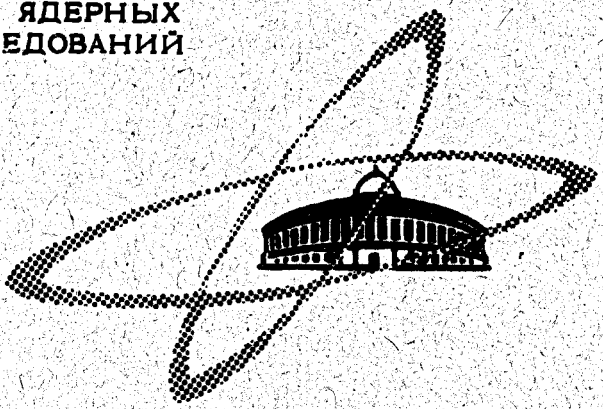
ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ
Дубна



E4 - 5006

N.M. Plakida

SELF-CONSISTENT PHONONS IN FERROMAGNETIC CRYSTAL

1970

ЛАБОРАТОРИЯ ТЕОРЕТИЧЕСКОЙ ФИЗИКИ

E4 - 5006

N.M. Plakida

SELF-CONSISTENT PHONONS IN FERROMAGNETIC CRYSTAL

Submitted to Phys. Lett.

A new approach to the theory of spin-phonon interaction which takes into account in a self-consistent manner the anharmonicity of lattice vibrations was proposed in [1] and [2]. In the present paper it is shown that the decoupling procedure for the Green's functions adopted in [1] and [2] is equivalent to the variational approach proposed in [3] for considering the self-consistent phonons in anharmonic crystals.

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

$$\mathcal{H} = H_{\ell} + H_{s} = \frac{1}{2M}\sum_{i} - \nabla_{i}^{2} + U(R_{i}) - \mu H \sum_{i} S_{i}^{z} - \frac{1}{2}\sum_{ij} J(R_{i} - R_{j}) S_{i} \cdot S_{j}, \qquad (1)$$

where $R_{i} = \ell_{i} + u_{i}$, u_{i} is the displacement and S_{i} is the spin operator of the atom in the lattice site $\ell_{i} = \langle R_{i} \rangle$. $U(R_{i})$ is the potential energy of the crystal and $J(R_{i} - R_{j})$ is the exchange integral. We assume that well-defined excitations - the self-consistent phonons [3], weakly coupled with magnetic excitations, can exist in the crystal. Then as an approximation we can adopt a trial Hamiltonian of the form

$$\mathcal{H}_0 = H_h + \tilde{\tilde{H}}_s \,, \quad H_h = \frac{1}{2M}\sum_i -\nabla_i^2 + \frac{1}{2}\sum_{ij} u_i \cdot \tilde{\tilde{\Phi}}_{ij} \cdot u_j \qquad (2)$$

and $\tilde{\tilde{H}}_s$ has the same form as H_s in (1) where the exchange integral is replaced by the function $\tilde{\tilde{J}}_{ij}$ depending only on equilibrium separation between atoms $\ell_{ij} = \ell_i - \ell_j$. The parameteres $\tilde{\tilde{\Phi}}_{ij}$ and $\tilde{\tilde{J}}_{ij}$ are determined variationally from the stationary condition for the trial free energy

$$F_{tr} = F_0 + \langle \mathcal{H} - \mathcal{H}_0 \rangle_0 \,, \quad F_0 = -\frac{1}{\beta} \ln Sp\{\exp(-\beta \mathcal{H}_0)\}. \qquad (3)$$

Using Taylor expansion in powers of displacements for $U(\ell_i + u_i)$ and $J(\ell_{ij} + u_i - u_j)$ and taking the thermal average $\langle \ldots \rangle_0$ with the Hamiltonian (2) we get for (3):

$$\langle U \rangle_0 = \exp\{\frac{1}{2}\sum_{ij} \langle u_i u_j \rangle : \nabla_i \nabla_j\} U_0(\ell_i)$$

$$\langle J \rangle_0 = \exp\{\frac{1}{2}\langle (u_i - u_j)(u_i - u_j) \rangle : \nabla_i \nabla_i\} J_0(\ell_{ij}). \qquad (4)$$

Variation of the free energy (3) with respect to $\langle S_i \cdot S_j \rangle_0$ and $\langle u_i u_j \rangle_0$ gives $\tilde{\tilde{J}}_{ij} = \langle J \rangle_0$ and the matrix $\tilde{\tilde{\Phi}}_{ij}$ which determines frequencies $\omega_{k\lambda}$ and polarization vectors $e_{k\lambda}$ of the trial harmonic phonons in (2) by the equation

$$e_{k\lambda}\omega^2_{k\lambda} = \frac{1}{MN}\sum_{ij}\{\exp(-ik\cdot\ell_{ij})\nabla_i\nabla_j\langle U\rangle_0 -$$

$$-\langle S_i S_j \rangle_0 [1 - \exp(-ik\cdot\ell_{ij})]\nabla_i\nabla_i \langle J \rangle_0\} \cdot e_{k\lambda} \qquad (5)$$

The displacement correlation function in the trial harmonic approximation (2) has the standard form

$$\langle u_i u_j \rangle_0 = \frac{1}{MN} \sum_{k\lambda} e_{k\lambda} e_{k\lambda} \exp(-ik \cdot \ell_{ij}) \frac{1}{2\omega_{k\lambda}} \coth\left(\frac{1}{2}\beta\omega_{k\lambda}\right). \qquad (6)$$

The spin correlation function $\langle S_i \cdot S_j \rangle_0 = -2\delta F_0 / \delta \tilde{J}_{ij}$ and can be obtained by the standart methods of the quantum theory of magnetism. The equilibrium positions of atoms $\ell_i = \langle R_i \rangle$ are determined by the equilibrium conditions for the crystal under external forces. In the case of the isotropic pressure P we get the following equation of state for the crystal with volume V [2]:

$$P = -\frac{1}{3V} \sum_i \ell_i \cdot \nabla_i \langle U \rangle_0 + \frac{1}{6V} \sum_{ij} \langle S_i \cdot S_j \rangle_0 \ell_{ij} \cdot \nabla_i \langle J \rangle_0 . \qquad (7)$$

The self-consistent system of equations (2) -(7) can describe the thermal, mechanic and magnetic properties of ferromagnetic crystals in a wide range of temperature and external pressure. The validity of the adopted approximations can be evaluated by taking into account the damping of the self-consistent phonons and magnetic excitations, e.g. by the Green's function method [4,5].

References

1. S.V. Tyablikov and H. Konwent. Phys.Lett., 27A, 130 (1968).
2. H. Konwent and N.M. Plakida. JINR Preprint, P4-4723, Dubna (1969); ТМФ, 3, 134 (1970).
3. N.S. Gillis and N.R. Werthamer and T.R. Koehler. Phys.Rev., 165, 951 (1968).
4. H. Konwent. Phys.Lett., 28A, 237 (1968).

5. N.M. Plakida and T. Siklos. phys.stat. sol., 33, 103 (1969).

Received by Publishing Department
on March 24, 1970.