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MOLECULAR BOND IN SUPERCONDUCTIVITY

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In the presence of a superconducting current an additional intermolecular bond appears, whose value determines the critical parameters.

The goal of the present work is to show that superconducting properties originate due to additional intermolecular interaction, stable below a critical temperature. The interaction to be found, affecting the orientation ordering of the whole system, is caused, in turn, by the original induced current.

This conclusion is based on consideration of superconductivity, including high-temperature superconductivity (HTSC), with the aid of the quantum-mechanical approach, including successive transformation of the number of particles, whose character is an inherent dynamic property of the system.

The essence of this approach can be described as follows: in its primary meaning, a system is understood as a continuum medium, in which the manifestation of any properties is caused by the appearance of traits of discreteness, which carry properties of individual objects (discreteness is identified with individuality); it is natural that the number of particles in the system is a variable that is not prescribed but, on the contrary, must be determined.

In the period $P = 1$ let there be a transformation of the number of particles in the medium $n_1^{(i)} \to n_2^{(i)} \to \ldots \to n_M^{(i)}$ ($n_M = n_1$) with the corresponding lifetimes $\Delta p_1^{(i)}$, $\Delta p_2^{(i)}$,..., $\Delta p_M^{(i)}$, the sum of which is unity (the superscript i indicates that this transformation is not unique). The Schrödinger equation with the eigenvalue of the total energy E_k is valid for each number of particles n_k. Then, for the whole period the discrete system is characterized by the average mechanical energy

$$\overline{E} = \sum_{k=1}^{M} E_{n_k} \Delta p_k , \tag{1}$$

where Δp_k is the probability of occurrence of the medium in the state with the number of particles n_k. The continuum medium successively "absorbs" and "gives" energy to the "discrete" system. Now, it is possible to speak about the "trajectory" of the natural development of the system (of electrons), which can be written as

$$B_{n_1\beta}^{N} \to B_{n_2\beta}^{N} \to \ldots \to B_{n_M\beta}^{N} , \tag{2}$$

where N is the basic number of particles and the subscript β indicates that these trajectories are multiple, and among them there are ones degenerate in dynamic characteristics and ones different in the sense of Eq. (1).

The physically observed process is a transition from one trajectory to another, involving absorption (emission) of a particle or a quantum of field energy. The average mechanical energy of the new trajectory differs from the average energy of the previous trajectory by the energy of the absorbed particle. The same can be said about the angular momentum. The absorption can take place with or without changes in the basic number N or without changes in both n_k and N but with changes in β. A real atom is considered as an inhomogeneous system AB. An element of the trajectory of this system is written as $(A_{n_i}^{N_1} B_{n_j}^{N_2})_{\alpha\beta}$. The formalism suggested is realized concretely in [2].

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Now, in considering an electronic subsystem with a variable number of particles, it is necessary to determine correspondingly the current vector j. To do this, we introduce the position vector $\mathbf{r}_{kc}$ of the center of inertia and annihilation (IA) for the time interval Δp_k in the form

$$\mathbf{r}_{kc} = \frac{1}{N} \sum_{\gamma=1}^{n_k} \mathbf{r}_{k\gamma} , \tag{3}$$

where $\mathbf{r}_{k\gamma}$ is the position vector of the center of the cell with the number γ, whose volume ΔV is much less than the effective volume V of the whole system (an atom), filled with a particle (quasikinematic equations of motion of the particle over the cells for its lifetime are formed in terms of the wave function). Then, the current vector is written for the same time interval Δp_k:

$$\mathbf{j}_k = e \frac{n_{k+1}\, \mathbf{r}_{k+1c} - n_k\, \mathbf{r}_{kc}}{\Delta p_k} . \tag{4}$$

If $n_k = N = \text{const}$ (there is no transformation of the number of particles in the electronic subsystem), then Eq. (4) becomes the well-known expression ($\mathbf{j} = eNd\mathbf{r}_{kc}/dt = eN\mathbf{v}$; in the volume V, N means the number density of particles).

As k changes (after a successive transformation of the discrete system), the current vectors form a broken line that changes its direction about some average orientation, along which we denote the unit vector $\mathbf{R}$ (director). This makes it possible to describe the additional molecular interaction that appears with the electric current. The necessity of determining the current in the sense of Eq. (4) is dictated by the effect of inner electrons of the atom on the ordinary current of conductance electrons, whose number is generally transformated but slightly.

We consider two neighboring atoms in the volumes V_1 and V_2, respectively. The force centers of the systems of electrons are at the centers of two cubes. Joint quantum-mechanical consideration with account for the conductance electrons leads to a certain orientation of the two directors $\mathbf{R}_1$ and $\mathbf{R}_2$ (the angle between them is denoted by φ). Upon a quantum transition of the system from one trajectory to another in the above formalism (as a result of an energy transformation induced by an external magnetic field) the angle φ changes (increases). Thus, it is this angle that reflects the presence of additional interaction of the two atoms (molecules), whose energy is $U(\varphi)$. In this case it is important to bear in mind that the angle φ is quantized. Therefore, the function U is written as the complex function $U(\varphi(\varepsilon))$, where ε is the energy of the transition from one energy level to another (an energy gap). But in this case the quantum transition is not unique and the energy gap is not unique, which is of basic importance for explanation of high-temperature superconductivity.

Since a real atom is an inhomogeneous system (AB), it is necessary that the presence of two energy quanta associated with the subsystems A and B, respectively, be included in the formalism considered. The quantum of the magnetic field ε_H absorbed by the subsystem A (the core) determines both the rearrangement of the electronic subsystem B with the transition energy ε_E and the induction of a current with the density j (electromagnetic induction). It is the quantum ε_E that determines the aforementioned additional intermolecular bond in the presence of the electric current.

The introduced energy quanta will be considered in more detail for magnetic and electric fields, respectively. The quanta will be expressed as

$$\varepsilon_H = \mathbf{h}_H \mathbf{H} \quad \text{and} \quad \varepsilon_E = \mathbf{h}_E \mathbf{E} . \tag{5}$$

In terms of h_H (h_E) corresponding units of length l_H (l_E) and time will be introduced. For example, for l_H and t_H, we write

$$l_H = \frac{h_H}{\sqrt{\hbar\, c}} , \quad t_H = \frac{h_H}{\sqrt{\hbar\, c^3}} . \tag{6}$$

If ε is assumed to be an energy quantum of an arbitrary physical field, the following expression can be written for it:

$$\boldsymbol{\varepsilon} = \mathbf{h}_g \Delta \mathbf{r}\,, \tag{7}$$

where $\Delta \mathbf{r}$ is the elementary displacement in the finite time interval Δt_g. Now, in terms of the three quantities $\hbar$, c, and h_g, it is possible to obtain a systems of units:
for the mass m_g

$$m_g = \sqrt{\left(\frac{\hbar h_g}{c^3}\right)}, \tag{8}$$

and for the length l_g and the time t_g, respectively,

$$l_g = \sqrt{\left(\frac{\hbar c}{h_g}\right)}, \quad t_g = \sqrt{\left(\frac{\hbar}{h_g c}\right)}. \tag{9}$$

Assuming $t_g = \Delta t_g$, the expression for the velocity $\mathbf{v} = \Delta \mathbf{r}/\Delta t_g$ is written as

$$v = \sqrt{\left(\frac{\varepsilon c \Delta r}{h}\right)}, \quad h = 2\pi\hbar\,. \tag{10}$$

The Planck-Einstein relations follow from Eq. (10), assuming $v = c$ and taking into consideration that $c\Delta t = \Delta r = \lambda$, which is the wavelength of the monochromatic wave (the frequency is ω). Indeed,

$$\varepsilon = \frac{ch}{\Delta r} = \frac{2\pi\hbar}{\Delta t} = \hbar\omega\,.$$

The expression for the momentum $p = \varepsilon/c$ can be obtained in the same way. It is also easy to obtain the de Broglie relations with the aid of Eq. (10). To do this, the initial triad h, c, and h_g is replaced by the triad h, u, and h_g, where u is the velocity of propagation of a monochromatic wave ($u = \omega/k = \lambda_u/\Delta t$; $\Delta r = u\Delta t$), and we assume $v = u$. If u is the velocity of propagation of a nonmonochromatic wave with the wavelength λ_v, then $\Delta r \neq \lambda_v$. If at $v = u$ (after substitution of u for c) ε from Eq. (10) is assumed to be equal to the kinetic energy of a particle with the mass m and its momentum p_v to be equal to $\hbar k_v$, the de Broglie relation is obtained for the length of the group wave ($u \neq \omega/k$).

Now, expressions (5) can be expressed in a form similar to that of Eq. (7):

$$\varepsilon_H = \mathbf{F}_H \Delta \mathbf{r}\,, \quad \varepsilon_E = \mathbf{F}_E \Delta \mathbf{r}\,, \tag{11}$$

where $\mathbf{F}_H$ is the Lorentz force:

$$\mathbf{F}_H = \frac{e}{c}(\mathbf{v}^* \times \mathbf{H})\,, \quad \mathbf{F}_E = e\mathbf{E}\,.$$

Here $\mathbf{v}^*$ is the fixed (averaged) velocity of an electron.

Then, the quantities h in Eq. (5) will be written as

$$\mathbf{h}_H = \frac{e}{c}(\mathbf{v}^* \times \Delta \mathbf{r})\,, \quad \mathbf{h}_E = e\Delta \mathbf{r}\,, \tag{12}$$

and the relation between them is

$$\mathbf{h}_H = \frac{1}{c}(\mathbf{v}^* \times \mathbf{h}_E)\,. \tag{13}$$

Let the three vectors **H**, $\mathbf{v}^*$, and $\Delta\mathbf{r}$ be mutually perpendicular (it is this case that while be of interest henceforth). According to Eq. (13), the vectors $\mathbf{h}_H$ and $\mathbf{h}_E$ are mutually perpendicular, and according to Eq. (12), the first of them is collinear to **H**, and, the second to $\Delta\mathbf{r}$. We consider the case where the vector **E** is also directed along $\Delta\mathbf{r}(\mathbf{H}\perp\mathbf{E})$. Then, Eq. (13) can be written as

$$h_H = \frac{v^*}{c} h_E \tag{14}$$

or in view of (6)

$$\frac{l_H}{l_E} = \frac{h_H}{h_E} = \frac{v^*}{c}. \tag{15}$$

At $v = c$ from general expression (10) we can write

$$\Delta r_E = \frac{\hbar c}{\varepsilon_E}. \tag{16}$$

On the other hand, using Eqs. (7), (9) and (14), (16) in definition (6), we can write

$$l_E^2 = \frac{e^2 \Delta r^2}{\hbar c} = \frac{e^2 \hbar c}{\varepsilon_E^2} \tag{17}$$

and, accordingly,

$$l_H^2 = \frac{v^{*2} \hbar e^2}{c \varepsilon_H^2}, \tag{18}$$

Consequently, an important relation is obtained:

$$\frac{\varepsilon_E}{\varepsilon_H} = \frac{v^*}{c} \leq 1. \tag{19}$$

Now, estimates necessary for the subsequent presentation will be given. In [2] the suggested quantum-mechanical program has been realized for the one-particle Hamiltonian of the Coulomb problem. In particular, for a system with $N_1 = 14$ and $N_2 = 8$ and $\Delta V_A = 0.6\Delta V_B$, there are three different energy levels and the energy qauntum $\varepsilon_E \sim 10^{-15}$ to 10^{-14} erg. Since the characteristic velocity of an electron $v^* \sim 10^8 - 19^9$ cm/sec, then according to Eqs. (18) and (19) the length $l_H \sim 10^{-6}$, which coincides with the value of the London length δ of penetration of the magnetic field in a superconductor. This is not a coincidence since the energy quantum has its own characteristic length and this characteristic of the field is δ and it is unlikely that these lengths are basically different.

The second characteristic scale of length l_E has the meaning of the correlation parameter ξ in the theory of superconductivity (see [1]). According to (15), their ratio δ/ξ must be of the order of magnitude of $10^{-2} - 10^{-1}$, which is the case for superconductors of the first kind (pure metals). Now in view of (19) Eqs. (17) and (18) can be written as

$$\varepsilon_E = \frac{e}{\xi} \sqrt{\hbar c}, \quad \varepsilon_H = \frac{e v^*}{\delta} \sqrt{\left(\frac{\hbar}{c}\right)}. \tag{20}$$

Rupture of the additional intermolecular bond $U(\varphi)$, which means breakdown of the SC (the angle φ becomes arbitrary), can occur due to the molecular kinetic energy kT_c. Since the energy U is proportional to ε_E, then assuming the latter to be equal to the kinetic energy, we find

$$T_c \simeq \frac{\bar{\varepsilon}_H}{k} \tag{21}$$

equal to ~ 10 K in order of magnitude. It is ε_E that is the known value of the energy gap Δ.

The breakdown of the SC is also attainable as ε_H rises, i.e., at a critical value of the magnetic intensity H_c. Indeed, in view of Eq. (21), kT_c and $\varepsilon_H = h_H H$ are related by (19), which means that as T_c rises, H_c also increases, as is found experimentally and by the BCS theory (see [1]).

Using the Maxwell equations, it is possible to find the relation between the energy quanta ε_H and ε_E and the current j (the last quantity is, of course, the averaged value of (4)). When the three vectors H, $\mathbf{v}^*$, and Δr are mutually perpendicular (as was mentioned above, the vectors $\mathbf{h}_H$ and $\mathbf{h}_E$ are mutually perpendicular too; $\mathbf{h}_H$ is collinear with H, and $\mathbf{h}_E$ and Δr), the following relation holds:

$$\frac{\partial \varepsilon_H}{\partial t} = \frac{\partial \varepsilon_E}{\partial t} + 4\pi \mathbf{h}_E \mathbf{j}\,, \tag{22}$$

which is important for the general theory of superconductivity. In the last case the derivative $\partial\varepsilon_H/\partial t$ becomes zero, while individual terms in the right-hand side of Eq. (22) are different from zero and increase substantially in the case of HTSC. This conclusion is supported by the fact that equations similar to Ginzburg-Landau ones follow from the equation

$$\frac{\partial \varepsilon_E}{\partial t} + 4\pi \mathbf{h}_E \mathbf{j} = 0 \tag{23}$$

(see [1], p. 217).

In the case of HTSC the situation is more pronounced due to greater manifestation of transformation properties of the electronic subsystem. In complex molecules, forming conductors with HTSC, more that one quantum transition is realized with a change in the energy level (there are at least two parameters Δ_1 and Δ_2 (gaps)), which leads inevitably to enhancement of the potential of intermolecular interaction and, consequently, to an increase in the critical parameters.

Although, just as in the above example, Δ_1 and Δ_2 are of the same order of magnitude, as the angle φ increases, the potential of the additional bond becomes proportional to the square of the gap Δ_2, and therefore the critical temperature becomes an order of magnitude higher than that in the case of low-temperature SC (the potential U can be conveniently approximated as a parabola of the function of the angle $\pi - \varphi$).

Superconductivity is a mixed state in a sense that some of the bound molecules have been formed by overcoming the gap Δ_1, and the other molecules the gap Δ_2. A two-component system is formed, which can be inferred from the changes in the critical current caused by an increase in the temperature. As the temperature rises, the bonds formed due to the gap Δ_1 are broken. This is confirmed qualitatively by experimental data of [3] (p. 279), although more detailed measurement of the current j as a function of temperature may be more informative.

In view of the aforesaid, the experimental values of the gap for HTSC are their averaged values in terms of Δ_1 and Δ_2 (the presence of a gap Δ_3 cannot be excluded).

To conclude the work, it should be noted that for HTSC the values or the parameters δ and ξ are inverted. In this case there should be a relation inverse to Eq. (15), single now, $\delta = l_g$ and $\xi = l_H$ and

$$\frac{\xi}{\delta} = \frac{v^*}{c} < 1\,. \tag{24}$$

A deeper energy transition (Δ_2) enhanceas the interaction of adjacent molecules and, accordingly, reduces substantially the coefficient of the correlation bond ($\xi \sim 10^{-7}$ cm).

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NOTATION

n, number of particles; r, position vector; j, current; e, electronic charge; v, velocity; ε, field energy quantum; k, Planck constant; c, velocity of light; H, magnetic field intensity; E, electric field intensity; ω, frequency; λ, wavelength; T_c, critical temperature; Δ, energy gap; t, time.

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