ISING MODEL WITH TRANSVERSE FIELD IN COMPRESSIBLE LATTICE IN THE SELF-CONSISTENT FIELD APPROXIMATION. NUMERICAL RESULTS

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The Ising model in a transverse field with an account of dependence of "exchange integral" on the mutual position of atoms which changes due to thermal motion, is investigated. Using the method developed recently by Konwent and Plakida in the theory of highly anharmonic ferromagnetic crystals, the system of selfconsistent equations describing the lattice and spin subsystem in the selfconsistent phonon and molecular fields approximations, respectively, is derived and numerically analysed for some values of the model parameters. Influences of the lattice vibrations and external pressure on the spin subsystem, and of the ordering in the spin subsystem on thermal expansion of the crystal, are investigated. It is found that the phase transition remains of the second order and the coefficient of thermal expansion exhibits discontinuity at the magnetic phase transition point, which is suppressed by external pressure.

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1. Introduction

In recent years the Ising model with transverse field (IMTF) was the subject of intensive investigations by means of different approximations [1–14]. For the extensive discussion of applications and properties of this model, we refer the reader to Refs. [1, 2, 5, 6]. One usually assumes [2–5] that all spins are located at the sites of the immobile lattice. We call this model the rigid Ising model with transverse field (RIMTF).

From the formal point of view, the compressible Ising model with transverse field (CIMTF) in the harmonic and weakly anharmonic lattices was investigated in Refs. [6–11] and [12–14], respectively.

The problem of spin-lattice coupling in the Ising and Heisenberg models was the subject of numerous studies in the past, e.g. in [15–31]. In the earlier works, compiled in Ref. [15], it was assumed that the exchange integral J depends on average interatomic

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distance. If we assume that J is an analytic function of the instantaneous distance between crystal atoms, we can expand J in the Taylor series with respect to thermal displacements of atoms, cf. [27–31]. Usually, a few lowest terms of this expansion were taken into consideration, [16–25].

In Refs. [26–31], the spin models with the infinite Taylor expansion of J were studied theoretically. The aim of the present paper is to investigate the CIMTF in isotropic anharmonic lattice. There will be taken into account all terms in the Taylor series expansion of crystal potential energy and exchange integral [31] with respect to the thermal displacement of crystal atoms. This is the essential feature, which differs our theoretical treatment of CIMTF from the previous approaches. We shall not consider the dependence of tunneling integral on the thermal vibrations of lattice, cf. [11]. In order to study the CIMTF, we shall apply the formalism of the spin-phonon interaction developed by Konwent and Plakida [27–31]. In this paper we have restricted ourselves to mean field approximation MFA and mean field phonon approximation for the spin and phonon subsystem, respectively. The paper is organized as follows: in Section 2 the Hamiltonian and the basic equations are introduced. In Section 3 the model of interactions and the system of self-consistent equations SSCE are presented. In Section 4 the numerical results are given. Conclusions are summarized in Section 5.

2. *Hamiltonian and the basic equations*

The total Hamiltonian of IMTF in compressible lattice can be written in the form

$$H = \tfrac{1}{2}\sum_{n}(P_n^2M^{-1}-2\Omega S_n^x)+\tfrac{1}{2}\sum_{n,m}{}'\,[\varphi(\boldsymbol{R}_n-\boldsymbol{R}_m)-J(\boldsymbol{R}_n-\boldsymbol{R}_m)S_n^zS_m^z], \tag{1}$$

where $\boldsymbol{P}_n$, $\boldsymbol{R}_n$ are the momentum and coordinate of atom with the spin S_n^z and mass M at the lattice site n; Ω is the tunneling integral.

We introduce the thermal displacement of atoms, u_n, from the equilibrium position n [31]

$$\boldsymbol{R}_n = \langle \boldsymbol{R}_n\rangle+\boldsymbol{u}_n = \boldsymbol{n}+\boldsymbol{u}_n, \tag{2}$$

where the average value $\langle\ldots\rangle$ is taken over canonical ensemble with the Hamiltonian, (1), $\langle\ldots\rangle = \mathrm{Tr}[\ldots\exp(-\beta H)]/\mathrm{Tr}[\exp(-\beta H)]$, $\beta = (k_BT)^{-1}$. The dynamical variables obey the usual, commutation relations [30, 31]

$$[u_l^\alpha, P_{l'}^\beta] = i\delta_{ll'}\delta_{\alpha\beta}, \quad [S_l^\alpha, S_{l'}^\beta] = i\varepsilon_{\alpha\beta\gamma}\delta_{ll'}S_l^\gamma,$$
$$[u_l^\alpha, S_{l'}^\beta] = [P_l^\alpha, S_{l'}^\beta] = 0.$$

According to Konwent and Plakida [31], the equation of state for the model under consideration takes the form

$$P = -\frac{1}{6V}\sum_{n,\alpha}\left\langle\frac{\partial\varphi(\boldsymbol{R}_n-\boldsymbol{R}_0)}{\partial R_n^\alpha}-S_n^zS_0^z\,\frac{\partial J(\boldsymbol{R}_n-\boldsymbol{R}_0)}{\partial R_n^\alpha}\right\rangle n^\alpha, \tag{3}$$

where P is the isotropic external pressure. Equation (3) defines the equilibrium parameters of lattice, which depends on the temperature T, external pressure P, and the correlation function $\langle S_n^z S_0^z \rangle$. Expanding $J(R_n - R_0)$ and $\varphi(R_n - R_0)$ in Taylor series of powers of the displacements $\boldsymbol{u}_n$, we write the Hamiltonian (1) in the form

$$H = \tfrac{1}{2} \sum_n (P_n^2 M^{-1} - 2\Omega S_n^x) + \tfrac{1}{2} \sum_{l=0}^{\infty} \frac{1}{l!} \sum_{n,m}{}' \sum_{1 \ldots l} (\Phi_{n-m}^{1 \ldots l} - J_{n-m}^{1 \ldots l} S_n^z S_m^z) \boldsymbol{u}_1 \ldots \boldsymbol{u}_l, \quad (4)$$

where

$$\Phi_{n-m}^{1 \ldots l} = \prod_{i=1}^{l} (\delta_{in} - \delta_{im}) \nabla_{nm}^{\alpha_1} \ldots \nabla_{nm}^{\alpha_n} \varphi(\boldsymbol{n} - \boldsymbol{m}).$$

The analogous expression is valid for $J_{n-m}^{1 \ldots l}$ [30].

To describe the thermodynamic properties of a system, we use the self-consistent phonon approximation[1] SCPA [29–31] for the lattice subsystem and MFA for the spin subsystem. We assume the trial Hamiltonian H_0 in the form

$$H_0 = H_{\mathrm{L}} + H_{\mathrm{S}} = \tfrac{1}{2} \sum_n (P_n^2 M^{-1} - 2\Omega S_n^x) + \tfrac{1}{2} \sum_{n,m}{}' (u_n^\alpha \tilde{\Phi}_{nm}^{\alpha\beta} u_m^\beta - \tilde{J}_{nm} S_n^z S_m^z), \quad (5)$$

where $\tilde{\Phi}_{nm}^{\alpha\beta}$ and $\tilde{J}_{nm}$ are the variational parameters. The trial free energy F_1 can be written as follows:

$$F_1 = F_0 + \langle H - H_0 \rangle_0, \quad (6)$$

$$F_0 = \beta^{-1} \{ \sum_{qj} \ln [2 \sinh (0.5 \beta \omega_{qj})] - \sum_n \ln [2 \cosh (0.5 \beta H_n^*)] \}, \quad (7)$$

where ω_{qj} are the solution of equations

$$e_{qj}^\alpha \omega_{qj}^2 = (MN)^{-1} \sum_{ll'\beta} e_{qj}^\beta \tilde{\Phi}_{ll'}^{\alpha\beta} \exp[-i\boldsymbol{q}(\boldsymbol{l} - \boldsymbol{l}')] \quad (8)$$

and

$$H_n^* = [\Omega^2 + (\sum_j \tilde{J}_{nj} \langle S_j^z \rangle)^2]^{1/2}. \quad (9)$$

The mean values of spin in ordered phase (OP), in MFA, are equal to

$$\langle S_n^x \rangle = \tfrac{1}{2} \Omega (H_n^*)^{-1} \tanh (\tfrac{1}{2} \beta H_n^*), \quad (10a)$$

$$\langle S_n^y \rangle = 0, \quad (10b)$$

$$\langle S_n^z \rangle = \tfrac{1}{2} \sum_j \tilde{J}_{nj} \langle S_j^z \rangle (H_n^*)^{-1} \tanh (\tfrac{1}{2} \beta H_n^*). \quad (10c)$$

Using the Bogolubov variational principle [29–31],

$$\frac{\delta F_1}{\delta \tilde{\Phi}_{nm}^{\alpha\beta}} = \frac{\delta F_1}{\delta \tilde{J}_{nm}} = 0 \text{ we have}$$

[1] This approximation is equivalent to pseudoharmonic approximation [27, 28].

$$\tilde{\Phi}^{\alpha\beta}_{nm} = \nabla^{\alpha}_{n}\nabla^{\beta}_{m}[\tilde{\varphi}(\boldsymbol{n}-\boldsymbol{m})-\tilde{J}(\boldsymbol{n}-\boldsymbol{m})\,\langle S^{z}_{n}\rangle_{0}\,\langle S^{z}_{m}\rangle_{0}], \tag{11}$$

$$\tilde{J}(\boldsymbol{n}-\boldsymbol{m}) = \exp\,[\tfrac{1}{2}\sum_{\alpha\beta}\langle(u^{\alpha}_{n}-u^{\alpha}_{m})\,(u^{\beta}_{n}-u^{\beta}_{m})\rangle_{0}\nabla^{\alpha}_{n}\nabla^{\beta}_{m}]J(\boldsymbol{n}-\boldsymbol{m}), \tag{12}$$

$$\tilde{\varphi}(\boldsymbol{n}-\boldsymbol{m}) = \exp\,[\tfrac{1}{2}\sum_{\alpha\beta}\langle(u^{\alpha}_{n}-u^{\alpha}_{m})\,(u^{\beta}_{n}-u^{\beta}_{m})\rangle_{0}\nabla^{\alpha}_{n}\nabla^{\beta}_{n}]\varphi(\boldsymbol{n}-\boldsymbol{m}), \tag{13}$$

$$\langle u^{\alpha}_{n}u^{\beta}_{m}\rangle_{0} = (MN)^{-1}\sum_{qj}(2\omega_{qj})^{-1}e^{\alpha}_{qj}e^{\beta}_{qj}\,\mathrm{cth}\,(\tfrac{1}{2}\,\beta\omega_{qj})\exp\,[-i\boldsymbol{q}(\boldsymbol{n}-\boldsymbol{m})]. \tag{14}$$

Substituting (11) for (8), we obtain the system of equations for the phonons frequencies. Let us note that the effective parameters of interactions φ and J, take into account the mutual influence of both subsystems [28–31]. Equations (3), (8), (10) form a closed basic system for ω_{qj}, n and $\langle S^{z}_{n}\rangle$ [29]. In the next Section we will consider this system for the chosen model of lattice and spin interactions.

3. *Model of interactions and the system of self-consistent equations (SSCE)*

In order to study the physical properties of CIMTF, we investigate the FCC lattice with the nearest-neighbour interactions. We assume, that atoms interact via the Morse potential [31]

$$\varphi(r) = D\{\exp\,[-2a(r-r_{0})]-2\exp\,[-a(r-r_{0})]\}. \tag{15a}$$

We choose the dependence of spin interactions on interatomic distances in the exponential form [29]

$$J(r) = J_{0}\exp\,[-b(r-r_{0})]. \tag{15b}$$

From (12) and (13), we get [27, 29]

$$\tilde{\varphi}(n) = D\{\exp\,[2(y-a(n-r_{0}))]-2\exp\,[\tfrac{1}{2}\,y-a(n-r_{0})]\}, \tag{15c}$$

$$\tilde{J}(n) = J_{0}\exp\left[\left(\tfrac{1}{2}\,\frac{b^{2}}{a^{2}}\right)y-b(n-r_{0})\right], \tag{15d}$$

where $y = \dfrac{a^{2}}{n^{2}}\langle[n(u_{n}-u_{0})]^{2}\rangle_{0}$ describes the correlation between displacements of atoms. Taking into account only leading terms for $\tilde{\varphi}''$ and $\tilde{J}''$, and using the Debye model for lattice vibrations [29], we obtain the following system of a self-consistent equations

$$\Delta^{2}y-\tfrac{3}{32}\,\Delta Q-\tfrac{1}{4}\,T_{0}WQF_{\mathrm{D}}[\Delta(WT_{0})^{-1}] = 0, \tag{16}$$

$$\tanh\,\{[Z^{2}+(\Gamma^{*})^{2}]^{1/2}/T^{*}\}-[Z^{2}+(\Gamma^{*})^{2}]^{1/2} = 0, \tag{17}$$

$$\Pi x^{2}-\exp\,\{2[y-A(x-1)]\}+\exp\,[\tfrac{1}{2}\,y-A(x-1)]$$

$$+\tfrac{1}{24}\,\frac{B}{A}\,WQZ^{2}\exp\left[\tfrac{1}{2}\,y\left(\frac{B}{A}\right)^{2}-B(x-1)\right] = 0. \tag{18}$$

The explicit expression for Δ reads

$$\Delta^2 = 2\exp\{2[y-A(x-1)]\}-\exp[\tfrac{1}{2}y-A(x-1)]$$
$$-\tfrac{1}{24}\left(\frac{B}{A}\right)^2 WQZ^2\exp\left[\tfrac{1}{2}\left(\frac{B}{A}\right)^2 y-B(x-1)\right]. \tag{19}$$

It has been introduced in (16)–(18) the following dimensionless variables: $x = n/r_0$, $z = 2\langle S^z\rangle$, $A = ar_0$, $B = br_0$, $T_c^0 = 3J_0$, $T_0 = T/T_c^0$, $W = T_c^0/T_D$, $Q = T_D/D$, $\Gamma_0 = \Omega/6J_0$, $\Pi = Pr_0^2(4.2^{1/2}Da)^{-1}$, $\Gamma^* = \Gamma_0\exp[2(x-y-1)]$, $T^* = T_0\exp[2(x-y-1)]$, T_D and F_D are respectively, the temperature and the Debye function

$$F_D(x) = 3\cdot x^{-3}\int_0^x t^3[\exp(t)-1]^{-1}dt.$$

Let us mention, that A, B, W, Q, Γ_0 are the external parameters of a model. We use the units ,where $n = k_B = 1$. Equations (16)–(18) form the algebraic, nonlinear system of equaions, which we solve numerically using standard methods [32, 33].

4. *Numerical results*

First we consider the case $z = \Pi = 0$. Then

$$x = n/r_0 = 1.0+1.5\cdot(y/A) \tag{20}$$

and equations (16)–(18) become greatly reduced. In this case, equation (16) is solved numerically for y only. The results of calculation for different, fixed values $Q = T_D/D$ are presented in Fig. 1a. They can be interpreted, if we consider two limiting cases:

1°. For $T \ll T_D$, $F_D(\Delta\cdot T_D/T) \simeq 0.0$ and $y \simeq 0.094\ Q$. These estimated values of y agree very well with the values obtained numerically.

2°. For $T \gg T_D$, we have $\exp(y) \simeq 4T_D y(QT)^{-1}$. When T is increasing the plots of both sides intersects at higher values of y. On the other hand, Eq. (16) for sufficiently high T has not any real solution.

For $Q \ll 1.0$, $\log_{10}(y)$ is a linear function of $\log_{10}(T/T_D)$. This indicates power dependence between y and T/T_D. For $Q = 0.001$ and $500 \leqslant T/T_D \leqslant 1.0$, we obtain: $y = 0.288\,[(T/T_D)\,10^{-3}]^{0.99}$, whereas for $Q = 0.01$, $50 \leqslant T/T_D \leqslant 1.0$, $y = 0.288\,[(T/T_D)10^{-2}]^{1.05}$. The obtained values of y can be now used to obtain the plots of x (20) versus T. From (20) we see, that with A increased, the lattice becomes more rigid. From the above it follows that for $\Pi = z = 0$ $(\partial y/\partial T)_Q > 0$ and $(\partial y/\partial Q)_T > 0$. Moreover, according to (20) we have $(\partial x/\partial T)_{Q,A} \geqslant 0$, $(\partial x/\partial Q)_{T,A} \geqslant 0$ and $(\partial x/\partial A)_{Q,T} < 0$. We notice, that the above results are the starting point for further numerical calculations. We choose the following values of the external parameters

$$A = 1.0,\quad B = 2.0,\quad W = 5.0,\quad Q = 0.1,\quad \Gamma_0 = 0.1. \tag{21}$$

In the numerical calculations T_0 varies from 0.0 to 2.0 and Π from 0.0 to 0.6. For $T^* < 1$, equations (16)–(18) were solved and for $T^* > 1$ only two first equations were solved at

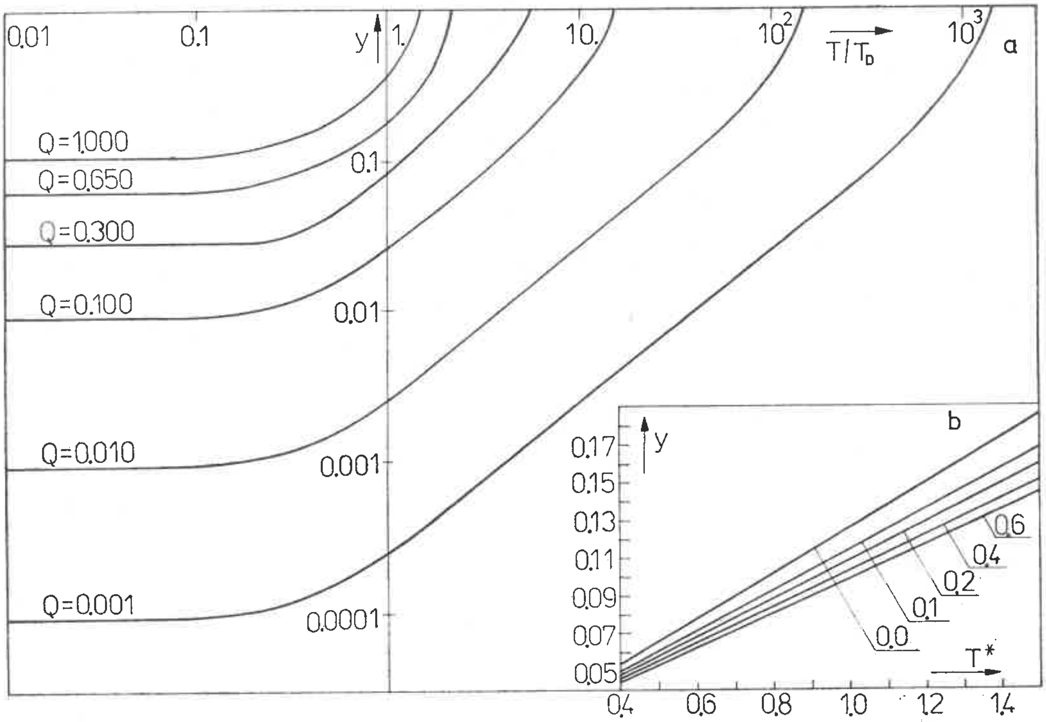

Fig. 1a. The $\log_{10}$–$\log_{10}$ plots of solutions for y, calculated from Eq. (16), against T/T_D for $\Pi = z = 0.0$. The actual values of Q are marked on each curve; b. The plots of numerical solutions of Eqs. (16)–(18): the values of y versus T^* for certain values of Π

$z = 0.0$. The plots of y versus T for a few values of Π in ordered (OP) and disordered (DP) phases have been given in Fig. 1b. The very weak influence of phase transition on the behaviour of y was observed in spin subsystem. The influence of $z \neq 0$ on y in OP is so weak, that it cannot be demonstrated in the scale used in Fig. 1b. More interesting results are shown in Fig. 2, where the dependences of $z = 2\langle S^z\rangle$ and $x = n/r_0$ on T^* for different of Π are demonstrated. In OP, $x = n/r_0$ depends strongly on $\langle S^z\rangle$. The value of x decreases in OP when compared its value in DP, owing to an appearance of $z \neq 0$ in ordered phase. Besides, x increases rapidly and approaches its value in DP in the vicinity of the phase transitin point. We notice, that x decreases with increasing Π. It should be added that increasing of Π causes the flatting of the curve shapes of n/r_0 near the Curie temperature T_c. In Fig. 3a we have illustrated the changes in the coefficient of thermal expansion, α

$$\alpha^* = [x(T_2^*) - x(T_1^*)]/[x(T_1^*)\,(T_2^* - T_1^*)]. \tag{22}$$

As was expected in Refs. [8, 18, 29] α^* jumps down at the phase transition point, and the magnitude of this jump decreases with increasing Π. The plots of $z = 2\langle S^z\rangle$ versus T have the same shape for the all Π just as in Fig. 2. This is a little misleading result. From

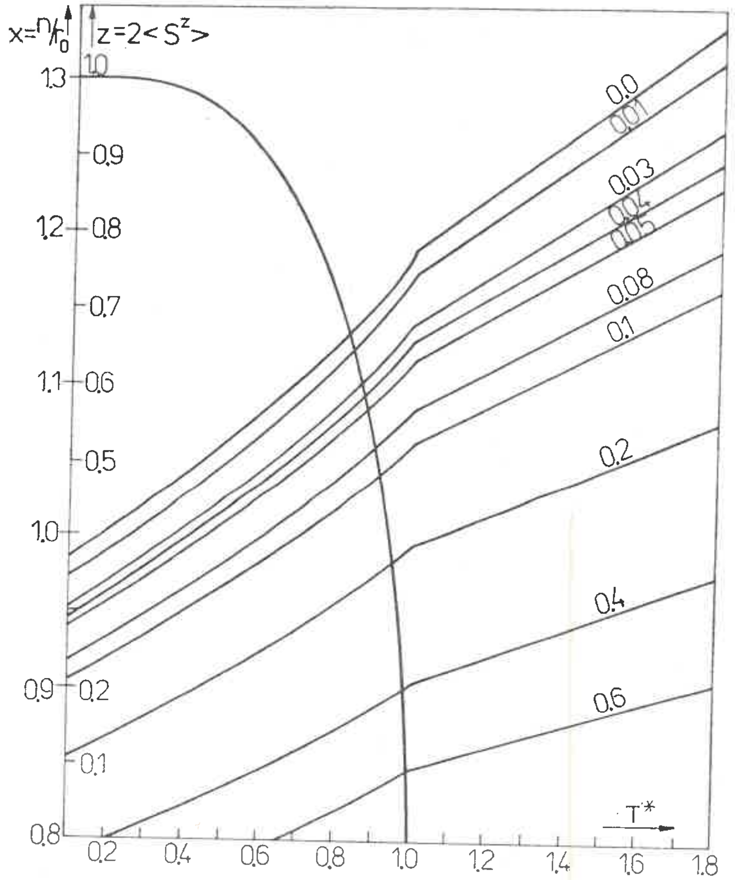

Fig. 2. The plots of numerical solutions of Eqs. 16)–(18): the values of $z = 2\langle S^z \rangle$ and $x = n/r_0$ against T^* for different fixed Π

Fig. 2 it seems that T_c is the same for the all Π. In fact T_c increases with Π, i.e. $(\partial T_c/\partial \Pi) > 0$, because of the explicit dependence of effective exchange integral $J(n)$ on x and y $J(n) = J_0 \exp [2(y+1-x)]$. For $\Gamma_0 > 0.5$, we can presumably obtain the different dependences of z on T for different Π, but this suggestion ought to be verified. For the qualitative discussion of the influences Γ_0, x and y on $\langle S^z \rangle$ we have performed the series of calculations, in which the equation (18) was solved only, for z at fixed, different values of Γ_0, x and y. In Fig. 3b we present some results of these calculations for values of Γ_0, x and y listed in Table I.

5. Discussion

In this paper we have presented results of numerical calculations for the compressible Ising model with transverse field. Using the standard numerical methods [32, 33], we have solved the system of the self-consistent equation (16)–(18) [29] for the certain values

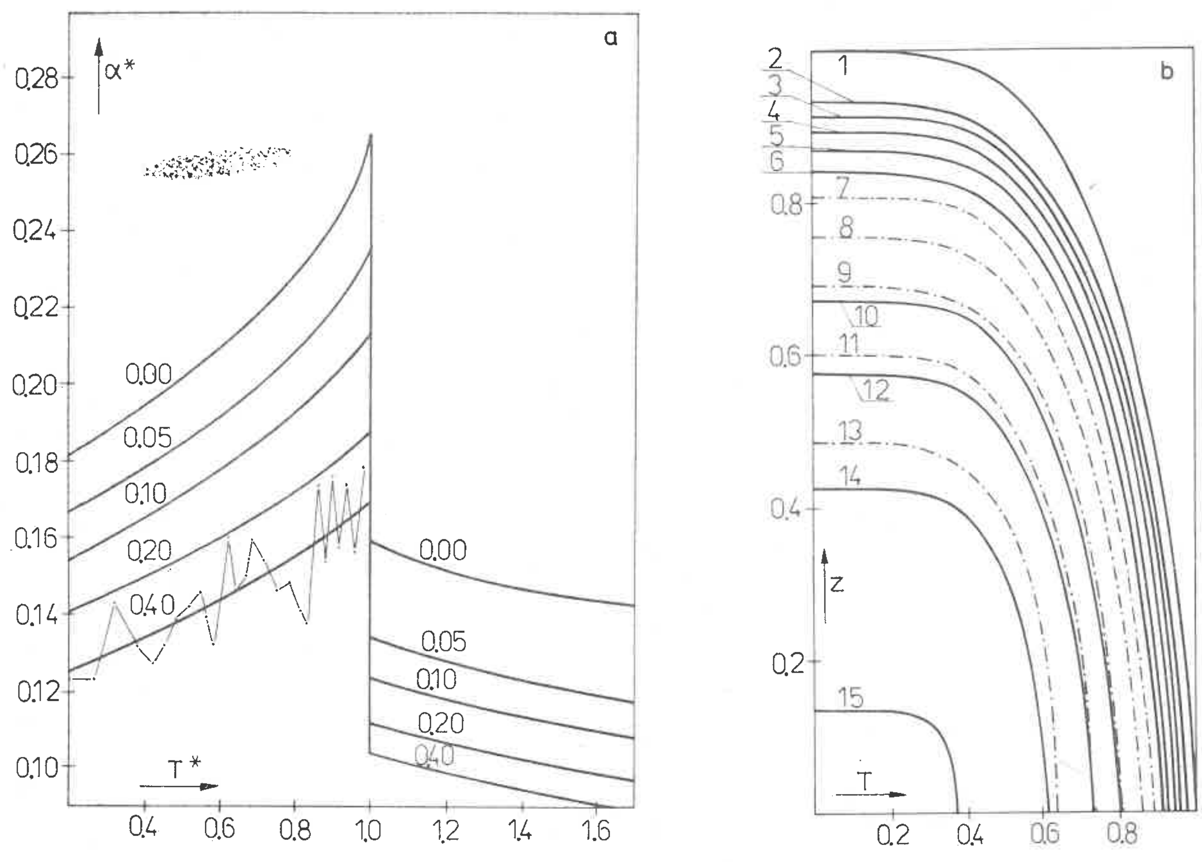

Fig. 3a. The plots of the coefficient of thermal expansion α^* against T^* for several fixed Π

Fig. 3b. The solutions of (18) for $z = 2\langle S^z \rangle$ versus T^* The numbers on the curves indicate the actual fixed values of x, y, Γ_0 in accordance with Table I

TABLE I

The number of curves	Γ_0	x	y
1	0.1	all combination	all combination
2	0.5	0.950	0.100
3	0.5	1.000 0.950	0.100 0.050
4	0.5	0.950 1.000 1.050	0.005 0.050 0.100
5	0.5	1.000 1.050	0.005 0.050
6	0.5	1.050	0.005
7	0.8	0.950	0.100
8	0.8	0.950 1.000	0.050 0.100
9	0.8	0.950 1.000 1.050	0.005 0.050 0.100
10	1.0	0.950	0.100
11	0.8	1.000 1.050	0.005 0.050
12	1.0	1.000 0.950	0.100 0.050
13	0.8	1.050	0.005
14	1.0	0.950 1.000 1.050	0.005 0.050 0.100
15	1.0	1.000	0.005

of model parameters A, B, Γ_0, Q, W in the wide range of reduced pressure Π and reduced temperature T^*.

The main results of the paper are as follows:

1. If the spin-phonon interaction is sufficiently weak[2], the phase transition in spin subsystem is of the second order.

2. Lattice vibration influence the properties of spin subsystem. (*i*) The Curie temperature T_c and the saturation values z_0 of the order parameter increase for the increasing values of y, whereas they decrease for the increasing values of the dimensionless interatomic distance x. This fact can be checked in Fig. 3b, e.g. for the curves labelled by 15, 14, 12 for T_c and 10, 12, 14 for z_0.

(*ii*) For $\Pi = 0.0$, T_c in CIMTF is lower than T_c^0 for RIMTF, e.g. $T_c \simeq 0.9\, T_c^0$. The Curie temperature T_c raises with increasing of Π and for $\Pi = 0.6$, $T_c \simeq 1.8\, T_c^0$. Therefore, $(\partial T_c/\partial \Pi) > 0$. In [20], it has been pointed out that the changes in T_c, for $\Pi = 0.0$ in the Ising model, depend on the range of the exchange integral. If it has the finite or infinite

[2] The value of model parameters used in our calculation are in the range of the second order phase transition of Zagrebnov and Fedyanin's paper [26]. Such a choice of the model parameters corresponds more adequately to the real physical situation.

ranges, T_c increases [16, 18, 21, 26] or decreases [20], respectively, as compared with its value for the rigid Ising model. In CIMTF the exchange integral has just an infinite range and the obtained changes in T_c for $\Pi = 0$ are in agreement with the results of Refs. [20, 29].

From our calculations it follows, that the Curie temperature T_c for CIMTF increases with the increasing of pressure. The same effect was first predicted by Konwent [29] for the compressible Heisenberg model.

In Section 3, it has been shown that dimensionless temperature is equal to $T^* = (T/3J_0) \exp[2(x-y-1)] \simeq T_c^0 \exp[2(x-y-1)]$ as $\Omega^2 \ll J^2$. We see that changes

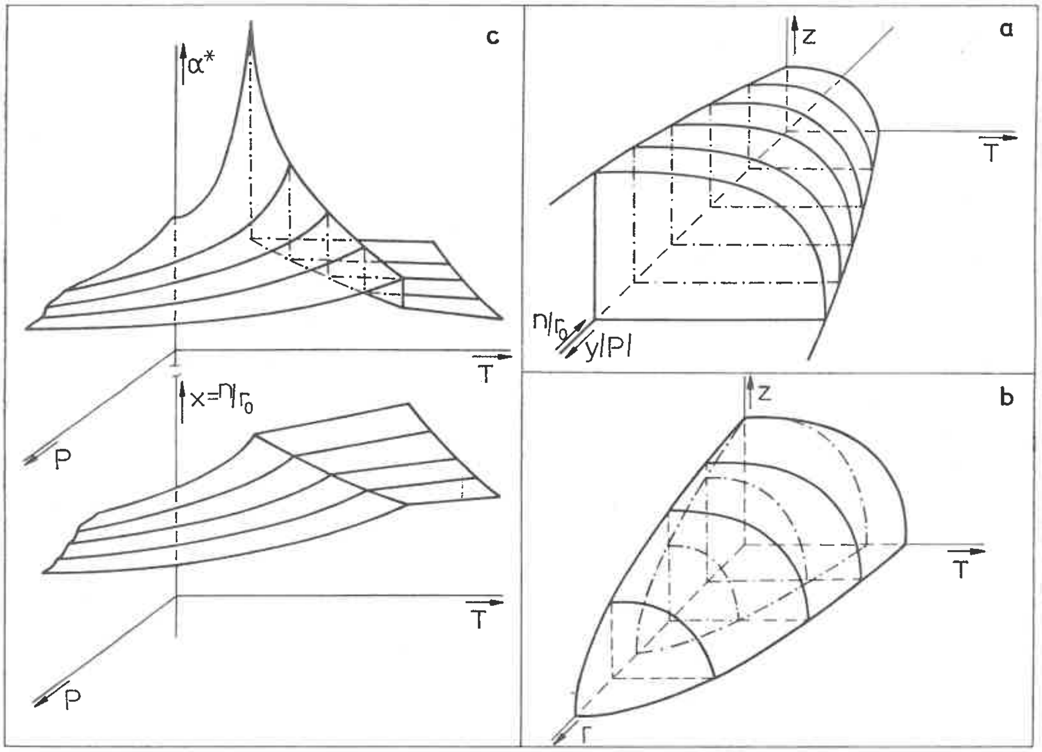

Fig. 4a. The qualitative picture of changes in z versus (T, y) or $(T, n/r_0)$ or (T, P); b. The qualitative presentations of the ordered phases (OP); for the RIMTF — the OP is placed under the surface, of which the cross-sections are marked as the point-dotted lines. For the CIMTF — the OP is placed under the surface, of which the cross-sections are marked as the solid lines; c. The qualitative picture of changes in α^* and n/r_0 versus T and P

in T_c are the results of competition between the temperature and pressure dependences of x and y. From the numerical calculations presented in Section 4 it follows, that in the vicinity of phase transition point for $\Pi > 0$, $x-y > 1.0$ and therefore $x-y-1 = c_1 > 0.0$ and $T = T_c^0 \exp(c_1)$, i.e. $T_c < T_c^0$. As x depends more strongly on Π than y when Π is increasing, we have $x-y < 1.0$. Thus, $x-y-1 = c_2 < 0.0$ and $T = T_c^0 \exp(c_2)$, i.e. $T_c > T_c^0$. The above conclusions are illustrated qualitatively in Fig. 4a.

3. The Curie temperature T_c and the saturation value z_0 of the order parameter for the rigid moddel [1, 2, 5, 6, 11] as well as for the compressible Ising model with transverse field [7, 11, 13] are the decreasing functions of Γ_0 i.e. $(\partial z_0/\partial \Gamma_0) < 0$ and $(\partial T_c/\Gamma_0) < 0$. However, for CIMTF the ordered can exist for $\Gamma_0 > 1.0$, whereas for RIMTF $T_c^0 = 0.0$ if $\Gamma_0 = 1.0$. This is a qualitatively new result, and it is the manifestation of the influences of x and y on T_c. It has been discussed above. This conclusion is presented qualitatively in Fig. 4b.

4. The appearance of z different from zero decreases the values of $x = n/r_0$ [29]. The influence of z on x is important for T near T_c and leads to discontinuity in the coefficient of thermal expansion at the transition point. We have shown this in Fig. 4c.

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