

SELF-CONSISTENT THEORY OF THE ELECTRON-PHONON INTERACTION IN TRANSITION METALS AND THEIR COMPOUNDS

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The renormalized electron and phonon spectra of the Barišić-Labbe-Friedel model of a transition metal are derived. Using the method of double-time thermal Green functions, the self-consistent system of equations including electron-phonon interaction is obtained. For the band and atomic limits of the Hubbard model the explicit solutions for the electron and phonon energies are obtained. The modified Stoner criterion is discussed. The energy gap, appearing between electron bands in the strong correlation limit, persists in the present calculations. The Eliashberg-type equations of superconductivity are obtained.

1. Introduction

In recent years, the problem of satisfactory description of the electron, thermal and superconducting properties of transition metals has evoked a great interest. A systematic, self-consistent treatment of the electron-phonon interaction plays an important role in this respect [1–3]. Particular properties of the transition metals, their alloys and compounds follow, to a great extent, from the dominant role of d-electrons. In the case of simple metals, where the approximation of almost free electrons is valid, efficient methods exist to carry the above task, based on pseudopotential concept [4, 5]. However, these methods cannot be applied to transition metals, since the d-electron wave functions are strongly localized and, therefore, a tight-binding scheme is more suitable.

Barišić, Labbe and Friedel [1] (BLF) proposed the Hamiltonian for a transition metal, in which they generalized the well-known Hubbard Hamiltonian [6] to include the lattice dynamics. The interaction of tightly bound d-electrons with lattice vibrations is constructed, in the BLF [1] Hamiltonian, within the "rigid ion" approximation, i.e. assuming that the d-electron wave function "rigidly" follows the moving ion. Contrary to other works [2, 3], the BLF Hamiltonian uses characteristic parameters of the transition metal in an explicit way. In the papers [1, 8–10] the squared matrix element of the electron-phonon interaction is calculated in the tight-binding approximation and many quantities connected with it are evaluated, e.g. cohesion energy [1, 8, 10], McMillan factor for superconducting transition temperature [1, 3, 8–10]. In the paper [9] the paramagnetic susceptibility is also calculated, while in [11] the phonon singularities in quasi-one-dimensional systems are studied.

In the present paper the BLF model is used for a self-consistent calculation of the renormalized electron and phonon spectra of the transition metals and their compounds, both in the band limit and in the strong Coulomb correlation limit. Single-particle densities of electrons and phonons, phonon damping and a modified Stoner criterion of magnetism are found. In the case of strong correlation, the usual Hubbard energy gap between two electron bands persists in our calculations too, despite of electron-phonon interaction included. The Eliashberg-type system of equations for superconductivity has also been obtained for the BLF model, allowing one the investigation of the superconducting properties of the transition metals within the same scheme.

2. The Hamiltonian of the model

Following [1] we consider a system of tightly-bound electrons in the one-band approximation, described by the Hubbard Hamiltonian [6]:

$$H_e = \sum_{i,j,\sigma} t_{ij} a_{i\sigma}^+ a_{j\sigma} + \frac{1}{2} U \sum_{i,\sigma} n_{i\sigma} n_{i-\sigma}, \quad (2.1)$$

where $a_{i\sigma}^+$, $a_{i\sigma}$ are creation and annihilation operators for electrons at the site \mathbf{R}_i , U is the Coulomb repulsion energy of the electrons at one site. The hopping integral t_{ij} is given by

$$t_{ij} = \int d^3r \phi^*(\mathbf{r} - \mathbf{R}_j) \left[\frac{p^2}{2m} + \sum_1 V_s(\mathbf{r} - \mathbf{R}_1) \right] \phi(\mathbf{r} - \mathbf{R}_i), \quad (2.2)$$

where $\{\phi(\mathbf{r} - \mathbf{R}_i)\}$ are a complete, orthonormal set of Wannier wave functions. Assuming $V_s(\mathbf{r})$ to be a short-range, self-consistent potential, eq. (2.2) may be rewritten as

$$t_{ii} \approx \int d^3r \phi^*(\mathbf{r}) \left[\frac{p^2}{2m} + V_s(\mathbf{r}) \right] \phi(\mathbf{r}) = t_0, \quad (2.3)$$

$$t_{ij} \approx T_{ij} + J_{ij} + J_{ji}^* = t(\mathbf{R}_j - \mathbf{R}_i), \quad i \neq j, \quad (2.4a)$$

where

$$T_{ij} = \int d^3r \phi^*(\mathbf{r} - \mathbf{R}_j + \mathbf{R}_i) \frac{p^2}{2m} \phi(\mathbf{r}), \quad (2.4b)$$

$$J_{ij} = \int d^3r \phi^*(\mathbf{r} - \mathbf{R}_j + \mathbf{R}_i) V_s(\mathbf{r}) \phi(\mathbf{r}). \quad (2.4c)$$

Note $t_0 \neq t(0)$. Considering small vibrations of ions in the ‘‘rigid ion’’ approximation, we replace in eq. (2.4) the ion position \mathbf{R}_i by $(\mathbf{R}_i + \mathbf{u}_i)$, i.e. its equilibrium position plus displacement. It is assumed that d-electron wave functions change very little under displacement of the ion. Also the orthogonality of the displaced wave functions is assumed:

$$\int d^3r \phi^*(\mathbf{r} - \mathbf{R}_j - \mathbf{u}_j) \phi(\mathbf{r} - \mathbf{R}_i - \mathbf{u}_i) \approx \delta_{ij}. \quad (2.5)$$

As it follows from eq. (2.5), the creation and annihilation operators $a_{i\sigma}^+$, $a_{i\sigma}$ may be introduced in the deformed lattice, and Hamiltonian (2.1) may be rewritten in terms of them:

$$H_e = t_0 \sum_{i\sigma} n_{i\sigma} + \sum_{\substack{ij\sigma \\ i \neq j}} t(\mathbf{R}_j + \mathbf{u}_j - \mathbf{R}_i - \mathbf{u}_i) a_{i\sigma}^+ a_{j\sigma} + \frac{1}{2} U \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}. \quad (2.6)$$

For small displacements \mathbf{u}_i we may expand $t(\mathbf{R})$ as

$$t(\mathbf{R}_j + \mathbf{u}_j - \mathbf{R}_i - \mathbf{u}_i) = t(\mathbf{R}_j - \mathbf{R}_i) + \left. \frac{\partial t(\mathbf{R})}{\partial \mathbf{R}} \right|_{\mathbf{R}=\mathbf{R}_j-\mathbf{R}_i} \cdot (\mathbf{u}_j - \mathbf{u}_i) + \dots \quad (2.7)$$

In the BLF paper [1] the following approximation, based on the nature of tight-binding functions, was introduced:

$$\frac{\partial t(\mathbf{R})}{\partial \mathbf{R}} = -q_0 \frac{\mathbf{R}}{|\mathbf{R}|} t(\mathbf{R}). \quad (2.8)$$

Here q_0 is a coefficient characterizing the exponential decrease of the radial part of the d-function, $\phi(|r|) \sim \phi_0 \exp(-q_0|r|)$, (usually q_0 is of the order of 1 \AA^{-1}).

Finally eq. (2.6) may be rewritten in the following form:

$$H_e = H_e^0 + H_{e-i}, \quad (2.9)$$

$$H_e^0 = t_0 \sum_{i\sigma} n_{i\sigma} + \sum_{\substack{ij\sigma \\ i \neq j}} t_{ij}^0 a_{i\sigma}^+ a_{j\sigma} + \frac{1}{2} U \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}, \quad (2.10)$$

where $t_{ij}^0 = t(\mathbf{R}_j - \mathbf{R}_i)$ at equilibrium positions,

$$H_{e-i} = q_0 \sum_{\substack{ij\sigma \\ i \neq j}} t_{ij}^0 \frac{(\mathbf{R}_j - \mathbf{R}_i)}{|\mathbf{R}_j - \mathbf{R}_i|} \cdot (\mathbf{u}_i - \mathbf{u}_j) a_{i\sigma}^+ a_{j\sigma}. \quad (2.11)$$

The operator H_{e-i} (2.11) describes the interaction between lattice vibrations and tightly-bound electrons in the localized Wannier basis.

The Hamiltonian for the ionic subsystem is assumed to have the usual form:

$$H_i = \sum_i \frac{P_i^2}{2M} + \frac{1}{2} \sum_{i\alpha\beta} u_i^\alpha \Phi_{ij}^{\alpha\beta} u_j^\beta. \quad (2.12)$$

The total Hamiltonian is a sum of (2.9) and (2.12). The localized basis representation, used above, underlines the tight-binding nature of d-electrons; besides, such form is necessary when disordered alloys or amorphous compounds [12–14] are to be described. In the case of the crystal it is convenient to introduce the normal coordinate operators $Q_{q\nu}$, $P_{q\nu}$, connected with the bare phonon (i.e. obtained without the d-electron influence [8]) of frequency $\omega_{0q\nu}$ and polarization $\mathbf{e}_{q\nu}$ at the wave vector \mathbf{q} and branch index ν . In terms of these H_i is diagonal:

$$H_i = \frac{1}{2} \sum_{q\nu} P_{q\nu}^+ P_{q\nu} + \omega_{0q\nu}^2 Q_{q\nu}^+ Q_{q\nu} \quad (2.13)$$

and the displacement is given by

$$\mathbf{u}_i = \frac{1}{\sqrt{MN}} \sum_{q\nu} Q_{q\nu} \mathbf{e}_{q\nu} e^{i\mathbf{q}\mathbf{R}_i} \quad (2.14)$$

(M is mass of the ion and N their number in the crystal). This leads to the following interaction operator

$$H_{e-i} = \sum_{\substack{ij\sigma q\nu \\ i \neq j}} A_{q\nu}(i, j) Q_{q\nu} a_{i\sigma}^+ a_{j\sigma}, \quad (2.15)$$

where

$$A_{q\nu}(i, j) = \frac{q_0}{\sqrt{MN}} t_{ij}^0 \frac{(\mathbf{R}_j - \mathbf{R}_i) \cdot \mathbf{e}_{q\nu}}{|\mathbf{R}_j - \mathbf{R}_i|} [e^{iq\mathbf{R}_i} - e^{iq\mathbf{R}_j}] \quad (2.16)$$

represents the matrix element of the electron-phonon interaction in terms of the parameters q_0 , t_{ij}^0 , M , \mathbf{R}_i characterizing the transition metal.

Because of the strong localization of the wave function it is reasonable to introduce the nearest neighbour (n.n.) approximation. Then the hopping integral $t(\mathbf{R}_\kappa)$ is related to the width W of the d band in a very simple way: $W = 2Zt(\mathbf{R}_\kappa)$ (Z is the number of n.n.). We introduce the notation \mathbf{R}_κ for the position of the n.n. with respect to the atom at the origin of the coordinate system. Then

$$\mathbf{R}_{i+\kappa} = \mathbf{R}_i + \mathbf{R}_\kappa = \sum_{\alpha=1}^3 (i_\alpha + \kappa_\alpha) \mathbf{a}_\alpha, \quad (2.17)$$

where \mathbf{a}_α are elementary translations of the lattice. Within the n.n. approximation and using (2.17), the hopping term in (2.10) may be written as

$$\sum_{i\kappa\sigma} t(\mathbf{R}_\kappa) a_{i\sigma}^+ a_{i+\kappa,\sigma} \quad (2.18)$$

while the electron-phonon part (2.15), (2.16) as

$$H_{e-i} = \sum_{i\kappa\sigma q\nu} A_{q\nu}(i, i + \kappa) Q_{q\nu} a_{i\sigma}^+ a_{i+\kappa,\sigma}, \quad (2.19)$$

$$A_{q\nu}(i, i + \kappa) = \frac{q_0}{\sqrt{MN}} t(\mathbf{R}_\kappa) \frac{\mathbf{R}_\kappa \cdot \mathbf{e}_{q\nu}}{|\mathbf{R}_\kappa|} e^{iq\mathbf{R}_i} [1 - e^{iq\mathbf{R}_\kappa}]. \quad (2.20)$$

Note that in the rigid-ion model of BLF [1] as well as in the Hubbard model [6], s-electrons are not accounted for explicitly, although their influence is taken into account in some indirect way. It is supposed that they participate in the determination of the bare phonon frequencies $\omega_{0q\nu}$ and that the Coulomb repulsion parameter U is renormalized due to the screening by the s-electrons.

3. Electron Green's function

We begin an investigation of our model from the so-called band limit for Hubbard Hamiltonian, $U \ll W$, a situation typical for a transition metal (e.g. $U/W = 0.14-0.16$ for Fe, Ni, Co). In this case it is convenient to use the momentum representation

$$H_e^0 = \sum_{k\sigma} \varepsilon_k a_{k\sigma}^+ a_{k\sigma} + \frac{U}{2N} \sum_{k_1 k_2 \sigma} a_{k_1 + q, \sigma}^+ a_{k_1 \sigma} a_{k_2 - q, -\sigma}^+ a_{k_2, -\sigma}. \quad (3.1)$$

The band energy is given by

$$\varepsilon_k = t_0 + \sum_{\kappa} t(\mathbf{R}_\kappa) e^{ik\mathbf{R}_\kappa}. \quad (3.2)$$

For lattices with the center of inversion, $t(\mathbf{R}_\kappa) = t(-\mathbf{R}_\kappa) = t^*(\mathbf{R}_\kappa)$, so that

$$\varepsilon_k = t_0 + \sum_{\kappa} t(\mathbf{R}_\kappa) \cos(\mathbf{k}\mathbf{R}_\kappa). \quad (3.2a)$$

The interaction in the momentum representation looks as

$$H_{e-i} = \sum_{k\sigma q\nu} V_\nu(\mathbf{k}, \mathbf{k} + \mathbf{q}) Q_{q\nu} a_{\mathbf{k}+\mathbf{q},\sigma}^+ a_{k\sigma}, \quad (3.3)$$

where

$$V_\nu(\mathbf{k}, \mathbf{k}') = \frac{q_0}{R_0 \sqrt{MN}} \sum_{\kappa} t(\mathbf{R}_\kappa) \mathbf{R}_\kappa \cdot \mathbf{e}_{\mathbf{k}'-\mathbf{k},\nu} [e^{i\mathbf{k}\mathbf{R}_\kappa} - e^{i\mathbf{k}'\mathbf{R}_\kappa}] \quad (3.4a)$$

$$= \frac{iq_0}{R_0 \sqrt{MN}} \sum_{\kappa} t(\mathbf{R}_\kappa) \mathbf{R}_\kappa \cdot \mathbf{e}_{\mathbf{k}'-\mathbf{k},\nu} [\sin(\mathbf{k}\mathbf{R}_\kappa) - \sin(\mathbf{k}'\mathbf{R}_\kappa)] \quad (3.4b)$$

$$= \frac{-iq_0}{R_0 \sqrt{MN}} \mathbf{e}_{\mathbf{k}'-\mathbf{k},\nu} \cdot \left[\frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}} - \frac{\partial \varepsilon_{\mathbf{k}'}}{\partial \mathbf{k}'} \right], \quad (3.4c)$$

with $R_0 = |\mathbf{R}_\kappa|$ as n.n. distance ((3.4b) is valid for the structures with a center of inversion). Summations over wave vectors in (3.1), (3.3) are limited to the first Brillouin zone.

We introduce now the double-time Green's function (GF) for electron and phonon operators [15]:

$$G_{p\sigma}(t-t') \equiv \langle\langle a_{p\sigma}(t), a_{p\sigma}^+(t') \rangle\rangle = -i\theta(t-t') \langle [a_{p\sigma}(t), a_{p\sigma}^+(t')] \rangle_+, \quad (3.5)$$

$$D_{q\nu}(t-t') \equiv \langle\langle Q_{q\nu}(t), Q_{q\nu}^+(t') \rangle\rangle = -i\theta(t-t') \langle [Q_{q\nu}(t), Q_{q\nu}^+(t')] \rangle_-. \quad (3.6)$$

We are going to calculate functions (3.5) and (3.6) using the equation of motion method for GF [15–17]. It leads to the following equation for an electron GF (Fourier transformed with respect to time)

$$(\omega - \varepsilon_{0p\sigma}) G_{p\sigma}(\omega) = 1 + \sum_{q\nu} V_\nu(\mathbf{p} - \mathbf{q}, \mathbf{p}) \langle\langle a_{\mathbf{p}-\mathbf{q},\sigma} Q_{q\nu} | a_{p\sigma}^+ \rangle\rangle_\omega, \quad (3.7)$$

where

$$\varepsilon_{0p\sigma} = \varepsilon_p + \frac{U}{N} \sum_{\mathbf{k}} \langle n_{\mathbf{k},-\sigma} \rangle. \quad (3.8)$$

As usually, the electron–electron scattering is limited here to the elastic processes:

$$\langle\langle a_{\mathbf{p}+\mathbf{q},\sigma} a_{\mathbf{k}+\mathbf{q},-\sigma}^+ a_{\mathbf{k},-\sigma} | a_{p,\sigma}^+ \rangle\rangle_\omega \approx \delta_{q,0} \langle n_{\mathbf{k},-\sigma} \rangle G_{p\sigma}(\omega). \quad (3.9)$$

Inelastic processes may be accounted for, in principle, by means of the irreducible GF method [16, 17].

In order to evaluate the GF occurring on the left-hand side of eq. (3.7), the GF is differentiated with respect to the second time variable t' . After some algebra one gets [16]:

$$G_{p\sigma}(\omega) = G_{p\sigma}^0(\omega) + G_{p\sigma}^0(\omega) P_{p\sigma}(\omega) G_{p\sigma}^0(\omega), \quad (3.10)$$

where the free-particle GF and the scattering operator are

$$G_{p\sigma}^0 = (\omega - \varepsilon_{0p\sigma})^{-1}, \quad (3.11)$$

$$P_{p\sigma}(\omega) = \sum_{qvq'\nu'} V_\nu(\mathbf{p} - \mathbf{q}, \mathbf{p}) V_{\nu'}(\mathbf{p}, \mathbf{p} - \mathbf{q}') \langle \langle a_{p-q,\sigma} Q_{q\nu} | Q_{q'\nu'}^+ a_{p-q',\sigma}^+ \rangle \rangle_\omega. \quad (3.12)$$

Following the works [16, 17] we introduce the mass operator $M_{p\sigma}(\omega)$ as the proper part of the operator P (without parts connected with the single G^0 line) according to the equation $P = M + MG^0P$. Then eq. (3.10) turns into the Dyson's equation $G = G^0 + G^0MG$, which can be solved immediately

$$G_{p\sigma}(\omega) = \{[G_{p\sigma}^0(\omega)]^{-1} - M_{p\sigma}(\omega)\}^{-1}. \quad (3.13)$$

In order to calculate the mass operator self-consistently, we express the GF from (3.12) in terms of its correlator:

$$\langle \langle a_{p+q,\sigma} Q_{q\nu} | Q_{q'\nu'}^+ a_{p-q',\sigma}^+ \rangle \rangle_\omega = \int_{-\infty}^{\infty} \frac{d\omega'}{\omega - \omega'} (e^{\omega'/\theta} + 1) \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{-i\omega't} \langle Q_{q'\nu'}^+(t) a_{p-q',\sigma}^+(t) a_{p-q,\sigma} Q_{q\nu} \rangle \quad (3.14)$$

(here the temperature T of the system enters as $\theta = k_B T$). Assuming that the renormalization of the electron–phonon interaction vertex may be neglected, (comp. Migdal's paper [18]), we decouple the two-particle correlator in the following way

$$\langle Q_{q'\nu'}^+(t) a_{p-q',\sigma}^+(t) a_{p-q,\sigma} Q_{q\nu} \rangle \approx \langle Q_{q'\nu'}^+(t) Q_{q\nu} \rangle \langle a_{p-q',\sigma}^+(t) a_{p-q,\sigma} \rangle. \quad (3.15)$$

Now, expressing one particle correlators in terms of the corresponding GFs, we get the final expression for the mass operator

$$M_{p\sigma}(\omega) = \sum_{q\nu} |V_\nu(\mathbf{p} - \mathbf{q}, \mathbf{p})|^2 \int \int \frac{d\omega_1 d\omega_2}{\pi^2} \frac{1 - n(\omega_1) + N(\omega_2)}{\omega - (\omega_1 + \omega_2)} \text{Im} G_{p-q,\sigma}(\omega_1) \text{Im} D_{q\nu}(\omega_2). \quad (3.16)$$

Here $n(\omega)$ and $N(\omega)$ are the Fermi- and Bose-distribution functions. Throughout the paper the argument ω of the functions G^0 , G , M , D etc. is to be understood as $\omega + i\delta$, with $\delta = 0^+$.

4. Phonon Green's function

Phonon GF $D_{p\nu}(\omega)$ obeys the following equation of motion:

$$(\omega^2 - \omega_{0p\nu}^2) D_{p\nu}(\omega) = 1 + \sum_{q\sigma} V_\nu(\mathbf{q}, \mathbf{q} - \mathbf{p}) \langle \langle a_{q-p,\sigma}^+ a_{q\sigma} | Q_{p\nu}^+ \rangle \rangle_\omega. \quad (4.1)$$

As in the previous section, by (double) differentiation of the higher GF, occurring in (4.1), with respect to the second time variable t' , the following equation is obtained:

$$D_{p\nu}(\omega) = D_{p\nu}^0(\omega) + D_{p\nu}^0(\omega) T_{p\nu}(\omega) D_{p\nu}^0(\omega), \quad (4.2)$$

where

$$D_p^0 = (\omega^2 - \omega_{0p\nu}^0)^{-1}, \quad (4.3)$$

$$T_{p\nu}(\omega) = \sum_{q\sigma q'\sigma'} V_\nu(\mathbf{q}, \mathbf{q} - \mathbf{p}) V_\nu(\mathbf{q}', \mathbf{q}' + \mathbf{p}) \langle\langle a_{q-p,\sigma}^+ a_{q\sigma} | a_{q'+p,\sigma'}^+ a_{q'\sigma'} \rangle\rangle_\omega. \quad (4.4)$$

Defining the mass operator Π as the proper part of the scattering operator T , i.e. by eq. $T = \Pi + \Pi D^0 T$, we get Dyson's equation for one-phonon GF:

$$D_{p\nu}(\omega) = D_{p\nu}^0(\omega) + D_{p\nu}^0(\omega) \Pi_{p\nu}(\omega) D_{p\nu}(\omega). \quad (4.5)$$

As previously, renormalization of the vertex is neglected, which corresponds to the decoupling:

$$\langle a_{q'+p,\sigma}^+(t) a_{q'\sigma}(t) a_{q-p,\sigma}^+ a_{q\sigma} \rangle \approx \langle a_{q'+p,\sigma}^+(t) a_{q\sigma} \rangle \langle a_{q'\sigma}(t) a_{q-p,\sigma}^+ \rangle. \quad (4.6)$$

Using (4.6), the mass operator for phonon GF obtained from (4.4) is

$$\Pi_{p\nu}(\omega) = \sum_{q\sigma} |V_\nu(\mathbf{q} - \mathbf{p}, \mathbf{q})|^2 \int \int \frac{d\omega_1 d\omega_2}{\pi^2} \frac{n(\omega_1) - n(\omega_2)}{\omega + \omega_1 - \omega_2} \text{Im} G_{q-p,\sigma}(\omega_1) \text{Im} G_{q\sigma}(\omega_2). \quad (4.7)$$

5. Renormalization of the electron and phonon spectra

The electron and phonon GFs are to be determined self-consistently from the following set of equations:

$$G_{k\sigma}(\omega) = [\omega - \varepsilon_{0k\sigma} - M_{k\sigma}(\omega)]^{-1}, \quad (5.1)$$

$$D_{q\nu}(\omega) = [\omega^2 - \omega_{0q\nu}^2 - \Pi_{q\nu}(\omega)]^{-1}, \quad (5.2)$$

$$M_{k\sigma}(\omega) = \sum_{p\nu} |V_\nu(\mathbf{k} - \mathbf{p}, \mathbf{k})|^2 \int \frac{d\omega_1 d\omega_2}{\pi^2} \frac{1 - n(\omega_1) + N(\omega_2)}{\omega - \omega_1 - \omega_2} \text{Im} G_{k-p,\sigma}(\omega_1) \text{Im} D_{p\nu}(\omega_2), \quad (5.3)$$

$$\Pi_{q\nu}(\omega) = \sum_{p\sigma} |V_\nu(\mathbf{p} - \mathbf{q}, \mathbf{p})|^2 \int \frac{d\omega_1 d\omega_2}{\pi^2} \frac{n(\omega_1) - n(\omega_2)}{\omega + \omega_1 - \omega_2} \text{Im} G_{p-q,\sigma}(\omega_1) \text{Im} G_{p\sigma}(\omega_2), \quad (5.4)$$

We solve (5.1)–(5.4) using “quasiparticle pole” approximation for the evaluation of M and Π (i.e. neglecting $\text{Im} M$, $\partial/\partial\omega \text{Re} M$, $\text{Im} \Pi$ and $\partial/\partial\omega \text{Re} \Pi$ in eqs. (5.1), (5.2) for G and D):

$$\text{Im} G_{k\sigma}(\omega) = -\pi \delta(\omega - \varepsilon_{k\sigma}), \quad (5.5)$$

$$\text{Im} D_{q\nu}(\omega) = -\pi \frac{1}{2\omega_{q\nu}} [\delta(\omega - \omega_{q\nu}) - \delta(\omega + \omega_{q\nu})], \quad (5.6)$$

where renormalized electron and phonon energies $\varepsilon_{k\sigma}$, $\omega_{q\nu}$ are self-consistent solutions of the equations:

$$\varepsilon - \varepsilon_{0k\sigma} - \text{Re } M_{k\sigma}(\varepsilon) = 0, \quad (5.7)$$

$$\omega^2 - \omega_{q\nu}^2 - \text{Re } \Pi_{q\nu}(\omega) = 0 \quad (5.8)$$

together with

$$M_{k\sigma}(\omega) = \sum_{q\nu} \frac{|V_\nu(\mathbf{k}-\mathbf{q}, \mathbf{k})|^2}{2\omega_{q\nu}} \left[\frac{1 + N(\omega_{q\nu}) - n(\varepsilon_{\mathbf{k}-\mathbf{q},\sigma})}{\omega - \omega_{q\nu} - \varepsilon_{\mathbf{k}-\mathbf{q},\sigma}} + \frac{N(\omega_{q\nu}) + n(\varepsilon_{\mathbf{k}-\mathbf{q},\sigma})}{\omega + \omega_{q\nu} - \varepsilon_{\mathbf{k}-\mathbf{q},\sigma}} \right], \quad (5.9)$$

$$\Pi_{q\nu}(\omega) = \sum_{k\sigma} |V_\nu(\mathbf{k}-\mathbf{q}, \mathbf{k})|^2 \left[\frac{n(\varepsilon_{\mathbf{k}-\mathbf{q},\sigma}) - n(\varepsilon_{\mathbf{k},\sigma})}{\omega + \varepsilon_{\mathbf{k}-\mathbf{q},\sigma} - \varepsilon_{\mathbf{k},\sigma}} \right]. \quad (5.10)$$

In this way energy shifts of electrons and phonons are to be calculated from the set of nonlinear integral equations (5.7–10) numerically, while electron and phonon damping is obtained from (5.1) and (5.2), using already calculated $\varepsilon_{k\sigma}$, $\omega_{q\nu}$, M , Π .

Theoretical calculations of the phonon linewidth in transition metals like Pd and Nb and comparison of the results with experimental values obtained by means of inelastic scattering of slow neutrons [19–23], have been of great interest in recent years. Following [15] we get from (5.2) the expressions for the phonon linewidth:

$$\tilde{\Gamma}_{q\nu} = \frac{\text{Im } \Pi_{q\nu}(\omega)}{2\omega - \frac{\partial}{\partial \omega} \text{Re } \Pi_{q\nu}(\omega)} \Big|_{\omega=\omega_{q\nu}}. \quad (5.11)$$

Contrary to the papers [21, 22] where the matrix element of the electron phonon interaction (for calculation of the phonon damping) was evaluated using RMTA [24], in a present paper, owing to the BLF model applied here, this matrix element is expressed in terms of the characteristic parameters of the transition metal: M , q_0 , $T(\mathbf{R}_\kappa)$. The last two, together with the Coulomb repulsion U , are phenomenological parameters of the model. Note that the anisotropy of the system is fully accounted in (5.9), (5.10), contrary to the Fröhlich model, where spherical Fermi surface is supposed. Owing to $N(\omega)$ and $n(\omega)$ occurring in (5.9), (5.10), the temperature dependence of M and Π may be investigated. In particular, for low temperatures one gets from (5.9):

$$[M_{k\sigma}(\omega; T) - M_{k\sigma}(\omega; 0)] \sim T^4 \quad (5.12)$$

which follows immediately from the estimation

$$|V_\nu(\mathbf{k}-\mathbf{q}, \mathbf{k})|^2 \sim q^2 \quad (5.13)$$

for small $|\mathbf{q}|$.

6. Renormalized spectrum of the Mott–Hubbard isolator

In many oxides and sulfides [25] of transition metal the Coulomb repulsion is much greater than the band width, $U \gg W$. In this case (opposite to the one assumed in the section 3) it is reasonable to work in the Wannier representation for all operators, as it was introduced in section 2. The one-electron GF:

$$G_{j'\sigma}(t, t') = \langle\langle a_{j\sigma}(t), a_{j'\sigma}^\dagger(t') \rangle\rangle \quad (6.1)$$

obeys the following equation of motion

$$(\omega - t_0) G_{jj'\sigma}(\omega) = \delta_{jj'} + \sum_{\kappa} t_{jj+\kappa} G_{j+\kappa,j'\sigma}(\omega) - U \Gamma_{jj'\sigma}(\omega) + \sum_{\kappa q\nu} A_{q\nu}(j, j + \kappa) \Phi_{q\nu,j+\kappa,j'\sigma}(\omega), \quad (6.2)$$

where

$$\Gamma_{jj_2\sigma}(\omega) = \langle\langle a_{j_1\sigma} n_{j_1-\sigma} | a_{j_2\sigma}^+ \rangle\rangle_{\omega}, \quad (6.3)$$

$$\Phi_{q\nu,j_1j_2\sigma}(\omega) = \langle\langle Q_{q\nu} a_{j_1\sigma} | a_{j_2\sigma}^+ \rangle\rangle_{\omega}. \quad (6.4)$$

Again, by means of time differentiation, the equation of motion for $\Gamma_{jj_2}(\omega)$ may be obtained as

$$\begin{aligned} \omega \Gamma_{jj_2}(\omega) &= \delta_{jj_2} \langle n_{j_1-\sigma} \rangle + (t_0 + U) \Gamma_{jj_2\sigma}(\omega) + \sum_{\substack{j_3 \\ j_3 \neq j_1}} \left\{ t_{jj_3} \langle\langle n_{j_1-\sigma} a_{j_3\sigma} | a_{j_2\sigma}^+ \rangle\rangle_{\omega} + t_{jj_3} \langle\langle a_{j_1-\sigma}^+ a_{j_3-\sigma} a_{j_1\sigma} | a_{j_2\sigma}^+ \rangle\rangle_{\omega} \right. \\ &\quad - t_{jj_3} \langle\langle a_{j_3-\sigma}^+ a_{j_1-\sigma} a_{j_1\sigma} | a_{j_2\sigma}^+ \rangle\rangle_{\omega} + \sum_{q\nu} [A_{q\nu}(jj_3) \langle\langle Q_{q\nu} n_{j_1-\sigma} a_{j_3\sigma} | a_{j_2\sigma}^+ \rangle\rangle_{\omega} \\ &\quad \left. + A_{q\nu}(jj_3) \langle\langle Q_{q\nu} a_{j_1-\sigma}^+ a_{j_3-\sigma} a_{j_1\sigma} | a_{j_2\sigma}^+ \rangle\rangle_{\omega} - A_{q\nu}(jj_3) \langle\langle Q_{q\nu} a_{j_3-\sigma}^+ a_{j_1-\sigma} a_{j_1\sigma} | a_{j_2\sigma}^+ \rangle\rangle_{\omega} \right\}. \quad (6.5) \end{aligned}$$

The electron subsystem in eqs. (6.2–5) is described according to Hubbard-I approximation. In the spirit of it, the following decouplings are performed:

$$\begin{aligned} \langle\langle Q_{q\nu} n_{j_1-\sigma} a_{j_3\sigma} | a_{j_2\sigma}^+ \rangle\rangle_{\omega} &\approx \langle n_{j_1-\sigma} \rangle \Phi_{q\nu,j_1j_2\sigma}(\omega), \\ \langle\langle Q_{q\nu} a_{j_1-\sigma}^+ a_{j_3-\sigma} a_{j_1\sigma} | a_{j_2\sigma}^+ \rangle\rangle_{\omega} &\approx \langle a_{j_1-\sigma}^+ a_{j_3-\sigma} \rangle \Phi_{q\nu,j_1j_2}(\omega), \\ \langle\langle Q_{q\nu} a_{j_3-\sigma}^+ a_{j_1-\sigma} a_{j_1\sigma} | a_{j_2\sigma}^+ \rangle\rangle_{\omega} &\approx \langle a_{j_3-\sigma}^+ a_{j_1-\sigma} \rangle \Phi_{q\nu,j_1j_2}(\omega). \end{aligned} \quad (6.6)$$

Using (6.6), eq. (6.2) may be rewritten as

$$\begin{aligned} (\omega - t_0) G_{jj_2\sigma}(\omega) &= \left\{ 1 + \frac{U n_{-\sigma}}{\omega - t_0 - U} \right\} \left\{ \delta_{jj_2} + \sum_{\kappa} \left[t_{jj_1+\kappa} G_{j_1+\kappa,j_2,\sigma}(\omega) \right. \right. \\ &\quad \left. \left. + \sum_{q\nu} A_{q\nu}(j_1, j_1 + \kappa) \Phi_{q\nu,j_1+\kappa,j_2,\sigma}(\omega) \right] \right\}. \quad (6.7) \end{aligned}$$

In a similar way, by time differentiation equation of motion for Φ is obtained, higher correlators are decoupled in the spirit of (6.6), and then, from (6.7), the final equation for $G_{jj'\sigma}$ obtained, which after Fourier transformation is

$$G_{k\sigma}(\omega) = G_{k\sigma}^0(\omega) + G_{k\sigma}^0(\omega) P_{k\sigma}(\omega) G_{k\sigma}^0(\omega), \quad (6.8)$$

where

$$G_{k\sigma}(\omega) = \frac{1}{N} \sum_{j_1j_2} e^{-ik(\mathbf{R}_{j_1} - \mathbf{R}_{j_2})} G_{j_1j_2\sigma}(\omega), \quad (6.9)$$

$$G_{k\sigma}^0(\omega) = [F_{\sigma}^0(\omega) - (\epsilon_k - t_0)]^{-1}, \quad (6.10)$$

$$F_{\sigma}^0(\omega) = \left[\frac{1 - n_{-\sigma}}{\omega - t_0} + \frac{n_{-\sigma}}{\omega - t_0 - U} \right]^{-1} \quad (6.11)$$

and the scattering operator

$$P_{k\sigma}(\omega) = \frac{1}{N} \sum_{q\nu q'\nu' j_1 j_2 j_3 j_4} A_{q\nu}(j_1 j_2) A_{q'\nu'}^*(j_3 j_4) e^{-i\mathbf{k}(\mathbf{R}_{j_1} - \mathbf{R}_{j_4})} \langle\langle Q_{q\nu} a_{j_2\sigma} | Q_{q'\nu'}^+ a_{j_3\sigma}^+ \rangle\rangle_{\omega}. \quad (6.12)$$

In terms of the mass operator $M_{k\sigma}(\omega)$, neglecting vertex renormalization, we get the following solution

$$G_{k\sigma}(\omega) = \{ [G_{k\sigma}^0(\omega)]^{-1} - M_{k\sigma}(\omega) \}^{-1}, \quad (6.13)$$

where

$$M_{k\sigma}(\omega) = \sum_{q\nu} |V_{\nu}(\mathbf{k} - \mathbf{q}, \mathbf{k})|^2 \int \int \frac{d\omega_1 d\omega_2}{\pi^2} \frac{1 - n(\omega_1) + N(\omega_2)}{\omega - \omega_1 - \omega_2} \text{Im} G_{\mathbf{k}-\mathbf{q},\sigma}(\omega_1) \text{Im} D_{q\nu}(\omega_2). \quad (6.14)$$

From the fact, that the mass operator (3.16) obtained in the region $U \ll W$ coincides with (6.14) obtained in the opposite case $U \gg W$, one can expect that the expression (6.14) is valid for any U, W . Of course, when calculating GF $G_{k\sigma}(\omega)$ in a self-consistent way by (3.13), (6.13), appropriate free-particle GF $G_{k\sigma}^0(\omega)$ must be used (e.g. (3.11) or (6.10) in the limiting cases).

Now let us solve the set of eqs. (6.13), (6.14) with (6.10), (6.11), (4.5) and (4.7) again in the quasiparticle pole approximation. Neglecting $\text{Im} M$ in (6.13) and inserting (6.10) and (6.11) we get

$$G_{k\sigma}(\omega) = \frac{\omega - E_{\sigma}^{(0)}}{(\omega - t_0)(\omega - t_0 - U) - U X_{k\sigma}(\omega)[\omega - E_{\sigma}^{(0)}]} = \frac{\omega - E_{\sigma}^{(0)}}{[\omega - E_{k\sigma}^{(1)}(\omega)][\omega - E_{k\sigma}^{(2)}(\omega)]}, \quad (6.15)$$

where

$$E_{\sigma}^{(0)} = t_0 + (1 - n_{-\sigma}) U, \quad (6.16)$$

$$X_{k\sigma}(\omega) = [\varepsilon_{\mathbf{k}} - \text{Re} M_{k\sigma}(\omega) - t_0]/U, \quad (6.17)$$

$$E_{k\sigma}^{(\alpha)}(\omega) = E_{\sigma}^{(0)} + \frac{U}{2} \{ [X_{k\sigma}(\omega) + 2n_{-\sigma} - 1] + (2\alpha - 3)[(X_{k\sigma}(\omega) + 2n_{-\sigma} - 1)^2 + 4n_{-\sigma}(1 - n_{-\sigma})]^{1/2} \}, \quad \alpha = 1, 2. \quad (6.18)$$

In terms of renormalized band energy $\tilde{E}_{\mathbf{k}}^{(\alpha)}$, defined as the solution of the equation

$$\omega - E_{k\sigma}^{(\alpha)}(\omega) = 0; \quad \alpha = 1, 2 \quad (6.19)$$

we get the following imaginary part of GF (compare with the Hubbard-I solution [6]):

$$\text{Im} G_{k\sigma}(\omega) = -\pi [A_{k\sigma}^{(1)} \delta(\omega - \tilde{E}_{k\sigma}^{(1)}) + A_{k\sigma}^{(2)} \delta(\omega - \tilde{E}_{k\sigma}^{(2)})], \quad (6.20)$$

where

$$A_{k\sigma}^{(\alpha)} = \left\{ \frac{\omega - E_{\sigma}^{(0)}}{[\omega - E_{k\sigma}^{(\beta-\alpha)}(\omega)] \left[1 - \frac{d}{d\omega} E_{k\sigma}^{(\alpha)}(\omega) \right]} \right\}_{\omega = \tilde{E}_k^{(\alpha)}} \quad (6.21)$$

In the limit of small X (i.e. $W \ll U$), the energies (6.18) and amplitudes (6.21) may be expanded into a power series:

$$E_{k\sigma}^{(1)}(\omega) = t_0 + (1 - n_{-\sigma})[\varepsilon_k - \text{Re } M_{k\sigma}(\omega) - t_0][1 + O(X)], \quad (6.22)$$

$$E_k^{(2)}(\omega) = t_0 + U + n_{-\sigma}[\varepsilon_k - \text{Re } M_{k\sigma}(\omega) - t_0][1 + O(X)],$$

$$A_{k\sigma}^{(1)} = (1 - n_{-\sigma}) \left\{ \frac{1 - 2n_{-\sigma} X_{k\sigma}(\omega)[1 + O(X)]}{1 - (1 - n_{-\sigma}) \frac{d}{d\omega} M_{k\sigma}(\omega)[1 + O(X)]} \right\}_{\omega = \tilde{E}_k^{(1)}}, \quad (6.23)$$

$$A_{k\sigma}^{(1)} = n_{-\sigma} \left\{ \frac{1 + 2(1 - n_{-\sigma}) X_{k\sigma}(\omega)[1 + O(X)]}{1 - n_{-\sigma} \frac{d}{d\omega} M_{k\sigma}(\omega)[1 + O(X)]} \right\}_{\omega = \tilde{E}_k^{(2)}}$$

The phonon GF in the pole approximation was already found (5.6). When (6.20) and (5.6) are inserted into (6.14) and (4.7), integrations over ω_1 and ω_2 may be immediately performed and expressions analogous to (5.9) and (5.10) (although two-times longer) are obtained.

From the expression (6.18) it is evident that $E_{k\sigma}^{(2)}(\omega) > E_{\sigma}^{(0)}$ and $E_{k\sigma}^{(1)}(\omega) < E_{\sigma}^{(0)}$ for any value of $X_{k\sigma}(\omega)$. This means that the finite gap between the two bands $\tilde{E}_k^{(1)}$ and $\tilde{E}_k^{(2)}$ exists despite of the fact that the electron-phonon interaction is included. Therefore our model is not capable of reproducing the metal-insulator transition for Hubbard-I solution.

7. Superconductivity in transition metals

The equations for superconductivity in transition metals were obtained in the Wannier representation in paper [14], for the following general form of the electron-phonon interaction:

$$H_{e-i} = \sum_{ij\sigma\alpha} T_{ij}^{\alpha} u_{ij}^{\alpha} a_{i\sigma}^{\dagger} a_{j\sigma}, \quad (7.1)$$

where

$$u_{ij}^{\alpha} = u_i^{\alpha} - u_j^{\alpha}. \quad (7.2)$$

These equations may be applied to the BLF model, considered in the present paper, for which (comp. (2.11))

$$T_{ij}^{\alpha} = q_0 t_{ij} (R_j^{\alpha} - R_i^{\alpha}) / |\mathbf{R}_j - \mathbf{R}_i|. \quad (7.3)$$

The GF appropriate for this problem has the matrix form:

$$\hat{G}_{ij}(\omega) = \begin{bmatrix} \langle\langle a_{i\uparrow} | a_{j\uparrow}^+ \rangle\rangle_\omega, \langle\langle a_{i\uparrow} | a_{j\downarrow} \rangle\rangle_\omega \\ \langle\langle a_{i\downarrow}^+ | a_{j\uparrow} \rangle\rangle_\omega, \langle\langle a_{i\downarrow}^+ | a_{j\downarrow} \rangle\rangle_\omega \end{bmatrix}. \quad (7.4)$$

It obeys the Dyson equation [14]:

$$\hat{G}_{ij2}(\omega) = \hat{G}_{ij2}^0(\omega) + \sum_{j3j4} \hat{G}_{ij3}^0(\omega) \hat{M}_{j3j4}(\omega) \hat{G}_{j4i2}(\omega), \quad (7.5)$$

where

$$\hat{M}_{j3j4}(\omega) = \hat{M}_{j3j4}^{e-ph}(\omega) + \hat{M}_{j3j4}^{e-e}(\omega) \quad (7.6)$$

is the mass operator. As obtained in a self-consistent way, with renormalization of the vertex neglected, its electron–phonon part looks [14]:

$$M_{j3j4}^{e-ph}(\omega) = \frac{-1}{\pi^2} \int \int_{-\infty}^{\infty} d\omega_1 d\omega_2 \frac{1 - n(\omega_1) + N(\omega_2)}{1 - \omega_1 - \omega_2} \sum_{\alpha\beta j1j2} T_{j3j1}^\alpha \text{Im} \langle\langle u_{j3j1}^\alpha u_{j2j4}^\beta \rangle\rangle_{\omega_2} \hat{\tau}_3 \text{Im} \hat{G}_{j1j2}(\omega_1) \hat{\tau}_3 T_{j2j4}^\beta, \quad (7.7)$$

where

$$\hat{\tau}_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \quad (7.8)$$

Now eqs. (7.4–7) may be rewritten in the momentum representation

$$\hat{G}_k(\omega) = \begin{bmatrix} \langle\langle a_{k\uparrow} | a_{k\uparrow}^+ \rangle\rangle_\omega, \langle\langle a_{k\uparrow} | a_{-k\downarrow} \rangle\rangle_\omega \\ \langle\langle a_{-k\downarrow}^+ | a_{k\uparrow} \rangle\rangle_\omega, \langle\langle a_{-k\downarrow}^+ | a_{-k\downarrow} \rangle\rangle_\omega \end{bmatrix}, \quad (7.9)$$

$$\hat{G}_k(\omega) = \hat{G}_k^0(\omega) + \hat{G}_k^0(\omega) \hat{M}_k(\omega) \hat{G}_k(\omega), \quad (7.10)$$

$$\begin{aligned} \hat{M}_k^{e-ph}(\omega) &= \sum_{q\nu} |V_\nu(\mathbf{k} - \mathbf{q}, \mathbf{k})|^2 \frac{1}{\pi^2} \int \int_{-\infty}^{\infty} d\omega_1 d\omega_2 \\ &\times \frac{\text{th}(\omega_1/2T) + \text{cth}(\omega_2/2T)}{2(\omega - \omega_1 - \omega_2)} \hat{\tau}_3 \text{Im} \hat{G}_{\mathbf{k}-\mathbf{q}}(\omega_1) \hat{\tau}_3 \text{Im} D_{q\nu}(\omega_2). \end{aligned} \quad (7.11)$$

When deriving (7.11), the following relation (see (2.14) and (3.6)) was used:

$$\langle\langle u_i^\alpha | u_i^\beta \rangle\rangle_\omega = \frac{1}{NM} \sum_{q\nu} D_{q\nu}(\omega) e_{q\nu}^\alpha e_{q\nu}^{*\beta} e^{iq(\mathbf{R}_i - \mathbf{R}_j)}. \quad (7.12)$$

Note that electron–phonon contribution to the mass operator (7.11) in the superconducting state has the same form as that obtained earlier (3.16), (6.14) for the normal state, except that the spin dependent GF $G_{k\nu}(\omega)$ is now replaced by the matrix $[\hat{\tau}_3 \hat{G}_k(\omega) \hat{\tau}_3]$, the distribution functions $n(\omega)$, $N(\omega)$ are written in terms of th and cth functions, as usual.

The electron–electron Coulomb part of M in the Hartree–Fock approximation is given by

$$\hat{M}_k^{e-e} = U \begin{bmatrix} \langle n_{k\downarrow} \rangle, & -\langle a_{-k\downarrow} a_{k\uparrow} \rangle \\ -\langle a_{k\uparrow}^\dagger a_{-k\downarrow}^\dagger \rangle, & -\langle n_{-k\uparrow} \rangle \end{bmatrix} = U \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \hat{\tau}_3 \text{Im } \hat{G}_k(\omega) \hat{\tau}_3 \text{th}\left(\frac{\omega}{2T}\right) \quad (7.13)$$

(the general expression may be found in [14]).

The self-consistent expressions (7.11) and (7.13) for the mass operator describe properties of the superconducting transition metal within the framework of the BLF [1] model. They are analogues of the Eliashberg equations [3] for simple metals. Owing to these one can investigate superconducting state within the same model as used for the description of the normal state, in terms of a few parameters of the transition metal, such as U , t_0 , $t(\mathbf{R}_\kappa)$, q_0 , M and the n.n. distance R_0 . Considering U to be a fitting parameter, the standard Eliashberg equations [3] may be derived:

$$[1 - Z(\omega)] \omega = - \int_{-\infty}^{\infty} dz K_{\text{ph}}(z, \omega) \text{Re} \frac{z}{\sqrt{z^2 - \Delta^2(z)}} \text{sign}(z), \quad (7.14)$$

$$Z(\omega) \Delta(\omega) = \int_{-\infty}^{\infty} dz K_{\text{ph}}(z, \omega) \text{Re} \frac{\Delta(z)}{\sqrt{z^2 - \Delta^2(z)}} \text{sign}(z) - UN(E_F) \int_0^{\omega_c} dz \text{th}\left(\frac{z}{2T}\right) \text{Re} \frac{\Delta(z)}{\sqrt{z^2 - \Delta^2(z)}}, \quad (7.15)$$

where

$$K_{\text{ph}}(z, \omega) = \int_0^{\infty} d\omega' \alpha^2(\omega') F(\omega') \frac{1}{2} \left[\frac{\text{th}(z/2T) + \text{cth}(\omega'/2T)}{z + \omega' - \omega + i\delta} - \frac{\text{th}(z/2T) - \text{cth}(\omega'/2T)}{z - \omega' - \omega + i\delta} \right] \quad (7.16)$$

while the electron-phonon spectral function [2, 3] is

$$\alpha^2(\omega) F(\omega) = \int_{S_F} \frac{d^2k}{v_k} \int_{S_F} \frac{d^2k'}{v_{k'}} \sum_{\nu} |V_{\nu}(\mathbf{k}', \mathbf{k})|^2 \left(\frac{-1}{\pi}\right) \text{Im } D_{\mathbf{k}-\mathbf{k}', \nu}(\omega + i\delta) / \left[\int_{S_F} \frac{d^2k}{v_k} \right]. \quad (7.17)$$

Eqs. (7.14) and (7.15) may be reduced to the linearized Eliashberg equations [3], defining the temperature of the superconducting transition. Results of the numerical evaluation of the $\alpha^2(\omega) F(\omega)$ for Nb, W, Mo, Ta, V, based on the expression (7.17), will be published elsewhere.

8. Conclusions

In the present paper a self-consistent theory of the electron-phonon interaction within the BLF [1] model was developed for the metallic case ($U \ll W$) as well for the Mott-Hubbard isolator case ($U \gg W$). The expressions (5.5 or 6.20) and (5.6) determine the renormalized one-particle densities of states for electrons and phonons:

$$\mathcal{N}^e(\omega) = -\frac{1}{\pi N} \sum_{\mathbf{k}\sigma} \text{Im } G_{\mathbf{k}\sigma}(\omega), \quad (8.1)$$

$$\mathcal{N}^{\text{ph}}(\omega) = -\frac{1}{3\pi N} \sum_{\mathbf{q}\nu} \text{Im } D_{\mathbf{q}\nu}(\omega). \quad (8.2)$$

Using (7.17), the electron-phonon enhancement parameter λ_{e-ph} may be expressed as [2, 3]

$$\lambda_{e-ph} = 2 \int_0^{\infty} \omega^{-1} \alpha^2(\omega) F(\omega) d\omega. \quad (8.3)$$

The renormalized electron density is

$$\mathcal{N}^e(E_F) = \mathcal{N}_0^e(E_F)(1 + \lambda_{e-ph}) \quad (8.4)$$

and therefore the Stoner criterion of magnetization may be written as

$$U\mathcal{N}_0^e(E_F)(1 + \lambda_{e-ph}) > 1. \quad (8.5)$$

Because of λ_{e-ph} occurring in (8.5) one may conclude that the electron-phonon interaction facilitates magnetic ordering at low temperatures, due to the dressing of the electron by the phonon cloud.

Superconducting properties of the model are handled by eqs. (7.14), (7.15), allowing investigation of the superconductivity in transition metals, their alloys and compounds within the framework of common system of equations [3, 14]. The BLF model has proved to be useful also in the case of the theory of electroconductivity for the one-band system, including shift of the Fermi surface and its deformation [26]. Essentially new temperature dependence of the electroresistance in the low temperature region was obtained there, in agreement with the results of ref. [24]. Using electron-phonon interaction in the form (3.3), magnon damping was obtained in the generalized RKKY model. The low temperature behaviour of the damping in a heavy rare-earth metal (like gadolinium) was previously determined [27]. The generalization of the electron-phonon interaction Hamiltonian for disordered binary alloy $A_x B_{1-x}$ of transition metals was earlier performed in [12]. Using methods of [12, 14] the theory for strong-coupling superconductivity in disordered transition metal alloys has been developed [31, 32].

It must be noted, however, that BLF model is not free of shortcomings and that it includes a number of assumptions. Nevertheless, all recent investigations [2, 3, 8, 10, 28, 30] show that in many interesting physical situations these assumptions are justified and lead to reasonable conclusions.

The results of the present paper demonstrate the effectiveness of the BLF model in the description of a variety of properties in the transition metals and their alloys.

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