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Electron-Phonon Interaction in Disordered Transition Metal Alloys

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The Hamiltonian of the electron-phonon interaction is derived and applied to the description of disordered transition metal alloys. The coupled set of equations for the electron and phonon Green functions is derived with the help of the equation-of-motion technique. Neglecting the vertex corrections in the self-energy operators the closed self-consistent system of equations is obtained. The relevant configurational averaging is performed in the framework of the CPA. The electronic specific heat in the low-temperature limit is calculated.

Выведен гамильтониан, описывающий сильно связанные электроны в разупорядоченном сплаве переходных металлов с учетом электрон-фононного взаимодействия. С помощью метода уравнений движения получена связанная система уравнений для электронной и фононной функций Грина. В пренебрежении вершинными поправками в массовом операторе получена замкнутая самосогласованная система уравнений. Конфигурационное усреднение проведено в рамках приближения когерентного потенциала. Вычислена низкотемпературная электронная теплоемкость сплава.

1. Introduction

In recent years there has been recognized that the microscopic description of certain unusual features [1, 2] of the disordered transition metal alloys requires the proper treatment of the electron-phonon interaction.

The electron-phonon interaction in disordered binary alloys has been studied by many authors. Chen et al. [3] introduced the model in which phonons were treated phenomenologically while electrons were described in CPA. The electron-phonon interaction was described by the local operator. The model was later generalized by Kolley and Kolley [4] and Wysokiński [5] for the off-diagonal disorder. Allen [6] attempted to develop the complete theory of the interacting electron-phonon system. He considered solids with weak static (impurities) and dynamic (phonons) disorder. The limitation of the theory is the weakness of disorder. The application of Allen's theory to the disordered transition metal alloys is not clear. Girvin and Jonson [7] used the same Hamiltonian as in [3] but developed a more complete many-body theory of the electron-phonon interaction in strongly disordered metal alloys. Sacchetti [8] introduced a very simple model for treating the electron-phonon interaction in the low-temperature region in random binary alloys. This author uses the results of the Migdal theory [9] of the electron-phonon interaction in simple metals for disordered alloys. However, the explicit form of the Hamiltonian as well as the derivation of the used formulae are not given in this paper.

The purpose of our paper is to develop the complete microscopic self-consistent theory of the electron-phonon interaction in substitutionally disordered transition

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metal alloys. For the description of the electron-phonon interaction we generalize the Barišić et al. [10] model to the case of alloys. Barišić et al. [10] (to be referred to as BLF) introduced a model of the electron-phonon interaction in the transition metals and their compounds. This model is a direct generalization of the well-known Hubbard model to the case of deformed lattice and is formulated in the language of the tight-binding (TB) approximation. Additionally the "rigid ion" approximation is used for the derivation of the BLF Hamiltonian.

The BLF model was successfully applied to the calculation of the superconducting transition temperature T_c , the McMillan parameter, cohesive energy and paramagnetic susceptibility of the transition metal [11 to 14]. The BLF's tight-binding approach to the problem was later clarified in papers [15 to 17]. Holas et al. [18] and Plakida et al. [19] used the BLF model to calculate the renormalized electron and phonon spectra in crystal in the band and the atomic limits, respectively. The present paper generalizes their results to alloys.

Because the method of irreducible Green's functions [22 to 24] we use here gives very successful self-consistent solution of the many-body part of the problem we present the derivation of Dyson equations for electrons and phonons in some detail. This approach is essentially equivalent to the so-called self-consistent many-body theory described recently in [34].

2. The Model

The total Hamiltonian of the electron-ion system in the substitutionally disordered alloy is written, for a given configuration of atoms, in the following form:

$$H = H_e^0 + H_{ee} + H_{e-i} + H_i, \quad (1)$$

where

$$H_e^0 = \sum_{i\sigma} \epsilon_i a_{i\sigma}^\dagger a_{i\sigma} + \sum'_{ij\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma}$$

is the one-particle Hamiltonian of an electron in an alloy. The parameters ϵ_i and t_{ij} are random quantities taking on the values ϵ_A, ϵ_B and $t_{ij}^{AA}, t_{ij}^{AB}, t_{ij}^{BB}$ depending on the type of atoms occupying sites i and j . The prime in the second sum indicates that summation over j is limited to the nearest neighbours of an atom located in site i . The electron-electron scattering is approximated here by the Hubbard [20] intrasite term with random parameters,

$$H_{ee} = \frac{1}{2} \sum_{i\sigma} U_i n_{i\sigma} n_{i-\sigma}; \quad n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma}. \quad (2)$$

The third term in (1) represents the electron-ion interaction in alloys. This part of the Hamiltonian is derived in the Appendix and it is a direct generalization of the BLF model,

$$H_{e-i} = \sum_{i,j,\sigma} \sum_{\alpha} T_{ij}^{\alpha} (u_i^{\alpha} - u_j^{\alpha}) a_{i\sigma}^\dagger a_{j\sigma}, \quad (3)$$

where

$$T_{ij}^{\alpha} = \frac{q_0^i + q_0^j}{2} t_{ij} \frac{R_{ji}^{\alpha}}{R_{ji}}. \quad (4)$$

In (3) and (4) u_i^{α} is the α -th component ($\alpha = x, y, z$) of the displacement of an ion placed in an i -th site. q_0^i is the Slater coefficient describing the exponential, $\exp(-q_0^i r)$, decrease of the d-function [10]. It is equal to $q_0^A(q_0^B)$ when an atom at a site i is of A(B) type. \mathbf{R}_{ji} is the relative position vector of two ions at i and j ,

$$\mathbf{R}_{ji} = \mathbf{R}_j - \mathbf{R}_i; \quad R_{ji} = |\mathbf{R}_{ji}|. \quad (5)$$

This simple form of the interaction Hamiltonian reduces to that given by BLF in the case of perfect crystal. However, it is not the only possible and unique extension of the BLF model.

The last part of the Hamiltonian represents the ion Hamiltonian and in the harmonic approximation, we use here, is given by

$$H_i = \sum_i \frac{P_i^2}{2M_i} + \frac{1}{2} \sum_{ij} \sum_{\alpha\beta} u_i^\alpha \Phi_{ij}^{\alpha\beta} u_j^\beta. \quad (6)$$

M_i denotes the mass of an ion at the i -th position, and it takes on two values M_A , M_B . The dynamical matrix $\Phi_{ij}^{\alpha\beta}$ is, in general, a random quantity taking on various values as a function of the occupation and distance between the sites i and j .

For our main interest is the description of the electron-phonon interaction, we use here the Hartree-Fock approximation for the Hubbard term

$$H_{cc}^{\text{HF}} = \sum_{i\sigma} U_{i\sigma} n_{i\sigma}; \quad U_{i\sigma} = U_i \langle n_{i-\sigma} \rangle. \quad (7)$$

Having this in mind we rewrite the Hamiltonian (1)

$$H = H_e + H_{e-i} + H_i, \quad (8)$$

where

$$H_e = \sum_{i\sigma} \epsilon_i^\sigma a_{i\sigma}^\dagger a_{i\sigma} + \sum'_{ij\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma}, \quad (9)$$

$$\epsilon_i^\sigma = \epsilon_i + U_i \langle n_{i-\sigma} \rangle \quad (10)$$

and H_{e-i} and H_i are given by (3) and (6), respectively.

3. Electron Green Functions

We use the two-time thermodynamic Green function (GF) [21]. In the site representation it is defined for electron operators by

$$G_{ij}^\sigma(t-t') \equiv \langle\langle a_{i\sigma}(t) | a_{j\sigma}^\dagger(t') \rangle\rangle = -i\theta(t-t') \langle [a_{i\sigma}(t), a_{j\sigma}^\dagger(t')]_+ \rangle. \quad (11)$$

The calculations of (11) will be done with the help of the equation-of-motion technique as developed and used in papers [18, 19, 22 to 24].

Proceeding in the standard way [21] we obtain the following equation for the Fourier transform of (11):

$$\sum_n h_{in}^\sigma(\omega) G_{nj}^\sigma(\omega) = \delta_{ij} + \sum_{n\alpha} T_{in}^\alpha \langle\langle u_{in}^\alpha a_{n\sigma} | a_{j\sigma}^\dagger \rangle\rangle_\omega, \quad (12)$$

where various symbols denote

$$u_{in}^\alpha = u_i^\alpha - u_n^\alpha, \quad h_{in}^\sigma(\omega) = (\omega - \epsilon_i^\sigma) \delta_{in} - t_{in}. \quad (13)$$

To obtain the formula for the GF $\langle\langle u_{in}^\alpha a_{n\sigma} | a_{j\sigma}^\dagger \rangle\rangle_\omega$ we differentiate it with respect to the second time variable t' . We get

$$\sum_m h_{mj}^\sigma(\omega) \langle\langle u_{in}^\alpha a_{n\sigma} | a_{m\sigma}^\dagger \rangle\rangle_\omega = \sum_{m\beta} T_{mj}^\beta \langle\langle u_{in}^\alpha a_{n\sigma} | u_{mj}^\beta a_{m\sigma}^\dagger \rangle\rangle_\omega. \quad (14)$$

Defining now the zeroth-order GF, $G_{ij}^{0\sigma}(\omega)$ by

$$\sum_n h_{in}^\sigma(\omega) G_{nj}^{0\sigma}(\omega) = \delta_{ij} \quad (15)$$

we can easily solve (12) and (14) for $G_{nj}^\sigma(\omega)$. To do this, we multiply both sides of equation (12) by $G_{ji}^{0\sigma}$ from the left and sum up over i , and similarly, multiply (14) by G_{jl}^σ from the right and sum up over j . We have

$$G_{jj}^\sigma(\omega) = G_{jj}^{0\sigma}(\omega) + \sum_{il} G_{ji}^{0\sigma} K_{il}^\sigma(\omega) G_{lj}^{0\sigma}(\omega). \quad (16)$$

The scattering operator K is equal to

$$K_{il}(\omega) = \sum_{nm} \sum_{\alpha\beta} T_{in}^\alpha \langle\langle u_{in}^\alpha a_{n\sigma} | u_{ml}^\beta a_{m\sigma}^+ \rangle\rangle_\omega T_{ml}^\beta. \quad (17)$$

Equation (16) can be written in the form of the Dyson equation

$$G_{jj}^\sigma(\omega) = G_{jj}^{0\sigma}(\omega) + \sum_{il} G_{ji}^{0\sigma}(\omega) M_{il}^\sigma(\omega) G_{lj}^\sigma(\omega) \quad (18)$$

if one introduces the massoperator $M_{il}^\sigma(\omega)$ related to the scattering operator (17) by the formula [22 to 24]

$$K_{il}^\sigma(\omega) = M_{il}^\sigma(\omega) + \sum_{jj'} M_{ij'}^\sigma(\omega) G_{jj'}^{0\sigma}(\omega) K_{j'l}^\sigma(\omega). \quad (19)$$

It follows from this equation that M is a "proper part" (pp) of the scattering operator (17). The proper part of an irreducible GF (in our case irreducible GF coincides with GF) does not contain inner parts connected by one G^0 -line. In the matrix notation we expressed this fact as

$$M(\omega) = \{K(\omega)\}^{\text{pp}}. \quad (20)$$

The solution of the Dyson equation (18) can be written in the matrix form as

$$G(\omega) = \{(G_0)^{-1} - M(\omega)\}^{-1}. \quad (21)$$

Hence, the determination of G has been reduced to the determination of G^0 and M .

Equations (20) and (17) give an exact representation of the mass operator in terms of higher-order GF for a given configuration of atoms in alloy. To find explicit expressions for $M(\omega)$ for different model parameters, suitable approximations to evaluate the higher-order GF in (17) should be used.

In order to calculate the mass operator (20) self-consistently, we have to express it approximatively by the lower-order GF. The mass operator describes the inelastic scattering processes of the electrons with phonons. Starting from this physical picture reasonable approximations for M can be found.

The GF standing in the r.h.s. of (17) can be written as

$$\langle\langle u_{in}^\alpha a_{n\sigma} | u_{ml}^{\beta'} a_{m\sigma}^+ \rangle\rangle_\omega = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega - \omega'} (e^{\beta\omega'} + 1) \int_{-\infty}^{\infty} dt e^{-i\omega't} \langle u_{ml}^{\beta'}(t) a_{m\sigma}^+(t) u_{in}^\alpha a_{n\sigma} \rangle_0. \quad (22)$$

Here $\beta = (k_B T)^{-1}$ with k_B the Boltzmann constant and T the absolute temperature. We decouple the correlation function in (22) in the following way:

$$\langle u_{ml}^{\beta'}(t) a_{m\sigma}^+(t) u_{in}^\alpha a_{n\sigma} \rangle \approx \langle u_{ml}^{\beta'}(t) u_{in}^\alpha \rangle \langle a_{m\sigma}^+(t) a_{n\sigma} \rangle. \quad (23)$$

The approximate expression (23) results from neglecting the vertex corrections. The used approximation of two interacting modes can be represented graphically [9]



where a straight line describes the propagation of the electron and the wavy line represents the phonon propagation.

Expressing the correlation functions in the r.h.s. of (23) through the GF's by means of the spectral theorem we obtain from (23), (22), and (19)

$$M_{ii}^{\sigma}(\omega) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\omega_1 d\omega_2 \frac{1 + N(\omega_2) - n(\omega_1)}{\omega - \omega_1 - \omega_2} \times \\ \times \sum_{nm} \sum_{\alpha\beta} \left\{ T_{in}^{\alpha} \left[-\frac{1}{\pi} \text{Im} G_{nm}^{\sigma}(\omega_1 + i\epsilon) \right] \left[-\frac{1}{\pi} \text{Im} \langle\langle u_{in}^{\alpha} | u_{mi}^{\beta} \rangle\rangle_{\omega_2 + i\epsilon} \right] T_{ml}^{\beta} \right\} \quad (24)$$

with

$$N(\omega) = [\exp(\beta\omega) - 1]^{-1}, \quad n(\omega) = [\exp(\beta\omega) + 1]^{-1}. \quad (25)$$

The equations (19) and (24) form a closed self-consistent system of equations for the electron GF. The total electron GF G_{ij}^{σ} depends on the massoperator M_{ii}^{σ} which in turn depends on the G . The phonon GF, entering into (24), also depends on the electron GF. Now we are going to find the solution for the phonon GF.

4. Phonon Green Functions

The general scheme of calculations is the same as in Section 3. Differentiating the phonon GF

$$D_{ij}^{\beta\alpha}(t - t') = \langle\langle u_i^{\beta}(t) | u_j^{\alpha}(t') \rangle\rangle = -i\theta(t - t') \langle [u_i^{\beta}(t), u_j^{\alpha}(t')]_- \rangle \quad (26)$$

twice with respect to the first time variable t we get for the Fourier transform

$$\omega^2 M_i D_{ij}^{\beta\alpha}(\omega) = \delta_{ij} \delta_{\alpha\beta} + \frac{1}{2} \sum_{n\alpha'} [\Phi_{in}^{\beta\alpha'} + \Phi_{ni}^{\alpha'\beta}] D_{nj}^{\alpha'\alpha}(\omega) - \\ - \sum_{n\sigma} [T_{ni}^{\beta} \langle\langle a_{n\sigma}^{\dagger} a_{i\sigma} | u_j^{\alpha} \rangle\rangle_{\omega} - T_{in}^{\beta} \langle\langle a_{i\sigma}^{\dagger} a_{n\sigma} | u_j^{\alpha} \rangle\rangle_{\omega}]. \quad (27)$$

The calculation of the GF $\langle\langle a_{n\sigma}^{\dagger} a_{i\sigma} | u_j^{\alpha} \rangle\rangle_{\omega}$ in the r.h.s. of (27) can be performed in the same way as in Section 3. We get

$$D_{ij}^{\alpha} = D_{ij}^{0\alpha} + \sum_{ij'} \sum_{\mu\mu'} D_{ii'}^{0\alpha\mu} P_{ij'}^{\mu\mu'} D_{j'j}^{0\mu'\alpha}, \quad (28)$$

where the zeroth-order phonon GF is given by

$$\sum_{n\alpha'} \{ \omega^2 M_i \delta_{in} \delta_{\mu\alpha'} - \frac{1}{2} [\Phi_{in}^{\mu\alpha'} + \Phi_{ni}^{\alpha'\mu}] \} D_{nj}^{0\alpha'\alpha}(\omega) = \delta_{ij} \delta_{\mu\alpha} \quad (29)$$

and

$$P_{ij}^{\mu\mu'}(\omega) = \sum_{n, m, \sigma} T_{in}^{\mu} [I_{injm}^{\sigma} - I_{inmj}^{\sigma} - I_{nijm}^{\sigma} + I_{nimj}^{\sigma}] T_{mj}^{\mu'}; \quad (30) \\ I_{inmj}^{\sigma}(\omega) = \langle\langle a_{i\sigma}^{\dagger} a_{n\sigma} | a_{j\sigma}^{\dagger} a_{m\sigma} \rangle\rangle_{\omega}.$$

Employing the same procedure (except of notation) as given by equations (17) to (20) we rewrite (28) in the form of the Dyson equation

$$D_{ij}^{\alpha}(\omega) = D_{ij}^{0\alpha}(\omega) + \sum_{ij'} \sum_{\mu\mu'} D_{ii'}^{0\alpha\mu}(\omega) H_{ij'}^{\mu\mu'}(\omega) D_{j'j}^{\mu'\alpha}(\omega). \quad (31)$$

The proper part of the operator P has been denoted by Π . In order to have a self-consistent expression for the "phonon" massoperator Π we use the same approximation as (23),

$$\langle a_{m\sigma}^\dagger(t) a_{j\sigma}(t) a_{i\sigma}^\dagger a_{n\sigma} \rangle \approx \langle a_{m\sigma}^\dagger(t) a_{n\sigma} \rangle \langle a_{j\sigma}(t) a_{i\sigma}^\dagger \rangle. \quad (32)$$

Proceeding in the same way as previously, we arrive at the following expression for Π :

$$\begin{aligned} \Pi_{ij}^{\mu\mu'}(\omega) = & \frac{1}{\pi^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\omega_1 d\omega_2 \cdot \frac{n(\omega_2) - n(\omega_1)}{\omega + \omega_2 - \omega_1} \times \\ & \times \sum_{nm\sigma} T_{in}^\mu \{ \text{Im } G_{im}^\sigma(\omega_1) \text{Im } G_{nj}^\sigma(\omega_2) - \text{Im } G_{nm}^\sigma(\omega_1) \text{Im } G_{ij}^\sigma(\omega_2) - \\ & - \text{Im } G_{ij}^\sigma(\omega_1) \text{Im } G_{nm}^\sigma(\omega_2) + \text{Im } G_{nj}^\sigma(\omega_1) \text{Im } G_{im}^\sigma(\omega_2) \} T_{mj}^{\mu'}. \quad (33) \end{aligned}$$

Equations (19), (24) and (31), (33) form a closed set of the self-consistent equations for electron (19) and phonon (31) GF's in substitutionally disordered alloys in the presence of electron-phonon interaction (3).

5. The Configurational Averaging

As we mentioned previously, all the calculations just presented have been done for a given (although for the sake of simplicity not explicitly specified) configuration of atoms in the alloy. All the quantities in our theory (G , D , M , Π as well as G^0 and D^0) depend on the whole configuration of the alloy. To obtain a theory of a real macroscopic sample, we have to average over various configurations of atoms in the sample [25 to 27]. The configurational averaging cannot be exactly made for a macroscopic sample. Hence we must resort to an additional approximation.

First, let us write equations (19) and (31) (to be averaged) in a short matrix notation (the meaning of symbols is obvious),

$$G^\sigma = G^{0\sigma} + G^{0\sigma} M^\sigma G^\sigma, \quad (34)$$

$$D = D^0 + D^0 \Pi D. \quad (35)$$

M and Π are in turn the functionals of G and D ,

$$M = M[G, D], \quad \Pi = \Pi[G]. \quad (36)$$

If the process of taking configurational averaging is denoted by $\langle \dots \rangle$, then we have

$$\langle G \rangle = \langle G^0 \rangle + \langle G^0 M G \rangle \quad (37)$$

with a similar equation for $\langle D \rangle$.

Few words are now appropriate for the description of general possibilities. The calculations of $\langle G^0 \rangle$ and $\langle D^0 \rangle$ can be performed with the help of an arbitrary available scheme. The best would be the self-consistent cluster theory valid for the off-diagonal disorder [27]. In the present work for the sake of simplicity, we chose another possibility and, at the cost of additional approximations in the model Hamiltonian, apply the single-site coherent potential approximation (CPA) as developed by Soven [28] (see also [29]) for calculation of the electron GF $\langle G^0 \rangle$, and by Taylor [30] for the phonon GF $\langle D^0 \rangle$. The necessary approximation is the periodicity (i.e. non-randomness) of the transfer integrals t_{ij} and dynamical matrix $\Phi_{ij}^{\alpha\beta}$. Thus the only random parameters in our model are now the energy levels ϵ_i , Coulomb correlations U_i , the ion masses M_i , and the Slater coefficients q_0^i .

The CPA method as applied to the calculation of the electron and phonon GF is described by Elliott et al. [26]. Here we write the relevant final formulae only. The matrix element of the $\langle G^0 \rangle$ in the site representation is expressed as

$$\langle G^0_{\sigma} \rangle = \bar{G}_{ij}^{0\sigma}(\omega) = \frac{1}{N} \sum_{\mathbf{k}} \frac{e^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)}}{\omega - \Sigma^{\sigma}(\omega) - \epsilon_{\mathbf{k}}}, \quad (38)$$

where

$$\epsilon_{\mathbf{k}} = \sum_{n=1}^z t_{n,0} e^{-i\mathbf{k}\mathbf{R}_n}. \quad (39)$$

z is the number of nearest neighbours of the site 0, and the coherent potential (or self-energy) $\Sigma^{\sigma}(\omega)$ is the solution of the CPA self-consistency equations. For the $A_x B_{1-x}$ alloy these read [29]

$$\Sigma^{\sigma}(\omega) = x\epsilon_A^{\sigma} + (1-x)\epsilon_B^{\sigma} - (\epsilon_A^{\sigma} - \Sigma^{\sigma}) F^{\sigma}(\omega, \Sigma) (\epsilon_B^{\sigma} - \Sigma^{\sigma}), \quad (40a)$$

$$F^{\sigma}(\omega, \Sigma) = \bar{G}_{ii}^{0\sigma}(\omega); \quad \sigma = \pm. \quad (40b)$$

On the other hand, the matrix elements of $\langle D^0 \rangle$ for the $A_x B_{1-x}$ alloy with B-type ions being the defects are given by [30]

$$\langle D^0 \rangle = \bar{D}_{ij}^{0\beta\alpha}(\omega) = \frac{1}{NM_A} \sum_{\mathbf{k}} \frac{e_{\mathbf{k}\nu}^{\beta} e_{\mathbf{k}\nu}^{\alpha} e^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)}}{\omega^2 [1 - \tilde{\epsilon}(\omega)] - \omega^2(\mathbf{k}, \nu)}, \quad (41)$$

where $\omega(\mathbf{k}, \nu)$ is the ν -branch of the phonon spectrum of the pure A-crystal, $e_{\mathbf{k}\nu}^{\alpha}$ is the α -th component of the relevant polarization vector, and $\tilde{\epsilon}(\omega)$ is a solution of equations [30],

$$\tilde{\epsilon}(\omega) = (1-x)\epsilon + \tilde{\epsilon}(\omega) [\epsilon - \tilde{\epsilon}(\omega)] \omega^2 D^0(\omega), \quad (42a)$$

$$D^0(\omega) = D_{ii}^{0\alpha\alpha}(\omega), \quad (42b)$$

$$\epsilon = \frac{M_A - M_B}{M_A}. \quad (43)$$

Now, let us return to the calculation of the configurationally averaged total GF's $\langle G \rangle$ and $\langle D \rangle$. To perform the remaining averages in (37), we use the approximation

$$\langle G^0 M G \rangle \rightarrow \langle G^0 \rangle \langle M \rangle \langle G \rangle. \quad (44)$$

The calculation of $\langle M \rangle$ and $\langle H \rangle$ requires further averaging of the product of matrices. We again use the prescription (44) there. However, the quantities like $\langle q_0^i q_0^j \rangle$ entering into $\langle M \rangle$ and $\langle H \rangle$ through $\langle T_{ij}^{\alpha} T_{mj}^{\beta} \rangle$ are averaged here according to

$$\langle q_0^i q_0^j \rangle = \begin{cases} Q_1 = x(q_0^A)^2 + (1-x)(q_0^B)^2 & \text{if } i = j, \\ Q_2 = x^2(q_0^A)^2 + 2x(1-x)q_0^A q_0^B + (1-x)^2(q_0^B)^2 & \text{if } i \neq j. \end{cases} \quad (45)$$

Equation (45) is written in a closed form as

$$\langle q_0^i q_0^j \rangle = Q_2 + (Q_1 - Q_2) \delta_{ij}. \quad (46)$$

The averaged quantities (in the following to be denoted by a bar, i.e. $\langle G \rangle = \bar{G}$) are periodic, so we can introduce the Fourier transform of them, i.e.

$$\bar{M}_{ij}^{\sigma}(\omega) = \frac{1}{N} \sum_{\mathbf{k}} \bar{M}_{\mathbf{k}}^{\sigma}(\omega) e^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)} \quad (47)$$

and similar formulae for \bar{G}_{ij}^σ and $\bar{G}_{ij}^{0\sigma}$. The "phonon functions", however, are additionally expanded over polarization vectors e_{kv} ,

$$\bar{D}_{ij}^{\mu\mu'}(\omega) = \frac{1}{MN} \sum_{kv} e_{kv}^\mu e_{kv}^{\mu'} \bar{D}_{kv}(\omega) e^{ik(\mathbf{R}_i - \mathbf{R}_j)}. \quad (48)$$

Performing the configurational averaging of (18), (20), (31), (33) and Fourier transforming the resulting expressions according to the above rules, we obtain

$$\bar{G}_{\mathbf{k}}^\sigma(\omega) = (\omega - \Sigma^\sigma(\omega) - \bar{M}_{\mathbf{k}}^\sigma(\omega) - \epsilon_{\mathbf{k}})^{-1}, \quad (49)$$

$$\bar{D}_{kv}(\omega) = (\omega^2 [1 - \tilde{\epsilon}(\omega)] - \bar{H}_{kv}(\omega) - \omega^2(kv))^{-1}, \quad (50)$$

where

$$\begin{aligned} \bar{M}_{\mathbf{k}}^\sigma(\omega) = & \\ & \frac{Q_1 - Q_2}{4M_A a^2 N^2} \sum_{\mathbf{p}q\alpha} (e_{\mathbf{q}\alpha}^\alpha)^2 (v_{\mathbf{k}}^\alpha - v_{\mathbf{k}-\mathbf{q}}^\alpha + v_{\mathbf{k}-\mathbf{p}}^\alpha - v_{\mathbf{k}-\mathbf{p}-\mathbf{q}}^\alpha)^2 A^\sigma(\omega, \mathbf{k} - \mathbf{p} - \mathbf{q}; \mathbf{q}\nu) + \\ & + \frac{Q_2}{M_A a^2 N} \sum_{\mathbf{q}\nu\alpha} (e_{\mathbf{q}\nu}^\alpha)^2 (v_{\mathbf{k}}^\alpha - v_{\mathbf{k}-\mathbf{q}}^\alpha)^2 A^\sigma(\omega, \mathbf{k} - \mathbf{q}; \mathbf{q}\nu) \end{aligned} \quad (51)$$

with

$$\begin{aligned} A^\sigma(\omega, \mathbf{k} - \mathbf{q}; \mathbf{q}\nu) = & \\ = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\omega_1 d\omega_2}{\pi^2} \frac{1 + \frac{N(\omega_2) - n(\omega_1)}{\omega - \omega_1 - \omega_2}}{\omega - \omega_1 - \omega_2} \text{Im} \bar{G}_{\mathbf{k}-\mathbf{q}}^\sigma(\omega_1) \text{Im} \bar{D}_{\mathbf{q}\nu}(\omega_2) \end{aligned} \quad (52)$$

and $v_{\mathbf{k}}^\alpha = \partial \epsilon_{\mathbf{k}} / \partial k_\alpha$,

$$\begin{aligned} \bar{H}_{kv}(\omega) = & \frac{Q_2}{M_A a^2 N} \sum_{\mathbf{p}\sigma\alpha} (e_{\mathbf{p}\sigma}^\alpha)^2 (v_{\mathbf{k}-\mathbf{p}}^\alpha - v_{\mathbf{p}}^\alpha)^2 B^\sigma(\omega, \mathbf{k} - \mathbf{p}, \mathbf{p}) + \\ & + \frac{Q_1 - Q_2}{4M_A a^2 N^2} \sum_{\mathbf{p}q\alpha} (e_{\mathbf{p}\alpha}^\alpha)^2 (v_{\mathbf{k}-\mathbf{p}}^\alpha - v_{\mathbf{p}}^\alpha + v_{\mathbf{k}-\mathbf{p}-\mathbf{q}}^\alpha - v_{\mathbf{p}-\mathbf{q}}^\alpha)^2 B^\sigma(\omega, \mathbf{k} - \mathbf{p} - \mathbf{q}, \mathbf{p}) \end{aligned} \quad (53)$$

with

$$B^\sigma(\omega, \mathbf{k} - \mathbf{p}, \mathbf{p}) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\omega_1 d\omega_2}{\pi^2} \frac{n(\omega_2) - n(\omega_1)}{\omega - \omega_1 + \omega_2} \text{Im} \bar{G}_{\mathbf{k}-\mathbf{p}}^\sigma(\omega_1) \text{Im} \bar{G}_{\mathbf{p}}^\sigma(\omega_2), \quad (54)$$

a is the distance between neighbouring atoms. For metals from the same row in the Periodic Table the q_0 -values are equal to [10] $q_0^A = q_0^B = q_0$. In this case we have $Q_1 = Q_2 = q_0^2$ and (51), (53) have greatly simplified forms with single sums only.

Equations (49) to (54) form a closed self-consistent system of equations. In principle, we can substitute in the r.h.s. of (52) and (54) any relevant initial Green functions and calculate the first approximation to mass operators H and M . The renormalized by the electron-phonon interaction electron and/or phonon spectrum of the alloy is determined by (49) and/or (50). Having obtained \bar{G} and \bar{D} we can, in principle, calculate by iteration the next approximations. This can be done with the help of a computer and is outside the scope of the present paper. The numerical results and farther discussion of averaging procedure and the role of vertex corrections are intended to be presented in near future. Another important point is the spin dependence of the electron-phonon self-energy and the size of magnetic consequences of electron-phonon interaction. This effect can in certain situations be much larger than expected [33].

6. The Electronic Specific Heat

As a simple application of the developed theory we consider the low-temperature electronic specific heat, c_v . Usually it is expressed as [31]

$$c_v = \gamma T, \quad (55)$$

where γ is the so-called low-temperature specific heat coefficient. The measurement of γ is one of the most important experimental techniques of looking at the electronic states of alloys. The specific heat c_v is defined as the temperature derivative of the electronic energy E of the system,

$$c_v = \frac{1}{N} \frac{\partial E}{\partial T}. \quad (56)$$

N is the number of particles and the energy E is given by

$$E = \langle H_e + H_{e-i} \rangle = \sum_{i\sigma} \epsilon_i^\sigma \langle a_{i\sigma}^\dagger a_{i\sigma} \rangle + \sum_{ij\sigma} t_{ij} \langle a_{i\sigma}^\dagger a_{j\sigma} \rangle - \sum_{ij\sigma\alpha} T_{ij}^\alpha \langle (u_j^\alpha - u_i^\alpha) a_{i\sigma}^\dagger a_{j\sigma} \rangle. \quad (57)$$

By the spectral theorem [21] we express the correlation functions entering into (57) through the GF's. Using then (12) and (14) we finally obtain

$$E = \int_{-\infty}^{\infty} d\omega \omega n(\omega) \sum_{i\sigma} \left[-\frac{1}{\pi} \text{Im} G_{ii}^\sigma(\omega + i\epsilon) \right]. \quad (58)$$

As is usually in alloys we take the configurational average of c_v and thus of E . So

$$\bar{E} = \int_{-\infty}^{\infty} d\omega \omega n(\omega) D(\omega), \quad (59)$$

where

$$D(\omega) = -\overline{\text{Im}} \frac{1}{\pi N} \sum_{k\sigma} \frac{1}{\omega - \Sigma^\sigma(\omega) - \bar{M}_k^\sigma(\omega) - \epsilon_k} \quad (60)$$

is the renormalized alloy density of states. Note, it is temperature dependent through $\bar{M}_k^\sigma(\omega)$. Performing the integral (59) by the well-known low-temperature expansion (cf. recent calculations of the specific heat of the disordered system with correlation performed in [32]) we obtain for γ

$$\gamma = \frac{1}{3} \pi^2 k_B^2 D(\epsilon_F) + \frac{1}{6} \pi^2 k_B^2 T \frac{\partial D(\epsilon_F)}{\partial T}$$

or in other form

$$\gamma = \frac{1}{3} \pi^2 k_B^2 D(\epsilon_F) \left(1 + \frac{1}{2} \frac{\partial \ln D(\epsilon_F)}{\partial \ln T} \right). \quad (61)$$

The second term in brackets comes from the electron-phonon interaction. This many-body interaction manifests itself in the term $D(\epsilon_F)$ as well. Equation (61) is a starting point for the study of the concentration dependence of γ . It can also be used to explain the nonlinear behaviour of the c_v vs T observed in some systems.

7. Conclusions

We have presented a microscopic theory of the electron-phonon interaction in strongly disordered transition metal alloys. The derived Hamiltonian contains explicitly the characteristic atomic parameters of both constituents. Working in the site representation we obtained the coupled set of exact equations for electron and phonon GF's by the equation-of-motion technique. The differentiation of the GF with respect to the first and second time variable enables us to derive the exact Dyson equations for the electrons and phonons. Neglecting the vertex corrections in the mass operators the closed self-consistent system of equations is obtained. We perform the configurational averaging so that the zeroth-order GF \bar{G}^0 has a simple single-site CPA form. The calculated low-temperature coefficient of the specific heat allows the comparison of the theory with experiment. To do this, however, it is necessary to perform the numerical calculations of the density of states. The results of such calculations will be presented elsewhere.

The developed theory can be applied, after some modifications, to the study of transition metal compounds. One can improve it using a more realistic Hamiltonian or going beyond the single-site CPA.

Appendix

We present here the short derivation of the alloy counterpart of the BLF Hamiltonian. As is usual in the tight-binding approximation, we define the localized atomic wave functions (for simplicity we take the nondegenerate d-band). In the binary A_xB_{1-x} disordered alloy we can define two sets of atomic functions: for the A-type ion potential and for the B one. So

$$\left[\frac{p^2}{2m} + V_\alpha(\mathbf{r} - \mathbf{R}_i) \right] \varphi_\alpha(\mathbf{r} - \mathbf{R}_i) = \epsilon_i^\alpha \varphi_\alpha(\mathbf{r} - \mathbf{R}_i). \quad (\text{A1})$$

In (A1) $\alpha = A(B)$ if the site i is occupied by an A(B)-type ion. We assume the d-functions $\varphi_\alpha(\mathbf{r} - \mathbf{R}_i)$ to form a complete and orthonormal set

$$\int \varphi_\alpha^*(\mathbf{r} - \mathbf{R}_i) \varphi_\beta(\mathbf{r} - \mathbf{R}_j) d^3r \approx \delta_{ij}. \quad (\text{A2})$$

Note, if $i = j$, then certainly $\alpha = \beta$, because a given site can be occupied by one atom only. Thus, we can introduce the operators a_i^\dagger and a_i creating and annihilating the electron in a state $\varphi_\alpha(\mathbf{r} - \mathbf{R}_i)$. The alloy one-electron Hamiltonian

$$H = \frac{p^2}{2m} + \sum_i V_\gamma(\mathbf{r} - \mathbf{R}_i) \quad (\text{A3})$$

can, therefore, be written in terms of these operators as

$$H = \sum_{ij\sigma} t_{ij}^{\alpha\beta} a_{i\sigma}^\dagger a_{j\sigma}, \quad (\text{A4})$$

where

$$t_{ij}^{\alpha\beta} = \int \varphi_\alpha^*(\mathbf{r} - \mathbf{R}_i) \left(\frac{p^2}{2m} + \sum_l V_\gamma(\mathbf{r} - \mathbf{R}_l) \right) \varphi_\beta(\mathbf{r} - \mathbf{R}_j) d^3r. \quad (\text{A5})$$

Writing the potential term of the Hamiltonian in (A5) in the form

$$\sum_l V_\gamma(\mathbf{r} - \mathbf{R}_l) = V_\alpha(\mathbf{r} - \mathbf{R}_i) + V_\beta(\mathbf{r} - \mathbf{R}_j) + \sum_{l \neq i, j} V(\mathbf{r} - \mathbf{R}_l)$$

we can doubly use equation (A1) with functions $\varphi_\alpha(\mathbf{r} - \mathbf{R}_i)$ and $\varphi_\beta(\mathbf{r} - \mathbf{R}_j)$. For $\alpha \neq \beta$ we have thus two possibilities

$$t_{ij}^{A(B)} = \int \varphi_A^*(\mathbf{r} - \mathbf{R}_i) \tilde{V}_A(\mathbf{r} - \mathbf{R}_i) \varphi_B(\mathbf{r} - \mathbf{R}_j) d^3r \quad (\text{A6})$$

and

$$t_{ij}^{(A)B} = \int \varphi_A^*(\mathbf{r} - \mathbf{R}_i) \tilde{V}_B(\mathbf{r} - \mathbf{R}_j) \varphi_B(\mathbf{r} - \mathbf{R}_j) d^3r, \quad (\text{A7})$$

where $\tilde{V}_{A(B)}(\mathbf{r} - \mathbf{R}_{i(j)})$ can be viewed as a "screened" potential attached to the site $i(j)$ occupied by an ion of the type A(B). In the present paper we take by definition

$$t_{ij}^{AB} = \frac{1}{2} (t_{ij}^{A(B)} + t_{ij}^{(A)B}). \quad (\text{A8})$$

However, other definitions of t_{ij}^{AB} are possible (e.g. $\overline{t_{ij}^{AB}} = xt_{ij}^{A(B)} + (1-x)t_{ij}^{(A)B}$). Thus, in the tight-binding approximation one can construct the various models of the electron hopping in disordered transition metal alloys.

In the deformed lattice, for small displacement \mathbf{u}_i , relation (A2) is still valid as it follows from the "rigid ion" approximation. So, the hopping integral in (A6), (A7) does not depend on $\mathbf{R}_i - \mathbf{R}_j$, but rather on $(\mathbf{R}_i - \mathbf{R}_j - \mathbf{u}_i + \mathbf{u}_j)$,

$$\begin{aligned} t_{ij}^{A(B)} &= \int \varphi_A^*(\mathbf{r}) \tilde{V}_A(\mathbf{r}) \varphi_B(\mathbf{r} + \mathbf{R}_i - \mathbf{R}_j + \mathbf{u}_i - \mathbf{u}_j) d^3r = \\ &= t_{ij}^{A(B)}(\mathbf{R}_i - \mathbf{R}_j + \mathbf{u}_i - \mathbf{u}_j), \end{aligned} \quad (\text{A9})$$

$$t_{ij}^{(A)B} = t_{ij}^{A(B)}(\mathbf{R}_j - \mathbf{R}_i + \mathbf{u}_j - \mathbf{u}_i). \quad (\text{A10})$$

Expanding (A9) and (A10) in a power series of $(\mathbf{u}_j - \mathbf{u}_i)$ and noting that for cubic lattices [10]

$$\frac{\partial t_{ij}^{(A)B}}{\partial \mathbf{R}_{ji}} \approx -q_0^A \frac{\mathbf{R}_{ji}}{R_{ji}} t_{ij}^{(A)B}(0) \quad (\text{A11})$$

we obtain from (A8)

$$t_{ij}^{\alpha\beta} \approx t_{ij}^{\alpha\beta}(0) - \frac{1}{2} \{q_0^\alpha t_{ij}^{\alpha(\beta)}(0) + q_0^\beta t_{ij}^{\alpha(\beta)}\} \frac{\mathbf{R}_{ji}}{R_{ji}} (\mathbf{u}_j - \mathbf{u}_i). \quad (\text{A12})$$

$t_{ij}^{\alpha\beta}(0)$ means the hopping integral of the undeformed lattice. In this paper we assume

$$t_{ij}^{\alpha(\beta)}(0) = t_{ij}^{(\alpha)\beta}(0) = t_{ij}.$$

So (A12) becomes

$$t_{ij}^{\text{def}} = t_{ij} - \frac{q_0^i + q_0^j}{2} t_{ij} \frac{\mathbf{R}_{ji}}{R_{ji}} (\mathbf{u}_j - \mathbf{u}_i). \quad (\text{A13})$$

In the last formula we use the single indices i, j to denote the site and type of an atom at that site. Thus, the electron-phonon interaction Hamiltonian suitable for disordered alloys has the form

$$H_{e-i} = \sum_{i\sigma} \frac{q_0^i + q_0^j}{2} t_{ij} \frac{\mathbf{R}_{ji}}{R_{ji}} (\mathbf{u}_i - \mathbf{u}_j) a_{i\sigma}^\dagger a_{j\sigma}. \quad (\text{A14})$$

The Hamiltonian (A14) reduces to the BLF model in the case of a pure crystal.

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