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INVESTIGATION OF THE SPIN-ONE ISING MODEL WITH BIQUADRATIC EXCHANGE INTERACTION WITHIN FUNCTIONAL INTEGRATION METHOD

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Spin-one Ising model with biquadratic exchange interaction is investigated within functional integration approach. Free energy in the approximation following random phase approximation (RPA) is calculated. Expression for ferromagnetic ordering temperature in RPA is obtained. Phase diagram of the system is studied by means of the free energy expansion. System's properties dependence on the ratio of bilinear to biquadratic exchange interaction constants is discussed. Structurally disordered model is considered. Ferromagnetic transition temperature change caused by structural disorder is found. Results of numerical simulations for hard core system's structural factors are presented.

Systems with both dipolar and quadrupolar types of interactions are now of current theoretical interest. Adequate examination of many magnetic systems also required more intricate than routine Ising and Heisenberg spin models to be considered. In ferromagnets and antiferromagnets the importance of biquadratic exchange interaction and its influence on the magnetic properties have been studied by many authors (rather detailed list of reference articles can be found in [1-3]. In this investigations the discussion mostly has been focused on regular Heisenberg ferromagnets. In the present paper we consider both structurally ordered and disordered spin-one Ising models with bilinear and biquadratic exchange interactions, using the functional integration formalism developed by one of the authors in cooperation with his collaboratours in [4-6]. Such approach allowed earlier to obtain important results in physics of magnetism more quickly and easily comparing with other methods.

Model

We consider the system with Hamiltonian of the form:

$$H = H_0 + H_{int}. \tag{1}$$

Term

$$H_{int} = -\frac{\lambda_1}{2}\sum_{\substack{i=1\\ i\neq j}}^{N}\sum_{j=1}^{N} J(|\mathbf{R}_i - \mathbf{R}_j|)S_i^z S_j^z - \frac{\lambda_2}{2}\sum_{\substack{i=1\\ i\neq j}}^{N}\sum_{j=1}^{N} J(|\mathbf{R}_i - \mathbf{R}_j|)Q_i^0 Q_j^0 \quad (2)$$

describes bilinear $\lambda_1 J(|\mathbf{R}_i - \mathbf{R}_j|)$ and biquadratic $\lambda_2 J(|\mathbf{R}_i - \mathbf{R}_j|)$ exchange interactions of the two atoms with spins S^z, localized in the sites of the crystal lattice with radius-vectors $\mathbf{R}_i$ and $\mathbf{R}_j$; $i, j = 1, ...N$; N is the number of the lattice sites. The quadrupolar operator in the case $S = 1$ is given by

$$Q_i^0 = \sqrt{3}\left[(S_i^z)^2 - 2/3\right]. \quad (3)$$

Reference system's hamiltonian

$$H_0 = -h\sum_{i=1}^{N} S_i^z - \Omega\sum_{j=1}^{N} Q_i^0 \quad (4)$$

describes the interaction of ideal system of spins and quadrupoles with the external magnetic field directed along z-axis and with the field of the single-ion anisotropy type affecting on quadrupoles. It is convenient to rewrite (2) in the form:

$$H_{int} = -\frac{1}{2}\sum_{\substack{i=1\\ i\neq j}}^{N}\sum_{j=1}^{N} J(|\mathbf{R}_i - \mathbf{R}_j|)\hat{L}_i\hat{L}_j, \quad (5)$$

here

$$\hat{L}_i\hat{L}_j = \sum_{\alpha=1}^{2} L_i^{(\alpha)}L_j^{(\alpha)}, \quad (6)$$

$$L_i^{(1)} = \sqrt{\lambda_1}S_i^z, \quad L_i^{(2)} = \sqrt{\lambda_2}Q_i^0. \quad (7)$$

After the Fourier-transformation in (5) we obtain for H_{int}:

$$H_{int} = -\frac{1}{2}\sum_{\mathbf{k}} \nu(k)\hat{L}_{\mathbf{k}}\hat{L}_{-\mathbf{k}}, \quad (8)$$

where Fourier-image of exchange integral

$$\nu(k) = \sum_{j=1}^{N} J(|\mathbf{R}_j|)e^{-\imath\mathbf{k}\mathbf{R}_j}, \quad (9)$$

wave vectors $\mathbf{k}$ belong to the first Brillouin zone;

$$\hat{L}_{\mathbf{k}} = \frac{1}{\sqrt{N}}\sum_{j=1}^{N} \hat{L}_j e^{-\imath\mathbf{k}\mathbf{R}_j}. \quad (10)$$

Free energy functional

Using well-known Stratonovich-Hubbard transformation and approach developed in [4-6] we obtain partition function of the system as the functional integral:

$$Z = \exp\Big(-\beta F_0\Big)\int (d\varphi)\exp\Big(F[\varphi]\Big), \tag{11}$$

here β is the inverse temperature; free energy of the reference system reads:

$$F_0 = -\frac{1}{\beta}\ln \mathrm{Sp}\exp\Big(-\beta H_0\Big); \tag{12}$$

integration is carried out over the real and imaginary parts of functional variables $\varphi_{\mathbf{k}}^{(\alpha)}$, conjugated to operators $L_{\mathbf{k}}^{(\alpha)}$:

$$\int (d\varphi) = \prod_{\alpha=1}^{2}\int_{-\infty}^{\infty} d\varphi_0^{(\alpha)}/\sqrt{2\pi}\prod_{\mathbf{k}\neq 0}{}'\int_{-\infty}^{\infty} d\varphi_{\mathbf{k}}^{(\alpha),c}/\sqrt{\pi}\int_{-\infty}^{\infty} d\varphi_{\mathbf{k}}^{(\alpha),s}/\sqrt{\pi}, \tag{13}$$

a prime near sign of product means that the wave vector $\mathbf{k} > 0$. Free energy functional reads

$$F[\varphi] = -\frac{1}{2}\sum_{\mathbf{k}}\hat{\varphi}_{\mathbf{k}}\hat{\varphi}_{-\mathbf{k}} + F_1[\varphi], \tag{14}$$

where

$$F_1[\varphi] = \ln\Big\langle \exp\Big\{\sum_{\mathbf{k}}\sqrt{\beta\nu(k)}\hat{\varphi}_{\mathbf{k}}\hat{L}_{-\mathbf{k}}\Big\}\Big\rangle_0 \tag{15}$$

and angle brackets $\Big\langle(...)\Big\rangle_0$ means averaging over the reference system

$$\Big\langle(...)\Big\rangle_0 = \mathrm{Sp}\exp\Big(-\beta H_0\Big)(...)/\mathrm{Sp}\exp\Big(-\beta H_0\Big). \tag{16}$$

Using cumulant expansion functional $F_1[\varphi]$ can be represented in the form of the functional series over $\varphi_{\mathbf{k}}^{(\alpha)}$

$$F_1[\varphi] = \sum_{l\geq 1}\frac{N^{1-l/2}}{l!}\sum_{\mathbf{k}_1\alpha_1}\cdots\sum_{\mathbf{k}_l\alpha_l}\mathcal{M}_{\alpha_1\ldots\alpha_l}(\mathbf{k}_1\ldots\mathbf{k}_l)\times$$
$$\times\sqrt{\beta\nu(k_1)\ldots\beta\nu(k_l)}\varphi_{\mathbf{k}_1}^{(\alpha_1)}\ldots\varphi_{\mathbf{k}_l}^{(\alpha_l)}, \tag{17}$$

coefficient functions $\mathcal{M}_{\alpha_1\ldots\alpha_l}(\mathbf{k}_1\ldots\mathbf{k}_l)$ are irreducible averages of the operators $L_{\mathbf{k}}^{(\alpha)}$ (symbols "c" means irreducible (cumulant) average):

$$\mathcal{M}_{\alpha_1\ldots\alpha_l}(\mathbf{k}_1\ldots\mathbf{k}_l) = N^{l/2-1}\Big\langle L_{\mathbf{k}_1}^{(\alpha_1)}\ldots L_{\mathbf{k}_l}^{(\alpha_l)}\Big\rangle_0^c =$$
$$= \delta(\mathbf{k}_1\ldots+\mathbf{k}_l)\Big\langle L_{j_1}^{(\alpha_1)}\ldots L_{j_l}^{(\alpha_l)}\Big\rangle_0^c \equiv \delta(\mathbf{k}_1\ldots+\mathbf{k}_l)\mathcal{M}_{\alpha_1\ldots\alpha_l}. \tag{18}$$

So with (11-18) free energy of the system can be represented as a functional integral:

$$F = F_0 - \frac{1}{\beta}\ln\int (d\varphi)\exp\Big(F[\varphi]\Big). \tag{19}$$

Calculation of the free energy

Let us calculate F_0 and coefficient functions. For the free energy of reference system is easy to obtain:

$$F_0 = \frac{N}{\beta}\frac{2\Omega\beta}{\sqrt{3}} - \frac{N}{\beta}\ln\left\{2\exp\left(\beta\Omega\sqrt{3}\right)\mathrm{ch}(\beta h)+1\right\}. \tag{20}$$

Formally generalizing (20) onto the case of nonhomogeneous fields h_i and Ω_i , we have

$$\left\langle L_i^{(1)}\right\rangle_0 = \sqrt{\lambda_1}\left\langle S_i^z\right\rangle_0, \quad \left\langle L_i^{(2)}\right\rangle_0 = \sqrt{\lambda_2}\left\langle Q_i^0\right\rangle_0 \tag{21}$$

and further:

$$\begin{aligned}
\left\langle S_i^z\right\rangle_0 &= \frac{1}{\beta}\frac{\partial}{\partial h_i}\Big(-\beta F_0[h_i,\Omega_i]\Big)|_{h_i\equiv h} \equiv M_1(h,\Omega),\\
\left\langle Q_i^0\right\rangle_0 &= \frac{1}{\beta}\frac{\partial}{\partial \Omega_i}\Big(-\beta F_0[h_i,\Omega_i]\Big)|_{\Omega_i\equiv\Omega} \equiv M_2(h,\Omega),\\
\left\langle S_{i_1}^z S_{i_2}^z\right\rangle_0^c &= \frac{1}{\beta^2}\frac{\partial}{\partial h_{i_1}}\frac{\partial}{\partial h_{i_2}}\Big(-\beta F_0[h_i,\Omega_i]\Big)|_{h_i\equiv h} = M_{11}(h,\Omega)\delta_{i_1,i_2},\\
\left\langle S_{i_1}^z Q_{i_2}^0\right\rangle_0^c &= \frac{1}{\beta^2}\frac{\partial}{\partial h_{i_1}}\frac{\partial}{\partial \Omega_{i_2}}\Big(-\beta F_0[h_i,\Omega_i]\Big)|_{h_i\equiv h,\Omega_i\equiv\Omega} = M_{12}(h,\Omega)\delta_{i_1,i_2}
\end{aligned} \tag{22}$$

and so on. We present here the expressions only for cumulants of the first and second order, which appeared in the expression for free energy in random phase (Gaussian) approximation:

$$M_1(h,\Omega) = \frac{2e^{\beta\Omega\sqrt{3}}\mathrm{sh}(\beta h)}{2e^{\beta\Omega\sqrt{3}}\mathrm{ch}(\beta h)+1}, \tag{23}$$

$$M_2(h,\Omega) = -\frac{2}{\sqrt{3}} + \frac{2\sqrt{3}e^{\beta\Omega\sqrt{3}}\mathrm{ch}(\beta h)}{2e^{\beta\Omega\sqrt{3}}\mathrm{ch}(\beta h)+1}, \tag{24}$$

$$M_{11}(h,\Omega) = \frac{2}{3} + \frac{1}{\sqrt{3}}M_2(h,\Omega) - M_1^2(h,\Omega), \tag{25}$$

$$M_{22}(h,\Omega) = \frac{2}{3} - \frac{1}{\sqrt{3}}M_2(h,\Omega) - M_2^2(h,\Omega), \tag{26}$$

$$M_{12}(h,\Omega) = \frac{1}{\sqrt{3}}M_1(h,\Omega) - M_1(h,\Omega)M_2(h,\Omega). \tag{27}$$

We note here that in the case $h\to 0, \Omega\to 0$ all irreducible averages containing odd number of indices "1" ($M_1(0,0)$, $M_{12}(0,0)$, $M_{111}(0,0)$, $M_{122}(0,0)$...) are equal to zero. Among cumulants from the first to the fourth order (which will be used for free energy analysis) only the following are nonzero ones:

$$\begin{aligned}
&M_{11}(0,0) = \frac{2}{3}, \quad M_{22}(0,0) = \frac{2}{3},\\
&M_{112}(0,0) = \frac{2}{3\sqrt{3}}, \quad M_{222}(0,0) = -\frac{2}{3\sqrt{3}},\\
&M_{1111}(0,0) = -\frac{2}{3}, \quad M_{1122}(0,0) = -\frac{2}{9}, \quad M_{2222}(0,0) = -\frac{2}{3}.
\end{aligned} \tag{28}$$

Let us rewrite free energy functional (14) in the form:

$$F[\varphi] = F_G[\varphi] + \Delta F[\varphi] = F_G[\varphi] + \sum_{l\geq 3} F_1^{(l)}[\varphi], \tag{29}$$

where Gaussian functional reads

$$F_G[\varphi] = -\frac{1}{2}\sum_{\mathbf{k}} \hat{\varphi}_{\mathbf{k}}\hat{\varphi}_{-\mathbf{k}} + F_1^{(2)}[\varphi] =$$
$$= \frac{1}{2}\sum_{\mathbf{k}} \beta\nu(k)\Big\{\lambda_1 M_{11}(h,\Omega)\varphi_{\mathbf{k}}^{(1)}\varphi_{-\mathbf{k}}^{(1)} + \lambda_2 M_{22}(h,\Omega)\varphi_{\mathbf{k}}^{(2)}\varphi_{-\mathbf{k}}^{(2)} +$$
$$+\sqrt{\lambda_1\lambda_2}M_{12}(h,\Omega)\Big(\varphi_{\mathbf{k}}^{(1)}\varphi_{-\mathbf{k}}^{(2)} + \varphi_{\mathbf{k}}^{(2)}\varphi_{-\mathbf{k}}^{(1)}\Big)\Big\}, \tag{30}$$

and

$$F_1^{(l)}[\varphi] = \frac{N^{1-l/2}}{l!}\sum_{\mathbf{k}_1\alpha_1} \ldots \sum_{\mathbf{k}_l\alpha_l} \mathcal{M}_{\alpha_1\ldots\alpha_l}(\mathbf{k}_1,\ldots\mathbf{k}_l) \times$$
$$\times\sqrt{\beta\nu(k_1)\ldots\beta\nu(k_l)}\varphi_{\mathbf{k}_1}^{(\alpha_1)}\ldots\varphi_{\mathbf{k}_l}^{(\alpha_l)}. \tag{31}$$

Considering non-Gaussian part of the functional integral as a small perturbation free energy can be represented as:

$$F = F_{mol} + F_G + \Delta F. \tag{32}$$

Component F_{mol} is obtained by integration the term with $l = 1$ in (31), also self-consistent fields y_1 and y_2 must be singled out with next substitution in expressions for F_0 and cumulants:

$$\beta h \to y_1 = \beta h + \beta\lambda_1\nu(0)\langle S^z\rangle, \tag{33}$$

$$\beta\Omega \to y_2 = \beta\Omega + \beta\lambda_2\nu(0)\langle Q^0\rangle, \tag{34}$$

$$F_0[h,\Omega] \to F_0[y_1,y_2]; \quad M_{\alpha_1\ldots\alpha_l}(h,\Omega) \to M_{\alpha_1\ldots\alpha_l}(y_1,y_2), \tag{35}$$

where $\langle\ldots\rangle$ means statistical averaging over Gibbs distribution with Hamiltonian (1). Finally

$$F_{mol} = \frac{N}{\beta}\frac{2y_2}{\sqrt{3}} - \frac{N}{\beta}\ln\Big\{2\exp(y_2\sqrt{3})\mathrm{ch}y_1 + 1\Big\} +$$
$$+\frac{N}{\beta}\frac{(y_1-\beta h)^2}{2\alpha_1(0)} + +\frac{N}{\beta}\frac{(y_2-\beta\Omega)^2}{2\alpha_2(0)}, \tag{36}$$

here

$$\alpha_1(k) \equiv \lambda_1\beta\nu(k), \quad \alpha_2(k) \equiv \lambda_2\beta\nu(k). \tag{37}$$

Integrating (19) with $F[\varphi] = F_G[\varphi]$, we obtain contribution into free energy in Gaussian approximation:

$$F_G = \frac{1}{2\beta}\sum_{\mathbf{k}}\ln\Big((1-\alpha_1(k)M_{11}(y_1,y_2)) \times (1-\alpha_2(k)M_{22}(y_1,y_2)) -$$
$$-\alpha_1(k)\alpha_2(k)M_{12}^2(y_1,y_2)\Big). \tag{38}$$

Contribution into free energy from non-Gaussian part of functional $\Delta F[\varphi]$ is taken into account by means of the expansion over the Gaussian moments with renormalized interaction. In the approximation following RPA, so called "two sums over k" approximation (corresponding second order of the perturbation theory over the cube of inverse effective exchange interaction range) we obtain:

$$F = \frac{N}{\beta}\frac{2y_2}{\sqrt{3}} - \frac{N}{\beta}\ln\left\{2\exp(y_2\sqrt{3})\mathrm{ch}y_1 + 1\right\} + \frac{N}{\beta}\frac{(y_1-\beta h)^2}{2\alpha_1(0)} +$$
$$+\frac{N}{\beta}\frac{(y_2-\beta\Omega)^2}{2\alpha_2(0)} + \frac{1}{2\beta}\sum_{\mathbf{k}}\ln\Big((1-\alpha_1(k)M_{11}(y_1,y_2))\times$$
$$\times(1-\alpha_2(k)M_{22}(y_1,y_2)) - \alpha_1(k)\alpha_2(k)M_{12}^2(y_1,y_2))\Big) -$$
$$-\frac{1}{\beta}\frac{M_{1111}(y_1,y_2)}{8N}\sum_{\mathbf{k}_1}\sum_{\mathbf{k}_2} g_1(k_1)g_2(k_2) -$$
$$-\frac{1}{\beta}\frac{M_{2222}(y_1,y_2)}{8N}\sum_{\mathbf{k}_1}\sum_{\mathbf{k}_2} g_2(k_1)g_2(k_2) -$$
$$-\frac{1}{\beta}\frac{M_{1122}(y_1,y_2)}{4N}\sum_{\mathbf{k}_1}\sum_{\mathbf{k}_2} g_1(k_1)g_2(k_2) -$$
$$-\frac{1}{\beta}\frac{M_{111}^2(y_1,y_2)}{12N}\sum_{\mathbf{k}_1}\sum_{\mathbf{k}_2}\sum_{\mathbf{k}_3} g_1(k_1)g_1(k_2)g_1(k_3)\delta(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3) -$$
$$-\frac{1}{\beta}\frac{M_{222}^2(y_1,y_2)}{12N}\sum_{\mathbf{k}_1}\sum_{\mathbf{k}_2}\sum_{\mathbf{k}_3} g_2(k_1)g_2(k_2)g_2(k_3)\delta(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3) -$$
$$-\frac{1}{\beta}\frac{M_{112}^2(y_1,y_2)}{4N}\sum_{\mathbf{k}_1}\sum_{\mathbf{k}_2}\sum_{\mathbf{k}_3} g_1(k_1)g_1(k_2)g_2(k_3)\delta(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3) -$$
$$-\frac{1}{\beta}\frac{M_{122}^2(y_1,y_2)}{4N}\sum_{\mathbf{k}_1}\sum_{\mathbf{k}_2}\sum_{\mathbf{k}_3} g_1(k_1)g_2(k_2)g_2(k_3)\delta(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3), \quad (39)$$

where

$$g_1(k) = \frac{\alpha_1(k)}{1-\alpha_1(k)M_{11}(y_1,y_2)}, \quad g_2(k) = \frac{\alpha_2(k)}{1-\alpha_2(k)M_{22}(y_1,y_2)}. \quad (40)$$

Landau free energy expansion

We first restrict ourselves to molecular field approximation and so consider the first four terms in the expression (39) for free energy. From the conditions $\frac{\partial F}{\partial y_1} = 0$ and $\frac{\partial F}{\partial y_2} = 0$ we obtain the system of self-consistent equations:

$$\langle S^z\rangle = \frac{2e^{y_2\sqrt{3}}\mathrm{sh}y_1}{2e^{y_2\sqrt{3}}\mathrm{ch}y_1 + 1}, \quad \langle Q^0\rangle = -\frac{2}{\sqrt{3}} + \frac{2\sqrt{3}e^{y_2\sqrt{3}}\mathrm{ch}y_1}{2e^{y_2\sqrt{3}}\mathrm{ch}y_1 + 1}. \quad (41)$$

Supposing external field to be equal to zero, let us consider first some particular cases.

1) $\lambda_2 = 0$, $\Omega = 0$;

below $T_d = 2/3\lambda_1\nu(0)$ phase transition from paramagnetic to ferromagnetic state occurs; dipolar ordering ($\langle S^z\rangle \neq 0$) is accompanied by the quadrupolar one ($\langle Q^0\rangle \neq 0$) even in the absense of biquadratic exchange as it usually takes place when multipolar moments of higher rank are taken into consideration [7].

2) $\lambda_2 = 0$, $\Omega \neq 0$;

for transition temperature into ferromagnetic state we obtain the following equation:

$$T_d = \frac{2}{3}\lambda_1\nu(0)\Big(1 + \frac{\Omega}{\sqrt{3}T_d}\Big). \tag{42}$$

For small values of single-ion anisotropy parameter Ω we find immediately:

$$T_d = \frac{2}{3}\lambda_1\nu(0)\frac{\Omega}{\sqrt{3}}, \tag{43}$$

which agrees with known results. From equations (41) under this conditions followes also possibility of transition to a state of nonzero quadrupolar but zero magnetic order in the system with only bilinear exchange interaction and single-ion anisotropy; the last fact was noted earlier, e. g. [8].

3) $\lambda_1 = 0$;

supposing $\Omega = 0$, we obtain transition temperature into the state with $\langle S^z\rangle = 0$, $\langle Q^0\rangle \neq 0$ (quadrupolar phase):

$$T_Q = \frac{2}{3}\lambda_2\nu(0). \tag{44}$$

We now come back to the general situation (equations (41)). Supposing $h = 0$, $\Omega = 0$ and $y_1 \to 0$, $y_2 \to 0$, we find:

$$T_d = \frac{2}{3}\lambda_1\nu(0), \quad T_Q = \frac{2}{3}\lambda_2\nu(0). \tag{45}$$

Pattern of possible phase transitions is determined by ratio of bilinear and biquadratic interactions constants. In the case $\lambda_1 > \lambda_2$ below T_d transition from paramagnetic to ferromagnetic phase occurs; in the case $\lambda_1 < \lambda_2$ - transition from paramagnetic to quadrupolar phase occurs below T_d.

System (41) also was solved graphically eliminating $\langle Q^0\rangle$ from the first equation. As a result, temperature dependences of $\langle S^z\rangle$ and $\langle (S^z)^2\rangle$ for different ratious of bilinear and biquadratic exchange constants are presented by Fig. 1-2.

For further detailed analysis we shall consider Landau expansion of the free energy. An expansion is made as a function of two order parameters $m \equiv \langle S^z\rangle$ and $Q \equiv \langle Q^0\rangle$ in the vicinity of transition temperatures. Rigorously, justification of such expansion, in general, remaines under the question, because m and Q are not fully independent order parameters. Indeed, if the state with $m = 0$, $Q \neq 0$ is possible, a state with $m \neq 0$, $Q = 0$ cannot exist; as noted above, when spins are ordered, all their higher rank multipolar moments are ordered too. That's why for following analysis usual theory of models with two coupled order parameters, e. g. [9], is not applicable.

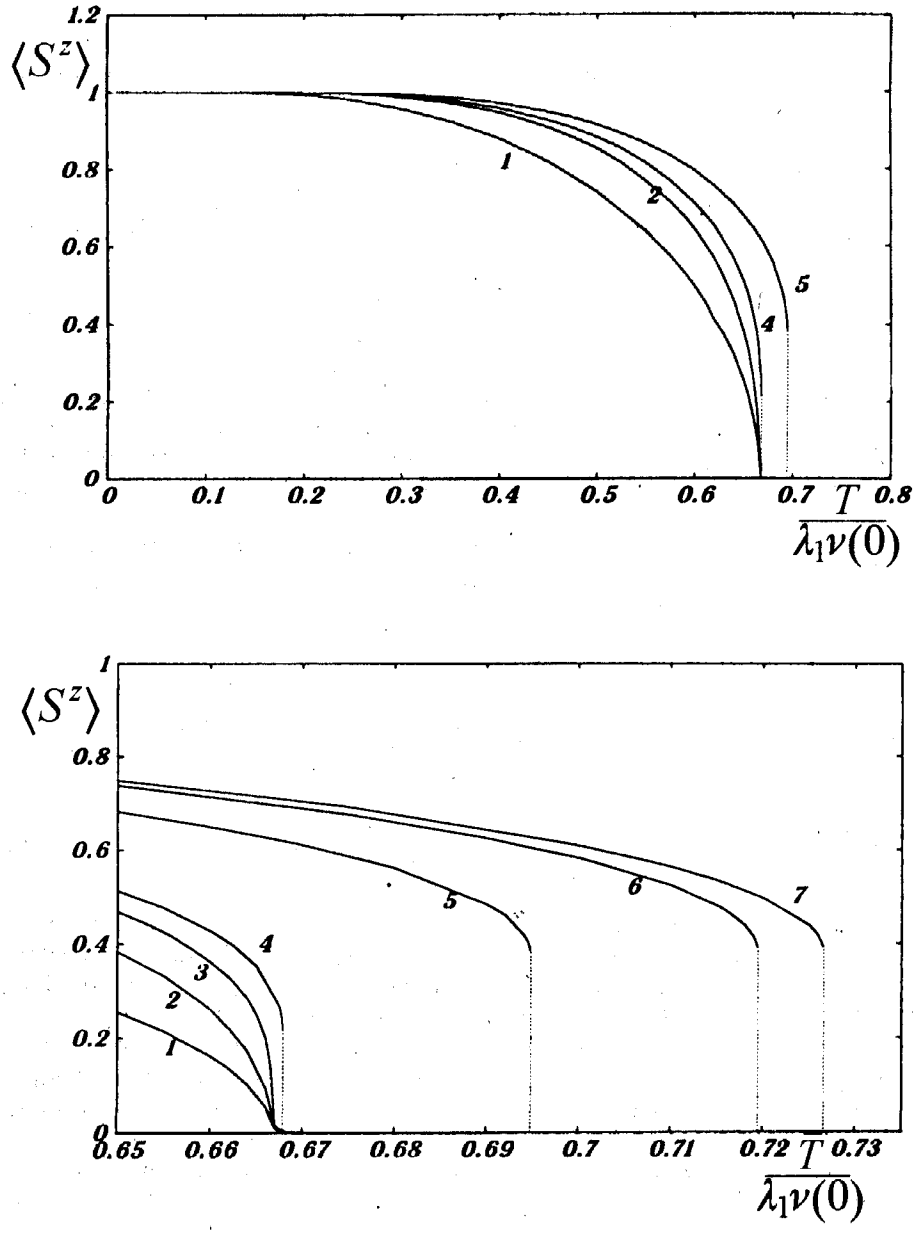

Figure 1. The temperature dependence of $\langle S^z \rangle$ for various values of biquadratic exchange interaction constant. Curves 1-7 correspond to $\lambda_2/\lambda_1 =$ 0,0.4, 0.5, 0.55, 0.8, 0.95, 0.99 respectively.

In molecular field approximation we obtain:

$$\frac{F}{N} = a_2(T)m^2 + b_2(T)Q^2 + a_3(T)m^2Q + b_3(T)Q^3 + a_4(T)m^4 + \\ + b_4(T)m^2Q^2 + c_4(T)Q^4, \quad (46)$$

where coefficients

$$a_2(T) = \frac{1}{2}\frac{\lambda_1\nu(0)}{T}\Big(T - \frac{2}{3}\lambda_1\nu(0)\Big),$$
$$b_2(T) = \frac{1}{2}\frac{\lambda_2\nu(0)}{T}\Big(T - \frac{2}{3}\lambda_2\nu(0)\Big),$$
$$a_3(T) = -\frac{\sqrt{3}}{9}\frac{\lambda_1^2\lambda_2\nu(0)^3}{T^2}, \quad b_3(T) = +\frac{\sqrt{3}}{27}\frac{\lambda_2^3\nu(0)^3}{T^2},$$
$$a_4(T) = \frac{1}{36}\frac{\lambda_1^4\nu(0)^4}{T^3}, \quad b_4(T) = \frac{1}{18}\frac{\lambda_1^2\lambda_2^2\nu(0)^4}{T^3},$$
$$c_4(T) = \frac{1}{36}\frac{\lambda_2^4\nu(0)^4}{T^3}. \quad (47)$$

Equations for finding m and Q are:

$$2m(a_2(T) + a_3(T)Q + 2a_4(T)m^2 + b_4(T)Q^2) = 0,$$
$$2b_2(T)Q + a_3(T)m^2 + 3b_3(T)Q^2 + 2b_4(T)m^2Q + 4c_4(T)Q^3 = 0. \quad (48)$$

We shall consider first the simplest case, retaining in (46) minimal quantity of terms which allowed to reveal phase transition from paramagnetic to ferromagnetic state:

$$\frac{F}{N} = a_2(T)m^2 + b_2(T)Q^2 + a_3(T)m^2Q + a_4(T)m^4. \quad (49)$$

After appropriate changes in (48), we obtain two solutions:

$$1)\ m = 0, \quad Q = 0; \quad (50)$$

$$2)\ m = \pm\sqrt{\frac{2a_2(T)b_2(T)}{a_3^2(T) - 4a_4(T)b_2(T)}}, \quad Q = \frac{-a_2(T)a_3(T)}{a_3^2(T) - 4a_4(T)b_2(T)}. \quad (51)$$

The first of this solutions corresponds to paramagnetic state and is stable for $T > 2/3\lambda_1\nu(0)$ and $T > 2/3\lambda_2\nu(0)$. The second exists and is stable for $T < 2/3\lambda_1\nu(0)$ and $\lambda_1 > 2\lambda_2$. Substituting in (49) value of the Q from (51)

$$Q = -\frac{a_3(T)}{2b_2(T)}m^2 \quad (52)$$

we obtain expression for the free energy as function of one order parameter m. Putting the coefficient of the m^4 term to be equal to zero we find the tricritical point $T = 4/3\lambda_2\nu(0)$ $(\lambda_1 = 2\lambda_2)$. So, if bilinear exchange is stronger than biquadratic are below $T = 2/3\lambda_1\nu(0)$ transition from paramagnetic to ferromagnetic phase occurs and for $\lambda_1 = 2\lambda_2$ it becomes of the second order. In ordered state

$$m \sim \sqrt{T_C - T}, \quad Q \sim T_C - T.$$

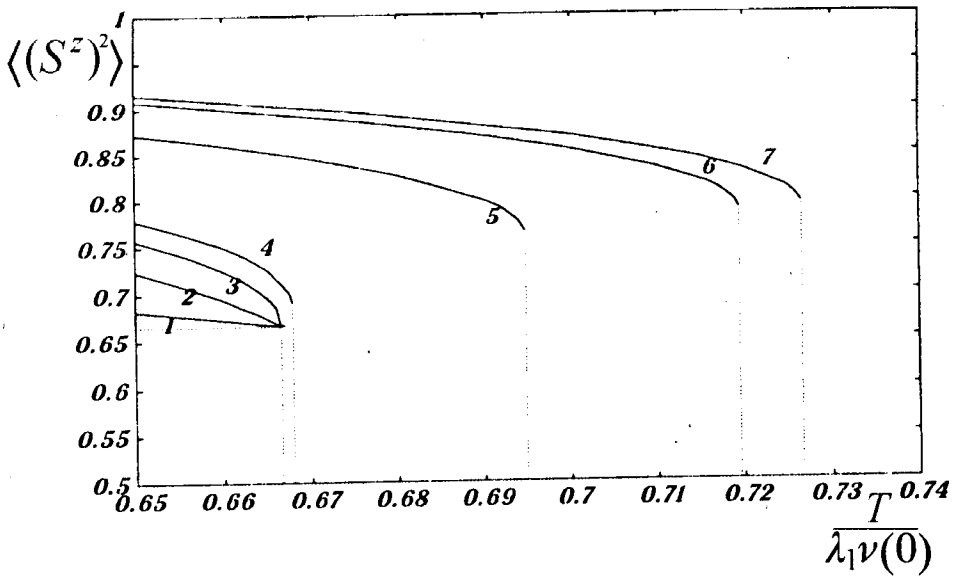

Figure 2. The temperature dependence of $\langle (S^z)^2 \rangle$ for various values of biquadratic exchange interaction constant. Curves 1-7 correspond to $\lambda_2/\lambda_1 =$ 0,0.4, 0.5, 0.55, 0.8, 0.95, 0.99 respectively.

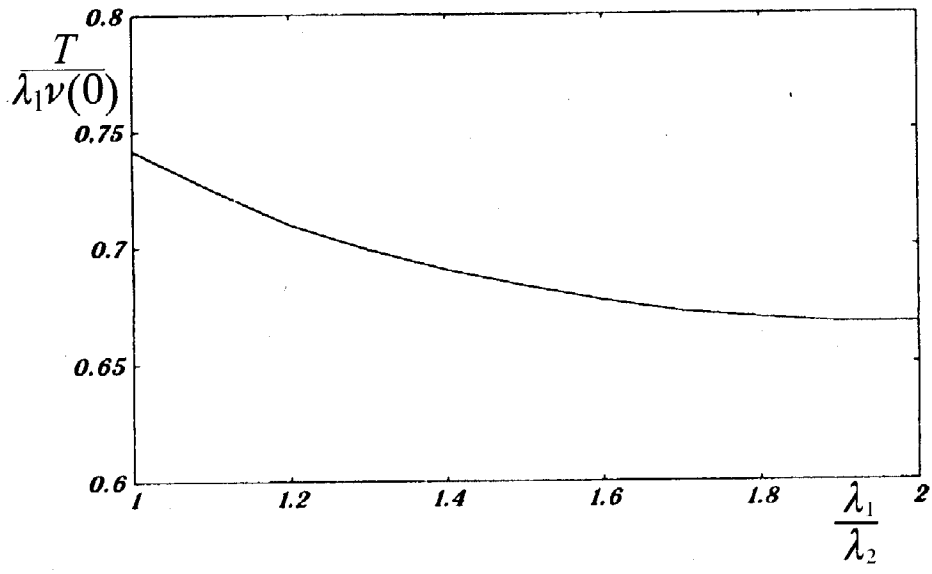

Figure 3. First order transition point's dependence on the ratio of bilinear to biquadratic exchange interaction constants.

For investigation of the ordered phase in the region $T < 2/3\lambda_1\nu(0)$, $\lambda_2 < \lambda_1 < 2\lambda_2$ we return to the expression (46). From equations (48) we have:

$$Q_{1,2} = -\frac{B(T)}{6A(T)}\left\{1 \pm \frac{1}{B(T)}\sqrt{B^2(T) - 12A(T)C(T)}\right\},$$
$$m^2 = -\frac{1}{2a_4(T)}\Big(a_2(T) + a_3(T)Q + b_4(T)Q^2\Big), \qquad (53)$$

where

$$A(T) = 2b_3(T)a_4(T) - a_3(T)b_4(T),$$
$$B(T) = 4b_2(T)a_4(T) - a_3^2(T) - 2a_4(T)b_4(T),$$
$$C(T) = -a_2(T)a_3(T). \qquad (54)$$

A matter of further interest is solution Q_2. In the case $\lambda_1 = \lambda_2$ it exists in the region $T \leq 3/4\lambda_1\nu(0)$ and is stable for $T < 3/4\lambda_1\nu(0)$; for $\lambda_1 = 2\lambda_2$: respectively for $T \leq 2/3\lambda_1\nu(0)$ and $T < 2/3\lambda_1\nu(0)$. In the region $\lambda_2 < \lambda_1 < 2\lambda_2$ stability bound quietly falles and for $\lambda_1 > \lambda_2$ become a straight line $T/\lambda_1\nu(O) = 2/3$. Stability bounds of paramagnetic ($T = 2/3\lambda_1\nu(0)$) and ferromagnetic phases in the interval $\lambda_2 < \lambda_1 < 2\lambda_2$ do not coincid. Free energy of these phases equalized in the points $T/\lambda_1\nu(O) = 60/81$ for $\lambda_1 = \lambda_2$ and $T/\lambda_1\nu(O) = 2/3$ for $\lambda_1 = 2\lambda_2$, in the last point transition becomes of the second order. Variation of first order transition point in indicated interval is shown on the figure 3.

Let us consider now quadrupolar phase with $m = 0$, $Q \neq 0$. Q is defined

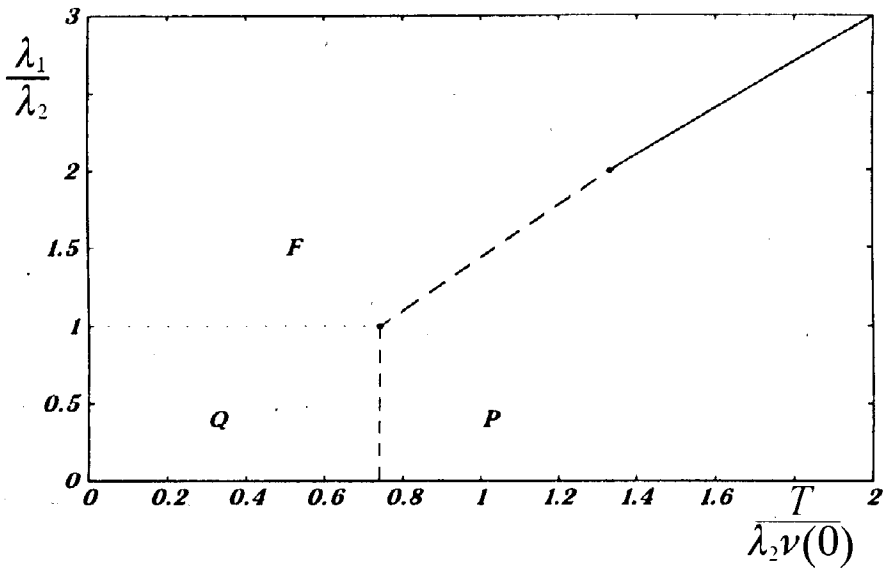

Figure 4. Phase diagram of the system; P, F and Q means paramagnetic, ferromagnetic and quadrupolar states respectively. Dashed lines indicats first-order transitions. (except the case of $\lambda_1 = \lambda_2$ required special studying).

from the second equation of (48). Non-trivial solutions are:

$$Q_{1,2} = -\frac{3b_3(T)}{8c_4(T)}\left\{1 \pm \frac{1}{3b_3(T)}\sqrt{9b_3^2(T) - 32b_2(T)c_4(T)}\right\}, \qquad (55)$$

Q_2 does not correspond to free energy minimum. Q_1 exists in the region $T \leq 3/4\lambda_2\nu(0)$ and is stable for $T < 3/4\lambda_2\nu(0)$. Stability bounds of paramagnetic ($T > 3/4\lambda_1\nu(0)$) and quadrupolar phases do not coincid; equalizing free energy in both states we obtain the point of first order phase transition; $T/\lambda_2\nu(0) = 60/81$. Finally phase diagram of the system in molecular field approximation is shown on the figure 4.

We shall find now transition temperature from paramagnetic to ferromagnetic state in random phase approximation. We obtained expression for $a_2(T)$ in this approximation and further equation for transition temperature. First iteration of such equation can be considered as its solution in this approximation; we obtain:

$$(T_d)^* = 1 - \frac{3}{4N}\sum_{\mathbf{k}}\left(1 - \frac{2}{3}\frac{l}{1-l}\frac{\gamma_k}{1-\gamma_k} + 1 + \frac{2}{3}\frac{l}{1-l}\frac{l\gamma_k}{1-l\gamma_k}\right) \qquad (56)$$

where $(T_d)^* = T_d^G/T_d^0$, $l = \lambda_2/\lambda_1$, $\gamma_k = \nu(k)/\nu(0)$, T_d^0 and T_d^G are "paramagnetic-ferromagnetic" transition temperatures respectively in molecular field and random phase approximations. Expression (56) can be found also by means of approach developed in [10].

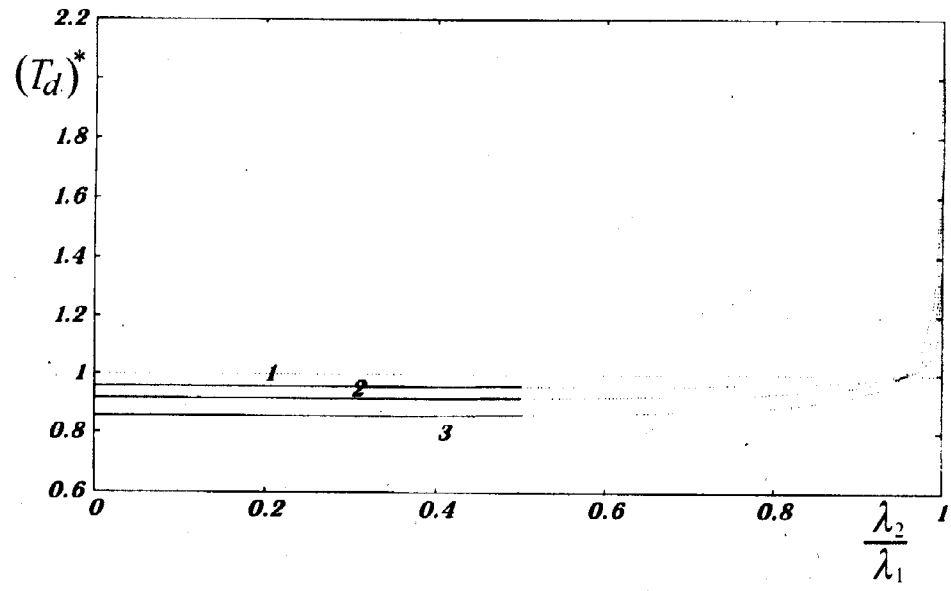

Figure 5. Correction for "paramagnetic-ferromagnetic" transition temperature in RPA. Curves 1-3 correspond to α =1, 5/4, 3/2 respectively.

For widely used model interaction potential

$$J(r) = J\exp\Big(-\alpha(r/a-1)\Big), \quad \nu(k) = \frac{\alpha^4}{(\alpha^2+k^2a^2)^2}, \tag{57}$$

passing from summation over $\mathbf{k}$ to integration and using integrals estimates of [11], we obtain dependencies $T^*(l)$, which are shown in the figure 5.

Behaviour of the system in the region $l > 0.5$ requirs further studying, using the conditions of phases equilibrium. $l \to 1$ must be considered as a special case because of the competition between small parameters $\alpha^3 = r_0^{-3}$ and $\frac{1}{1-l}$. In the similar manner, expression in RPA for transition temperature from paramagnetic to quadrupolar state is obtained, which requirs further studying.

Disordered system

Let us consider now system of N randomly distributed and fixed in volume V magnetically active atoms, which coordinates are $(\mathbf{R}_i ... \mathbf{R}_N) \equiv \{\mathbf{R}^N\}$. In this case Hamiltonian $H = H[\{\mathbf{R}^N\}]$ is dependent on the configuration $\{\mathbf{R}_N\}$ of atoms. $J(|\mathbf{R}_i - \mathbf{R}_j|)$ we shall treat as theory parameter which can be chosen in convenient manner from physical considerations. We suggest that $J(R)$ can be expanded in Fourier series in cube with volume V:

$$J(R) = \frac{1}{V}\sum_{\mathbf{k}} \nu(k) e^{i\mathbf{kR}}, \tag{58}$$

here $\nu(k)$ is defined as

$$\nu(k) = \int d\mathbf{R} J(R) e^{\imath \mathbf{k}\mathbf{R}} \tag{59}$$

and wave vector $\mathbf{k}$ in contrast with the case of crystal lattice is not restricted to the first Brillouin zone and can vary in the infinite space of its values. Free energy of the system is given by

$$F^{am} = -\frac{1}{\beta}\Big\langle \ln Z[\{\mathbf{R}^N\}]\Big\rangle_{av}, \tag{60}$$

here $\Big\langle (...)\Big\rangle_{av}$ means configurational averaging with normalized disribution function of variables $\mathbf{R}_N$ probabilities $P(\mathbf{R}_1, ..., \mathbf{R}_N) \equiv P[\{\mathbf{R}^N\}]$; by means of $P[\{\mathbf{R}^N\}]$ structure disorder of the model is specified; choice of $P[\{\mathbf{R}^N\}]$ proceeds from the considerations about disorder system structure in each particular case.

By similar transformations as for crystalline magnetic we obtain:

$$Z[\{\mathbf{R}^N\}] = \exp\Big(-\beta F_0\Big) \int (d\varphi) \exp\Big(F[\varphi; \{\mathbf{R}^N\}]\Big), \tag{61}$$

where

$$F[\varphi; \{\mathbf{R}^N\}] = -\frac{1}{2}\sum_{\mathbf{k}} \hat{\varphi}_{\mathbf{k}} \hat{\varphi}_{-\mathbf{k}} + \sum_{l\geq 1} \frac{N^{1-l/2}}{l!} \sum_{\mathbf{k}_1 \alpha_1} ... \sum_{\mathbf{k}_l \alpha_l} \mathcal{M}_{\alpha_1 ... \alpha_l} \times$$

$$\times \sqrt{\beta\nu(k_1)N/V ... \beta\nu(k_l)N/V} \frac{1}{N} \sum_{j=1}^{N} e^{-\imath(\mathbf{k}_1 + ... + \mathbf{k}_l)\mathbf{R}_j} \varphi_{\mathbf{k}_1}^{(\alpha_1)} ... \varphi_{\mathbf{k}_l}^{(\alpha_l)}. \tag{62}$$

All the configurational dependence of $Z[\{\mathbf{R}^N\}]$ is included in the factor $N^{-1}\sum_{j=1}^{N} \exp\Big(-\imath(\mathbf{k}_1 + ... + \mathbf{k}_l)\mathbf{R}_j\Big)$ of functional (62), which in the case of crystal lattice coincids with Kronecker δ-symbol. For structurally disordered system

$$\frac{1}{N}\sum_{j=1}^{N} e^{-\imath(\mathbf{k}_1 + ... + \mathbf{k}_l)\mathbf{R}_j} = \frac{1}{\sqrt{N}} \rho_{\mathbf{k}_1 + ... + \mathbf{k}_l} + \delta(\mathbf{k}_1 + ... + \mathbf{k}_l), \tag{63}$$

where

$$\rho_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{-\imath \mathbf{k}\mathbf{R}_j}, \quad \mathbf{k} \neq 0 \tag{64}$$

is the Fourier-image of density fluctuations. $F[\varphi; \{\mathbf{R}^N\}]$ can be represented in the form:

$$F[\varphi; \{\mathbf{R}^N\}] \equiv F[\varphi; \rho] = F[\rho] + \Delta F[\varphi; \rho]. \tag{65}$$

First component formally coincides with the free energy functional for crystalline magnetic, taking into account the difference noted about the manifold of possible values for wave vectors and new definitions of $\alpha_1(k)$ and $\alpha_2(k)$:

$$\alpha_1(k) = \lambda_1 \beta\nu(k)N/V, \quad \alpha_2(k) = \lambda_2 \beta\nu(k)N/V. \tag{66}$$

All the information about structural disorder is included in the second term:

$$\Delta F[\varphi;\rho]=\sum_{l\geq 1}\frac{N^{1-l/2}}{l!}\sum_{\mathbf{k}_1\alpha_1}\ldots\sum_{\mathbf{k}_l\alpha_l}\mathcal{M}_{\alpha_1\ldots\alpha_l}\sqrt{\beta\nu(k_1)N/V\ldots\beta\nu(k_2)N/V}$$
$$\times\frac{1}{\sqrt{N}}\rho_{\mathbf{k}_1+\ldots+\mathbf{k}_l}\varphi^{(\alpha_1)}_{\mathbf{k}_1}\ldots\varphi^{(\alpha_l)}_{\mathbf{k}_l},\quad \mathbf{k}_1+\ldots+\mathbf{k}_l\neq 0. \quad (67)$$

(67) is the functional both of variables $\varphi^{(\alpha)}_{\mathbf{k}}$, connected with spin fluctuations and of collective variables $\rho_{\mathbf{k}}$, which described structure fluctuations.

Using (66), we separate in explicit form $Z[\{\mathbf{R}^N\}]$ dependence of $\rho_{\mathbf{k}}$:

$$Z[\{\mathbf{R}^N\}]=e^{-\beta F^{or}}\overline{\exp(\Delta F[\varphi;\rho])}=e^{-\beta F^{or}}e^{U[\rho]}, \quad (68)$$

here $\overline{(\ldots)}$ - means functional averaging over Gibbs distribution with configurationally independent functional $F[\varphi]$. F^{or} formally coincides with earlier obtained expression for free energy of the cfystalline model taking into account noted above differences. Functional

$$U[\rho]=\ln\overline{\exp(\Delta F[\varphi;\rho])}=\sum_{l\geq 1}\frac{1}{l!}\overline{\{\Delta F[\varphi;\rho]\}^l}^c \quad (69)$$

is represented by infinite functional expansion in series over the structural variables $\rho_{\mathbf{k}}$:

$$U[\rho]=\sum_{l\geq 1}\frac{N^{1-l/2}}{l!}\sum_{\mathbf{k}_1}\ldots\sum_{\mathbf{k}_l}a_l(\mathbf{k}_1,\ldots,\mathbf{k}_l)\delta(\mathbf{k}_1+\ldots+\mathbf{k}_l)\rho_{\mathbf{k}_1}\ldots\rho_{\mathbf{k}_l},\ \mathbf{k}_i\neq 0. \quad (70)$$

Coefficients

$$a_l(\mathbf{k}_1,\ldots,\mathbf{k}_l)\delta(\mathbf{k}_1+\ldots+\mathbf{k}_l)=\frac{1}{N}\overline{\left\{\Delta[\varphi;\mathbf{k}_1]\ldots\Delta[\varphi;\mathbf{k}_l]\right\}}^c \quad (71)$$

are irreducible averages of products of

$$\Delta[\varphi;\mathbf{k}]=\sum_{l\geq 1}\frac{N^{1-l/2}}{l!}\sum_{\mathbf{k}_1\alpha_1}\ldots\sum_{\mathbf{k}_l\alpha_l}\delta(\mathbf{k}_1+\ldots+\mathbf{k}_l-\mathbf{k})\mathcal{M}_{\alpha_1\ldots\alpha_l}\times$$
$$\sqrt{\beta\nu(k_1)N/V\ldots\beta\nu(k_l)N/V}\,\varphi^{(\alpha_1)}_{\mathbf{k}_1}\ldots\varphi^{(\alpha_l)}_{\mathbf{k}_l}. \quad (72)$$

Finally the free energy of disordered system is given by:

$$F^{am}=F^{or}-\frac{1}{\beta}\sum_{l\geq 1}\frac{N^{1-l/2}}{l!}\sum_{\mathbf{k}_1}\ldots\sum_{\mathbf{k}_l}a_l(\mathbf{k}_1,\ldots,\mathbf{k}_l)\delta(\mathbf{k}_1+\ldots+\mathbf{k}_l)\times$$
$$\left\langle\rho_{\mathbf{k}_1}\ldots\rho_{\mathbf{k}_l}\right\rangle_{av},\quad \mathbf{k}_i\neq 0. \quad (73)$$

The influence of structural fluctuations on the system's behaviour is determined in (73) by the configurational averages of $\rho_{\mathbf{k}}$ products. Let us introduce l-particle irreducible structure functions:

$$S^{am}_l(\mathbf{k}_1,\ldots,\mathbf{k}_l)\delta(\mathbf{k}_1+\ldots+\mathbf{k}_l)=N^{l/2-1}\left\langle\rho_{\mathbf{k}_1}\ldots\rho_{\mathbf{k}_l}\right\rangle^c_{av}. \quad (74)$$

Such approach ("liquid approximation") developed in [12] is one of the most successful methods of structure disorder modeling. It allows to represent thermodynamical features of the system by means of experimentally observable values. Among these values the most important is pair structure factor $S_2^{am}(k) \equiv S_2^{am}(\mathbf{k}, -\mathbf{k})$. So structure factors $S_l^{am}(\mathbf{k}_1, ..., \mathbf{k}_l)$ can be considered as parameters, which may be taken from experimental results in each particular case. From the other hand, they may be approximated by corresponding structure factors of hard cores system.

Further calculation of the free energy is reduced to the calculation of coefficients $a_l(\mathbf{k}_1, ..., \mathbf{k}_l)$. Functional integrals can be found by the expansion over the Gaussian moments considering the non-Gaussian part as a small perturbation. We have obtained the expression for the free energy in "two sums over $\mathbf{k}$" - approximation [13], but it is too cumbersome to be presented here. In the Gaussian approximation:

$$F_G^{am} = F_G^{or} - \frac{1}{2\beta} M_1^2(y_1, y_2) \sum_{\mathbf{k}} g_1(k) S_2^{am}(\mathbf{k}, -\mathbf{k}) - \\ - \frac{1}{2\beta} M_2^2(y_1, y_2) \sum_{\mathbf{k}} g_2(k) S_2^{am}(\mathbf{k}, -\mathbf{k}). \qquad (75)$$

Let us find in this approximation expression for ferromagnetic transition temperature. From the appropriate expression for $a_2(T)$ and $b_2(T)$ we obtain:

$$\left(T_d^{dis}\right)^* = 1 - \frac{3}{4N} \sum_{\mathbf{k}} \left[\left(1 - \frac{2}{3} \frac{l}{1-l} - \frac{4}{3} S_2^{am}(\mathbf{k}, -\mathbf{k}) \right) \frac{\gamma_k}{1-\gamma_k} + \right. \\ \left. \left(1 + \frac{2}{3} \frac{l}{1-l} \right) \frac{l\gamma_k}{1-l\gamma_k} \right], \qquad (76)$$

For noted earlier model interaction potential (57) we calculated numerically (76). Structure factor was simulated by solution of Percus-Yevick equation for hard cores system. The results are presented in Figures 6a, 6b.

For the figure 6 we must repeat once more all the precautions noted above for the figure 5. Competition noted between small parameters r_0^{-3} and $\frac{1}{1-l}$ especially can be observed in the region $0 < \alpha^{-1} < 0.25$ of the figure 7. Further studying is required for the expression obtained for "paramagnetic-quadrupolar" transition temperature. It would also be interesting to find the change of tricritical point in random phase approximation and carry out numerical calculations for other model interaction potentials.

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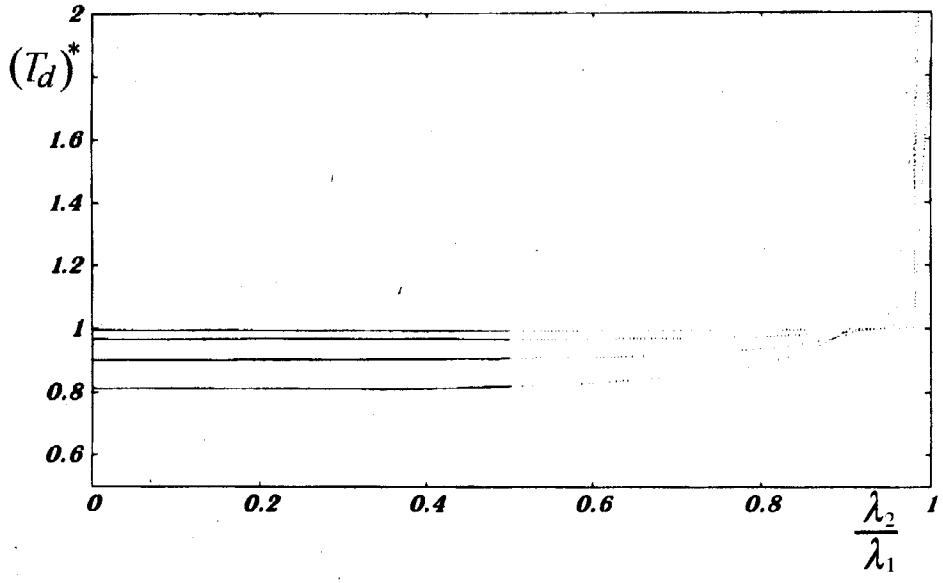

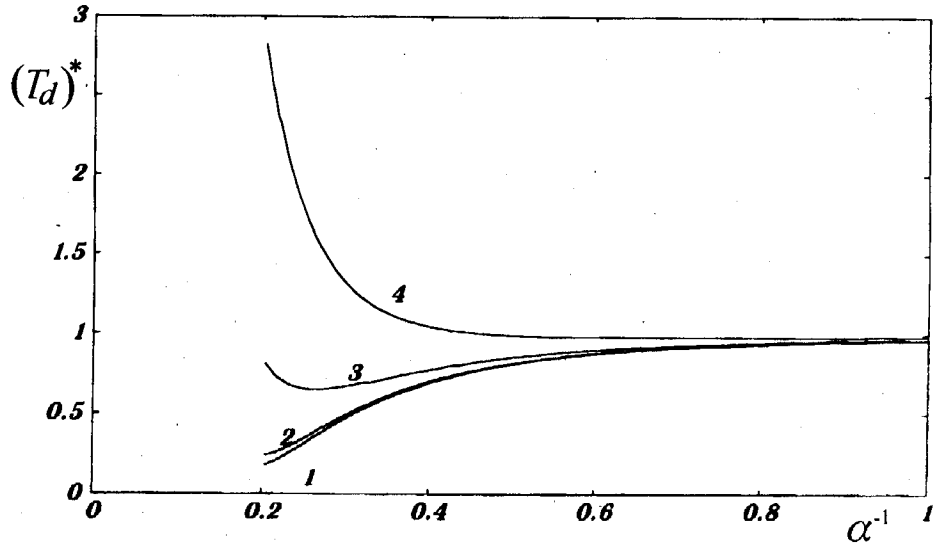

Figure 6. Influence of the structural disorder on the "paramagnetic - ferromagnetic" transition temperature. On the figure 6 curves moving down corresponded for α = 0.5, 1, 1.5, 2 respectively. On figure 6 curves 1-4 correspond to l =0, 0.4, 0.7, 0.9 respectively.

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ДОСЛІДЖЕННЯ ІЗІНГІВСЬКОЇ МОДЕЛІ З ОДИНИЧНИМ СПІНОМ З БІКВАДРАТИЧНОЮ ОБМІННОЮ ВЗАЄМОДІЄЮ МЕТОДОМ ФУНКЦІОНАЛЬНОГО ІНТЕГРУВАННЯ

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В рамках методу функціонального інтегрування досліджується ізінгівська модель з одиничним спіном та біквадратичною обмінною взаємодією. Обчислюється вільна енергія моделі в наближенні хаотичних фаз (НХФ). У цьому ж наближенні отримано вираз для температури феромагнітного впорядкування. Вивчається фазова діаграма системи, отримана при допомозі розкладу вільної енергії. Обговорюються властивості системи в залежності від значення констант білінійної й біквадратичної обмінної взаємодії. Розглядається випадок структурно невпорядкованої системи. Знайдено зміну температури феромагнітного переходу, спричинену структурним безладом. Представлено результати чисельних розрахунків для структурних факторів системи твердих сфер.