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ENERGY OF MAGNETIC EXCITATIONS AND MAGNETIZATION IN COMPRESSIBLE FERROMAGNET

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In ref. [1] a new approach to the theory of the spin-phonon interaction, taking into account in a self-consistent manner the anharmonicity of the lattice vibrations, was proposed. In ref. [2] the equation of state of the anharmonic ferromagnetic crystal under external pressure was derived.

In the present paper some of the preliminary results obtained, when studying the temperature dependence of the lattice constant in the anharmonic ferromagnetic crystal at low temperatures, and its influence on the magnetic excitation spectrum and magnetization are given.

Let us consider a ferromagnetic crystal which can be described by the Hamiltonian [2]:

$$H = H_L + H_S = -\frac{1}{2M}\sum_i \nabla_i^2 + U(\vec{R}_i) - \mu H \sum_i S_i^z - \frac{1}{2} J(\vec{R}_i - \vec{R}_j)\vec{S}_i \vec{S}_j , \quad (1)$$

where $\vec{R}_i = \vec{\ell}_i + \vec{u}_i$, $\vec{u}_i$ is the displacement operator and $\vec{S}_l$ is the spin operator of the atom in the lattice point $\vec{\ell}_i = \langle \vec{R}_l \rangle$, $U(\vec{R}_l)$ is the potentional energy of the crystal and $J(\vec{R}_l - \vec{R}_j)$ is the exchange integral.

We assume that well-defined excitations, the self-consistent phonons, weakly coupled with magnetic excitations can exist in the crystal [3]. Then considering the spin system in the mean field approximation [4] and using the Holstein-Primakoff approximation at low temperatures the magnetic excitation spectrum can be written in the form:

$$E_q = S(\tilde{J}_0 - \tilde{J}_q) - \frac{1}{N}\sum_{q'} N_{q'}(\tilde{J}_0 + \tilde{J}_{q-q'} - \tilde{J}_q - \tilde{J}_{q'}), \quad (2)$$

where $N_q=[\exp\frac{\mu H+E_q}{T}-1]^{-1}$ and $\tilde{J}_q$ is the Fourrier-transform of the renormalized exchange integral $\tilde{J}_{ij}=\langle J(\vec{R}_i-\vec{R}_j)\rangle_0$. The symbol $\langle - - - \rangle_0$ denotes the thermal average in the pseudoharmonic approximation [3].

Let us suppose that the potential is a central-force one: $U(\vec{R}_1,\ldots,\vec{R}_N)=\frac{1}{2}\sum_{n\neq m}\phi(\vec{R}_n-\vec{R}_m)$. In the nearest neighbours approximation the equation of state takes the form [2]:

$$P=-\frac{z\ell}{6V}\{\tilde{\phi}'(\ell)-\tilde{J}'(\ell)\langle\vec{S}_\ell\cdot\vec{S}_0\rangle\}, \qquad (3)$$

where P is the pressure, V is the volume of the elementary cell, ℓ is the separation between the nearest neighbours, z is the number of the nearest neighbours, the prime emplies differentiation with respect to ℓ. $\tilde{J}(\ell)$ can be written in the form [3]:

$$\tilde{J}(\ell)=\langle J(\vec{R}_\ell-\vec{R}_0)\rangle=\exp[\frac{\overline{u^2}}{2}\nabla_\ell\nabla_\ell]J(\ell), \qquad (4)$$

where $\overline{u^2}=\overline{u_\ell^2}=\langle[\vec{\ell}\cdot(\vec{u}_\ell-\vec{u}_0)]^2\rangle/\ell^2$ and $\tilde{\phi}(\ell)$ has an analogous form.

If we take $\ell\equiv\ell(T)=\ell_0+\delta\ell(T)$ where ℓ_0 is the equilibrium separation at zero pressure and zero temperature, from the equation of state we get for the simple cubic lattice up to T^4:

$$\delta\ell(T)=AT^{\frac{5}{2}}+BT^4, \qquad (5)$$

where

$$A=-2\pi SZ_{\frac{5}{2}}(\frac{\mu H}{T})\tilde{J}'(\ell_0)/[4\pi S\tilde{J}_0(\ell_0)]^{\frac{5}{2}}f(\ell_0);$$

$$B=\pi^4[S^2\tilde{J}_0'''(\ell_0)-\tilde{\phi}_0(\ell_0)]/10\omega_D^3\phi''(\ell_0)f(\ell_0);$$

$$f(\ell_0)=\phi_0''(\ell_0)-S^2\tilde{J}_0''(\ell_0);\quad Z_p(n)=\sum_{n=1}^{\infty}n^{-p}e^{-nx};$$

$\omega_D=1{,}05\sqrt{8\phi''(\ell_0)/M}$ and $\tilde{J}_0(\ell_0)$, $\tilde{\phi}_0(\ell_0)$ can be obtained from (4) substituting $\ell=\ell_0$ and $\overline{u^2}=\overline{u^2_{T=0}}$.

From (5) for the thermal expansion coefficient we get:

$$\eta=\frac{1}{\ell_0}\frac{d}{dT}\delta\ell(T)=\frac{1}{\ell_0}(\frac{5}{2}AT^{\frac{3}{2}}+4BT^3). \qquad (6)$$

The expression (6) indicates that at low temperatures $(\theta=T/4\pi S\tilde{J}_0(\ell_0)\ll 1)$ the spin system exerts an essential influence on the thermal expansion. In the considered case for fertomagnet in (5) and (6) we have $A>0$ and $B>0$. This is a consequence of the fact that usually $\tilde{J}_0'(\ell_0)<0$, $f(\ell_0)>0$ (because $\tilde{\phi}_0''(\ell_0)>0$ and $\tilde{\phi}_0''(\ell_0)>S^2\tilde{J}_0''(\ell_0)$) and $\tilde{\phi}_0'''(\ell_0)<0$.

In the nearest neighbours approximation for a simple cubic lattice when $q\to 0$ and $T\to 0$ the spectrum (2) takes the form:

$$E_q=Sq^2\ell_0^2\tilde{J}_0(\ell_0)[1+\delta\ell(T)\frac{\tilde{J}_0'(\ell_0)}{\tilde{J}_0(\ell_0)}][1-\pi\frac{Q(s)}{s}Z_{\frac{5}{2}}(\frac{\mu H}{T})(\frac{T}{4\pi S\tilde{J}_0(\ell_0)})^{\frac{5}{2}}], \qquad (7)$$

where $Q(s)=(1+0{,}03S^{-1})/(1-0{,}1S^{-1})+0{,}17S^{-1}$.

From (5) and (7) taking into account only the terms up to T^4 for the relative magnetization we obtain:

$$\sigma=1-\alpha\theta^{\frac{3}{2}}-\beta\theta^4-\gamma\theta^4, \qquad (8)$$

where $\alpha=\frac{1}{s}Z_{\frac{3}{2}}(\frac{\mu H}{T})$, $\beta=\frac{3}{2}\pi\frac{Q(s)}{s^2}Z_{\frac{3}{2}}(\frac{\mu H}{T})Z_{\frac{5}{2}}(\frac{\mu H}{T})$,

$$\gamma=3\pi Z_{\frac{3}{2}}(\frac{\mu H}{T})Z_{\frac{5}{2}}(\frac{\mu H}{T})[\tilde{J}_0'(\ell_0)]^2/\tilde{J}_0(\ell_0)f(\ell_0).$$

We note that the temperature dependence in (5) is in accordance with the expression derived in ref. [5] in a phenomenological way. There the term proportional to

$T^{5/2}$ is obtained from the consideration of the Green functions $\langle\langle us^+|s^-\rangle\rangle$ which lead to a renormalization in the magnetic excitation spectrum similar to that given by $\delta\ell(T)$.

We also note that the coefficients for T^4 and $T^{\frac{5}{2}}$ in (5) are explicitly expressed in terms of the spin and phonon interaction constant. The last term of (5) introduces in the magnetization (8) an addition proportional to T^4, the coefficient γ of which contains the factor $[\tilde{J}_0'(\ell_0)]^2$ playing in our case the role of the spin-phonon coupling constant.

The influence of the thermal expansion on the magnetization at low temperatures can be comparable with the spin-spin interaction effect. It is seen from (8) that $\gamma \approx \beta$ if the condition $[\tilde{J}_0'(\ell_0)]^2 \approx \tilde{J}_0(\ell_0) f(\ell_0)$ is fulfilled, i.e. if the spin-phonon interaction is intensive enough.

Analogous investigations for the temperatures in the vicinity of the Curie point will be carried out elsewhere.

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