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THE THEORY FOR STRONG-COUPLING SUPERCONDUCTIVITY IN DISORDERED TRANSITION METAL ALLOYS

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1. INTRODUCTION

Modern microscopic theory of superconductivity has been given a rigorous mathematical formulation in the classical works of N.N.Bogolubov[1-3] and others[4-8]. It was shown that the equations for superconductivity can be derived from the fundamental electron-ion and electron-electron interactions. The obtained set of equations is known as the Eliashberg equations. It enables us to investigate the electronic and lattice properties of the metal in both the normal and superconducting states. Moreover, the Eliashberg equations are appropriate for the description of the strong coupling superconductors, contrary to the so-called Gorkov equations valid in the weak coupling regime and describing the electron subsystem in the superconducting state only.

The extensions of the theory to the disordered superconductors have been given for the "dirty"[9] and dilute alloys[10] limits. Since then still increasing interest in the theoretical and experimental study of the disordered superconductors[11] is observed. A lot of effort has been devoted to the transition metal compounds and substitutionally disordered alloys[12,13].

The Gorkov weak coupling approach and the coherent potential approximation (CPA), to treat disorder, have been used in a number of papers[14-21] to describe concentrated superconducting alloys. They used the following model Hamiltonian with the Cooper pair sources Δ_i

$$H = \sum_{i\sigma} \varepsilon_i n_{i\sigma} + \sum'_{ij\sigma} t_{ij} a^+_{i\sigma} a_{j\sigma} - \sum_i (\Delta_i a^+_{i\uparrow} a^+_{i\downarrow} + \Delta^*_i a_{i\downarrow} a_{i\uparrow}) . \qquad (1.1)$$

This group of papers discussed the influence of the disorder on the electron subsystem. The phonon-mediated parameters of the effective electron-electron interaction in alloys entering the definition of Δ_i in (1.1) have been recently derived [22] on the basis of the random contact model. On the other hand in paper[23] there has been studied the effect of the force constant disorder on the electron-phonon spectral function, while in[24] the influence of atomic ordering in alloys on their T_c by means of the integral equation for the vertex part was investigated.

The Eliashberg-type theories have also been proposed for superconducting alloys[25,26]. Kerker and Bennemann[25] have used

the Fröhlich-type Hamiltonian for the electron-phonon interaction and neglected the effect of disorder on the phonon Green function (GF). Lustfeld[26] has obtained the expression for T_c on the basis of the phenomenological ansatz for averaged anomalous self-energy (c.f. the equation (16) for $\hat{\sigma}_{eff}$ in[26]).

The purpose of the present paper is to develop the microscopic selfconsistent theory for strong-coupling superconductivity in disordered transition metal alloys. The alloy version[27] of the Barisic, Labbe and Friedel (BLF) tight-binding model[28,29] is used for the electron-ion interaction. As has been shown in[30-32] the BLF phonon induced d-d coupling is the dominant mechanism for superconductivity in such systems. We derive the equations for superconductivity in the site representation by means of the irreducible Green function method[33-35] in section 2. We employ there the ideas developed previously in connection with the derivation of Eliashberg-type equations for pure transition metals in the Wannier representation[35]. Various attempts at configurational averaging are discussed in section 3, where the formula for T_c is also obtained. Section 4 contains the discussion and conclusions.

2. GENERAL THEORY

When studying the superconductivity in transition metal alloys, one must take care of at least three facts of major importance:

i) The d-electrons responsible for superconductivity in these systems have an atomic character (section 2.1).

ii) These materials usually belong to the class of strong-coupling superconductors (sections 2.2 and 2.3).

iii) They are very often disordered so the obtaining of meaningful results requires the proper averaging (section 3).

2.1. The Hamiltonian

In the so-called modified tight-binding method we write the Hamiltonian for a given configuration of atoms in an alloy, as[27]

$$\mathcal{H} = \sum_{i\sigma} \varepsilon_i n_{i\sigma} + \frac{1}{2}\sum_{i\sigma} U_i n_{i\sigma} n_{i-\sigma} + \sum'_{ij\sigma} t_{ij} a^+_{i\sigma} a_{j\sigma} + H_{e-i} + H_i \,. \quad (2.1)$$

Here $n_{i\sigma} = a^+_{i\sigma} a_{i\sigma}$, and $a^+_{i\sigma}(a_{i\sigma})$ creates (annihilates) the d-electron in Wannier state $|i>$ with spin σ. The t_{ij} are the hopping matrix elements, and the prime indicates that the sum over j is limited to nearest neighbours of i. ε_i and U_i are the random

"energy levels" and intrasite Coulomb matrix elements, respectively. H_{e-i} stands for the electron-ion interaction Hamiltonian. This part of $\mathcal{H}$ was derived previously[27] and is a direct generalization of the BLF[28] model,

$$H_{e-i} = \sum_{ij\alpha} \sum_{\alpha} T^{\alpha}_{ij} (u^{\alpha}_i - u^{\alpha}_j) a^+_{i\sigma} a_{j\sigma} \quad (2.2)$$

with

$$T^{\alpha}_{ij} = \frac{q^i_0 + q^j_0}{2} t_{ij} \frac{R^{\alpha}_j - R^{\alpha}_i}{|\vec{R}_j - \vec{R}_i|} \,. \quad (2.3)$$

Here u^{α}_i is the α-th component of the displacement of an ion at i-th site, q^i_0 is the Slater coefficient describing an exponential, $\exp(-q^i_0 r)$, decrease of the d-electron wave function[28]. It takes on value $q^A_0(q^B_0)$ when atom at site i is of an A(B)-type. $\vec{R}_j - \vec{R}_i = \vec{R}_{ji}$ is the relative position vector of two ions at i and j. The last part of the Hamiltonian represents the ion subsystem and in the harmonic approximation, we use here, is given by

$$H_i = \sum_i \frac{P_i^2}{2M_i} + \frac{1}{2}\sum_{ij}\sum_{\alpha\beta} u^{\alpha}_i \Phi^{\alpha\beta}_{ij} u^{\beta}_j \,. \quad (2.4)$$

M_i denotes the mass of an ion at i-th site. It is equal to M_A or M_B. The dynamical matrix $\Phi^{\alpha\beta}_{ij}$ is in general a random quantity too.

2.2. Electron Green Function and Mass-Operator

In disordered systems, where the distance between "impurities" is comparable to the interatomic distance of the host[10], the coherence length (or the Cooper pair size) is greatly reduced. The proper description of superconductivity in such circumstances requires the proper description of the Cooper pairs. The pairing in general takes place between time-reversal states but these cannot be represented as $|\vec{k}\downarrow>$ and $|-\vec{k}\uparrow>$ in disordered alloys, for $\vec{k}$ is not a good quantum number in these systems. Therefore, we have to start from the states in the site representation, describe the pairing (i.e., obtain an expression for the anomalous electron GF and mass-operator) and *only then average over various configurations* in order to obtain quantities comparable to the experimental ones.

To solve for the mass-operator, we use the equation of motion method for the two-time thermodynamic Green functions[36,37].

The Green function $\hat{\mathcal{G}}^{\sigma}_{ij}(\omega)$ is a matrix in Nambu representation and is defined for a fixed configuration of ions in space by

$$\hat{\mathcal{G}}^{\sigma}_{ij}(\omega) = \begin{bmatrix} \ll a_{i\sigma} | a^{+}_{j\sigma} \gg_{\omega} & \ll a_{i\sigma} | a_{j-\sigma} \gg_{\omega} \\ \ll a^{+}_{i-\sigma} | a^{+}_{j\sigma} \gg_{\omega} & \ll a^{+}_{i-\sigma} | a_{j-\sigma} \gg_{\omega} \end{bmatrix} = \ll \psi_{i\sigma} | \psi^{+}_{j\sigma} \gg_{\omega}, \tag{2.5}$$

where $\psi^{+}_{i\sigma} = (a^{+}_{i\sigma}, a_{i-\sigma})$ is the so-called Nambu field spinor /5/. Differentiation of the $\hat{\mathcal{G}}^{\sigma}_{ij}(t-t')$ over the first time variable t gives the following equation for GF (2.5):

$$\sum_{m} \hat{A}_{im} \hat{\mathcal{G}}^{\sigma}_{mj}(\omega) = \hat{I}_{ij} + U_i \hat{r}_3 \hat{B}_{ij} + \sum_{m\beta} T^{\beta}_{im} \hat{C}_{im,j}, \tag{2.6}$$

where the sign "$\hat{}$" denotes matrices in spin indices, $\hat{r}_i$, i=1,2,3 are the Pauli matrices and

$$\hat{A}_{im} = \omega \hat{r}_0 - (\varepsilon_i \delta_{im} + t_{im}) \hat{r}_3 ; \quad \hat{I}_{ij} = \delta_{ij} \hat{r}_0 ;$$

$$\hat{B}_{ij} = \begin{bmatrix} \ll a_{i\sigma} n_{i-\sigma} | a^{+}_{j\sigma} \gg_{\omega} & \ll a_{i\sigma} n_{i-\sigma} | a_{j-\sigma} \gg_{\omega} \\ \ll a^{+}_{i-\sigma} n_{i\sigma} | a^{+}_{j\sigma} \gg_{\omega} & \ll a^{+}_{i-\sigma} n_{i\sigma} | a_{j-\sigma} \gg_{\omega} \end{bmatrix}$$

$$\hat{C}_{im,j} = \begin{bmatrix} \ll u^{\beta}_{im} a_{m\sigma} | a^{+}_{j\sigma} \gg_{\omega} & \ll u^{\beta}_{im} a_{m\sigma} | a_{j-\sigma} \gg_{\omega} \\ \ll u^{\beta}_{mi} a^{+}_{m-\sigma} | a^{+}_{j\sigma} \gg_{\omega} & \ll u^{\beta}_{mi} a^{+}_{m-\sigma} | a_{j-\sigma} \gg_{\omega} \end{bmatrix}$$

$$u^{\alpha}_{im} = u^{\alpha}_{i} - u^{\alpha}_{m} .$$

To proceed we define the "irreducible" operators as in /33-35/

$$\ll {}^{ir}(a_{i\sigma} n_{i-\sigma}) | a^{+}_{j\sigma} \gg_{\omega} = \ll a_{i\sigma} n_{i-\sigma} | a^{+}_{j\sigma} \gg_{\omega} - \langle n_{i-\sigma} \rangle \ll a_{i\sigma} | a^{+}_{j\sigma} \gg_{\omega} + \langle a_{i\sigma} a_{i-\sigma} \rangle \ll a^{+}_{i-\sigma} | a^{+}_{j\sigma} \gg_{\omega} \tag{2.7}$$

giving rise to new equations of the form (2.6) with $\hat{B}_{im}$ replaced by ${}^{ir}(\hat{B}_{im})$ and $\hat{A}_{im}$ replaced by

$$\hat{A}^{1}_{im} = \hat{A}_{im} - U_i \begin{bmatrix} \langle n_{i-\sigma} \rangle & -\langle a_{i\sigma} a_{i-\sigma} \rangle \\ -\langle a^{+}_{i-\sigma} a^{+}_{i\sigma} \rangle & -\langle n_{i\sigma} \rangle \end{bmatrix} \delta_{im} . \tag{2.8}$$

It means that we have extracted from the original GF the Hartree-Fock-Bogolubov /3/ mean field given here by the difference $(\hat{A}^{1}_{im} - \hat{A}_{im})$. To proceed we write down the equations of motion for the GF's ${}^{ir}(\hat{B}_{ij})$ and $\hat{C}_{im,j}$ differentiating them over the second time variable t' (see /29,33-35/). Then again we go over to "irreducible" GFs but with respect to the rhs operators (c.f. (2.7)). The obtained set of equations for various GFs can be solved exactly. To this end we define the zeroth order GF as

$$\sum_{m} \hat{A}^{1}_{im} \hat{\mathcal{G}}^{0\sigma}_{mj} = \hat{I}_{ij} \tag{2.9}$$

and obtain the following exact equation:

$$\hat{\mathcal{G}}^{\sigma}_{ij}(\omega) = \hat{\mathcal{G}}^{0\sigma}_{ij}(\omega) + \sum_{nm} \hat{\mathcal{G}}^{0\sigma}_{in}(\omega) \hat{K}^{\sigma}_{nm}(\omega) \hat{\mathcal{G}}^{0\sigma}_{mj}(\omega), \tag{2.10}$$

where the "scattering" operator $\hat{K}^{\sigma}$ is given by

$$\hat{K}^{\sigma}_{i\ell}(\omega) = \sum_{mn} \hat{r}_3 \begin{bmatrix} \ll {}^{ir}(\rho^{-\sigma}_{im} a_{m\sigma}) | \rho^{-\sigma}_{\ell n} a^{+}_{n\sigma})^{ir} \gg_{\omega} & \ll {}^{ir}(\rho^{-\sigma}_{im} a_{m\sigma}) | (\rho^{\sigma}_{\ell n} a_{n-\sigma})^{ir} \gg_{\omega} \\ \ll {}^{ir}(\rho^{\sigma}_{im} a^{+}_{m-\sigma}) | \rho^{-\sigma}_{\ell n} a^{+}_{n\sigma})^{ir} \gg_{\omega} & \ll {}^{ir}(\rho^{\sigma}_{im} a^{+}_{m-\sigma}) | \rho^{\sigma}_{\ell n} a_{n-\sigma})^{ir} \gg_{\omega} \end{bmatrix} \hat{r}_3 \tag{2.11}$$

$$\rho^{\sigma}_{ij} = U_i n_{i\sigma} \delta_{ij} + \sum_{\alpha} T^{\alpha}_{ij} (u^{\alpha}_{i} - u^{\alpha}_{j}) . \tag{2.12}$$

Equation (2.10) can be written in the form of the Dyson equation /33,34/

$$\hat{\mathcal{G}}^{\sigma}_{nj}(\omega) = \hat{\mathcal{G}}^{0\sigma}_{nj}(\omega) + \sum_{i\ell} \hat{\mathcal{G}}^{0\sigma}_{ni}(\omega) \hat{\mathfrak{M}}^{\sigma}_{i\ell}(\omega) \hat{\mathcal{G}}^{\sigma}_{\ell i}(\omega) \tag{2.13}$$

if one introduces the mass-operator $\hat{\mathfrak{M}}^{\sigma}_{i\ell}$ being the "proper part" /33,34/ of the scattering operator $\hat{K}^{\sigma}_{i\ell}(\omega)$. Denoting the random matrices in site-space by $\hat{\mathcal{G}}$, $\hat{\mathcal{G}}^{0}$, $\hat{\mathfrak{M}}$ one can write the formal solution of (2.13) as

$$\hat{\mathcal{G}} = \{ (\hat{\mathcal{G}}^{0})^{-1} - \hat{\mathfrak{M}} \}^{-1} . \tag{2.14}$$

To find an expression for the mass operator $\hat{\mathfrak{M}}$ we proceed in the same way as previously [29,35], and express the GFs entering the operator $\hat{K}^{\sigma}$ through the correlation functions by means of the spectral theorem [36,37]. These correlation functions are decoupled in the following way:

$$\langle u^{\beta}_{m\ell}(t)\, a^{+}_{m\sigma}(t)\, u^{\alpha}_{in}\, a_{n\sigma}\rangle \approx \langle u^{\beta}_{m\ell}(t)\, u^{\alpha}_{in}\rangle \langle a^{+}_{m\sigma}(t)\, a_{n\sigma}\rangle ,$$
$$\langle n_{\ell-\sigma}(t)\, a^{+}_{\ell\sigma}(t)\, n_{i-\sigma}\, a_{i\sigma}\rangle \approx \langle n_{\ell-\sigma}(t)\, n_{i-\sigma}\rangle \langle a^{+}_{\ell\sigma}(t)\, a_{i\sigma}\rangle \qquad (2.15)$$

by neglecting the vertex corrections according to the Migdal-Eliashberg approach [4,6,29]. Using again the spectral theorem to the rhs of (2.15), we obtain for the mass-operator $\hat{\mathfrak{M}}$ (cf. [35])

$$\hat{\mathfrak{M}}^{\sigma}_{i\ell}(\omega) = \hat{\mathfrak{M}}^{e\ell-ph}_{i\ell,\sigma}(\omega) + \hat{\mathfrak{M}}^{c}_{i\ell,\sigma}(\omega) \qquad (2.16)$$

with the electron-phonon part given by

$$\hat{\mathfrak{M}}^{e\ell-ph}_{i\ell,\sigma}(\omega) = \frac{1}{2}\iint_{-\infty}^{\infty} d\omega_1\, d\omega_2\, \frac{\mathrm{cth}\frac{\beta\omega_1}{2} + \mathrm{th}\frac{\beta\omega_2}{2}}{\omega-\omega_1-\omega_2} \sum_{mn} T^{\alpha}_{im}\left(-\frac{1}{\pi}\right)\mathrm{Im}\langle\langle u^{\beta}_{im} | u^{\alpha}_{n\ell}\rangle\rangle_{\omega_1+i\epsilon} \times \qquad (2.17)$$
$$\times \hat{r}_3\left(-\frac{1}{\pi}\right)\mathrm{Im}\,\hat{\mathcal{G}}^{\sigma}_{mn}(\omega_2+i\epsilon)\,\hat{r}_3\,\hat{T}^{\alpha}_{n\ell}$$

and energy dependent Coulomb part

$$\hat{\mathfrak{M}}^{c}_{i\ell}(\omega) = \frac{U_i U_\ell}{2\pi^2}\iint_{-\infty}^{\infty} d\omega_1\, d\omega_2\, \frac{\mathrm{cth}\frac{\beta\omega_1}{2} + \mathrm{th}\frac{\beta\omega_2}{2}}{\omega-\omega_1-\omega_2} \times \qquad (2.18)$$
$$\times\left(\Gamma^{\sigma,\sigma}_{i\ell}(\omega_1)\, g^{n}(\omega_2) - \Gamma^{\sigma,-\sigma}_{i\ell}(\omega_1)\, g^{s}(\omega_2)\right)$$

with

$$\Gamma^{\sigma,\sigma}_{i\ell}(\omega) = \mathrm{Im}\begin{bmatrix} \langle\langle n_{i-\sigma} | n_{\ell-\sigma}\rangle\rangle_{\omega} & 0 \\ 0 & \langle\langle n_{i\sigma} | n_{\ell\sigma}\rangle\rangle_{\omega} \end{bmatrix}$$

$$g^{n}_{i\ell}(\omega) = \mathrm{Im}\begin{bmatrix} \langle\langle a_{i\sigma} | a^{+}_{\ell\sigma}\rangle\rangle_{\omega} & 0 \\ 0 & \langle\langle a^{+}_{i-\sigma} | a_{\ell-\sigma}\rangle\rangle_{\omega} \end{bmatrix}; \quad g^{s}_{i\ell}(\omega) = \mathrm{Im}\begin{bmatrix} 0 & \langle\langle a_{i\sigma} | a_{\ell-\sigma}\rangle\rangle_{\omega} \\ \langle\langle a^{+}_{i-\sigma} | a^{+}_{\ell\sigma}\rangle\rangle_{\omega} & 0 \end{bmatrix}.$$

The elastic or Hartree-Fock-Bogolubov part of the Coulomb mass-operator, not included into (2.16) and (2.18), can be written as (c.f. its definition in (2.8))

$$\hat{\mathfrak{M}}^{HF}_{i\ell} = \frac{U_i}{2}\delta_{i\ell}\,\hat{r}_3 - \frac{U_i}{2}\int_{-\infty}^{\infty} d\omega\, \mathrm{th}\frac{\beta\omega}{2}\hat{r}_3\left\{-\frac{1}{\pi}\mathrm{Im}\hat{G}^{-\sigma}_{ii}(\omega+i\epsilon)\right\}\hat{r}_3\,\delta_{i\ell}\,. \qquad (2.19)$$

The equations (2.13), (2.16)-(2.19) form a set of self-consistent equations for the determination of the random GF and mass-operator. The calculation of the phonon GF entering the electron-phonon part of the mass operator is discussed in the following section.

2.3. The Renormalized Phonon GF

The general scheme of calculations is the same as for the electron GF. The phonon GF is defined as

$$D^{\alpha\beta}_{ij}(t-t') = \langle\langle u^{\alpha}_{i}(t)\, u^{\beta}_{j}(t')\rangle\rangle = -i\theta(t-t')\langle[u^{\alpha}_{i}(t)\, u^{\beta}_{j}(t')]_{-}\rangle . \qquad (2.20)$$

We differentiate it twice over the time t and then twice over the time t'. The zeroth order GF defined as

$$\sum_{n\gamma}\left[M_i\omega^2\delta_{in}\delta_{\alpha\gamma} - \Phi^{\alpha\gamma}_{in}\right]D^{0\gamma\beta}_{nj}(\omega) = \delta_{ij}\,\delta_{\alpha\beta} \qquad (2.21)$$

enables us to write down the Dyson equation

$$D^{\alpha\beta}_{ij}(\omega) = D^{0\alpha\beta}_{ij}(\omega) + \sum_{mn}\sum_{\gamma\gamma'} D^{0\alpha\gamma}_{im}(\omega)\,\Pi^{\gamma\gamma'}_{mn}(\omega)\,D^{\gamma'\beta}_{nj}(\omega) \qquad (2.22)$$

with the phonon mass-operator (polarization operator) Π given by

$$\Pi^{\gamma\gamma'}_{mm'}(\omega) = \frac{1}{2\pi^2}\sum_{n\ell}\sum_{n'\ell'}\sum_{\sigma\sigma'}(\delta_{mn}-\delta_{m\ell})\,T^{\gamma}_{n\ell}\left\{\langle\langle a^{+}_{n\sigma}\, a_{\ell\sigma} | a^{+}_{n'\sigma'}\, a_{\ell'\sigma'}\rangle\rangle_{\omega}\right\}^{pp}\times \qquad (2.23)$$
$$\times\, T^{\gamma'}_{n'\ell'}(\delta_{n'm'} - \delta_{\ell'm'}) .$$

The method of calculation Π we use here is the same as for $\mathfrak{M}$. Neglecting the vertex corrections, we obtain

$$\Pi^{\gamma\gamma'}_{mm'}(\omega) = \frac{1}{2\pi^2}\iint_{-\infty}^{\infty} d\omega_1\, d\omega_2\, \frac{\mathrm{th}\frac{\beta\omega_1}{2} - \mathrm{th}\frac{\beta\omega_2}{2}}{\omega-\omega_1+\omega_2}\sum_{n\ell}\sum_{n'\ell'}\sum_{\sigma}\times \qquad (2.24)$$
$$\times\left\{(\delta_{mn}-\delta_{m\ell})\,T^{\gamma}_{n\ell}\left[\mathrm{Im}\langle\langle a_{\ell\sigma} | a^{+}_{n'\sigma}\rangle\rangle_{\omega_1}\mathrm{Im}\langle\langle a_{\ell'\sigma} | a^{+}_{n\sigma}\rangle\rangle_{\omega_2} - \right.\right.$$
$$\left.\left. - \mathrm{Im}\langle\langle a^{+}_{n-\sigma} | a^{+}_{n'\sigma}\rangle\rangle_{\omega_1}\mathrm{Im}\langle\langle a_{\ell'\sigma} | a_{\ell\sigma}\rangle\rangle_{\omega_2}\right] T^{\gamma}_{n'\ell'}(\delta_{n'm'} - \delta_{\ell'm'})\right\} .$$

Note, the phonon spectrum in the superconducting state is additionally renormalized as compared to the normal state [27,32,38].

3. CONFIGURATIONAL AVERAGING

In this section we discuss different attempts at averaging. Our main task is to obtain the averaged system of equations describing the superconducting alloy. For a given, fixed configuration of atoms in a lattice these are given by the set of equations (2.13), (2.16)-(2.19). Roughly speaking we need the configurationally averaged GF $\langle\hat{\mathcal{G}}(\omega)\rangle=\hat{\bar{G}}(\omega)$ and total mass-operator $\langle\hat{\mathfrak{M}}^t(\omega)\rangle=\hat{\bar{M}}^t(\omega)$, where

$$\hat{\bar{M}}^t = \langle \hat{\mathfrak{M}}^t(\omega)\rangle = \hat{\bar{M}}^{HF} + \hat{\bar{M}}^{e\ell-ph}(\omega) + \hat{\bar{M}}^c(\omega). \tag{3.1}$$

For the later convenience we rewrite equation (2.13) as

$$\sum_\ell (\omega\hat{\tau}_0\delta_{i\ell} - (\varepsilon_i\delta_{i\ell} + t_{i\ell})\hat{\tau}_3 - \hat{\mathfrak{M}}^t_{i\ell,\sigma}(\omega))\hat{\mathcal{G}}^\sigma_{\ell j}(\omega) = \delta_{ij}. \tag{3.2}$$

In this paper we are not interested in the dynamical effect of the electron-electron interaction and neglect the mass-operator $\hat{\mathfrak{M}}^c_{i\ell}(\omega)$ [4,6,12]. Thus, the electron correlations are treated in the Hartree-Fock approximation.

We start the discussion of averaging with the simplest possibility where only the random energy levels ε_i are described in the CPA and other random parameters U_i, T_{ij} are averaged to the lowest order of concentrations x.

3.1. The Simplest Method of Averaging

In the following we assume the hopping integrals t_{ij} to be nonrandom, periodic quantities, or replace the actual parameters by an average, i.e.,

$$t_{ij} \to \bar{t}_{ij} = x^2 t^{AA}_{ij} + 2xy\, t^{AB}_{ij} + y^2 t^{BB}_{ij}. \tag{3.3}$$

The average of the alloy Green function $\hat{\mathcal{G}} = \hat{\mathcal{G}}^0 + \hat{\mathcal{G}}^0\hat{\mathfrak{M}}^1\hat{\mathcal{G}}$, where $\hat{\mathfrak{M}}^1 = \hat{\mathfrak{M}}^{HF} + \hat{\mathfrak{M}}^{e\ell-ph}$ and $\hat{\mathcal{G}}^0_{ij}$ is defined by

$$\sum_\ell (\omega\hat{\tau}_0\delta_{i\ell} - \varepsilon_i\hat{\tau}_3\delta_{i\ell} - \bar{t}_{i\ell}\hat{\tau}_3)\hat{\mathcal{G}}^0_{\ell j}(\omega) = \delta_{ij}, \tag{3.4}$$

is assumed to be

$$\hat{\bar{G}} = \hat{\bar{G}}^0_{CPA} + \hat{\bar{G}}^0_{CPA}\langle\hat{\mathfrak{M}}^1\rangle\hat{\bar{G}}. \tag{3.5}$$

Here $\hat{\bar{G}}^0_{CPA}$ means the CPA averaged GF defined in eq. (3.4). In order to obtain the lowest order estimation to $\langle\hat{\mathfrak{M}}^1\rangle$ we replace the GFs entering the definition of $\hat{\mathfrak{M}}^1$ by their averaged values, while the remaining random single site parameters $a_i = U_i$, q^r_0, ... etc., or their products average in the following manner:

$$\langle a_i a_j\rangle = \begin{cases} \langle a_i^2\rangle = x a_A^2 + y a_B^2, & \text{if } i=j \\ \langle a_i\rangle\langle a_j\rangle = (x a_A + y a_B)^2, & \text{if } i\neq j. \end{cases} \tag{3.6}$$

The above scheme of averaging is rather crude but workable. It gives some insight into the problem, and moreover, enables us to derive the nonlinearized Eliashberg equations of superconductivity in alloys. In some sense this scheme resembles the so-called Anderson limit of constant order parameter studied in the CPA in papers [14,20].

Fourier transforming the averaged equation (3.5) and expressing the averaged mass-operator $\hat{\bar{M}}^1(\omega)$ in terms of the Pauli matrices $\hat{\tau}_i$ in a standard way [4-8,12]

$$\hat{\bar{M}}(\omega) = [1-\hat{Z}(\omega)]\omega\tau_0 + \chi(\omega)\hat{\tau}_3 + \phi(\omega)\hat{\tau}_1 \tag{3.7}$$

we arrive to equations [12]

$$[1-Z(\omega)]\omega = -\int_{-\infty}^{\infty} d\omega' K(\omega',\omega)\,\mathrm{Re}\frac{\omega'}{\sqrt{\omega'^2-\Delta^2(\omega')}}\,\mathrm{sign}\,\omega', \tag{3.8}$$

$$\Delta(\omega)Z(\omega) = \int_{-\infty}^{\infty} d\omega' K(\omega',\omega)\,\mathrm{Re}\frac{\Delta(\omega')}{\sqrt{\omega'^2-\Delta^2(\omega')}}\,\mathrm{sign}\,\omega' - V_c\int_0^{\omega_c} d\omega'\,\mathrm{th}\frac{\beta\omega'}{2}\,\mathrm{Re}\frac{\Delta(\omega')}{\sqrt{\omega'^2-\Delta^2(\omega')}}, \tag{3.9}$$

where $\Delta(\omega)=\phi(\omega)/Z(\omega)$ and [12]

$$V_c = N(\epsilon_f)\langle U_i\rangle / (1-N(\epsilon_f)\langle U_i\rangle \ln\frac{\epsilon_f}{\omega_c}) \tag{3.10}$$

$N(\epsilon_f)$ is the density of states of an alloy at the Fermi energy ϵ_f, and the kernel $K(\omega',\omega)$ is given by

$$K(\omega',\omega) = \int_{-\infty}^{\infty} dz\,\alpha^2(z)F(z)\frac{\mathrm{th}\frac{\beta\omega'}{2} + \mathrm{cth}\frac{\beta z}{2}}{\omega - z - \omega' + i\epsilon}.$$

Here $\alpha^2(\omega)F(\omega)$ is the electron-phonon spectral (or Eliashberg) function

$$\alpha^2(\omega)F(\omega) = \int_{S_F} \frac{d^2k}{v_k} \int_{S_F} \frac{d^2q}{v_q} \sum_\lambda \{ |g_1^\lambda(\vec{k},\vec{q})|^2 \{ -\frac{1}{\pi} \mathrm{Im} \bar{D}_{\vec{k}-\vec{q},\lambda}(\omega+i\epsilon) \} +$$

$$+ \int_{S_F} \frac{d^2p}{v_p} |g_2^\lambda(\vec{k},\vec{q},\vec{p})|^2 \{ -\frac{1}{\pi} \mathrm{Im} \bar{D}_{\vec{k}-\vec{p}-\vec{q},\lambda}(\omega+i\epsilon) \} \} / \int_{S_F} \frac{d^2k}{v_k} \quad . \tag{3.11}$$

All the information about the system needed to calculate T_c and $\Delta(\omega)$ is contained in this function.

$$|g_1^\lambda(\vec{k},\vec{q})|^2 = \frac{Q_2}{2M_A a^2} \sum_\alpha [e^\alpha_{\vec{k}-\vec{q},\lambda} (v^\alpha_k - v^\alpha_q)]^2$$

$$|g_2^\lambda(\vec{k},\vec{q},\vec{p})|^2 = \frac{Q_1 - Q_2}{8M_A a^2} \sum_\alpha [e^\alpha_{\vec{k}-\vec{p}-\vec{q},\lambda} (v^\alpha_k - v^\alpha_{p+q} + v^\alpha_{k-p} - v^\alpha_q)]^2 \tag{3.12}$$

$$Q_1 = x q_A^2 + y q_B^2 ; \quad Q_2 = x^2 q_A^2 + 2xy q_A q_B + y^2 q_B^2$$

$$\epsilon_k = N^{-1} \sum_{ij} \bar{t}_{ij} \exp[ik(R_i - R_j)] ; \quad v^\alpha_k = \frac{\partial \epsilon_k}{\partial k^\alpha} .$$

Here a denotes the distance between nearest neighbours in a cubic lattice, $\vec{e}_{k,\lambda}$ and $\bar{D}_{k,\lambda}(\omega)$ denote, respectively, the phonon polarization vector and the averaged GF of a phonon branch λ /27/. The phonon GF $\bar{D}_{k\lambda}(\omega)$ itself is a solution of the equation (shorthand notation is used)

$$\bar{D} = \bar{D}^\circ + \bar{D}^\circ \bar{\Pi} \bar{D} , \tag{3.13}$$

where $\bar{D}^\circ$ as defined in (2.21) is calculated in the CPA, but the phonon mass-operator $\bar{\Pi}(\omega)$ giving the renormalization of the phonon spectrum in an alloy is calculated here in a similar way as $\hat{\bar{M}}$ (c.f. /27/). In general, it is important to use the fully renormalized phonon GF, for the anomalous phonon contribution to the high T_c comes mainly from the phonon linewidth ($\sim \mathrm{Im}\,\bar{\Pi}(\omega)$) /32/ .The renormalization can remarkably change the spectrum of the superconductor giving rise to a new localized phonon mode /38/.

3.2. General Scheme of Averaging

All the quantities of the theory developed in Sec.2 such as mass-operators $\hat{\mathfrak{M}}^\sigma_{i\ell}(\omega)$, $\Pi_{i\ell}(\omega)$, GFs, etc. depend on the configurations of the whole alloy. The most important, however, is the dependence on the occupancy of the so-called terminal points i,ℓ. The rest of the atoms can be replaced by an effective medium. It means that we replace the functions $\hat{\mathfrak{M}}^\sigma_{i\ell}(\omega)$, $\hat{\mathcal{G}}^\sigma_{i\ell}(\omega)$, etc., by their conditionally averaged counterparts

$$\hat{M}^\sigma_{i\ell}(\omega) = \langle \hat{\mathfrak{M}}_{i\ell,\sigma} \rangle^{\{j\}}_{i\ell} ; \qquad \hat{G}^\sigma_{i\ell} = \langle \hat{\mathcal{G}}^\sigma_{i\ell}(\omega) \rangle^{\{j\}}_{i\ell} \quad \ldots \tag{3.14}$$

Here $\langle \ldots\ldots \rangle^{\{j\}}_{i\ell}$ means the configurational conditional averaging over all lattice sites $\{j\}$ different from i and ℓ, the condition being the fixed types of atoms at site i and ℓ. Evaluation of various conditional averaged $M^{AA}_{i\ell}$, $M^{AB}_{i\ell}$ ... requires in turn the knowledge of conditionally averaged electron and phonon GFs. The best way to calculate them is to use the off-diagonal CPA developed in /39/ for electrons and its extension to phonons /40/. The resulting set of equations is difficult to solve numerically, and therefore, we shall not discuss it further.

To make the problem tractable we resort in the next subsection to additional approximation leading to the single-site description.

3.3. The Random Contact Model

In the contact model the electron scattering processes, caused by the electron-electron and electron-phonon interactions, are taken into account only if the two electrons are initially both at the same site i and finally both at the other site j /24-26/. In our tight-binding approach it means that we neglect all off-diagonal (in site indices) matrix elements of the electron and phonon GFs and of the mass-operator. Thus, we obtain

$$\hat{\mathfrak{M}}^\sigma_{ii}(\omega) = \epsilon_i \hat{\tau}_3 - \frac{U_i}{2} \int_{-\infty}^{\infty} d\omega_2 \mathrm{th}\frac{\beta\omega_2}{2} \hat{\tau}_3 \{ -\frac{1}{\pi} \mathrm{Im}\, \hat{\mathcal{G}}^{-\sigma}_{ii}(\omega_2 + i\epsilon) \} \hat{\tau}_3 -$$

$$- \frac{1}{2} \iint_{-\infty}^{\infty} d\omega_1 d\omega_2 \frac{\mathrm{cth}\frac{\beta\omega_1}{2} + \mathrm{th}\frac{\beta\omega_2}{2}}{\omega - \omega_1 - \omega_2} \sum_{m\alpha} T^\alpha_{im} \{ -\frac{1}{\pi} \mathrm{Im}(D^\alpha_{ii}(\omega_1 + i\epsilon) + D^\alpha_{mm}(\omega_1 + i\epsilon)) \} \tag{3.15}$$

$$\times \hat{\tau}_3 \{ -\frac{1}{\pi} \mathrm{Im}\, \hat{\mathcal{G}}^\sigma_{mm}(\omega_2 + i\epsilon) \} \hat{\tau}_3 T^\alpha_{mi} \quad .$$

Note, that we have incorporated the random energy levels into the definition of the mass-operator matrix. The sum over m

is limited here to nearest neighbouring sites to i (c.f. the definition of T^{α}_{im}). Denoting the distance between neighbouring sites as previously by $a=|\vec{R}_m-\vec{R}_i|$ and $a_\alpha=|R^\alpha_m-R^\alpha_i|$, we can rewrite equation (3.15) as

$$\hat{M}^{\sigma}_{A}(\omega)=\epsilon_A\hat{\tau}_3-\frac{U_A}{2}\int_{-\infty}^{\infty}d\omega_2 th\frac{\beta\omega_2}{2}\hat{\tau}_3\{-\frac{1}{\pi}Im\hat{G}^{-\sigma}_{A}(\omega_2+i\epsilon)\}\hat{\tau}_3-$$

$$-\frac{1}{2\pi^2}\iint_{-\infty}^{\infty}d\omega_1 d\omega_2\frac{cth\frac{\beta\omega_1}{2}+th\frac{\beta\omega_2}{2}}{\omega-\omega_1-\omega_2}\sum_{\alpha}\frac{\bar{t}^2a^2_\alpha}{a^2}\{2xq^2_A ImD^{\alpha}_{A}(\omega_1+i\epsilon)\times \tag{3.16}$$

$$\times\hat{\tau}_3 Im\hat{G}^{\sigma}_{A}(\omega_2+i\epsilon)\hat{\tau}_3+\frac{1}{4}(q_A+q_B)^2y(ImD^{\alpha}_{A}(\omega_1+i\epsilon)+ImD^{\alpha}_{B}(\omega_1+i\epsilon))\times$$

$$\times\hat{\tau}_3 Im\hat{G}^{\sigma}_{B}(\omega_2+i\epsilon)\hat{\tau}_3\}$$

with a similar formula for $\hat{M}^{\sigma}_{B}(\omega)$. Here $\bar{t}$ denotes the value of the hopping integral for neighbouring atoms in a cubic lattice (cf. eq. (3.3)). According to the discussion in Sec.3.2 and in order to have true single-site description of $\hat{M}$, we have conditionally averaged equation (3.15) with a condition i=A. $G_A(D_A)$ means conditionally averaged electron (phonon) GFs. The third term in (3.16) resulting from the electron-phonon interaction has exactly the same form as an expression for $\sigma_{1,A}$ in /26/.

The above defined single-site matrices $\hat{M}^{\sigma}_{i}(\omega)$, i = A,B are the only random quantities in our model and serve as input parameters in the matrix CPA equations. The output of these equations are: i) the coherent potential matrix $\hat{\Sigma}^{\sigma}(\omega)$ replacing $\hat{M}^{\sigma}_{i}(\omega)$ in an effective medium, and ii) the Green function $\hat{\bar{G}}^{\sigma}(\omega)$ describing the properties of the averaged system. As usual the existence of the nonzero solution for the off-diagonal in spin indices (i.e., anomalous) part of the $\hat{\Sigma}(\omega)$ matrix determines the superconducting transition temperature.

The model as stated above is appropriate for the discussion of possible coexistence between superconductivity and magnetism, but this is outside the scope of the present paper. Therefore, in the following we omit the spin index σ .

3.4. CPA Equations for Superconductivity in the Contact Model

Here we briefly discuss the calculations of the averaged electron GF $\hat{\bar{G}}(\omega)$ and $\hat{G}_i(\omega)$, i=A,B. The averaged GF $\hat{\bar{G}}(\omega)$ is related to the configuration dependent one $\hat{G}$ by /41/

$$\hat{\mathcal{G}}(\omega)=\hat{\bar{G}}(\omega)+\hat{\bar{G}}(\omega)\hat{\mathcal{T}}(\omega)\hat{\bar{G}}(\omega) \tag{3.17}$$

where the scattering operator $\hat{\mathcal{T}}$ refers to the whole system. In the single-site CPA the condition $\langle\hat{\mathcal{T}}\rangle=0$ determining the averaged GF is replaced by the following /41/

$$\langle\hat{T}_i\rangle=x\hat{T}_A+y\hat{T}_B=0;\qquad \hat{T}_i=\langle\mathcal{T}\rangle_{\{j\}\neq i} \tag{3.18}$$

with the single-site T-matrix

$$\hat{T}_i=\hat{V}_i+\hat{T}_i\hat{V}_i\hat{\bar{G}}. \tag{3.19}$$

Here

$$\hat{V}_i=\begin{bmatrix} M_{11}(\omega)-\Sigma_{11}(\omega), & M^{i}_{12}(\omega)-\Sigma_{12}(\omega) \\ M^{*i}_{12}(\omega^*)-\Sigma^*_{12}(\omega^*), & -M^{i}_{11}(-\omega)+\Sigma_{11}(-\omega)\end{bmatrix}, \tag{3.20}$$

$$\hat{\bar{G}}(\omega)=\begin{bmatrix} \bar{G}_{11}(\omega), & \bar{G}_{12}(\omega) \\ \bar{G}^*_{12}(\omega^*), & -\bar{G}_{11}(-\omega)\end{bmatrix} \tag{3.21}$$

and

$$\bar{G}_{11}(\omega)=\frac{1}{N}\sum_{k}\frac{\omega+\epsilon_k+\Sigma_{11}(-\omega)}{[\omega-\epsilon_k-\Sigma_{11}(\omega)][\omega+\epsilon_k+\Sigma_{11}(-\omega)]-\Sigma_{12}(\omega)\Sigma^*_{12}(\omega^*)},$$

$$\bar{G}_{12}(\omega)=\frac{1}{N}\sum_{k}\frac{\Sigma_{12}(\omega)}{[\omega-\epsilon_k-\Sigma_{11}(\omega)][\omega+\epsilon_k+\Sigma_{11}(-\omega)]-\Sigma_{12}(\omega)\Sigma^*_{12}(\omega^*)}. \tag{3.22}$$

A very important relation, connecting the anomalous and normal part of (3.21), follows from the last two equations, namely

$$\bar{G}_{12}(\omega)=\frac{\bar{G}_{11}(\omega)-\bar{G}_{11}(-\omega)}{2\omega+\Sigma_{11}(-\omega)-\Sigma_{11}(\omega)}\Sigma_{12}(\omega). \tag{3.23}$$

To close the set of equations (3.15), (3.17)-(3.23) we need the expression for the single-site GF, $\hat{G}_i(\omega)$. In the CPA it is given by /41/:

$$\hat{G}_i(\omega)=\hat{\bar{G}}(\omega)+\hat{\bar{G}}(\omega)\hat{T}_i(\omega)\hat{\bar{G}}(\omega)=[1-\hat{\bar{G}}(\hat{M}_i-\hat{\Sigma})]^{-1}\hat{\bar{G}}, \quad (i=A,B). \qquad (3.24)$$

The resulting set can be solved numerically and the transition temperature T_c determined. At this temperature there appear the nonzero solution for the anomalous part of these equations. Therefore we expect at $T\to T_c$, $\Sigma_{12}(\omega)\to 0$ and $M^i_{12}(\omega)\to 0$, thus making possible the linearization and the simplification of the problem. It is a subject of the next section.

3.5. Linearized Equations and the Transition Temperature

The simplest way to obtain the linearized, with respect to $\Sigma_{12}(\omega)$ and $M^i_{12}(\omega)$, equations of the previous sections is to write every matrix $\hat{F}$ as a sum of normal $\hat{F}^n$ (diagonal) and anomalous (i.e., purely off-diagonal, superconducting) $\hat{F}^s$ parts and use the matrix identity $(A-B)^{-1}=A^{-1}+A^{-1}B(A-B)^{-1}$ repeatedly. Up to linear order in Σ_{12} the diagonal part of (3.10) gives the so-called Soven equation/42/

$$\Sigma_{11}(\omega)=xM^A_{11}(\omega)+yM^B_{11}(\omega)-(M^A_{11}(\omega)-\Sigma_{11}(\omega))\bar{G}_{11}(\omega)(M^B_{11}(\omega)-\Sigma_{11}(\omega)) \qquad (3.25)$$

$$\bar{G}_{11}(\omega)=\frac{1}{N}\sum_k \frac{1}{\omega-\epsilon_k-\Sigma_{11}(\omega)}$$

while the off-diagonal part can be written as

$$\bar{G}_{12}(\omega)=\langle G^i_{11}(\omega)[\frac{\bar{G}_{12}(\omega)}{\bar{G}_{11}(\omega)\bar{G}_{11}(-\omega)}+\Sigma_{12}(\omega)-M^i_{12}(\omega)]G^i_{11}(-\omega)\rangle. \qquad (3.26)$$

Noting the definition $G^i_{11}(\omega)=(G^{-1}_{11}(\omega)-M^i_{11}(\omega)+\Sigma_{11}(\omega))^{-1}$ and the identity

$$G^i_{11}(\omega)-G^i_{11}(-\omega)=G^i_{11}(\omega)[\frac{\bar{G}_{11}(-\omega)-\bar{G}_{11}(\omega)}{\bar{G}_{11}(\omega)\bar{G}_{11}(-\omega)}+\Sigma_{11}(\omega)-\Sigma_{11}(-\omega)+ \qquad (3.27)$$

$$+M^i_{11}(-\omega)-M^i_{11}(\omega)]G^i_{11}(-\omega)$$

and defining the auxiliary function $\tilde{\Sigma}_{12}(\omega)$ (cf./17,21,25/),

$$\tilde{\Sigma}_{12}(\omega)=\Sigma_{12}(\omega)\frac{2\omega}{2\omega+\Sigma_{11}(-\omega)-\Sigma_{11}(\omega)} \qquad (3.28)$$

we obtain from (3.26) and (3.23) the CPA equation for $\tilde{\Sigma}_{12}(\omega)$

$$\langle G^i_{11}(\omega)\tilde{\Sigma}_{12}(\omega)\frac{2\omega-M^i_{11}(-\omega)+M^i_{11}(\omega)}{2\omega}G^i_{11}(-\omega)\rangle = \qquad (3.29)$$

$$=\langle G^i_{11}(\omega)M^i_{12}(\omega)G^i_{11}(-\omega)\rangle .$$

Note, equation (3.28) has the structure of the so-called Abrikosov-Gorkov relation/10,21,26/. It expresses the additional changes of the $\Sigma_{12}(\omega)$ due to the disorder in the normal part of the problem. It is easy to verify that

$$G^i_{12}(\omega)=\frac{G^i_{11}(\omega)-G^i_{11}(-\omega)-G^i_{11}(\omega)[2\omega+M^i_{11}(\omega)-M^i_{11}(-\omega)]G^i_{11}(-\omega)}{2\omega+\Sigma_{11}(-\omega)-\Sigma_{11}(\omega)}\tilde{\Sigma}_{12}(\omega)+ \qquad (3.30)$$

$$+G^i_{11}(\omega)M^i_{12}(\omega)G^i_{11}(\omega).$$

Equation (3.15) or (3.16) and (3.30) determine the input parameters, $M^i_{12}(\omega)$, for (3.29). It is worth while to note the presence of the terms $(M^i_{11}(-\omega)-M^i_{11}(\omega))$ in (3.29) and (3.30). They express some additional influence of the electron-phonon disorder (only the electron-phonon part of $\hat{M}_i$ is energy dependent in our treatment) on the superconducting behaviour of an alloy. However, we expect this effect to be weak and neglect it (cf./25,26/).

Combining equations (3.27), (3.30) and (3.15) we obtain from (3.29) the equation

$$\tilde{\Sigma}_{12}(\omega)=\int_{-\infty}^{\infty}d\omega' K_{eff}(\omega',\omega)\mathrm{Re}\{\frac{\tilde{\Sigma}_{12}(\omega'+i\epsilon)}{\omega'}\}- \qquad (3.31)$$

$$-N(\epsilon_f)U_{eff}\int_0^{\infty}d\omega'\,\mathrm{th}\frac{\beta\omega'}{2}\mathrm{Re}\{\frac{\tilde{\Sigma}_{12}(\omega'+i\epsilon)}{\omega'}\}$$

replacing the Eliashberg equation for the order parameter $\Delta(\omega)$ (cf. eq. (3.9)). The kernel K_{eff} is defined as usually/12/

$$K_{eff}(\omega',\omega)=\int_{-\infty}^{\infty}dz\,\alpha^2(z)F(z)\frac{\mathrm{cth}\frac{\beta z}{2}+\mathrm{th}\frac{\beta\omega'}{2}}{z+\omega'-\omega-i\epsilon} \qquad (3.32)$$

where the Eliashberg function

$$\overline{\alpha^2(\omega)F(\omega)} = 2\sum_{\alpha}\bar{t}^2\frac{a_\alpha^2}{a^2}\{x^2q_A^2N_A^2(\epsilon_f)(-\frac{1}{\pi}\mathrm{Im}D_A^\alpha(\omega+i\epsilon)) +$$

$$+\frac{1}{4}xy(q_A+q_B)^2N_A(\epsilon_f)N_B(\epsilon_f)(-\frac{1}{\pi}\mathrm{Im}D_A^\alpha(\omega+i\epsilon)-\frac{1}{\pi}\mathrm{Im}D_B^\alpha(\omega+i\epsilon))+ \qquad (3.33)$$

$$+y^2q_B^2N_B^2(\epsilon_f)(-\frac{1}{\pi}\mathrm{Im}D_B^\alpha(\omega+i\epsilon))\}/N(\epsilon_f)$$

$$N(\epsilon_f)U_{eff} = \langle U_i N_i^2(\epsilon_f)/N(\epsilon_f)\rangle , \qquad (3.34)$$

$N_i(\epsilon_f)$ and $N(\epsilon_f)$ denote, respectively, the partially and totally averaged electron densities of states at the Fermi level

$$N_i(\epsilon_f) = -\frac{1}{\pi}\mathrm{Im}G_{11}^i(\epsilon_f), \quad i=A,B$$

$$N(\epsilon_f) = -\frac{1}{\pi}\mathrm{Im}\bar{G}_{11}(\epsilon_f) = xN_A(\epsilon_f)+yN_B(\epsilon_f) . \qquad (3.35)$$

Following the work of McMillan[8], we can write down the formula for T_c

$$T_c = \frac{\theta}{1.45}\exp\{-\frac{1.04(1+\lambda_{eff})}{\lambda_{eff}-\mu^*_{eff}(1+0.62\lambda_{eff})}\} , \qquad (3.36)$$

where the electron-phonon coupling constant

$$\lambda_{eff} = \sum_{\alpha}\bar{t}^2\frac{a_\alpha^2}{a^2}\{xN_A(\epsilon_f)\tilde{D}_A^\alpha[xq_A^2N_A(\epsilon_f)+\frac{1}{4}y(q_A+q_B)^2N_B(\epsilon_f)]+$$

$$+yN_B(\epsilon_f)\tilde{D}_B^\alpha[yq_B^2N_B(\epsilon_f)+\frac{1}{4}x(q_A+q_B)^2N_A(\epsilon_f)]\}/N(\epsilon_f) \qquad (3.37)$$

and the Coulomb pseudopotential

$$\mu^*_{eff} = N(\epsilon_f)U_{eff}/(1+N(\epsilon_f)U_{eff}\ln\frac{W}{\theta}). \qquad (3.38)$$

both depend on the alloy parameters, particularly on the concentration x, thus giving rise to the concentration dependence of the transition temperature T_c. The calculation of T_c versus x for various transition metal alloys will be a subject of the next paper.

In the above formulae θ is of the order of the Debye temperatire of an alloy, W is the alloy band width[25] and $\tilde{D}_i^\alpha$ is

$$\tilde{D}_i^\alpha = -\frac{2}{\pi}\int d\omega\,\frac{\mathrm{Im}D_i^\alpha(\omega+i\epsilon)}{\omega}, \qquad i=A,B. \qquad (3.39)$$

To obtain T_c for various alloys one has to solve the CPA equation (3.25) then calculate $N_i(\epsilon_f)$, $N(\epsilon_f)$. The phonon GFs $D(\omega)$ and $\tilde{D}_i^\alpha$ are calculated from the equation similar to (3.25)[27,43]

4. DISCUSSION AND CONCLUSIONS

We have developed the theory for strong coupling superconductivity in disordered transition metal alloys. The use of the alloy version of the BLF model ensures the proper treatment of an atomic character of d-electrons responsible for superconductivity in such systems. We were able to obtain the closed set of equations determining the electron and phonon GFs and mass operator. These equations give the general microscopic description of an alloy in the spirit of the Migdal-Eliashberg approach. Written in a Wannier space they refer to the fixed configuration of atoms in an alloy. Therefore, the averaging is needed. This was performed in two different ways. First, in section 3.1, we used very simple approximation for the averaged GFs. As it was mentioned previously this approximation gives the workable scheme for the derivation of the usual nonlinear Eliashberg equations written in terms of alloy microscopic parameters. The second approach is fully based on the CPA. We take into account the randomness not only through the parameters of the Hamiltonian, but also, in a self-consistent way through the configuration dependence of the single site electron mass-operator. Although similar to[25,27] our paper contains further developments of these theories for strong-coupling superconductivity in disordered alloys. Contrary to[25] we take into account the effect of disorder on the phonon GF, and we do not replace, as already mentioned, the single-site GFs G_A, G_B in mass operator by the averaged GF $\bar{G}$. In paper[26] the electron-phonon interaction Hamiltonian is not expressed through the microscopic parameters like q_q^i, t_{ij}, etc. The expression for the self-energy in[26] is limited to the contact model only, and in order to average the GF over configuration this author resorts to some phenomenological ansatz for the anomalous self-energy. Contrary to that we derived the mass-operator in the general way by means of the "irreducible" GFs, which permit the derivation of the exact expression for $\mathfrak{M}$ by the separation of the Hartree-Fock-Bogolubov mean-field terms. It must be emphasized that for the random con-

tact model limit we derived and exploited the exact general relatioship between normal and anomalous parts of the electron GF, performing the configurational averaging in the spirit of the CPA without any additional ansatz.

The present theory in its general, as well as contact model version, will be used in the near future for the discussion of the concentration dependence of T_c in some transition metal alloys.

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Высокиньски К.И., Куземский А.Л. E17-82-649
Теория сильносвязанных сверхпроводящих разупорядоченных сплавов переходных металлов

Выведены уравнения сверхпроводимости для разупорядоченных сплавов переходных металлов с сильной связью. Использовалась обобщенная для случая сплавов модель БЛФ электрон-ионного взаимодействия и метод "неприводимых" функций Грина. Конфигурационное усреднение выполнено в рамках приближения когерентного потенциала. Получены выражения для температуры сверхпроводящего перехода и эффективного параметра электрон-фононного взаимодействия, которые выражаются через микроскопические параметры сплава.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Wysokiński K.I., Kuzemsky A.L. E17-82-649
The Theory for Strong-Coupling Superconductivity in Disordered Transition Metal Alloys

The equations for strong-coupling superconductivity in disordered transition metal alloys have been derived by means of "irreducible" Green functions and on the basis of the alloy version of the BLF model for the electron-ion interaction. The configurational averaging has been performed by means of the CPA. Making some approximations we have obtained the formulae for the transition temperature T_c and for the electron-phonon coupling constant λ. The coupling λ depends on the alloy component and total densities of states, the phonon GF and the parameters of the model.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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