RESEARCH ARTICLES

J. Sci. Soc. Thailand, **2** (1976), 103-116

s-ELECTRON CURRENTS IN d-BAND SUPERCONDUCTORS*

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(Received 23 July 1976)

Summary

Using the Anderson Hamiltonian with an additional term for the electron-phonon coupling between the d-electrons to describe the d-band superconductors, the s-electron current density is calculated by the Green's function method. It is shown that the s-electron current density is proportional to a vector potential and is therefore part of the supercurrent.

I. Introduction

The band structures of the transition-metals (TM) are characterized by the appearance of a broad s-band and a narrow d-band.[1] At the Fermi energy, the density of states of the d-band is much greater than that of the s-band. The s-band is composed of free electrons which are described by plane wave functions while the d-band is composed of electrons which are localized about the lattice sites and which are therefore best described by Wannier functions or d-electron orbitals. Because the s-electrons are free to move through the metal while the d-electrons are not, most models[2] for the electrical conduction in the transition-metals have the s-electrons as the carriers of the current. Webb[3] has measured the low temperature behavior of the resistivity of a very pure niobium wire and has seen temperatures behaviors which are consistent with Mott's two band model for electrical conduction in the transition metals. In Mott's model, the electric current is carried mainly by the s-electrons. The main role of the d-band is that of providing a sea into which the

* Based in parts on a Master degree thesis submitted by Montree Yamvong in partial fulfilment of the requirements for the Degree of Master of Science (Physics) in the Faculty of Graduate Studies of Chulalongkorn University.

s-electrons can be scatterred. The existence of this type of scattering process leads to a T^3 temperature dependence in the resistivity which was seen by Webb.

It is generally accepted that the mechanism most likely responsible for superconductivity is the electron phonon interaction between pairs of electrons having opposite spins.[4] Therefore, the mechanism for superconductivity in the pure transition-metals should be the electron-phonon interaction between d-electron pairs since they are localized about the nuclei located on the lattice sites and would therefore be affected by the motion of the nuclei more than the freely moving s-electrons. Theories[5] based on this assumption have been worked out and appear to be able to explain many of the observed thermodynamical properties of the pure TM superconductors. In these d-band theories of superconductivity, the electric current and the other transport currents are carried by the BCS pairs formed by the d-electrons when the transition metals go into the superconducting phase. One would therefore expect that the transport currents would show an abrupt change at the critical temperature T_c since the s-electrons are the carriers when the transition metals are in the normal phase, while the d-electrons are the carriers when the transition metals are in the superconducting phase. However, the observed behavior of the transport currents[6] show the changes to be continuous at T_c. This points to the likelihood that the same set of electrons are the transport carriers in both the normal and superconducting phases.

The purpose of this paper is to show that in the transition-metals having some overlap of the s-and d-band (most of the transition-metals fall into this category), the electric current composed of s-electrons goes into the supercurrent state even though the mechanism for superconductivity in the pure transition metals is the BCS electron phonon interaction between d-electrons. We shall show that the quantum mechanical expression for the s-band electrical current density leads to a current density proportional to a vector potential $\vec{A}$ when the d-electrons start to form BCS pairs. We will then show that a current density which is proportional to the vector potential is a supercurrent, i.e. a current which exist even when there is no applied voltage across the metal.

II. Green's Functions

The double-time retarded temperature dependent Green's function is defined as[7]

$$\ll A(t)j\ B(t')\gg\ =\ -i\ \theta(t-t')\ \langle\{A(t),\ B(t')\}\rangle \tag{II.1}$$

where the operators A(t) and B(t') are products of creation and destruction operators of Fermion particles or fields in the generalized Heisenberg representation; $\theta(t-t')$ is the Heaviside step function; $\langle\ldots\ldots\rangle$ denotes a grand canonical ensemble average and $\{\ldots\ldots\}$ indicates an anti-commutation of the two operators. Since the time derivative of the step function is a delta function, we find that the derivative with respect to the time t of the above function leads to the differential equation

$$i\frac{d}{dt} \ll A(t); B(t') \gg = \delta(t-t') \langle \{A(t), B(t')\} \rangle + \ll [A(t), H]; B(t') \gg \tag{II.2}$$

where the commutation between the operator A (t) and the Hamiltonian of the system of particles arises because

$$i\frac{d\ A(t)}{dt} = [A(t), H] \tag{II.3}$$

in the Heisenberg representation. The reason for calling (II.1) a Green's function is that eq. (II.2) is called the "Green's differential equation".

If we now introduce the Fourier transform of the Green's function and

$$\ll A; B \gg_\omega = \frac{1}{2\pi} \int_{-\infty}^{\infty} \ll A(t); B(t') \gg e^{i\omega(t-t')}\, d(t-t') \tag{II.4}$$

substitute it into Green's differential equation, we obtain the algebraic equation

$$\omega \ll A; B \gg_\omega = \frac{1}{2\pi} \langle \{A, B\} \rangle + \ll [A, H]; B \gg_\omega . \tag{II.5}$$

In general, the commutation of the operator A (t) with the Hamiltonian will produce a new operator C (t) which will be a polynomial in the creation and destruction operators of a higher order than the operator A (t). Therefore, the equation for the Green's function $\ll A; B \gg_\omega$ requires that a second Green's function $\ll C; B \gg_\omega$ be known. However, the equation defining this second Green's function requires that a third function be known; the third function requires a fourth to be known and so on. Thus a hierarchy of coupled equations connecting the Green's functions of higher order is obtained.

In order that a "closed form" Green's function be obtainable, one usually introduces at some point an approximation which will trunicate the hierarchy of equations. To trunicate the hierarchy of equations arising in our study, we have used the Hartree Fock approximation.[8]

$$A^+B^+CD = \langle A^+B^+ \rangle CD + \langle CD \rangle A^+B^+ - \langle A^+C \rangle B^+D - \langle B^+D \rangle A^+C \tag{II.6}$$

The above approximation is used to treat both the BCS term and the coulomb repulsion term appearing in the Hamiltonian used in this study. The Hartree Fock treatment of the BCS term leads[8] to the same results as those obtained in the original theory of superconductivity of BCS.[4] The Hartree Fock treatment of the coulomb term has been shown[9] to be equivalent to the neglect of correlations between electrons of opposite spins. The approximation has also been used to treat both terms simultaneously[10] in the study of transition metal impurities in simple superconductors.

III. Transition Metal Hamiltonian

As was mentioned in the Introduction, there are two or more groups of electrons (i.e., s, d and f electrons) present in the transition metals. One of these groups, the s-electrons, behave like free electrons while the others are localized about the nuclei located at the lattice sites. Anderson has introduced a model Hamiltonian,[11] which takes into account the presence of both free electron states and localized states. Included in his Hamiltonian are terms for the hybridization of the conduction electrons with localized d electrons and for the coulomb interaction between electrons of opposite spins occupying the localized orbital state. While the model proposed by Anderson was intended for the study of the occurrence of a localized magnetic moments on iron-group atoms which are dissolved as dilute impurities in nonmagnetic metal, it contains the essential features of the narrow d-band transition metals.

In its simplest form, the Anderson model is described by the Hamiltonian

$$H = \sum_{k,\sigma} \varepsilon_k C_{k\sigma}^{+} C_{k\sigma} + \sum_{j,\sigma} E_j d_{j\sigma}^{+} d_{j\sigma} + \sum_{j,k,\sigma} V_{kj} C_{k\sigma}^{+} d_{j\sigma}$$

$$+ \sum_{j,k,\sigma} V_{jk}^{+} d_{j\sigma}^{+} C_{k\sigma} + \tfrac{1}{2} U \sum_{j,\sigma} d_{j\sigma}^{+} d_{j\sigma} d_{j-\sigma}^{+} d_{j-\sigma} \tag{III.1}$$

where σ labels the spin orientation; $c_{k\sigma}^{+}$ and $c_{k\sigma}$ are the creation and destruction operators for a s-electrons of momentum k, respectively, and ε_k is its energy; $d_{j\sigma}^{+}$ and $d_{j\sigma}$ are the creation and destruction operators for a d-orbital electron or Wannier function, respectively, and E_j is its energy. The last three terms are the hybridization terms and the coulomb repulsion term. If we now carry out the Hartree Fock approximation (II.6), we get

$$H = \sum_{k,\sigma} \varepsilon_k C_{k\sigma}^{+} C_{k\sigma} + \sum_{j,\sigma} (E_j + U \langle n_{\sigma} \rangle) d_{j\sigma}^{+} d_{j\sigma}$$

$$+ \sum_{j,k,\sigma} (V_{kj} C_{k\sigma}^{+} d_{j\sigma} + V_{jk}^{*} d_{j\sigma}^{+} C_{k\sigma}) - \tfrac{1}{2} \Delta_d \sum_{j} d_{j\sigma}^{+} d_{j\sigma}^{+}$$

$$- \tfrac{1}{2} \Delta_d^{*} \sum_{j} d_{j-\sigma} d_{j\sigma} \tag{III.2}$$

where

$$\Delta_d = - U \langle d_{j-\sigma} d_{j\sigma} \rangle \tag{III.3}$$

is the fluctuation due to the coulomb repulsion. As was mentioned in the Section II, the Hartree Fock approximation leads to an overestimate of the effect of the Coulomb correlation energy, U, on the production of a localized magnetic moment. Since the occurrence of a localized magnetic moment precludes the possiblility of

superconductivity and since we are only interested in those transition metals which can go superconducting, the criterion for the occurrence of the localized magnetic moment will not be met in the transition metals we are interested and therefore should not be of any concern to this study.

Most of the recent theories of superconductivity in the transition metals[5, 12] assume that superconductivity in these metals arises from the virtual exchange of phonons between the d-electrons. Appel and Kohn[5] have shown that the vertex function constructed with Wannier function representation of the d-orbital electrons exhibit the singularities which indicate an instability against the formation of Cooper pairs.[13] Bennermann and Garland[12] have shown that the electron-phonon matrix element between localized d-orbitals leads to an expression for the critical temperature which allows for the variation in T_c seen in three transition metal series. They have also shown that the McMillan equation,[14] which is based on the virtual exchange of the phonons between the d-electrons, can explain the pressure dependence of the transition temperatures seen in the transition metal superconductors. With the above in mind, we add to the Anderson Hamiltonian, the term

$$- \tfrac{1}{2} g \sum_{j,m,\sigma} d_{j\sigma}^{+} d_{j-\sigma}^{+} d_{m-\sigma} d_{m\sigma} \qquad \text{(III.4)}$$

where g is the strength of the electron-phonon interaction between d-orbitals located on the j-th and m-th site and is taken to be the electron-phonon coupling constant in McMillan's work. We have called (III.4) H_{BCS} since it is similar to the term in the BCS theory which leads to the formation of Cooper pairs in simple metal superconductors.

Applying the Hartree Fock approximation to eq. (III.4), we obtain the following Hamiltonian.

$$\begin{aligned} H = & \sum_{k,\sigma} \varepsilon_k C_{k\sigma}^{+} C_{k\sigma} + \sum_{j,\sigma} (E_j + V\langle n_\sigma \rangle) d_{j\sigma}^{+} d_{j\sigma} \\ & + \sum_{j,k,\sigma} (V_{kj} C_{k\sigma}^{+} d_{j\sigma} + V_{jk}^{*} d_{j\sigma}^{+} C_{k\sigma}) \\ & - \tfrac{1}{2} \sum_{j,\sigma} (\Delta_g^{*} d_{j-\sigma} d_{j\sigma} + \Delta_g d_{j\sigma}^{+} d_{j-\sigma}^{+}) \end{aligned} \qquad \text{(III.5)}$$

where

$$\Delta_g = g \sum_{j\sigma} \langle d_{j-\sigma} d_{j\sigma} \rangle + \Delta_d \qquad \text{(III.6)}$$

For the reasons we have mentioned previously, the above Hamiltonian (III.5) should be a fairly good description of the superconducting phase of the transition metals.

IV. Self-Consistent Solutions.

To obtain the Green's functions or propagators for the s-electrons, the commutations of the four operators $c_{k\sigma}^{+}$, $c_{k\sigma}$, $d_{j\sigma}^{+}$ and $d_{j\sigma}$ with the Hamiltonian must be evaluated. Using the relationship

$$[A, BC] = \{A, B\}C - B\{A, C\} \tag{IV.1}$$

where [ ] denotes the commutation and { }, the anticommutation, we obtain

$$[C_{k\sigma}^{+}, H] = -\varepsilon_k C_{k\sigma}^{+} - \sum_j V_{kj}^{*} d_{j\sigma}^{+}, \tag{IV.2a}$$

$$[C_{k\sigma}, H] = \varepsilon_k C_{k\sigma} + \sum_j V_{jk} d_{j\sigma}, \tag{IV.2b}$$

$$[d_{j\sigma}, H] = (E_j + U\langle n_{\sigma}\rangle) d_{j\sigma} - \Delta_g d_{j-\sigma}^{+} + \sum_l V_{lj}^{*} C_{l\sigma}, \tag{IV.2c}$$

and

$$[d_{j-\sigma}^{+}, H] = -(E_j + U\langle n_{\sigma}\rangle) d_{j-\sigma}^{+} - \Delta_g^{*} d_{j\sigma} - \sum_l V_{jl} C_{l-\sigma}^{+} \tag{IV.2d}$$

where $\Delta_g = \Delta_o + \Delta_d$. Substituting the commutation relations (IV.2a) and (IV.2b) into the algebraic equations (II.5) for the Green's function $\hat{G}(k, k')$, we get

$$\hat{G}(k, k') = \tfrac{1}{2\pi} \hat{G}_o(k) S_{kk'} + \sum_j \hat{G}_o(k) \hat{V}(k, j) \hat{M}(j, k') \tag{IV.3}$$

where the matrices $\hat{G}(k, k')$, $\hat{G}_o(k)$, $\hat{V}(k, j)$ and $\hat{M}(j, k)$ are defined as

$$\hat{G}(k, k') = \begin{pmatrix} \ll C_{k\sigma};\ C_{k'\sigma}^{+} \gg & \ll C_{k\sigma};\ C_{-k'-\sigma} \gg \\ \ll C_{-k-\sigma}^{+};\ C_{k'\sigma}^{+} \gg & \ll C_{-k-\sigma}^{+};\ C_{-k'-\sigma} \gg \end{pmatrix} \tag{IV.4}$$

$$\hat{G}_o(k, k') = \begin{pmatrix} \omega - \varepsilon_k & 0 \\ 0 & \varepsilon + \omega_k \end{pmatrix} \tag{IV.5}$$

$$\hat{V}(kj) = \begin{pmatrix} V_{jk} & 0 \\ 0 & -V_{-kj}^{*} \end{pmatrix} \tag{IV.6}$$

and

$$\hat{M}(j, k) = \begin{pmatrix} \ll d_{j\sigma};\ C_{k\sigma}^{+} \gg & \ll d_{j\sigma};\ C_{-k-\sigma} \gg \\ \ll d_{j-\sigma}^{+};\ C_{k\sigma}^{+} \gg & \ll d_{j-\sigma}^{+};\ C_{-k-\sigma} \gg \end{pmatrix}. \tag{IV.7}$$

The matrix Green's function M(j, k) is obtained by substituting the commutation relations (IV.2c) and (IV.2d) into the algebraic equation (II.5) for M(j, k). The results of these substitutions is the new matrix equation

$$[\hat{M}_o(j)]^{-1}\ \hat{M}(j, k) = \sum V^{+}(j, l)\ \hat{G}(l, k) \tag{IV.8}$$

where

$$[\hat{M}_o(j)]^{-1} = \begin{pmatrix} \omega - E_j - U\langle n_\sigma \rangle & \Delta_g \\ \Delta_g^{*} & \omega + E_j + U\langle n_\sigma \rangle \end{pmatrix} \tag{IV.9}$$

where $\hat{V}^{+}(l, j)$ is the complex conjugate of the matrix (IV.6). Substituting the matrix equation (IV.3) into the matrix equation (IV.8) we obtain

$$[\hat{M}_o(j)]^{-1}\ \hat{M}(j, k) = \tfrac{1}{2\pi}\ \hat{V}^{+}(j, k)\ \hat{G}_o(k) + \sum_{j'l} \left|\hat{V}_{lj'}\right|^2\ \hat{G}_o(l)\ \hat{M}(j, k). \tag{IV.10}$$

To obtain the above, we have used the fact that V(l, j) and $G_o(l)$ commute with each other since they are both diagonal matrices. Substituting the matrix equation (IV.10) into the equation (IV.3), we get

$$\begin{aligned} \hat{G}(k, k') &= \tfrac{1}{2\pi}\ \hat{G}_o(k)\ S_{kk'} + \sum_{j} \hat{G}_o(k)\ \hat{V}(kj) \tfrac{1}{2\pi}\ \hat{M}_o'\ \hat{V}^{+}(k'j)\ \hat{G}_o(k') \\ &+ \sum \hat{G}_o(k)\ \hat{V}(kj) \tfrac{1}{2\pi}\ \hat{M}_o'(j) \sum_{j'j} \sum_{l} \left|\hat{V}_{lj'}\right|^2\ \hat{G}_o(l)\ \hat{M}_o'(j')\ \hat{V}^{+}(k', j')\ \hat{G}_o(k') \\ &+ \text{higher order terms} \end{aligned} \tag{IV.11}$$

where

$$[\hat{M}_o'(j)]^{-1} = [\hat{M}_o(j)]^{-1} - \sum_{l} \left|V(l, j)\right|^2\ \hat{G}_o(l). \tag{IV.12}$$

The matrix equation (IV.11) can be rewritten in the form of a Dyson equation

$$[\hat{G}(k, k')]^{-1} = [\hat{G}_o(k)]^{-1} - \mathcal{T}(k, k') \tag{IV.13}$$

where $\mathcal{T}(k, k')$ is the energy correction

$$\mathcal{T}(k, k') = \tfrac{1}{2\pi} \sum_j \hat{V}(kj)\, \hat{M}_o'(j)\, \hat{V}^+(j, k). \tag{IV.14}$$

Letting M_{11}, M_{12}, M_{21} and M_{22} be the elements of $\hat{M}_o'(j)$, i.e.,

$$\hat{M}_o'(j) = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}, \tag{IV.15}$$

the energy correction matrix is

$$\mathcal{T}(k, k') = \tfrac{1}{2\pi} \sum_j \begin{pmatrix} |V_{kj}|^2 M_{11} & - V_{kj} V^*_{j-k} M_{12} \\ - V_{kj} V_{j-k} M_{21} & |V_{-kj}|^2 M_{22} \end{pmatrix}. \tag{IV.16}$$

Substituting (IV.16) into (IV.13), we find that the inverse of the matrix Green's function $\hat{G}(k, k')$ is

$$[\hat{G}(k, k)]^{-1} = \begin{pmatrix} \omega - \varepsilon_k - \tfrac{1}{2\pi} \sum_j |V_{kj}|^2 M_{11} & \tfrac{1}{2\pi} \sum_j |V_{kj}|^2 M_{12} \\ \tfrac{1}{2\pi} \sum_j |V_{kj}| M_{21} & \omega + \varepsilon_k - \tfrac{1}{2\pi} \sum_j |V_{kj}|^2 M_{22} \end{pmatrix} \tag{IV.17}$$

where we have assumed $\hat{V}_{kj} = \hat{V}^*_{-k,\, j}$. Inverting (IV.17), we get

$$\hat{G}(k, k) = \frac{1}{\mathrm{Det}\ \hat{G}^{-1}} \begin{pmatrix} \omega + \varepsilon_k - \tfrac{1}{2\pi} \sum_j |V_{kj}|^2 M_{22} & - \tfrac{1}{2\pi} \sum_j |V_{kj}|^2 M_{21} \\ - \tfrac{1}{2\pi} \sum_j |V_{kj}|^2 M_{12} & \omega - \pi_k - \tfrac{1}{2\pi} \sum_j |V_{kj}|^2 M_{11} \end{pmatrix} \tag{IV.18}$$

where

$$\det \hat{G}^{-1} = (\omega - \varepsilon_k - \tfrac{1}{2\pi} \sum_j |V_{kj}|^2 M_{11})\ (\omega + \varepsilon_k - \tfrac{1}{2\pi} \sum_j |V_{kj}|^2 M_{22}) - \tfrac{1}{4\pi^2} \sum_{jj'} |V_{kj}|^2\, |V_{kj'}|^2\, M_{21}\, M_{12}. \tag{IV.19}$$

Since

$$[M_o'(j)]^{-1} = \begin{pmatrix} \omega - E_j - U\langle n_\sigma \rangle - \sum_j \frac{|V_{ij}|^2}{\omega - \varepsilon_i} & \Delta_g \\ \Delta_g^* & \omega + E_j + U\langle n_\sigma \rangle - \sum_j \frac{|V_{ij}|^2}{\omega + \varepsilon_i} \end{pmatrix} \tag{IV.20}$$

we find that

$$M_{11} = \frac{\omega + E_j + U\langle n_\sigma\rangle - \sum_{\bar{l}} \frac{|V_{lj}|^2}{\omega+\varepsilon}}{\det\,[\hat{M}_o']^{-1}} \tag{IV.21a}$$

$$M_{21} = \frac{-\Delta_g^*}{\det\,[\hat{M}_o']^{-1}} \tag{IV.21b}$$

$$M_{21} = \frac{-\Delta_g}{\det\,[\hat{M}_o']^{-1}} \tag{IV.21c}$$

and

$$M_{22} = \frac{\omega - E_j - U\langle n_\sigma\rangle - \sum_{\bar{l}} \frac{|V_{lj}|^2}{\omega+\varepsilon}}{\det\,[\hat{M}_o']^{-1}} \tag{IV.21d}$$

where

$$\det\,[\hat{M}_o'^{-1}]^{-1} = \left(\omega + E_j + U\langle n_\sigma\rangle - \sum_{\bar{l}} \frac{|V_{lj}|^2}{\omega-\varepsilon}\right) \left(\omega - E_j - U\langle n_\sigma\rangle - \sum_{\bar{l}} \frac{|V_{lj}|^2}{\omega-\varepsilon}\right) - |\Delta_g|^2. \tag{IV.22}$$

By assuming that V_{jl} is a constant and by replacing the summation over $\bar{l}$ by an integration over d^3l, the above eqns. (IV.21a) to (IV.21d) become

$$M_{11} = \frac{\omega + B}{\omega^2 - B^2 - \Delta_g^2} \tag{IV.23a}$$

$$M_{12} = \frac{-\Delta_g^*}{\omega^2 - B^2 - \Delta_g^2} \tag{IV.23b}$$

$$M_{21} = \frac{-\Delta_g}{\omega^2 - B^2 - \Delta_g^2} \tag{IV.23c}$$

$$M_{22} = \frac{\omega - B}{\omega^2 - B^2 - \Delta_g^2} \tag{IV.23d}$$

where

$$B = E_j + U\langle n_\sigma\rangle + \frac{2mP_F\,V^2}{(2\pi)^3} \text{ in } \frac{\omega - \omega_D}{\omega + \omega_D} \tag{IV.24}$$

Because the integral diverges, a cutoff at the Debye frequency has been introduced.

V. Response Kernel

Starting with the quantum mechanical expression for the current density operator in the second quantized representation

$$\vec{j}(x) = \frac{ie}{2m}\left[\nabla_{x'} - \nabla_x\right]_{x\to x'} \psi^+(x')\ \psi(x) - \frac{C^2\ \vec{A}(x)}{m}\ \psi^+(x)\ \psi(x) \tag{V.1}$$

where $\psi+(x)$ and $\psi(x)$ are the particle field operators for the s-electrons, it can be easily shown that the above expression leads to the following expression for the fourier transformed current density

$$\vec{j}(k) = -\frac{2c^2\ T}{(2\pi)^3\ m^2}\sum_{\omega}\int d^3p\ \vec{p}[\vec{p}\ \vec{A}(k)]\left\{\eta_\omega(\vec{p}_+)\eta_\omega(\vec{p}_-) + \Im_\omega(\vec{p}_+)\Im_\omega(\vec{p}_-)\right\} - \frac{Nc^2}{m}A(k) \tag{V.2}$$

where $\vec{p}_+ = \vec{p} \pm \frac{1}{2}\vec{k}$ and $\eta_\omega(p)$ and $\Im_\omega(p)$ are the continuations of the Green's functions $\ll C_{p\sigma};\ C^{+}_{p\sigma}\gg_\omega$ and $\ll C_{p\sigma};\ C_{-p-\sigma}\gg_\omega$, respectively, into the complex ω plane. Procceeding in a manner similar to that of section 37.1 of reference 8, we find that for our model, the response kernel for the s-electron current density is given by

$$Q(k) = \frac{3T}{4}\sum_{\omega}\int_0^{\pi}\sin^3\theta\ d\theta\int_{-\infty}^{\infty}d\varepsilon\ \frac{N^2V^4\ \Delta_g^2\ g^{-2}(i\omega)}{[\mathrm{Det}\ G]_+\ [\mathrm{Det}\ G]_-} \tag{V.3}$$

where

$$[\mathrm{Det}\ G]_\pm = (i\omega - \varepsilon_\pm - \frac{V^2}{2\pi}\sum_j M_{11})\ (i\omega + \varepsilon_\pm - \frac{V^2}{2\pi}\sum_j M_{22}) - N^2V^1\ \Delta_g^2\ g^{-2}(i\omega) \tag{V.4}$$

with

$$\varepsilon_\pm = \varepsilon_k \pm \tfrac{1}{2}\ \vec{v}\text{–}\vec{k}$$
$$g(i\omega) = -(\omega^2 + B^2 + \Delta_g^2). \tag{V.5}$$

The integrand of eqn. (V.3) has four singularities in the complex plane. They are located at

$$\varepsilon_1 = \frac{NV^2\ B}{2\pi\ (\omega^2 + B^2 + \Delta_g^2)} - \tfrac{1}{2}\ vk\beta + i\sqrt{\omega^2 + |\Delta'|^2 + C^2} \tag{V.6a}$$

$$\varepsilon_2 = \frac{NV^2\ B}{2\pi\ (\omega^2 + B^2 + \Delta_g^2)} - \tfrac{1}{2}\ vk\beta + i\sqrt{\omega^2 + |\Delta'|^2 + C^2} \tag{V.6b}$$

$$\varepsilon_3 = \frac{NV^2\ B}{2\pi\ (\omega^2 + B^2 + \Delta_g^2)} + \tfrac{1}{2}\ vk\beta + i\sqrt{\omega^2 + |\Delta'|^2 + C^2} \tag{V.6c}$$

and

$$\varepsilon_4 = \frac{NV^2\, B}{2\pi\,(\omega^2 + B^2 + \Delta_g^2)} + \tfrac{1}{2}\, vk\beta - i\sqrt{\omega^2 + |\Delta'|^2 + C^2} \tag{V.6d}$$

where

$$|\Delta'|^2 = \frac{N^2\, V^2\, \Delta_g^2}{\omega^2 + B^2 + \Delta_g^2} \tag{V.7}$$

$$C^2 = -\left\{\frac{NV^2\,\omega^2}{\pi\,(\omega^2 + B^2 + \Delta_g^2)} - \frac{N^2\, V^4}{4\pi^2\,(\omega^2 + B^2 + \Delta_g^2)^2}\right\} \tag{V.8}$$

and where β is the cosine of the angle between k and v. The singularities, ε_1 and ε_3, lie in the upper half of the complex ε plane, while the singularities, ε_2 and ε_4, lie in the lower half plane. Converting the ε integration from $-\infty$ to $+\infty$ into a line integration over a closed contour enclosing the upper half plane, we get

$$Q(k) = \tfrac{3\pi}{8}\, T \sum_{\omega} \int_0^{\pi} \sin^3\theta\, d\theta\, \frac{N^2V^4\, \Delta_g^2\, g^{-2}(i\omega)}{\sqrt{\omega^2 + |\Delta'|^2 + C^2}\left(\frac{v^2k^2\beta^2}{4} + \omega^2 + |\Delta'|^2 + C^2\right)}. \tag{V.9}$$

Since most of the transition metal superconductors are type-II or London superconductors, the integration over the angle θ gives

$$Q(k) = \tfrac{\pi}{2}\, T \sum_{\omega} \int_0^{\pi} \sin^3\theta\, d\theta\, \frac{N^2V^4\, \Delta_g^2}{(\omega^2 + B^2 + \Delta_g^2)^2\,(\omega^2 + |\Delta'|^2 + C^{3/2}}. \tag{V.10}$$

In order that the summation may be done, we shall assume that $B^2 \geqslant \frac{\sqrt{2}-1}{2}\,\frac{NV^2}{\pi}$. With this assumption, we may neglect the C^2 term appearing in the denominator of (V.10). Close to the critical temperature, the Δ_g^2 and $|\Delta'|^2$ terms appearing in the denominator may also be neglected. Therefore, close to T_c, the response kernel is

$$Q(k) = \tfrac{\pi}{2}\, N^2V^2\, \Delta_g^2 T \sum_{\omega} \frac{1}{(\omega^2 + B^2)^2\, \omega^3} \tag{V.11}$$

If we assume that B^2 is very small, the summation over $\omega = (2n + 1)\pi T$ gives

$$Q(k) = \tfrac{\pi}{2}\left(\frac{NV^2}{T^2}\right)^2 \left(\frac{\Delta_g}{T}\right)^2 \zeta\,(7) \tag{V.12}$$

where $\zeta(\ )$ is the Riemann Zeta function. However, if we assume that B^2 is large, the summation over ω gives

$$Q(k) = \frac{\pi}{2}\left(\frac{NV^2}{B^2}\right)^2\left(\frac{\Delta_g}{T}\right)^2 \frac{7}{8}\,\zeta(3). \tag{V.13}$$

In both cases, the response kernel is independent of $\vec{k}$. Therefore, if we take the fourier inverse of

$$\vec{j}(k) = Q(k)\,\vec{A}(k), \tag{V.14}$$

we get

$$\vec{j}(r) = \text{Constant}\ \vec{A}(r) \tag{V.15}$$

where the constant is (V.12) if B^2 is small and is (V.13) if B^2 is large.

VI. Supercurrent

In Section V., we showed that the s-electron current density in a d-band superconductor is proportional to a vector potential $\vec{A}(x)$. In one of the first theoretical studies of superconductivity, London[15] showed that if a current is proportional to a vector potential, the current is a supercurrent, i.e., the current can exist without there being an applied voltage (or an electric field present). We shall now repeat his argument and show that the s-electron current density, eqn. (V.15) is a supercurrent.

We being by noting that both the local magnetic field $\vec{h}$ and local electric field $\vec{e}$ are related to the vector potential via

$$\vec{h}/c = -\,\text{curl}\ \vec{A} \tag{VI.1a}$$

and

$$\vec{e}/c = \frac{1}{c}\frac{\partial \vec{A}}{\partial t}. \tag{VI.1b}$$

Since the s-electron current density j_s (eqn. (V.15)) is proportional to the vector potential, we get the two London relations

$$\frac{\vec{h}}{c} = -\,\text{curl}\ \Lambda\ \vec{j}_s \tag{VI.2}$$

and

$$\vec{e} = \frac{\partial}{\partial t}\,\Lambda\,\vec{j}_s \tag{VI.3}$$

where $\Lambda = Q^{-1}$ (where Q is given by either eqn. (V.12) or eqn. (V.13)). Introducing the total current density as the sum of the currents formed by the s-electrons which form into BCS pairs and by the s-electrons which remain in the normal state, $\vec{j}_{total} = \vec{j}_s + \vec{j}_n$, we can write down the following to Maxwell equations

$$\text{curl } \vec{h} = \frac{4\pi}{c} \vec{j}_{total} + \frac{1}{c} \frac{\partial \vec{e}}{\partial t} \tag{VI.4a}$$

and

$$\text{curl } \vec{e} = -\frac{1}{c} \frac{\partial \vec{h}}{\partial t}. \tag{VI.4b}$$

Taking the curl of eqn. (IV.4b), we obtain

$$C^2 \text{ curl curl } \vec{e} + 4\pi \frac{\partial}{\partial t} j_{total} + \frac{\partial^2}{\partial t^2} \vec{e} = O. \tag{VI.5}$$

Since $j_n = \sigma \vec{e}$ (where σ is the normal state conductivity) and $\frac{\partial}{\partial t} j_s = \Lambda^{-1} e$, equation (VI.5) becomes

$$C^2 \text{ curl curl } \vec{e} + 4\pi \Lambda^{-1} + 4\pi\sigma \frac{d}{dt} \vec{e} + \frac{\partial^2}{\partial t^2} \vec{e} = O. \tag{VI.6}$$

If we now assume that we have static conditions, then all the terms in the above equation which involve time derivatives (this includes the first term in the above equation since curl $\vec{e} = -\frac{1}{c} \frac{\partial \vec{h}}{\partial t}$) vanish. This leaves us with the result that $\vec{e} = O$ inside the superconductor even though there is a current density given by eqn. (V.15) flowing through the superconductor. Thus the s-electric current density is a supercurrent.

We finally note that there will be no supercurrent in the normal metal since Δ_g vanishes and Q(k) would therefore be zero.

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บทคัดย่อ

โดยการใช้ Anderson Hamiltonian ร่วมกับเทอมสำหรับ electron-phonon coupling ระหว่าง d-electrons อธิบายถึง d-band superconductors (pure-transition metal superconductors) และคำนวณหา s-electron current density โดยวิธี Green's Function บทความนี้แสดงให้เห็นว่า s-electron current density แปรผันกับ vector potential ดังนั้นจึงเป็นส่วนหนึ่งของ supercurrent.