ON TAKING CRYSTAL STRUCTURE INTO ACCOUNT IN THE THEORY OF SUPERCONDUCTIVITY

PHYSICS

1969

SovietRxiv

Abstract

Full Text

UDC 537.312.62

PHYSICS

E. E. TAREEVA

ON TAKING CRYSTAL STRUCTURE INTO ACCOUNT IN THE THEORY OF SUPERCONDUCTIVITY

(Presented by Academician N. N. Bogolyubov on 8 IV 1969)

In a number of works (see, for example, ([1–3])) the matrix element of the effective electron–electron interaction arising from phonon exchange and apparently responsible for superconductivity in most metals was calculated. In this way, success was achieved in a qualitative description of the phenomenon. A number of effects, however, in principle cannot be described within the approximation of almost free electrons used by the authors cited. Such effects include, first of all, phenomena connected with anisotropy of the gap, with the influence of pressure and of the type of crystal lattice on the critical temperature. In this connection we undertook an attempt to investigate the approximation of strongly bound electrons, bearing in mind the introduction into the theory of the atomic and structural characteristics of the substance. In work ([4]) the simplest case of the effective-mass approximation for strongly bound electrons was considered, which made it possible to introduce into the exponent determining the critical temperature new characteristics of the metal, namely, the ionization potential and the radius of the electron shell of the atom.

In the present work we do not restrict ourselves to the effective-mass approximation, but consider the general case of strongly bound electrons, when the one-particle energy $E_{\mathbf{k}}$ is represented by some sum over the lattice, invariant with respect to transformations of the crystal group. This invariance makes it possible to use the energy as a variable and to avoid the difficulties mentioned in ([4]), which arise in obtaining the superconductivity criterion in the anisotropic case.

As in ([4]), we shall use the Hamiltonian of the electron–phonon interaction written in the second-quantization representation with the aid of orthogonalized functions ([5])

$$\Phi_\alpha(x) = \sum_{\alpha'} U_{\alpha\alpha'} \Psi_{\alpha'}(x), \tag{1}$$

where $\Psi_\alpha(x)$ are atomic one-electron functions; $\alpha = \{f, \nu, \sigma\}$; f is the number of the lattice site; ν is the number of the function in the atom; σ is the electron spin;

$$U_{\alpha\alpha'} = \delta_{\alpha\alpha'} - \frac{1}{2}(1-\delta_{\alpha\alpha'})S_{\alpha\alpha'} + \frac{3}{8}\sum_{\alpha_1}(1-\delta_{\alpha\alpha_1})(1-\delta_{\alpha_1\alpha'})S_{\alpha'\alpha_1}S_{\alpha_1\alpha} + \cdots; \quad (2)$$

$$S_{\alpha\alpha'} = \int \Psi^*_\alpha(x)\Psi_{\alpha'}(x)\,dx$$

are overlap integrals.

Following works ([6–7]), it is not difficult to obtain the secular equations for pair excitations over the normal Fermi state. To terms of second order in the electron-phonon interaction, in the case of one band the secular equations for excitations with zero total momentum and energy E have the form

$$2|\xi_{\mathbf{k}}|\,\vartheta(\mathbf{k}) - \sum_{\mathbf{k}'} J(\mathbf{k},\mathbf{k}')\frac{\xi_{\mathbf{k}}\xi_{\mathbf{k}'}}{|\xi_{\mathbf{k}}|\,|\xi_{\mathbf{k}'}|}\vartheta(\mathbf{k}') = E\theta(\mathbf{k}), \quad (3)$$

$$2|\xi_{\mathbf{k}}|\,\theta(\mathbf{k}) - \sum_{\mathbf{k}'} J(\mathbf{k},\mathbf{k}')\theta(\mathbf{k}') = E\vartheta(\mathbf{k}).$$

Here

$$\xi_{\mathbf{k}} = E_{\mathbf{k}} - E_F; \qquad J(\mathbf{k},\mathbf{k}') = \frac{2\,|V(\mathbf{k}-\mathbf{k}'-\mathbf{k})|^2}{|\xi_{\mathbf{k}}| + |\xi_{\mathbf{k}'}| + \omega_{\mathbf{k}-\mathbf{k}'}}, \quad (4)$$

$$V(\mathbf{k},\mathbf{p}) = 4\pi Zie^2\sqrt{\frac{N}{2M\omega_k}}\,\frac{(\mathbf{e}_{\mathbf{k}},\mathbf{k})}{k^2}\,\mathfrak{A}(\mathbf{k}\mid\mathbf{p});$$

$\omega_{\mathbf{k}}$ is the phonon frequency; $\mathbf{e}_{\mathbf{k}}$ is its polarization; Z, M, and N are, respectively, the charge, mass, and density of the ions;

$$\mathfrak{A}(\mathbf{k}\mid\mathbf{p}) = \sum_{\mathbf{f}} e^{i\mathbf{pf}}\mathfrak{A}(\mathbf{k}\mid\mathbf{f}), \qquad \mathfrak{A}(\mathbf{k}\mid\mathbf{f}) = \int \Phi^*_0(\mathbf{r})e^{i\mathbf{kr}}\Phi_{\mathbf{f}}(\mathbf{r})\,d\mathbf{r}.$$

Using further the invariance of the energies $\xi_{\mathbf{k}}$ under transformations of the group, we can write the expansion of the functions $J(\mathbf{k},\mathbf{k}')$ in crystal harmonics $\Psi^{(L)}_{j\mu}$ (j is the number of the irreducible representation; μ is the row number) in the form

$$J(\mathbf{k},\mathbf{k}') = \sum_{j\mu L} J_j^{(L)}(\xi,\xi')\,\Psi_{j\mu}^{(L)}(\hat{k})\,\Psi_{j\mu}^{*(L)}(\hat{k}'). \tag{5}$$

This makes it possible to seek solutions of equations (3) in the form

$$\vartheta(\mathbf{k}) = \sum_{j\mu L} \vartheta_{j\mu}^{(L)}(\xi)\Psi_{j\mu}^{(L)}(\hat{k}), \qquad \theta(\mathbf{k}) = \sum_{j\mu L} \theta_{j\mu}^{(L)}(\xi)\Psi_{j\mu}^{(L)}(\hat{k}). \tag{6}$$

We next pass from summation over the momentum to integration over the energy and introduce functions, not explicitly dependent on the angles,

$$C_{j\mu}^{1(L)}(\xi) = \int d\xi'\, J_j^{(L)}(\xi,\xi') \sum_{\substack{j_1\mu_1 L_1\\ j_2\mu_2 L_2}} \langle j\mu \mid j_1\mu_1 j_2\mu_2\rangle\, \theta_{j_1\mu_1}^{(L_1)}(\xi')\, N_{j_2\mu_2}^{(L_2)}(\xi'),$$

$$C_{j\mu}^{2(L)}(\xi) = \int d\xi'\, J_j^{(L)}(\xi,\xi')\,\frac{\xi'}{|\xi'|} \sum_{\substack{j_1\mu_1 L_1\\ j_2\mu_2 L_2}} \langle j\mu \mid j_1\mu_1 j_2\mu_2\rangle\, \vartheta_{j_1\mu_1}^{(L_1)}(\xi')\, N_{j_2\mu_2}^{(L_2)}(\xi'). \tag{7}$$

Here

$$\langle j\mu \mid j_1\mu_1 j_2\mu_2\rangle = \int \Psi_{j\mu}^{*}(\hat{k})\,\Psi_{j_1\mu_1}(\hat{k})\,\Psi_{j_2\mu_2}(\hat{k})\,d\Omega,$$

and $N_{j\mu}^{(L)}(\xi)$ are determined from the expansion

$$\frac{1}{(2\pi)^3}\,\frac{k^2}{|d\xi/dk|} = \sum_{j\mu L} N_{j\mu}^{(L)}(\xi)\Psi_{j\mu}^{(L)}(\hat{k}). \tag{8}$$

Now from equations (3) we obtain

$$2|\xi|\vartheta_{j\mu}^{(L)}(\xi) - \frac{\xi}{|\xi|}C_{j\mu}^{2(L)}(\xi) = E\theta_{j\mu}^{(L)}(\xi),$$

$$2|\xi|\theta_{j\mu}^{(L)}(\xi) - C_{j\mu}^{1(L)}(\xi) = E\vartheta_{j\mu}^{(L)}(\xi), \tag{9}$$

which, together with definition (7), leads to the equation

$$C_{j\mu}^{2(L)}(\xi) = \int d\xi'\, J_j^{(L)}(\xi,\xi')\,\frac{\xi}{|\xi'|} \sum_{\substack{j_1\mu_1 L_1\\ j_2\mu_2 L_2}} \frac{\xi}{|\xi'|}\,\frac{2\xi' C_{j_1\mu_1}^{2(L_1)}(\xi') + E C_{j_1\mu_1}^{1(L_1)}(\xi')}{4\xi'^2 - E^2}\, N_{j_2\mu_2}^{(L_2)}(\xi'). \tag{10}$$

Taking into account that the interaction (4) is concentrated near the Fermi surface, we can, as usual, replace $J_j^{(L)}(\xi, \xi')$ by $J_j^{(L)}(0,0) = J_j^{(L)}$,

and $N_{j\mu}^{(L)}(\xi)$ by $N_{j\mu}^{(L)}(0) = N_{j\mu}^{(L)}$, and rewrite (10) in the form

$$C_{j\mu}^{2(L)} = J_j^{(L)} \sum_{\substack{j_1\mu_1 L_1 \\ j_2\mu_2 L_2}} \langle j\mu \mid j_1\mu_1 j_2\mu_2\rangle N_{j_2\mu_2}^{(L_2)} \int d\xi' \, \frac{2\xi'^2}{|\xi'|} \, \frac{C_{j_1\mu_1}^{2(L_1)}}{4\xi'^2 - E^2}, \qquad (11)$$

where the integration over energy is now limited to a region of width $2\tilde{\omega}$, where $\tilde{\omega}$ is some mean phonon energy.*

The equation (11) assumes its simplest form in the case when the density of states on the Fermi surface is taken to be independent of the point on the Fermi surface, which apparently is admissible in the case of some *sp*-superconductors. Then

$$-E^2 = 4\tilde{\omega}^2 \exp(-2/J_j N_0), \qquad (12)$$

where $N_0 = N_{00}^0(0)$.

Relation (12) means that attraction in any one representation is sufficient for the occurrence of superconductivity, and the transition temperature will be determined by the corresponding coefficient J_j. In the case when several coefficients J_j correspond to attraction, several gaps will already be needed to describe the superconductor. It is possible that such a situation occurs in tin, [8]. It is interesting that, since the angular dependence of the gaps is different, the character of the angular dependence of anisotropic quantities (for example, the ultrasound absorption coefficient) will in this case change with temperature.

One may, however, not restrict oneself to the case of a density of states constant on the Fermi surface. If in the expansions (5) and (8) one takes into account only those basis functions of the representations which are constructed from spherical harmonics with the lowest L, then the solution of the system (11) presents no difficulty.

Let us give some of the simplest results for the group T_d. Suppose that only one coefficient J_j differs from zero. For $j = 0$ or 1, relation (12) is valid; for $j = 2$ we obtain

$$-E^2 = 4\tilde{\omega}^2 \exp(-2/J_2 N_2),$$

where**

$$N_2 = \frac{N_0^2 + N_{10}^2 - \frac{1}{2}\left(N_{21}^2 + N_{2,-1}^2\right)}{N_0 \pm \sqrt{\frac{1}{2}\left(N_{21}^2 + N_{2,-1}^2\right) - N_{10}^2}}.$$

If J_0 and J_1 differ from zero, then

$$-E^2 = 4\tilde{\omega}^2 e^{-2/\rho},$$

where

$$\rho = \frac{2J_0J_1\left(N_0^2 - N_{10}^2\right)}{N_0(J_0 + J_1) \pm \sqrt{N_0^2(J_0 - J_1)^2 + 4J_0J_1N_{10}^2}}.$$

In conclusion I express my gratitude to Acad. N. N. Bogolyubov for useful discussions and interest in the work, and to E. N. Yakovlev for a number of valuable remarks.

Institute of High-Pressure Physics
Academy of Sciences of the USSR

Received
8 IV 1969

References

[1] D. Pines, Phys. Rev., **109**, 280 (1958).
[2] P. Morel, P. W. Anderson, Phys. Rev., **125**, 1263 (1962).
[3] McMillan, Phys. Rev., **167**, 331 (1968).
[4] E. E. Tareyeva, Phys. Lett., **25A**, 252 (1967).
[5] N. N. Bogolyubov, *Lectures on Quantum Statistics*, Kiev, 1949.
[6] R. Brout, Phys. Rev., **108**, 515 (1957).
[7] N. N. Bogolyubov, V. V. Tolmachev, D. V. Shirkov, *A New Method in the Theory of Superconductivity*, Moscow, 1958.
[8] A. J. Bennett, Phys. Rev., **153**, 482 (1967).
[9] D. T. Sviridov, Yu. F. Smirnov, V. E. Troitskii, *Kristallografiya*, **9**, 807 (1964).

* To obtain quantitative results one should use different values of $\tilde{\omega}_j$ for different representations; moreover, $\tilde{\omega}_j$ apparently cannot substantially exceed $\tilde{\omega}$.

** The notation and numerical Clebsch-Gordan coefficients are taken from Ref. [9].

Note: Figure translations are in progress. See original paper for figures.