EQUATIONS OF SUPERCONDUCTIVITY FOR TRANSITION METALS IN THE WANNIER REPRESENTATION

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In the Wannier representation, a system of equations of the superconductivity is obtained for strongly bound electrons in a transition metal, which is described by the Hubbard Hamiltonian. The electron–phonon interaction is written down using the rigid-ion model. A closed system of equations is obtained when the renormalization of the vertex in the mass operator is ignored.

1. Introduction

In recent years, there has been much interest in the investigation of the superconducting properties of transition metals, their alloys, and compounds [1]. In contrast to simple metals, transition metals have not only a broad s band but also a partly filled relatively narrow d band. It has been shown on a number of occasions [2-5] that strongly bound d electrons are to a large degree responsible for the superconducting properties of transition metals. Even in the case of strong correlation, the Coulomb interaction between strongly bound electrons can lead to the formation of Cooper pairs in a Mott–Hubbard semiconductor [6].

The simplest model that describes the correlation of strongly bound electrons in transition metals and their alloys is the Hubbard model [7], by means of which it is possible to explain numerous electric and magnetic properties of transition metals, their alloys, and compounds [8, 9]. It should be noted that the Hubbard Hamiltonian is a strongly simplified variant of the Shubin–Vonsovskii–Bogolyubov polar model of a metal [10] and in this sense is a first step in the construction of a systematic microscopic theory of transition metals and their compounds.

In the present paper, we derive a system of equations of the superconductivity for strongly bound electrons of a transition metal interacting with the phonons. The equations of superconductivity are written down in a basis of localized Wannier wave functions. Such a representation emphasizes the strongly bound nature of the d electrons and, in addition, is necessary to describe the superconducting properties of disordered alloys of transition metals [1, 11-14] and amorphous superconductors [14, 15].

To derive the superconductivity equations, we use the equations of motion for the two-time Green's functions [16], in which the decoupling procedure is carried out only for approximate calculation of the mass operator of the matrix electron Green's function. A closed system of equations is obtained when the renormalization of the vertex in the electron–ion interaction is ignored, as in [17, 18]. The obtained system of superconductivity equations for strongly bound electrons in the localized basis is analogous to Éliashberg's equations [18] for Bloch electrons and makes it possible to study the superconducting properties of transition metals and their alloys in the framework of a unified system of equations.

2. Hamiltonian of the Electron–Ion Model of a Narrow-Band Metal

We represent the total Hamiltonian of the electron–ion system in the form of the sum

$$H=H_e+H_i+H_{e\text{-}i}, \tag{1}$$

where H_e is the electron part of the Hamiltonian representing the Hubbard operator [7]:

$$H_e=\sum_{ij\sigma} t_{ij}a_{i\sigma}^{+}a_{j\sigma}+\frac{U}{2}\sum_{i\sigma} n_{i\sigma}n_{i-\sigma}. \tag{2}$$

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The operators $a_{i\sigma}^+$ and $a_{i\sigma}$ are the Fermi operators of creation and annihilation of electrons at site i; U is the energy of the Coulomb repulsion of the electrons with opposite spins at one site, $t_{ij}=N^{-1}\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \exp[i\mathbf{k}(\mathbf{R}_i-\mathbf{R}_j)]$ is the hopping integral, and $\varepsilon_{\mathbf{k}}$ is the band energy.

The ion subsystem is described by the operator

$$H_i=\frac{1}{2}\sum_n \frac{P_n^2}{2M_n}+\frac{1}{2}\sum_{nm}\Phi_{nm}^{\alpha\beta}u_n^{\alpha}u_m^{\beta}, \tag{3}$$

where $\mathbf{P}_n$ is the momentum operator, M_n is the mass of an ion, and $\mathbf{u}_n$ is the displacement of the atom from the equilibrium position at the lattice site $\mathbf{R}_n$.

The operator of the electron–ion interaction has the form

$$H_{e\text{-}i}=\sum_{\sigma}\sum_{n,i\neq j} V_{ij}^{\alpha}(\mathbf{R}_n^0)\,a_{i\sigma}^+a_{j\sigma}u_n^{\alpha}, \tag{4}$$

where

$$\sum_n V_{ij}^{\alpha}(\mathbf{R}_n^0)\,u_n^{\alpha}=\frac{\partial t_{ij}(\mathbf{R}_{ij}^0)}{\partial \mathbf{R}_{ij}^0}(\mathbf{u}_i-\mathbf{u}_j). \tag{5}$$

It is convenient to rewrite the operators (2) and (4) by means of Nambu operators and Pauli matrices:

$$H_e=\sum_{ij} t_{ij}\psi_i^+\tau_3\psi_j+\frac{U}{2}\sum_i(\psi_i^+\tau_3\psi_i)(\psi_i^+\tau_3\psi_i), \tag{6}$$

$$H_{e\text{-}i}=\sum_{n,\,i\neq j} V_{ijn}\psi_i^+\tau_3\psi_j u_n, \tag{7}$$

where

$$\psi_i=\begin{pmatrix} a_{i\uparrow}\\ a_{i\downarrow}^+\end{pmatrix},\quad \psi_i^+=(a_{i\uparrow}^+,a_{i\downarrow});\quad \tau_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix},\quad \tau_0=\begin{pmatrix}1&0\\0&1\end{pmatrix}. \tag{8}$$

Note that in the model of a metal considered here the s electrons are not taken into account explicitly. Instead of two bands of s and d electrons, as in the Hubbard model, we consider a single "effective" band of electrons interacting with phonons. However, the influence of the s electrons is taken into account indirectly. It is assumed that all three normal frequencies of the phonons $\omega^0(q\nu)$ without allowance for the d electrons correspond to acoustic frequencies, and the magnitude of the Coulomb repulsion U is renormalized by the screening by the s electrons [3, 19].

3. Equations for the Electron Green's Functions

We consider the equations of motion for the electron Green's functions, which we represent in the matrix form

$$G_{ij}(\omega)=\begin{bmatrix}\langle\langle a_{i\uparrow}|a_{j\uparrow}^+\rangle\rangle_\omega & \langle\langle a_{i\uparrow}|a_{j\downarrow}\rangle\rangle_\omega\\ \langle\langle a_{i\downarrow}^+|a_{j\uparrow}^+\rangle\rangle_\omega & \langle\langle a_{i\downarrow}^+|a_{j\downarrow}\rangle\rangle_\omega\end{bmatrix}=\langle\langle\psi_i|\psi_j^+\rangle\rangle_\omega. \tag{9}$$

Differentiation of $G_{ij}(t-t')$ with respect to the first time gives for the Fourier components the equation of motion

$$\sum_j(\omega\tau_0\delta_{ij}-t_{ij}\tau_3)\langle\langle\psi_j|\psi_{i'}^+\rangle\rangle_\omega=\delta_{ii'}\tau_0+\sum_{nj}V_{ijn}\langle\langle u_n\tau_3\psi_j|\psi_{i'}^+\rangle\rangle_\omega+U\langle\langle(\psi_i^+\tau_3\psi_i)\tau_3\psi_i|\psi_{i'}^+\rangle\rangle_\omega. \tag{10}$$

As in [17], we separate the renormalization of the electron energy in the Hartree–Fock–Bogolyubov average field approximation (with allowance for anomalous mean values) from the renormalization in higher orders due to inelastic scattering. For this, we introduce irreducible (ir) parts of the Green's functions in accordance with the definition (as an example, we take two of the four Green's functions)

$$\langle\langle a_{i\uparrow}a_{i\downarrow}^+a_{i\downarrow}|a_{i\uparrow}^+\rangle\rangle_\omega=\langle\langle(a_{i\uparrow}n_{i\downarrow})^{ir}|a_{i'\uparrow}^+\rangle\rangle_\omega+\langle n_{i\downarrow}\rangle\langle\langle a_{i\uparrow}|a_{i'\uparrow}^+\rangle\rangle_\omega-\langle a_{i\uparrow}a_{i\downarrow}\rangle\langle\langle a_{i\downarrow}^+|a_{i'\uparrow}^+\rangle\rangle_\omega, \tag{11}$$

$$\langle\langle a_{i\uparrow}a_{i\downarrow}^+a_{i\downarrow}|a_{i'\downarrow}\rangle\rangle_\omega=\langle\langle(a_{i\uparrow}n_{i\downarrow})^{ir}|a_{i'\downarrow}\rangle\rangle_\omega+\langle n_{i\downarrow}\rangle\langle\langle a_{i\uparrow}|a_{i'\downarrow}\rangle\rangle_\omega-\langle a_{i\uparrow}a_{i\downarrow}\rangle\langle\langle a_{i\downarrow}^+|a_{i'\downarrow}\rangle\rangle_\omega. \tag{12}$$

The choice of the irreducible parts of the Green's functions in (11) and (12) is specified by the conditions

$$\langle [(a_{i\uparrow}n_{i\downarrow})^{ir},\ \psi_i^+]_+\rangle=0. \tag{13}$$

The relation (13) makes it possible to introduce unambiguously the irreducible parts and make the inhomogeneous terms in the equations for them vanish. Using (11) and (12), we rewrite Eq. (10) in the form

$$\sum_j (\omega\tau_0\delta_{ij}-t_{ij}\tau_3-\Sigma^a_{i\sigma})\langle\langle\psi_j|\psi_{i'}^+\rangle\rangle=\delta_{ii'}\tau_0+\sum_j\langle\langle(\rho_{ij}\tau_3\psi_j)^{ir}|\psi_{i'}^+\rangle\rangle, \tag{14}$$

where

$$\rho_{ij}=U\rho_i\delta_{ij}+\sum_n V_{ijn}u_n(1-\delta_{ij}),\quad \rho_i=\psi_i^+\tau_3\psi_i=\sum_\sigma a_{i\sigma}^+a_{i\sigma}=\sum_\sigma n_{i\sigma}. \tag{15}$$

Here, $\Sigma_{i\sigma}^a$ is the mass operator in the average field approximation:

$$\Sigma^a_{i\sigma}=U\begin{pmatrix} n_{i-\sigma} & -\langle a_{i\sigma}a_{i-\sigma}\rangle \\ -\langle a^+_{i-\sigma}a_{i\sigma}^+\rangle & -n_{i\sigma}\end{pmatrix}. \tag{16}$$

In the representation of the Nambu operators

$$\psi_{i,-\sigma}=\begin{pmatrix} a_{i-\sigma}\\ a_{i\sigma}^+\end{pmatrix},\qquad \psi^+_{i,-\sigma}=(a^+_{i-\sigma},\ a_{i\sigma})$$

the mass operator (16) can be written in the form

$$\Sigma^a_{i\sigma}=-U\tau_3\langle\psi_{i,-\sigma}\psi^+_{i,-\sigma}\rangle\tau_3+\frac{U}{2}(\tau_0+\tau_3). \tag{17}$$

To calculate the irreducible matrix Green's function in (14), we write down for it the equation of motion with respect to the second time t' (see, for example, [17]). For the Fourier component of the Green's function, we obtain the equation

$$\sum_{j'}\langle\langle(\rho_{kj}\tau_3\psi_j)^{ir}|\psi_{j'}^+\rangle\rangle_\omega(\omega\tau_0\delta_{i'j'}-t_{j'i'}\tau_3)=\sum_{mj'}V_{j'i'm}\langle\langle(\rho_{kj}\tau_3\psi_j)^{ir}|\psi_{j'}^+\tau_3u_m\rangle\rangle_\omega+\frac{U}{2}\langle\langle(\rho_{kj}\tau_3\psi_j)^{ir}|(\psi_{i'}^+\tau_3\rho_{i'}+\rho_{i'}\psi_{i'}^+\tau_3)\rangle\rangle_\omega. \tag{18}$$

The procedure for separating the irreducible part with respect to the operators on the right-hand of the Green's function in (17) can be done in the same way as in [14]. This gives

$$\sum_{j'}\langle\langle(\rho_{kj}\tau_3\psi_j)^{ir}|\psi_{j'}^+\rangle\rangle(\omega\tau_0\delta_{i'j'}-t_{j'i'}\tau_3-\Sigma^e_{i'\sigma})=\sum_{j'}\langle\langle(\rho_{kj}\tau_3\psi_j)^{ir}|(\psi_{j'}^+\tau_3\rho_{j'i'})^{ir}\rangle\rangle. \tag{19}$$

To solve the system of equations (14), (19), we introduce the zeroth Green's function

$$\sum_j(\omega\tau_0\delta_{ij}-t_{ij}\tau_3-\Sigma^a_{i\sigma})G_{ji'}^0(\omega)=\delta_{ii'}. \tag{20}$$

Using (20) in (14) and (18), we obtain

$$G_{ii'}(\omega)=G_{ii'}^0(\omega)+\sum_{kk'}G_{ik}^0(\omega)T_{kk'}(\omega)G^0_{k'i'}(\omega). \tag{21}$$

The S matrix is determined by the irreducible part of the many-particle Green's function in (19):

$$T_{kk'}(\omega)=\sum_{jj'}\langle\langle(\rho_{kj}\tau_3\psi_j)^{ir}|(\psi_{j'}^+\tau_3\rho_{j'k'})^{ir}\rangle\rangle_\omega. \tag{22}$$

If we introduce the mass operator $M_{kk'}$, which is the connected part of the S matrix,

$$T_{kk'}(\omega)=M_{kk'}(\omega)+\sum_{mn}M_{km}(\omega)G_{mn}^0(\omega)T_{nk'}(\omega), \tag{23}$$

then Eq. (21) can be represented in the form of the Dyson equation

$$G_{ii'}(\omega)=G_{ii'}^{0}(\omega)+\sum_{kk'}G_{ik}^{0}(\omega)M_{kk'}(\omega)G_{k'i'}(\omega). \tag{24}$$

The mass operator $M_{kk'}=\{T_{kk'}\}^{p}$ does not contain parts that can be cut with respect to a G_0 line, which is indicated by the superscript p (proper part):

$$M_{kk'}=\sum_{jj'}\langle\!\langle(\rho_{kj}\tau_3\psi_j)^{1r}|(\psi_{j'}^{+}\tau_3\rho_{j'k'})^{1r}\rangle\!\rangle_{\omega}^{p}. \tag{25}$$

Thus, the most general expression for the electron Green's function in the localized basis with allowance for the electron–phonon interaction in the form (4) can be written in the matrix form

$$\overline{G}^{-1}=\overline{G}_0^{-1}-\overline{M}. \tag{26}$$

The calculation of the total Green's function $\overline{G}$ is reduced to the finding of $\overline{G}_0$ and $\overline{M}$.

4. Approximate Calculation of the Mass Operator

The explicit expression for the mass operator in (26) has the form

$$M_{ii'}(\omega)=\sum_{jj'}\int_{-\infty}^{\infty}\frac{d\omega'}{\omega-\omega'}(e^{\beta\omega'}+1)\int_{-\infty}^{\infty}\frac{dt}{2\pi}e^{-i\omega' t}\times\begin{bmatrix}\langle\rho_{j'i\uparrow}(t)a_{j'\uparrow}^{+}(t)a_{j\uparrow}\rho_{ij\uparrow}\rangle^{p,1r} & -\langle a_{j'\downarrow}(t)\rho_{i'j'\downarrow}(t)a_{j\uparrow}\rho_{ij\uparrow}\rangle^{p,1r}\\ -\langle\rho_{j'i'\uparrow}(t)a_{j'\uparrow}^{+}(t)\rho_{ji\downarrow}a_{j\downarrow}^{+}\rangle^{p,1r} & \langle a_{j'\downarrow}(t)\rho_{i'j'\downarrow}(t)\rho_{ji\downarrow}a_{j\downarrow}^{+}\rangle^{p,1r}\end{bmatrix}. \tag{27}$$

To obtain a closed self-consistent system of equations for the mass operator (27), it is necessary to use an approximation in order to express it in terms of the Green's function (9). The mass operator (27) describes inelastic scattering of electrons (the elastic part is contained in $\Sigma_{i\sigma}^{a}$ (16)) on fluctuations of the density of the total electron–ion charge in the lattice. By analogy with [17] (see also [19,21]), we find an analytic expression for the mass operator in the approximation of "two interacting modes." This approximation consists of ignoring the renormalization of the vertex, i.e., the correlation in the propagation of the distinguished electron (hole) and the propagation of charge density fluctuations. To this approximation there corresponds the following representation in (27) of the higher correlation functions in terms of the lower:

$$\langle\rho_{j'i'\uparrow}(t)a_{j'\uparrow}^{+}(t)a_{j\uparrow}\rho_{ij\uparrow}\rangle^{p,1r}\approx\langle\rho_{j'i'\uparrow}(t)\rho_{ij\uparrow}\rangle\langle a_{j'\uparrow}^{+}(t)a_{j\uparrow}\rangle. \tag{28}$$

We note that the one-time mean values are already taken into account in the mass operator $\Sigma_{i\sigma}^{a}$ (16).

Writing down further spectral representations for the correlation functions in (28), we represent the mass operator (27) with allowance for the definition (15) in the form of the sum

$$M_{ii'}(\omega)=M_{ii'}^{1}(\omega)+M_{ii'}^{2}(\omega), \tag{29}$$

where

$$M_{ii'}^{1}=\sum_{nn'}\sum_{jj'}V_{ijn}V_{j'i'n'}\int\!\!\int_{-\infty}^{\infty}\frac{d\omega_1\,d\omega_2}{\omega-(\omega_1+\omega_2)}\frac{1}{2}\left(\operatorname{th}\frac{\beta\omega_1}{2}+\operatorname{cth}\frac{\beta\omega_2}{2}\right)\times$$

$$\left[-\frac{1}{\pi}\operatorname{Im}\langle\!\langle u_n|u_{n'}\rangle\!\rangle_{\omega_2+i\varepsilon}\right]\left(-\frac{1}{\pi}\right)\tau_3\operatorname{Im}\langle\!\langle\psi_j|\psi_{j'}^{+}\rangle\!\rangle_{\omega_1+i\varepsilon}\tau_3. \tag{30}$$

The mass operator (30) has a form characteristic of an interacting electron–phonon system [18,19,21]. The contribution $M_{ii'}^{2}$ has a more complicated structure:

$$M_{ii'}^{2}=U^2\int\!\!\int_{-\infty}^{\infty}\frac{d\omega_1\,d\omega_2}{\omega-(\omega_1+\omega_2)}\frac{1}{2}\left(\operatorname{th}\frac{\beta\omega_1}{2}+\operatorname{cth}\frac{\beta\omega_2}{2}\right)\begin{bmatrix}A & B\\ C & D\end{bmatrix}, \tag{31}$$

where

$$A=\left[-\frac{1}{\pi}\operatorname{Im}\langle\!\langle n_{i\downarrow}|n_{i'\downarrow}\rangle\!\rangle_{\omega_2}\right]\left[-\frac{1}{\pi}\operatorname{Im}\langle\!\langle a_{i\uparrow}|a_{i'\uparrow}^{+}\rangle\!\rangle_{\omega_1}\right];\quad B=\left[\frac{1}{\pi}\operatorname{Im}\langle\!\langle n_{i\downarrow}|n_{i'\uparrow}\rangle\!\rangle_{\omega_2}\right]\left[-\frac{1}{\pi}\operatorname{Im}\langle\!\langle a_{i\uparrow}|a_{i'\downarrow}\rangle\!\rangle_{\omega_1}\right];$$

$$C=\left[\frac{1}{\pi}\operatorname{Im}\langle\!\langle n_{i\uparrow}|n_{i'\downarrow}\rangle\!\rangle_{\omega_2}\right]\left[-\frac{1}{\pi}\operatorname{Im}\langle\!\langle a_{i\downarrow}|a_{i'\uparrow}^{+}\rangle\!\rangle_{\omega_1}\right];\quad D=\left[-\frac{1}{\pi}\operatorname{Im}\langle\!\langle n_{i\uparrow}|n_{i'\uparrow}\rangle\!\rangle_{\omega_2}\right]\left[-\frac{1}{\pi}\operatorname{Im}\langle\!\langle a_{i\downarrow}|a_{i'\downarrow}\rangle\!\rangle_{\omega_1}\right].$$

It can be seen from Eqs. (30) and (31) that, in contrast to the electron–ion model of a simple metal with allowance for the direct Coulomb interaction of the electrons [17], the effective electron–electron interaction determined in (31) by the Green's function of the charge density fluctuations, cannot be expressed in simple approximations in terms of the total permittivity of the electron–ion system for the Hubbard model.

This is a reflection of one of the shortcomings of the Hubbard model – the neglect of the exchange interaction at different sites. The permittivity for the Hubbard model can be formally expressed for k, $\omega \neq 0$ in terms of the longitudinal dynamic conductivity [22]. However, for k, $\omega \to 0$ the resulting expression for the permittivity is not defined. In the polar model of a metal [10], the electron system is described in a more consistent manner. Therefore, the derivation of the equations of superconductivity for the polar model of a metal (with allowance for the electron–phonon interaction) is of particular interest.

The well-known difficulties associated with calculating the frequency dependence of the correlation function $\langle n_{i\sigma}(t) n_{j\sigma'} \rangle$ for the Hubbard model are associated with this circumstance. Essentially, these difficulties are analogous to those that arise in the calculation of the correlation function $\langle S_i^z(t) S_j^z \rangle$ in an isotropic Heisenberg ferromagnet [23, 24]. When the Green's function $\langle\langle S_i^+ | S_j^- \rangle\rangle$ is calculated, the Green's function $\langle\langle \delta S^z S^+ | \delta S^z S^- \rangle\rangle$ (where $\delta S^z = S^z - \langle S^z \rangle$) arises. When $\langle \delta S_i^z(t) \delta S_j^z \rangle \langle\langle S^+ | S^- \rangle\rangle$ is decoupled, the static approximation [24, 25] is usually employed for the correlation function $\langle \delta S_i^z \delta S_j^z \rangle$. An approximate method for calculating the correlation function $\langle n_{i\sigma} n_{j\sigma'} \rangle$ in the static limit is discussed, for example, in [26]. The system of equations (26) and (29) obtained for strongly coupled electrons in a transition metal can be analyzed further by the well-known methods (see, for example, [27, 28]).

In conclusion, we note that for strongly bound electrons of a transition metal the operator of the electron–phonon interaction can be expressed in terms of a small number of characteristic parameters of the transition metal [3, 19, 21]:

$$\frac{\partial t(\mathbf{R}_i - \mathbf{R}_j)}{\partial (\mathbf{R}_i - \mathbf{R}_j)} = q_0 t_{ij} \frac{\mathbf{R}_i - \mathbf{R}_j}{|\mathbf{R}_i - \mathbf{R}_j|}.$$

Here, q_0 is the Slater coefficient that characterizes the exponential decrease of the d functions [3]. The hopping integral t_{ij} for the z nearest neighbors can be expressed in terms of the band width W = 2tz. Thus, the self-consistent system of superconductivity equations (26) and (29) obtained in the present paper in the Wannier representation makes it possible to investigate real transition metals, their alloys, and compounds from a unified point of view.

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INFLUENCE OF s–d HYBRIDIZATION ON THE ELECTRICAL CONDUCTIVITY OF LIQUID TRANSITION METALS

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Retarded Green's functions are used to develop a theory of the electrical conductivity of liquid transition metals with systematic allowance for the hybridization of the s and d states of the conduction electrons. It is shown that the conductivity can be represented as a sum of three terms, one of which is due to the scattering of s electrons by ions, including resonance scattering by d states, the second is due to tunneling of d electrons through d states, and the third is due to transitions of almost localized d electrons to delocalized s states and reverse transitions from s to d states. Expressions for each of the contributions are obtained in the framework of perturbation theory with respect to the pseudopotential of the electron–ion interaction, the hybridization potential, and the resonance integral.

1. Introduction

In recent years, there has been an appreciable increase in the interest shown toward study of transport phenomena in disordered systems. Among the most important systems of this type are liquid transition metals, which occupy an intermediate position between simple liquid metals, whose properties can be well described in the approximation of almost free electrons, and amorphous semiconductors, for which the tight-binding approximation is more adequate. In transition metals, there are not only almost free s electrons but also almost bound d electrons. The approaches – based on a modified Ziman formula [1,2] – used at the present time to interpret the experimental data on the static conductivity take into account the contribution to the conductivity due solely to the s electrons. The role of the d states is reduced merely to resonance scattering of the s electrons by them. In the case of [1], the modification consists of replacing the pseudopotential of the electron–ion interaction by the single-particle t matrix; in the case of [2], it consists of replacing it by the potential of the s–d hybridization. Such an approach does not enable one to describe even qualitatively many properties of these metals, in particular, their electrical conductivity in the optical frequency range and the Hall effect. Moreover, it has not yet been established to what extent the approach is applicable even for the description of the static conductivity of liquid transition metals. It is therefore necessary to take into account more systematically all the effects associated with the presence of the d electrons.

In the present paper, the electrical conductivity of liquid transition metals will be obtained in the framework of a model that takes into account explicitly the presence of the d electrons and the hybridization of the s and d states.

2. Formulation of the Problem

Apart from the electron–electron interaction of the s electrons, which makes an appreciable contribution to the resistivity of both simple and transition metals only at very low temperatures [3,4], it is necessary to take into account in transition metals the electron–electron interaction of the d electrons and the s and d electrons. If we proceed from a model of d electrons localized at atoms, the interaction of the

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