SOME EXACT RESULTS FOR THE ISING MODEL WITH SPIN--PHONON INTERACTION

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The magnetization for the Ising model with a renormalized exchange integral due to the spin-phonon interaction is evaluated in the following situations: (a) the case of nearest neighbours interaction; (b) the case of long-range interaction of infinite radius. The conditions of the change of phase transition order are obtained. The exact temporal evolution of the statistical expectation value of magnetization is also considered for situation (b).

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The problem of the influence of the lattice vibrations on the thermodynamical behaviour of magnetic crystals was examined by many authors (see, e.g., [1, 2]). But the only exact result, as far as we know, was obtained by Wagner [3] for the Ising model with the spin-phonon interaction in the harmonic approximation. He has shown that the influence of spin displacements can be described by means of the supplementary term of the fourth order in the spin variables, which is introduced into the Hamiltonian of the spin subsystem.

The same result may be also obtained for the general case of the Heisenberg model with the spin-phonon interaction under the assumption of strong correlations between the spin and phonon subsystems [4]. In this case only a finite number of phonon modes has to be considered. It should be emphasized that the restrictions on the number of phonon modes is used as a standard approach to the description of a strong bond between the phonon and the atomic subsystems in crystals [5, 6].

In this paper we continue the investigation of the models with strong bond between phonon and spin subsystems and consider a case of the Ising Hamiltonian with spin-phonon interaction in harmonic approximation.

Let $J(f,f')$ be an exchange integral in the "ideal" system, i.e. in the system without lattice vibrations. Then the spin-phonon influence on the spin subsystem may be taken into consideration effectively in the general case by means of the following renormalization [4].

$$J(f,f') \rightarrow G(f,f') = J(f,f')+B(f,f') \lim_{N\rightarrow\infty} \left\langle \frac{1}{N^2} \sum_{f,f'} S_f S_{f'} \right\rangle, \tag{1}$$

where

$$B(f,f') = 2\,\mathrm{Re}\left\{ \sum_{k=k_1}^{kn} \frac{\vec{\tau}_k}{\omega_k \sqrt{2m\omega_k}} (e^{ikf}-e^{ikf'}) \nabla_{ff'} J(f,f') \right\}.$$

Here n is the number of modes, m is the mass of the atom with spin S_f, ω_k is the energy of the k-th mode, $\vec{\tau}_k$ is the unit vector of polarization and N is the number of lattice sites.

Such a renormalization leads to the exact result in the thermodynamical limit when $N \rightarrow \infty$. At the same time in the phonon subsystem the following renormalization of free phonons takes place [7]

$$a_k^\dagger \rightarrow \alpha_k^\dagger \equiv a_k^\dagger + \frac{\sqrt{N}}{2\omega_k} \sum_{f,f'} B(f,f') \lim_{N\rightarrow\infty} \left\langle \frac{1}{N^2} \sum_{f,f'} S_f S_{f'} \right\rangle. \tag{2}$$

It should be noted that the renormalizations (1) and (2) are independent of the form of exchange integral $J(f,f')$.

Let us consider the case of the two-dimensional Ising model with the nearest neighbours interaction. Then, taking into account the definition of the spontaneous magnetization per spin of paper [8], one may obtain the following form of the renormalized exchange integral instead of (1)

$$G(f,f') = J(f,f')+B(f,f')M^2, \tag{3}$$

where M is the magnetization per spin. For the case of zero magnetic field one can use the well-known Onsager's solution for the spontaneous magnetization. Then we get

$$M = \left(1-\mathrm{sh}^{-4}\frac{G}{\theta}\right), \tag{4}$$

where θ is the temperature and $G = J+BM^2$, $J(f,f') = J$, $B(f,f') = B$ for the nearest neighbours and $J(f,f') = B(f,f') = 0$ for all other pairs. Unlike the usual Onsager's result (4) has the magnetization M on both sides. The solution of equation (4) for the function $M = M(\theta)$ is presented in figure 1.

Expressing now the temperature θ from (4) as a function of M and expanding it near $M = 0$ one may obtain

$$\theta = \frac{J}{\mathrm{arcsh}\ 1} + \frac{B}{\mathrm{arcsh}\ 1} M^2 + O(M^4). \tag{5}$$

From expansion (5) it is evident that for any $B > 0$ the phase transition of the continuous type into the ferromagnetic state at the critical point $\theta_c = \dfrac{J}{\mathrm{arcsh}\ 1}$ is impossible. The

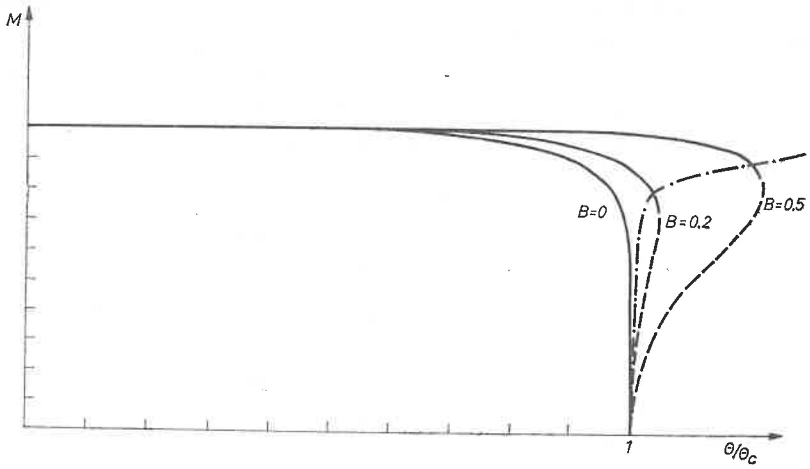

Fig. 1

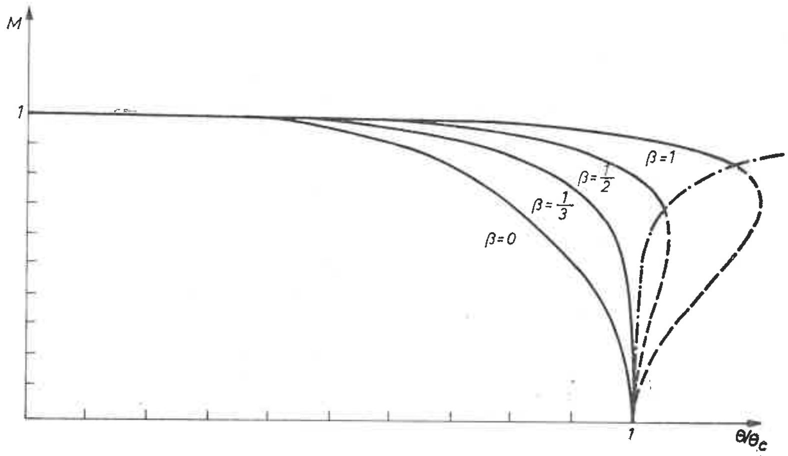

Fig. 2

Fig. 1 and 2. Magnetization plotted against temperature for the cases of short range and long range interaction correspondingly. The dashed-and-dotted line separates the stable nontrivial solutions for the magnetization from the instable ones (dashed lines)

phase transition of the first order takes place. The point of transition θ_0 is calculated from the condition of continuity for Gibbs free energy

$$\int_0^\pi d\omega \int_0^\pi d\omega' \ln\left[\operatorname{ch}^2 \frac{J+BM^2(\theta_0)}{\theta_0} - \operatorname{sh} \frac{J+BM^2(\theta_0)}{\theta_0} (\cos\omega + \cos\omega')\right]$$

$$= \int_0^\pi d\omega \int_0^\pi d\omega' \ln\left[\operatorname{ch}^2 \frac{J}{\theta_0} - \operatorname{sh} \frac{J}{\theta_0} (\cos\omega + \cos\omega')\right].$$

It lies above the critical point of the usual Onsager's solution. It should be noted that the obtained result is in compliance with the conclusions of papers [9, 10], obtained on the basis of an approximate examination of the Ising model with the total set of phonon modes.

Now we consider a case of long-range interaction. For this purpose let us choose an exchange integral of an "ideal" system in the form

$$J(f,f') = N^{-1}\gamma(f,f'), \tag{6}$$

where $\gamma(f,f') > 0$ for all f, f' and is a bounded function. Then, taking into account expression (3) for the renormalized exchange integral and the definition of "phonon function" $B(f,f')$, one can obtain the following expression of long range type instead of (3)

$$G(f,f') = N^{-1}g(f,f') = N^{-1}\left[\gamma(f,f')+\beta(f,f')\lim_{N\to\infty}\left\langle\frac{1}{N^2}\sum_{f,f'}S_fS_{f'}\right\rangle\right], \tag{7}$$

where

$$\beta(f,f') \equiv 2\,\mathrm{Re}\left\{\sum_{k=k_1}^{k_n}\frac{\vec{\tau}_k}{\omega_k\sqrt{2m\omega_k}}(e^{ikf}-e^{ikf'})\nabla_{ff'}\gamma(f,f')\right].$$

For the systems with long-range interaction the exact solution may be obtained on the basis of the trial Hamiltonian method [11], established for the spin models of general form in paper [12]. In the framework of this method the bilinear in spin operators form of the Ising Hamiltonian with the exchange integral (7) may be approximated by the following trial Hamiltonian

$$H_{\mathrm{trial}} = -\tfrac{1}{2}\sum_{f,f'}G(f,f')(2S_f-M)M-\mu\sum_f hS_f, \tag{8}$$

where M is the magnetization per spin for the trial Hamiltonian (8) and h is an external magnetic field. It may be proved [12] that the Hamiltonian (8) describes correctly the thermodynamical behaviour of the system with long-range renormalized interaction (7).

The correlation function on the right-hand side of (7) may be estimated on the basis of theorem 2 of paper [13]. Then we get the form of the type of (3)

$$G(f,f') \to \bar{G}(f,f') = N^{-1}[\gamma(f,f')+\beta(f,f')M^2]. \tag{9}$$

Magnetization M for the trial Hamiltonian (8) is defined by the following equation of the Curie-Weiss type

$$M = \mathrm{th}\frac{(\gamma+\beta M^2)M+\mu h}{\theta}, \tag{10}$$

where $\gamma = \frac{1}{N}\sum_g \gamma(g)$; $\beta = \frac{1}{N}\sum_g \beta(g)$ and $\gamma(f,f') = \gamma(f-f')$; $\beta(f,f') = \beta(f-f')$ [4].

Expressing now the temperature as a function of M from (10) and expanding it near $M = 0$ for the case of zero magnetic field one may obtain

$$\theta = \gamma+(\beta-\tfrac{1}{3}\gamma)M^2-\left(\tfrac{13}{45}\gamma-\frac{\beta}{3}\right)M^4+O(M^6). \tag{11}$$

From the expansion (11) one can see that as long as the phonon parameter β is less than $\gamma/3$, equation (10) with $h = 0$ describes the phase transition of the second order at the critical point $\theta_c = \gamma$ as in the usual molecular field theory. The critical index for the magnetization is $\frac{1}{2}$. For $\beta = \gamma/3$ the phase transition of the second order takes place, which is close to the transition of the first order. The corresponding critical index is $\frac{1}{2}$. For the case $\beta > \gamma/3$ only the phase transition of the first order occurs (see Fig. 2). The corresponding phase transition points for every β are determined from the condition of the continuity of Gibbs free energy per spin, as in the previous case:

$$-\theta \ln 2 = -\theta \ln 2 \operatorname{ch} \frac{(\gamma+\beta M^2)M}{\theta} + \tfrac{1}{2}(J+\beta M^2)M^2.$$

It should be emphasized that the renormalized exchange integrals (3) and (9) are some functions of temperature θ. Their dependence on the temperature is presented in Fig. 3.

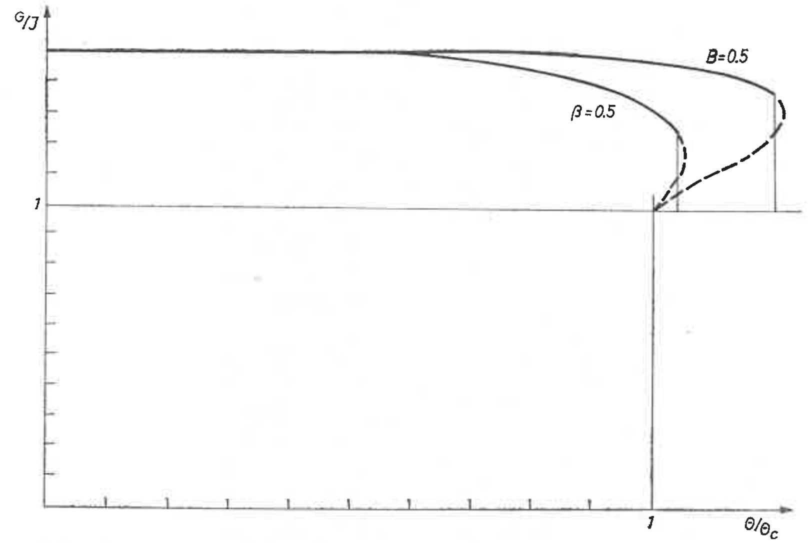

Fig. 3. The temperature dependence of the exchange integral for the cases of short range and long range interaction

For the case of the Ising model with the long-range interaction one may obtain also the dynamical behaviour of the order parameter $\langle s_j \rangle$ on the basis of the Glauber stochastic approach and the trial Hamiltonian method [14]. In this connection it should be noted that [14]:

(*i*) the ground state energies for the model Ising renormalized Hamiltonian with the long-range interaction and the trial Hamiltonian (8) coincide for any N, i.e. the model and trial systems have identical states with the total spin ordering;

(*ii*) Gibbs free energies per site for the model and trial systems coincide in the thermodynamical limit at any closed set

$$O = \{\theta, h : 0 \leqslant \theta < \infty, 0 \leqslant h < \infty\};$$

(*iii*) the complete sets of thermodynamical parameters for the model and trial systems asymptotically coincide (when $N \to \infty$) if they are determined as the quasiaverages [15], so the model and trial systems are thermodynamically equivalent and their Gibbs distributions in the thermodynamic limit coincide also, then the probability of the transition from the state with the spin configuration $\{s_1, \ldots, s_j, \ldots, s_N\}$ to the state $\{s_1, \ldots, -s_j, \ldots, s_N\}$ per unit time is determined by the detailed balance principle as in [14]

$$w_1(s_j) = \frac{1}{2\alpha}\left[1 - s_j \,\mathrm{th}\, \frac{\mu h + (\gamma + \beta\langle s_j\rangle^2)\langle s_j\rangle}{\theta}\right],$$

where α is a constant having the dimension of time.

Now taking into account the Pauli Master Equation we may obtain the equation of motion for the order parameter in the following form

$$2\alpha \frac{d}{dt} M(t) = -M + \mathrm{th}\, \frac{[\gamma + \beta M^2(t)]M(t) + \mu h}{\theta}; \qquad M(t) = \langle s_j(t)\rangle.$$

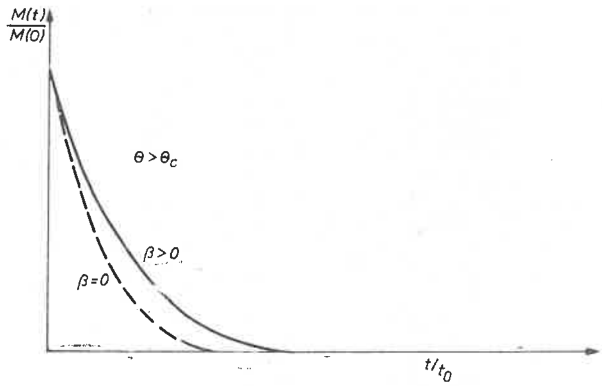

Fig. 4. The temporal dependence of the magnetization for the case of long range interaction

Its numerical solutions are presented in Fig. 4. One can see that the relaxation to the equilibrium state reduces speed with the increase of the parameter β. In other words, the influence of atomic vibrations leads to the strengthening of the stochasticity of the system under consideration.

Discussion

So, as we have shown, the renormalization of the exchange integral due to the atomic vibrations leads to the essential change of the properties of the spin subsystem near the point of the phase transition. First, the influence of the phonon subsystem may change the order of the transition. However, there is a significant difference between the two cases considered above. In the case of the nearest neighbour interaction in the planar Ising model the infinitesimally weak influence of the phonon subsystem makes the phase transition of the continuous type in the system impossible.

When we consider the system with the long-range interaction, i.e. every particle of the system interacts with all the particles with infinitesimally weak intensity, in order to change the character of the transition the phonon contribution must be sufficiently large and must be of the order of the critical temperature (it should be noted that the results for the model with long-range interaction are valid for any dimension of the lattice).

The second case is, probably, more realistic, for near the phase transition point the real potential of the interaction should have both short-range and long-range parts [16]. Moreover, the numerical computations for magnetic models [17] demonstrate that the long-range interaction leads to more adequate coincidence with the experimental data.

Since we use the harmonic approximation and restrict ourselves to the linear term in the expansion of the exchange integral with respect to the atomic displacements [4], the phonon parameter B should be thought less than the critical temperature. Therefore, we believe that the explanation of the existence of the magnets with the phase transition of the first order should not be based only on the taking into account of the phonon contribution (compare with Ref. [9]).

Alternatively, it is of interest that the introduction of term bilinear in magnetization into the exchange integral may change the critical index for magnetization in the theory of molecular field type from $\frac{1}{2}$ to $\frac{1}{4}$.

Our last result (the decrease of the speed of relaxation to equilibrium) is quite evident from the physical point of view.

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