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SUPERCONDUCTIVITY OF TRANSITION ELEMENTS

by

J. PERETTI

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Joint Nuclear Research Center
Ispra establishment - Italy
Reactors Physics Department

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SUPERCONDUCTIVITY OF TRANSITION ELEMENTS

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Since the discovery that no isotope effect exists for transition metals like Ru and Os [1], there has been some speculation as to whether, in some instances, the electron-phonon interaction is or is not completely responsible for superconductivity. Empirical evidence has led Matthias [2] to propose that there should be two types of superconductivity, one valid for non-transition metals and due to the electron-phonon interaction, the other suitable for transition metals and based on another mechanism, producing no isotope effect (Ru and Os), or a partial one (Mo [3]). His views seem to be supported also by the recent observations of Bucher et al. [4] and of Blaugher et al. [5] that the parameter $V' = N(0)V/\gamma$ is increasing very rapidly with the electronic concentration for Nb-Ru and Nb-Mo alloys. These findings are at variance with the ideas expressed by Pines [6] based on the BCS theory [7] of superconductivity. Garland [8] has thus suggested that the Coulomb interaction between the s electrons is screened in transition metals by the s-d electron cloud. He introduces a dielectric constant $\epsilon(q,\omega)$ and using a very specific model, he is able to prove that in a certain domain $\epsilon(q,\omega)$ is negative, giving thus an attractive interaction between the s electrons. Unfortunately, his model leads to an energy gap much too large (0.03 eV) and to a first order transition at T_c.

The purpose of this note is to show that generally s-d interaction leads to superconductivity, and thus to support the idea of Garland. We use the Hamiltonian of Suhl [9]:

$$H = H_0 + H_s + H_d + H_{sd} , \qquad (1)$$

where

$$H_0 = \sum_{k,\sigma} \epsilon_{ks}\, c^*_{k\sigma}\, c_{k\sigma} + \epsilon_{kd}\, d^*_{k\sigma}\, d_{k\sigma} ,$$

$$H_s = - \sum_{k,k'} V_s(k,k')\, c^*_{+k+}\, c^*_{-k-}\, c_{-k'-}\, c_{+k'+} ,$$

$$H_d = - \sum_{k,k'} V_d(k,k')\, d^*_{+k+}\, d^*_{-k-}\, d_{-k'-}\, d_{+k'+} ,$$

$$H_{sd} = - \sum_{k,k'} [V_{sd}(k,k')\, c^*_{k+}\, c^*_{-k-}\, d_{-k'-}\, d_{+k'+} + V_{ds}(k,k')\, d^*_{+k+}\, d^*_{-k-}\, c_{-k'-}\, c_{+k'+}] ,$$

where $V(k,k')$ are the matrix elements (real) for the different interactions, c, c^*, d, d^* the Fermi operators for the s and d bands. $V < 0$ means a repulsion, $V > 0$ an attraction. The ϵ's are the Bloch energies. We perform the Bogoliubov canonical transformation as in ref. [9]:

$$c_{k+} = u_k\, e_{k0} + v_k\, e^*_{k1} ,$$

$$c_{-k-} = - v_k\, e^*_{k0} + u_k\, e_{k1} ,$$

$$d_{k+} = \alpha_k\, f_{k0} + \beta_k\, f^*_{k1} ,$$

$$d_{-k-} = - \beta_k\, f_{k0} + \alpha_k\, f_{k1} ,$$

and write that at the absolute zero the coefficients of $e_{k0}e_{k1}$ and $f_{k0}f_{k1}$ are zero, thus obtaining

$$\epsilon_{ks}\, 2u_k v_k - (S_k + N_k)(u_k^2 - v_k^2) = 0 ,$$

$$\epsilon_{kd}\, 2\alpha_k \beta_k - (D_k + M_k)(\alpha_k^2 - \beta_k^2) = 0 ,$$

where

$$S_k = \sum_{k'} V_s(k,k')\, u_{k'}\, v_{k'} ,$$

$$D_k = \sum_{k'} V_d(k,k')\, \alpha_{k'}\, \beta_{k'} ,$$

$$M_k = \sum_{k'} V_{ds}(k,k')\, u_{k'}\, v_{k'} , \qquad (3)$$

$$N_k = \sum_{k'} V_{sd}(k,k')\, \alpha_{k'}\, \beta_{k'} .$$

The compatibility equations obtained from eqs. (2) and (3) are:

$$S_k = \sum_{k'} V_s(k,k')\, \frac{S_{k'} + N_{k'}}{2\Omega_{k's}} , \qquad (4a)$$

$$D_k = \sum_{k'} V_d(k,k') \frac{D_{k'} + M_{k'}}{2\Omega_{k'd}} ,$$

$$M_{k'} = \sum_{k'} V_{ds}(k,k') \frac{S_{k'} + N_{k'}}{2\Omega_{k's}} , \qquad (4b)$$

$$N_{k'} = \sum_{k'} V_{sd}(k,k') \frac{D_{k'} + M_{k'}}{2\Omega_{k'd}} ,$$

$$\Omega_{ks} = [\epsilon_{ks}^2 + (S_k + N_k)^2]^{\frac{1}{2}} > 0 ,$$
$$\Omega_{kd} = [\epsilon_{kd}^2 + (D_k + M_k)^2]^{\frac{1}{2}} > 0 . \qquad (5)$$

The ground state energy is

$$H^{(0)} = -\tfrac{1}{2} \sum_{k\sigma} \Omega_{k\sigma}^{-1} (\epsilon_{k\sigma} - \Omega_{k\sigma})^2 \qquad (6)$$

and the elementary excitations are

$$H^{(1)} = \sum_k \Omega_{ks} (e_{k0}^* e_{k0} + e_{k1}^* e_{k1}) + \Omega_{kd} (f_{k0}^* f_{k0} + f_{k1}^* f_{k1}) , \qquad (7)$$

In the limit of weak interactions S_k, D_k, M_k, N_k are independent of k and given by:

$$S = (S + N) V_s N_s \ln [\epsilon_1 |S+N|^{-1}] ,$$
$$D = (D + M) V_d N_d \ln [\epsilon_2 |D+M|^{-1}] ,$$
$$M = (S + N) V_{sd} N_s \ln [\epsilon_3 |D+N|^{-1}] , \qquad (8)$$
$$N = (D + M) V_{sd} N_d \ln [\epsilon_3 |D+M|^{-1}] ,$$

where V_s, V_d, V_{sd} are averages of the interactions over the Fermi surface, N_s, N_d the density of s and d levels at the Fermi surface, ϵ_1, ϵ_2, ϵ_3, the distance from Fermi surface where interactions become negligible. By a careful inspection it is possible to show that, provided that $N_s V_s$ and $N_d V_d$ are of the order of 10^{-1}, or less, eqs. (8) admit always a non-trivial solution, whatever the sign of the interactions *. Because of eq. (6), a non-trivial solution gives always a ground state of lower energy than the normal state. This shows that on the basis of the Hamiltonian (1) one can predict that all the transition elements are superconductors. The argument fails naturally for those elements which exhibit a magnetic ordering since in this case it is not possible to perform the Bogoliubov transformation (see, e.g., Vonsovskii and Svirskii [10]).

An order of magnitude for the energy gaps can be calculated for the simple case where $V_s = V_d = 0$ It is found that the solution of eqs. (8) is

$$S = D = 0 ,$$
$$|M| = (N_d/N_s)^{\frac{1}{4}} \epsilon_3 \exp(-1/|V_{sd}|\sqrt{N_s N_d}) ,$$
$$|N| = (N_s/N_d)^{\frac{1}{4}} \epsilon_3 \exp(-1/|V_{sd}|\sqrt{N_s N_d}) . \qquad (9)$$

Assuming that V_{sd} is a Coulomb interaction, it is roughly equal to $-4\pi e^2 K_F^{-2} v_d/v_s$, where v_d is the "effective" volume occupied by d electrons in each shell, and v_s the volume of each cell. For $v_d/v_s = 10^{-2}$ we find that $|V_{sd}|\sqrt{N_s N_d}$ is of the order of 0.1, which gives a reasonable value for the energy gaps.

Finally we notice that in eq. (9), ϵ_3 is not proportional to any vibration frequency, i.e., no isotope effect is predicted; that $|V_{sd}|\sqrt{N_s N_d}$ is not proportional to γ since the latter is proportional to $N_s + N_d$. By the usual procedure of Bogoliubov et al. [11] the transition at T_c can be proved to be a second order transition.

* We assume that $V_{sd} \neq 0$; $V_{sd}^2 \neq V_s V_d$; $N_s V_s \ln \epsilon_1/\epsilon_3 \neq 1$ and $N_d V_d \ln \epsilon_2/\epsilon_3 \neq 1$.

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