $\Theta = 0$. Then it can be easily seen that a sufficient condition for the validity of the inequalities

$$f_2(0) < f_1(0), \quad f_2(0) < f_4(0) < f_3(0), \quad f_1(0) < f_3(0)$$

is the following relation:

$$A_1 + A_2 + 2A < 0. \tag{13}$$

Thus, if (13) is valid, the usual solution is thermodynamically more preferable, and the hybrid solution can be realized as a metastable state. The equation $A_1 + A_2 + 2A = 0$ determines a plane tangent to the cone (12). Below this plane the solutions are (at $\Theta = 0$) for sure metastable.

In the case when the temperature has values near the critical one, we can apply the phase probability convexity conditions for the investigation of the stability of the system. For the stability of the hybrid solution the validity of the following relations is necessary:

$$\frac{\partial^2 f_1}{\partial w_1^2} > 0, \quad \frac{\partial^2 f_1}{\partial w_2^2} > 0.$$

We have

$$\frac{\partial^2 f_1}{\partial w_1^2} = A_1 - J_1 C_1^2 - \frac{2S_1^2}{\Theta} (2J_1 w_1 C_1 - J w_2 C_2)^2 \frac{\mathrm{d}B_{S_1}(x_1)}{\mathrm{d}x_1} -$$

$$- \frac{2S_2^2}{\Theta} (J w_2 C_1)^2 \frac{\mathrm{d}B_{S_2}(x_2)}{\mathrm{d}x_2},$$

$$\frac{\partial^2 f_1}{\partial w_2^2} = A_2 - J_2 C_2^2 - \frac{2S_1^2}{\Theta} (J w_1 C_2)^2 \frac{\mathrm{d} B_{S_1}(x_1)}{\mathrm{d} x_1} -$$

$$- \frac{2S_2^2}{\Theta} (2J_2 w_2 C_2 - J w_1 C_1)^2 \frac{\mathrm{d} B_{S_2}(x_2)}{\mathrm{d} x_2}.$$

When $\Theta \to \Theta_N$, then $\frac{\partial^2 f_1}{\partial w_1^2} \to A_1$, $\frac{\partial^2 f_1}{\partial w_2^2} \to A_2$. Thus, near the critical point the metastable states will correspond to the negative values of A_1 and A_2.

The condition of the normalization of the phase probability $0 \leqslant w_1 \leqslant 1$ under $\Theta = 0$ and $S_1 = S_2 = S$ (for the simplicity we consider this case in A_1, A_2, A axes) leads to the inequalities

$$(A - \alpha)^2 - (A_1 - \alpha_1)(A_2 - \alpha_2) \gtreqqless \frac{1}{4} (J + J_2)^2 S^4,$$

$$(A - \beta)^2 - (A_1 - \beta_1)(A_2 - \beta_2) \gtreqqless \frac{1}{4} (J + J_2) S^4, \tag{14}$$

where one must take either the upper or the lower inequality signs in the both lines,

$$\alpha = \frac{1}{2} (3J + J_2) S^2, \quad \alpha_1 = (J + 2J_1) S^2, \quad \alpha_2 = J_2 S^2,$$

$$\beta = \frac{1}{2} (J - J_2) S^2, \quad \beta_1 = -J S^2, \quad \beta_2 = J_2 S^2.$$

The normalization condition of the phase probability w_2 under the same conditions gives, respectively,

$$(A - \gamma)^2 - (A_1 - \gamma_1)(A_2 - \gamma_2) \gtreqqless \frac{1}{4} (J + J_1)^2 S^4,$$

$$(A - \delta)^2 - (A_1 - \delta_1)(A_2 - \delta_2) \gtreqqless \frac{1}{4} (J + J_1)^2 S^4, \tag{15}$$

where

$$\gamma = \frac{1}{2} (3J + J_1) S^2, \quad \gamma_1 = (J + 2J_2) S^2, \quad \gamma_2 = J_1 S^2,$$

$$\delta = \frac{1}{2} (J - J_1) S^2, \quad \delta_1 = -J S^2, \quad \delta_2 = J_1 S^2.$$

The simultaneous equality of right and left-hand sides in relations (14), (15) is excluded. Let us give the geometrical interpretation of the conditions (14), (15). For this purpose we do the following change of variables:

$$A_1 = a_1 + a_2, \qquad A_2 = a_1 - a_2,$$

that corresponds to the 45° rotation in the A_1A_2 plane. As a result, we have

$$\begin{aligned}
&(A - \tilde{\alpha})^2 - (a_1 - \tilde{\alpha}_1)^2 + (a_2 - \tilde{\alpha}_2)^2 \gtreqqless \frac{1}{4}(J + J_2)^2\, S^4,\\
&(A - \tilde{\beta})^2 - (a_1 - \tilde{\beta}_1)^2 + (a_2 - \tilde{\beta}_2)^2 \gtreqqless \frac{1}{4}(J + J_2)^2\, S^4,\\
&(A - \tilde{\gamma})^2 - (a_1 - \tilde{\gamma}_1)^2 + (a_2 - \tilde{\gamma}_2)^2 \gtreqqless \frac{1}{4}(J + J_1)^2\, S^4,\\
&(A - \tilde{\delta})^2 - (a_1 - \tilde{\delta}_1)^2 + (a_2 - \tilde{\delta}_2)^2 \gtreqqless \frac{1}{4}(J + J_1)^2\, S^4,
\end{aligned} \tag{16}$$

where

$$\tilde{\alpha} = \frac{1}{2}(3J + J_2)\, S^2, \quad \tilde{\alpha}_1 = \frac{1}{2}(J + 2J_1 + J_2)\, S^2, \quad \tilde{\alpha}_2 = \frac{1}{2}(J + 2J_1 - J_2)\, S^2,$$

$$\tilde{\beta} = \frac{1}{2}(J - J_2)\, S^2, \quad \tilde{\beta}_1 = \frac{1}{2}(J_2 - J)\, S^2, \quad \tilde{\beta}_2 = -\frac{1}{2}(J + J_2)\, S^2,$$

$$\tilde{\gamma} = \frac{1}{2}(3J + J_1)\, S^2, \quad \tilde{\gamma}_1 = \frac{1}{2}(J + J_1 + 2J_2)\, S^2, \quad \tilde{\gamma}_2 = \frac{1}{2}(J + J_2 - J_1)\, S^2,$$

$$\tilde{\delta} = \frac{1}{2}(J - J_1)\, S^2, \quad \tilde{\delta}_1 = \frac{1}{2}(J_1 - J)\, S^2, \quad \tilde{\delta}_2 = -\frac{1}{2}(J + J_1)\, S^2.$$

Let us now put $a_1 = \text{const}$. So, we shall have a section in the A, a_2 plane. The normalization conditions will lead to some set of circumferences. More exactly, if Q_α, Q_β, Q_γ, Q_δ are interiors of sircumferences defined by equalities in (16) at $a_1 = \text{const}$, then normalization conditions are not valid in the regions

$$Q_1 = Q_\alpha \cup Q_\beta / Q_\alpha \cap Q_\beta, \qquad Q_2 = Q_\gamma \cup Q_\delta / Q_\gamma \cap Q_\delta.$$

In these regions we have to put the corresponding $w_j = 1$ $(j = 1, 2)$ at $\Theta = 0$. So in $Q_1 \cap Q_2$ the ground state is completely ordered.

Consider as an example the case $a_1 = \dfrac{A_1 + A_2}{2} = 0$, $J_1 = J_2 = 0$, $S_1 = S_2 = \dfrac{1}{2}$. Let us draw the corresponding curves in the $\dfrac{a_2}{J}$, $\dfrac{A}{J}$ axes (see Fig. 2).

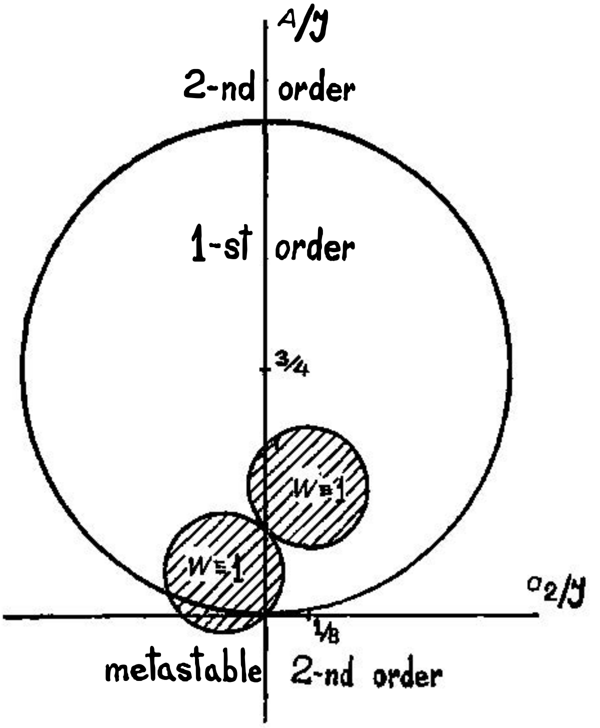

Fig. 2. The phase diagram for the case $J_1 = 0$, $J_1 = J_2 = 0$, $S_1 = S_2 = \frac{1}{2}$.

The Eqs. (11) and (12) will give only one circumference with the centre at the point $B = \left\{0, \frac{3}{4}\right\}$ and with the radius $R = \frac{3}{4}$. The points inside this circle will correspond to the 1-st order phase transition, those which are outside to the 2-nd order phase transition. The straight line $\frac{A}{J} = 0$ defined by the condition (13) will be the boundary of stability — below it the heterophase solutions will be for sure metastable at zero temperature. The condition (16) in this case will give a pair of eircumferences described by the equations

$$\left(\frac{A}{J} - \frac{3}{8}\right)^2 + \left(\frac{a_2}{J} - \frac{1}{8}\right)^2 = \frac{1}{32},$$

$$\left(\frac{A}{J} - \frac{1}{8}\right)^2 + \left(\frac{a_2}{J} + \frac{1}{8}\right)^2 = \frac{1}{32}.$$

The hatched interior of these circles (see Fig. 2) corresponds to the violation of the normalization conditions for the phase probabilities, and we put there $w_1 = w_2 = 1$. Thus, in these regions only the homophase ground state is possible.

The boundary of the circles corresponds to the values of parameters for which the system becomes a mixture at $\Theta = 0$ (the points of nucleation). Let us consider qualitatively the situation when $\Theta \neq 0$. In this case the position of the centres and the values of radii of the circumferences corresponding to the phase probabilities normalization are changed. The requirement for the circle corresponding to $\Theta \neq 0$ to stay into the circle corresponding to $\Theta = 0$ can be written as follows

$$R(\Theta) + \Delta(\Theta) \leq R(0),$$

where $R(\Theta)$, $R(0)$ are radii of the circles defined by the equalities from (16) at $a_1 = \text{const}$ and $\Theta \neq 0$ or $\Theta = 0$, respectively, $\Delta(\Theta)$ is the displacement of the circle centre at the temperature changing from zero to Θ. For the case considered ($a_1 = 0$, $J_1 = J_2 = 0$) this condition reduces to the inequality

$$\sqrt{\frac{1}{2}}\, C^2 + \sqrt{\frac{5}{2}}\,(S^2 - C^2) \leq \frac{1}{2}\, S^2,$$

which obviously is not valid. Therefore, the values of parameters are possible for which at $\Theta = 0$ the probabilities satisfy the normalization conditions $0 \leq w_j < 1$ ($j = 1, 2$), and at some temperature becomes equal to 1, i. e. the nuclei of paramagnetic phase disappear. It is possible that with further increasing the temperature the nucleation will again occur.

Fig. 3 corresponds to the case $a_1 = \frac{J}{2}$, $J_1 = J_2 = 0$, $S_1 = S_2 = 1$. For this case we have 4 circles on the $\frac{a_2}{J}, \frac{A}{J}$ plane. The circumferences

$$\left(\frac{A}{J}\right)^2 + \left(\frac{a_2}{J}\right)^2 = \frac{1}{4},$$

$$\left(\frac{A}{J} - \frac{8}{3}\right)^2 + \left(\frac{a_2}{J}\right)^2 = \frac{169}{36},$$

are obtained by the intersection of the cones (11), (12) by the plane $a_1 = \frac{2}{J}$. The values of parameters which are inside these circles correspond to the transition of 1-st order, if not, to the transition of 2-nd order. The hatched parts of circumferences determined by the equalities (16)

$$\left(\frac{A}{J} - \frac{3}{2}\right)^2 + \left(\frac{a_2}{J} - \frac{1}{2}\right)^2 = \frac{1}{4},$$

$$\left(\frac{A}{J} - \frac{1}{2}\right)^2 + \left(\frac{a_2}{J} + \frac{1}{2}\right)^2 = \frac{5}{4},$$

give us the regions where phase probability normalization conditions are violated. The boundary of the hatched regions corresponds to the nucleation points at zero

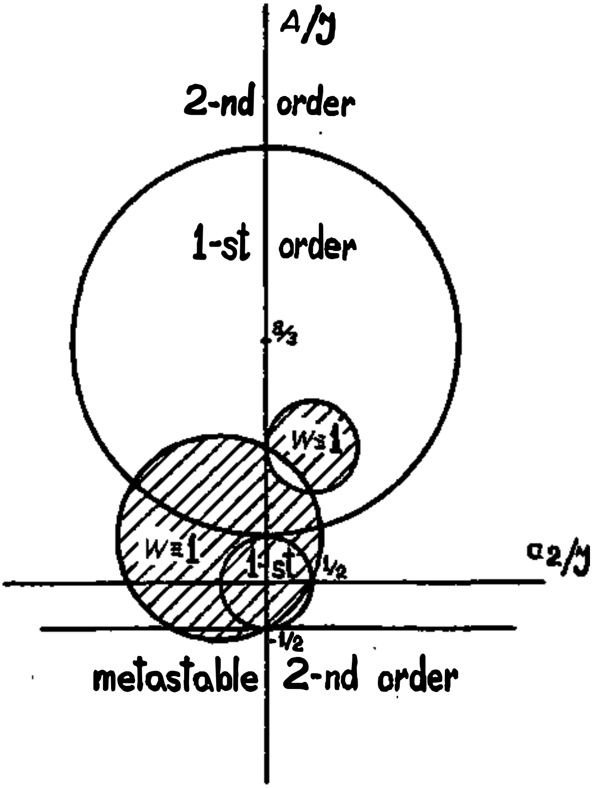

Fig. 3. The phase diagram for the case $a_1 = \frac{J}{2}$, $J_1 = J_2 = 0$, $S_1 = S_2 = 1$.

temperature. At the points below the straight line $\frac{A}{J} = -\frac{1}{2}$ defined from (13) the hybrid solutions are for sure metastable. As well as in the previous case the nucleation can occur in the regions with the transitions both of 1-st and 2-nd orders and also in the region where heterophase states are metastable. Moreover Fig. 3. indicates that the 1-st order phase transitions can be realized in the metastable region.

3. *Equivalent sublattices*

Let now the conditions $A_1 = A_2$, $J_1 = J_2$, $S_1 = S_2 = S$ be satisfied, but at the same time $A_1 \neq A$, $J_1 \neq J$. Thus, we have completely equivalent sublattices. In this case

$$C = C_1 = -C_2 = SB_s(x), \qquad x = \frac{2S}{\Theta}(J + J_1)\, w^2 C,$$

$$w = w_1 = w_2 = \frac{1}{2}\, \frac{A_1^2 - A^2 - (A_1 + A)(J_1 - J)\, C^2}{A_1^2 - A^2 - 2(A_1 J_1 - AJ)\, C^2 + (J_1^2 - J^2)\, C^4}.$$

The Neel temperature is $\Theta_N = \frac{1}{6} S(S+1)(J_1 + J)$. The equations (11), (12) will transform into the following equations in the A_1, A plane, respectively,

$$\left(A - \frac{J+J_1}{\frac{3}{10}L}\right)^2 - \left(A_1 - \frac{J+J_1}{\frac{3}{10}L}\right)^2 = 0,$$

$$A_1^2 - A^2 = 0.$$

The regions with different kinds of transitions are presented for this case in Fig. 4 (the hatched region corresponds to the transitions of 1-st order). The necessary condition of the stability will be $A + A_1 > 0$, which gives one of the boundaries of the 1-st order phase transitions (see Fig. 4).

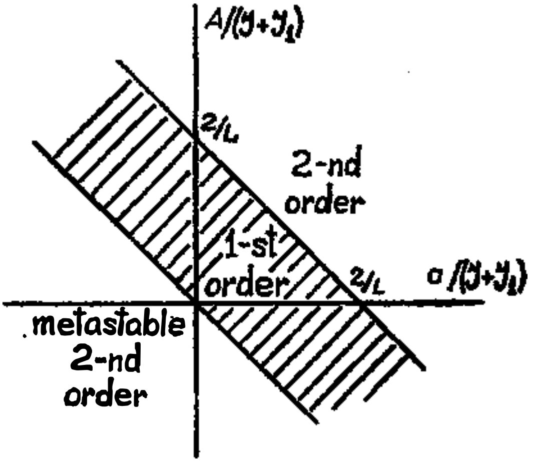

Fig. 4. The phase diagram of the model with equivalent sublattices.

4. Neel model

Let us now consider in more detail the case when the interactions in sublattices are absent, and only the interaction between sublattices exists (the Neel model). That is, we have $A_1 = A_2 = J_1 = J_2 = 0$, $S_1 = S_2 = S$, and

$$C = C_1 = -C_2 = SB_S(x), \qquad x = \frac{2Jw^2CS}{\Theta},$$

$$w = w_1 = w_2 = \frac{A}{2(A - JC^2)},$$

$$\Theta_N = \frac{S(S+1)J}{6}.$$

The condition for the phase transition to be of 1-st order will be $\frac{2J}{A} > \frac{3}{10}L$. The probability will be normalized when the following relations are valid:

$$A \geqslant 2JC^2, \qquad A \leq 0.$$

The temperature when the nucleation occurs ($w = 1$) is determined by the relation

$$\Theta' = \frac{S\sqrt{2AJ}}{B_s^{-1}\left(\frac{\sqrt{A}}{S\sqrt{2J}}\right)},$$

where $B_s^{-1}(x)$ is the inverse Brillouin function. When $A < 0$, the solutions will be metastable.

Let us see now, which physical situations will be realized in the system depending on parameters. For the Neel model we can change $\frac{A}{J}$ from $+\infty$ to $-\infty$. Such a change for $S = \frac{1}{2}$ corresponds to the movement along $\frac{A}{J}$ axis in Fig. 2.

a) When $\frac{2}{\frac{3}{10}L} < \frac{A}{J} < +\infty$, the phase transition of 2-nd order occurs in the system (the temperature dependence of the order parameter C is shown in Fig. 5a). When $\frac{A}{J} = \frac{2}{\frac{3}{10}L}$, the critical indices change from $\alpha = 0$, $\beta = \frac{1}{2}$ to $\alpha = \frac{1}{2}$, $\beta = \frac{1}{4}$ for phase transition of 2-nd order; the transition is of 2-nd order since the coefficient of C^4 in expansion series (9) is negative.

b) The next region is $2S^2 < \frac{A}{J} < \frac{2}{\frac{3}{10}L}$ (remember that the region where the probability normalization conditions are violated in Fig. 2 corresponds to the zero temperature; for $\Theta \neq 0$ the inequality will be $2C^2 < \frac{A}{J} < \frac{2}{\frac{3}{10}L}$), here the phase transition is of 1-st order (see Fig. 5b). When $\frac{A}{J} = 2S^2$, there is the phase transition of 1-st order, and at zero temperature the nucleation occurs in the system.

c) In the region of parameter values $\frac{A'}{J} < \frac{A}{J} < 2S^2$ the nucleation will occur in the system for some value of the temperature Θ' in the interval $0 < \Theta' < \Theta_{tr}$, A' being defined by the equation

$$A' = 2 \frac{S\sqrt{2A'J}}{B_S^{-1}\left(\frac{1}{S}\sqrt{\frac{A'}{2J}}\right)} \ln \left(\frac{\operatorname{sh}\left(\frac{2S+1}{2S} B_S^{-1}\left(\frac{1}{S}\sqrt{\frac{A'}{2J}}\right)\right)}{\operatorname{sh}\left(\frac{1}{2S} B_S^{-1}\left(\frac{1}{S}\sqrt{\frac{A'}{2J}}\right)\right)} \right).$$

The temperature dependence of the order parameter in this case is depicted in Fig. 5c. In this case the phase transition of 1-st order is realized again.

d) When $\frac{A}{J}$ is on the interval $0 \leq \frac{A}{J} \leq \frac{A'}{J}$, the normalization of the phase probability is violated for any temperature $\Theta < \Theta_{tr}$, and we must put $w = 1$. So, in this case the paramagnetic nuclei are absent in the system. The order parameter has a jump again, since we have the transition of 1-st order (see Fig. 5d).

e) When $\frac{A}{J} < 0$, the system will be metastable. For the hybrid solution we always have $w \leq \frac{1}{2}$, and paramagnetic nuclei will dominate in the system, if this solution is realized. In this case the phase transition is of 2-nd order (see Fig. 5a).

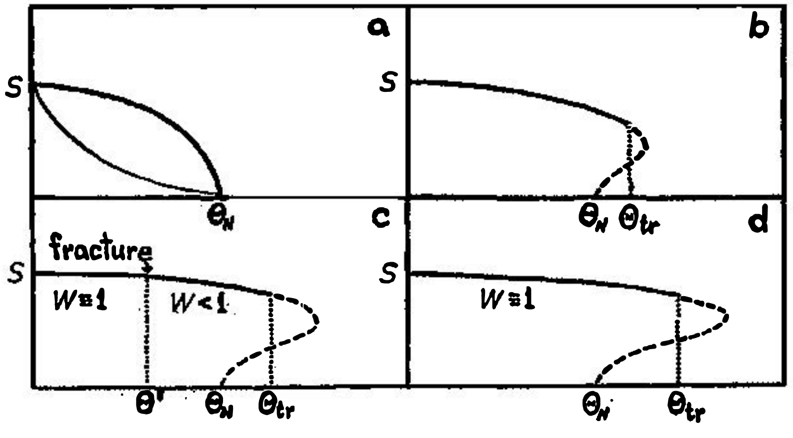

Fig. 5. The temperature dependence of the order parameter C in the Neel model: a) the 2-nd order phase transition for the cases $\frac{20}{3L} \leqslant \frac{A}{J}$, $\frac{A}{J} < 0$; b) the 1-st order phase transition for the case $2S^2 < \frac{A}{J} < \frac{20}{3L}$; c) the 1-st order phase transition with $\Theta' < \Theta_{tr}$ for the case $\frac{A'}{J} < \frac{A}{J} \leqslant 2S^2$; d) the 1-st order phase transition for the case $0 \leqslant \frac{A}{J} \leqslant \frac{A'}{J}$.

In the region c), where the nucleation occurs, the temperature dependence of the specific heat

$$C_H = \frac{4S^2J^2w^4C^2\frac{\mathrm{d}B_S(x)}{\mathrm{d}x}}{\Theta\left[\Theta - 2S^2Jw^2\left(1 + \frac{8JwC^2}{A}\right)\frac{\mathrm{d}B_S(x)}{\mathrm{d}x}\right]}$$

has two jumps (one of them corresponds to the nucleation, the other to the phase transition). Such a behaviour is in qualitive agreement with some experimental data[25,26].

5. *Discussion*

From the consideration presented it can be seen that assuming the existence of the heterophase state in the system and taking into account the competition between direct and exchange interactions, we arrive to physically different situations. That is, depending on the values of the parameters A_1, A_2, A, J_1, J_2, J eight different cases are possible:

1) The phase transition is of 2-nd order;
2) The phase transition is of 2-nd order with the nucleation;
3) The phase transition is of 2-nd order in the metastable region;
4) The phase transition is of 2-nd order with the nucleation in the metastable region;
5—8) The same, but for the phase transition of 1-st order.

Let us remark now that if we consider the usual Heisenberg model in the molecular field approximation, we shall have only the phase transition of 2-nd order (see, for example Ref. 27). Thus, one of the advantages of the proposed approach is the inclusion into the model the possibility for the change of the transition order. In this connection let us mention the set of papers considering the possibility of phase transitions of 1-st and 2-nd order for different substances with the use of the renormgroup technique[28-33]. In these papers an idea due to Wilson and Fisher[34] has been used, that for a certain relation between parameters of a model the transition of 2-nd order becomes impossible and transforms into the transition of 1-st order as a result of a sharp increase of fluctuations. In the set of papers mentioned the Landau-Ginzbourg-Wilson Hamiltonian has been built for isotropic systems[28,29], or for the systems with anisotropy[30,33] with the dimension of order parameter $n \geqslant 4$. The existence of the phase transition of 2-nd order in the system was identified with the existence of the stable point in the renormgroup equations for the dimension $d = 4$. The absence of the stable point was identified with the phase transition of 1-st order. It was supposed that the structure of the renormgroup equations was not changed when the dimension was varied from $d = 4$ to the real one $d = 3$. Decreasing of the order parameter dimension to $n = 4$ and below as a consequence of decreasing the symmetry due to some reasons, for example, to a stress along the diagonal [111] in the cubic lattice MnO[28] leads to the appearing of the stable point; the phase transition of 1-st order occuring under usual conditions transforms into the phase transition of 2-nd order. Let us underline, that in our case the change of the relation between parameters of the system due to the stress, for example, can lead to such a change of the order of transition (it is supposed that we can take into account the dependence of the parameters on such a stress). The argument for this explanation is the fact that a finite (but not infinitesimal) stress is necessary for changing the order of transition. We can suppose also that the corresponding parameters for Cr, for which under usual conditions the phase transition of 1-st order occurs, are near the boundary between the transitions of 1-st and 2-nd order, since adding of a certain amount of impurities (with the threshold concentration) leads to the phase transition of 2-nd order[35,36].

A similar situation takes place in the ferromagnets[37] (where the analogous consideration can be done) of the R_aCo_b type, where R are rare-earths or yttrium. Here for some elements under certain relations between a and b the 1-st order transition can occur instead of 2-nd order one.

In Ref. 38 the Ising model was considered with competing interactions for a body-centered cubic lattice. The nearest-neighbour coupling was supposed to be ferromagnetic, the next-nearest-neighbour one was antiferromagnetic. In this paper, with the parallel use of the renormgroup and Monte-Carlo technique it was shown that the paramagnet-antiferromagnet phase transition is of 1-st order (in contrast to molecular field theory predictions).

An analysis of other possible mechanisms of changing a phase transition in ferromagnets and antiferromagnets (the volume-striction mechanism, the consideration of the biquadratic term in the isotropic indirect exchange, and so on) can be found in Ref. 39 (see also Ref. 40).

The advantage of our model of a heterophase antiferromagnet is in the fact that this model not only describes a possible change of the phase transition order but it better corresponds to those experiments[4,5] where the existence of a paramagnetic fraction in magnets has been observed.

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MODEL ANTIFEROMAGNETA S HETEROFAZNIM FLUKTUACIJAMA

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Razmatran je model antiferomagneta s paramagnetskom jezgrom. Posebno je analizirano ponašanje fazne vjerojatnosti u okolišu apsolutne nule i okolišu Neelove temperature. Uvjeti stabilnosti pokazuju kada je takav antiferomagnet stabilan, metastabilan ili nestabilan. Također je ispitivano ponašanje toplinskog kapaciteta u okolišu kritične točke. Heterofazne fluktuacije mogu promijeniti red faznog prijelaza sa $n = 2$ na $n = 3$. Kriterij za tu promjenu je ustanovljen i prodiskutiran.