Proc. Estonian Acad. Sci. Phys. Math., 1991, 40, N 4, 337—340
https://doi.org/10.3176/phys.math.1991.4.12

УДК 538.945

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DEFORMATIONAL INTERACTION OF CURRENT CARRIERS IN SUPERCONDUCTORS

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Владимир ХИЖНЯКОВ, Эрнст СИГМУНД. ДЕФОРМАЦИОННОЕ ВЗАИМОДЕЙСТВИЕ НОСИТЕЛЕЙ ТОКА В СВЕРХПРОВОДНИКАХ

It is shown that in superconductors with several atoms in the elementary cell there exists a pairing attraction of all the current carriers of all wave vectors. This attraction is of a deformational origin: the attraction of the carriers occurs as a result of the carrier-induced distortions of the elementary cells of the crystal, and it exists already within the range of weak electron-phonon interaction. This pairing mechanism of current carriers may lead to a high temperature of a superconducting transition.

It is usually considered that electron-phonon interaction within weak limits causes the attraction of only those current carriers whose wave vector $\vec{k}$ is close to the Fermi surface [1]. If restricted to the above attraction mechanism, the critical temperature of the superconductivity T_c remains small — $kT_c \ll \hbar\bar{\omega}$, where $\bar{\omega}$ is the mean phonon frequency. In contrast to the weak electron-phonon interaction, the strong interaction ensures the attraction of particles irrespective of the value of $\vec{k}$. However, the particles will thereby become autolocalized and heavy, which does not allow for a high T_c either. For these reasons often other — nonelectron-phonon mechanisms — are applied to explain the high critical temperature of oxide superconductors. However, as will be shown below, the role of electron-phonon interaction in high-T_c superconductivity may be more essential than commonly considered. It turns out that within the weak electron-phonon interaction, on fulfilling simple symmetry conditions the attraction of the Cooper pairs appears for all wave vectors $\vec{k}$. Such attraction may result in relatively high values of T_c.

Let us consider a crystal with several atoms in the elementary cell. Suppose that particles (electrons, holes) move along the atoms not lacated in centro-symmetrical positions. If a particle occurs on such an atom, a force may appear that moves the atom out of equilibrium position. In this case the electron-phonon (hole-phonon) interaction contains the term

$$H_{eph}^{(0)} = W \sum_l c_l^+ c_l Q_l, \tag{1}$$

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where $Q_l = \sum_{l'r} \Phi \begin{pmatrix} l-l' \\ r_0, r \end{pmatrix} x \begin{pmatrix} l' \\ r \end{pmatrix}$, Φ is the element of the dynamic matrix of the crystal [2]; $x \begin{pmatrix} l \\ r \end{pmatrix}$ is the displacement of the atom r in the l-th elementary cell (r includes the indices of the Cartesian components x, y, z); r_0 labels the atom on which the particle resides; the direction of the appearing force is chosen along one of the coordinate axes. The full Hamiltonian of the system is as follows: $H = H_e + H_L + H_{eph}$, where

$$H_e = \sum_k \varepsilon(k) c_k^+ c_k,$$

$$H_L = H_{kin} + \frac{1}{2} \sum_{il'} \sum_{rr'} \Phi \begin{pmatrix} l-l' \\ r, r' \end{pmatrix} x \begin{pmatrix} l \\ r \end{pmatrix} x \begin{pmatrix} l' \\ r' \end{pmatrix} = \sum_{qv} \hbar \omega_{vq} \left(b_{vq}^+ b_{vq} + \frac{1}{2} \right),$$

H_{kin} is the operator of the kinetic energy of vibrations, $b_{vq}^+ (b_{vq})$ is the operator of creation (annihilation) of the phonon of the branch v of the wave vector q and frequency ω_{vq}, $c_k^+ (c_k)$ is the operator of creation (annihilation) of the electron (hole) with the wave vector k, $\varepsilon(k)$ is its kinetic energy, $H_{eph} = H_{eph}^{(0)} + H_{eph}^{(1)}$,

$$H_{eph}^{(1)} = \sum_l c_l^+ c_l Q_{1l}, \tag{2}$$

Q_{1l} is the displacement operator of the atoms not containing $x \begin{pmatrix} l \\ r_0 \end{pmatrix}$.

By a unitary transformation the linear electron-phonon interaction H_{eph} can be eliminated by replacing it with a number of electron-electron and nonlinear electron-phonon interactions. In this model it can be made in two ways: 1) as usual, by proceeding to the k-representation of H_{eph} and performing a unitary Fröhlich transformation [3]; 2) by first performing the unitary transformation of the coordinate displacement shift $x \begin{pmatrix} l \\ r_0 \end{pmatrix}$, that would fully or partially eliminate $H_{eph}^{(0)}$ at $\varepsilon(k) = 0$, and then proceeding to the k-representation and by the unitary Fröhlich transformation eliminating the rest of the linear electron-phonon interaction operators as well as those appearing (at $\varepsilon(k) \neq 0$) as the result of the first transformation. The Hamiltonian obtained this way has a different but, naturally, an equivalent form. The electron-electron interaction of interest here is of a much simpler form in case the second way is used, whereby at first half of the $H_{eph}^{(0)}$ is excluded.

The first unitary transformation in this case is of the form

$$H_1 = e^{s_1} H e^{-s_1} = H + [s_1, H] + \frac{1}{2} [s_1, [s_1, H]] + \ldots,$$

where $s_1 = (W/2) \sum_l c_l^+ c_l \partial / \partial x \begin{pmatrix} l \\ r_0 \end{pmatrix}$. With the accuracy up to the terms of the order W^2 we obtain

$$H_1 \simeq H_e + H_{ph} - \frac{3}{4} \overline{W}^2 \sum_l (c_l^+ c_l)^2 + \tilde{H}_{eph}, \tag{3}$$

$$\tilde{H}_{eph} = \sum_{kq} \sum_{v} g_v(k, q) b_{vq}^+ c_k^+ c_{k+q} + \text{h. c.}, \tag{4}$$

$$g_\nu(k,q)=\frac{W}{2}\left(\frac{M_{r_0}\omega_{\nu q}}{2\hbar}\right)^{1/2}\xi(r_0;\nu,q)\times$$

$$\times[\varepsilon(k+q)-\varepsilon(k)+\hbar\omega_{\nu q}]+Vg_\nu^{(1)}(q), \qquad (5)$$

$\overline{W}^2=\frac{1}{2}W^2\Phi\begin{pmatrix}0\\ r_0,\ r_0\end{pmatrix}$, $\xi(r;\nu,q)$ is the amplitude of the phonon on the atom r_0, $g_\nu^{(1)}(q)$ are the coefficients of the expansion Q_{ll} by the operators of phonon creation and annihilation.

In formula (5) we took into account that (see [2])

$$\sum_{lr} M_r^{-1/2}\Phi\begin{pmatrix}l\\ r_0,\ r\end{pmatrix}\xi(r;\nu,q)\,e^{iql}=\omega_{\nu q}^2 M_{r_0}^{1/2}\xi(r_0;\nu,q).$$

The second unitary transformation is of the form $H_2=e^{s_2}H_1e^{-s_2}$, where

$$s_2=-\sum_{kq}\sum_{\nu} g_\nu(k,q)\,[\varepsilon(k+q)-\varepsilon(k)-\hbar\omega_{\nu q}]^{-1}b_{\nu q}^{+}c_k^{+}c_{k+q}-\text{h. c.} \qquad (6)$$

Transformation (6) gives, with the accuracy up to the terms $\sim W^2$,

$$H_2\simeq H_e+H_{ph}-\frac{3}{4}\overline{W}^2\sum_{kk'n''}c_k^{+}c_{k'}c_{k-k'+k''}+H', \qquad (7)$$

$$H'=\frac{1}{4}M_{r_0}W^2\sum_{q\nu}\omega_{\nu q}^2\,|\xi(r_0;\nu,q)|^2[(\varepsilon(k+q)-\varepsilon(k))^2-(\hbar\omega_{\nu q})^2]^{-1}\times \qquad (8)$$

$$\times R_\nu(k,q)R_\nu^*(k',q)\left(c_k^{+}c_{k+q}c_{k'+q}^{+}c_{k'}+\delta_{kk'}\left(b_{\nu q}^{+}b_{\nu q}+\frac{1}{2}\right)(c_{k+q}^{+}c_{k+q}-c_k^{+}c_k)\right),$$

where

$$R_\nu(k,q)=\varepsilon(k+q)-\varepsilon(k)+\hbar\omega_{\nu q}+$$

$$+2VW^{-1}|\xi(r_0;\nu,q)|^{-1}g_\nu^{(1)}(q)\,(2\hbar/M_{r_0}\omega_{\nu q}^3)^{1/2}$$

(the terms $\sim b_{\nu q}^{+}b_{\nu' q'}^{+}$ at $\nu\neq\nu'$, $q\neq q'$ are not included).

As is known [1] it is the electron-electron interaction $\sim c_k^{+}c_{-k}^{+}c_{-k'}c_{k'}$ that leads to superconduction. In the case under consideration this interaction is equal to

$$H_{sc}=-\sum_{kq}c_k^{+}c_{-k}^{+}c_{-k-q}c_{k+q}\left[\overline{W}^2+\frac{VG(\nu,q)\hbar\omega_{\nu q}}{(\hbar\omega_{\nu q})^2-(\varepsilon(k+q)-\varepsilon(k))^2}+\right.$$

$$\left.+VW\sqrt{\frac{\omega_{\nu q}}{2\hbar^3}}\,\mathrm{Re}\,\xi^*(r_a;\nu,q)g_\nu^{(1)}(q)\right], \qquad (9)$$

where

$$G(\nu,q)=V|g_\nu^{(1)}(q)|^2+\overline{W}(M_{r_0}\omega_{\nu q}^3/2\hbar)^{1/2}\mathrm{Re}\,\xi^*(r_0;\nu,q)g_\nu^{(1)}(q).$$

Here it has been taken into account that in the nearest neighbours interaction approximation $\sum_\nu \omega_{\nu q}^2\,|\xi(r_0;\nu,q)|^2=M_{r_0}^{-1}\Phi(r_0^0\ r_0)$.

We can see that the $\sim V$ term in formula (9) has a common sign-variable form; it causes attraction only in the region $|\varepsilon(k+q)-\varepsilon(k)|\lesssim\hbar\bar{\omega}$.

In contrast to that the $\sim\overline{W^2}$ term gives attraction for all wave vector particles. If this term prevails, then the superconducting gap Δ, satisfying the equation of [1],

$$1=\overline{W^2}\sum_{\varepsilon<\varepsilon_F}(\varepsilon^2+\Delta^2)^{-1/2}$$

in a two-dimensional case actual for oxyde superconductors, at $\varepsilon_F<B/2$, is equal to

$$\Delta=2\sqrt{\varepsilon_F B}\exp(-1/2\varrho\overline{W^2}), \qquad (10)$$

where ϱ is the density of states, ε_F is the Fermi energy and B the zone width. This formula, proposed earlier in [4], differs from the corresponding theory of *BCS* [1] by its preexponential multiplier, which in the last formula equals $2\hbar\overline{\omega}$. As usually $\sqrt{\varepsilon_F B}$ exceeds $\hbar\overline{\omega}$ by at least an order of magnitude, and then the superconducting gap given by formula (10) as well as the critical temperature T_c are also considerably larger than in the *BCS* theory. In the deduction presented above the interaction $\sim\overline{W^2}$ responsible for such high values of Δ and T_c has within the factor 3/4 been obtained as the result of local shifts of the atoms r_0, that lead to the deformation of elementary cells. Therefore we call this interaction deformational.

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Received
April 3, 1991