Bragg-Coulomb double-flow mechanism for high-T_c superconductivity

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A mechanism for a high-temperature superconductivity based on the Bragg reflection of electron pairs from a lattice of conducting atomic layers is proposed. The Coulomb repulsion screened by these layers is shown to lead to a high-T_c superconductivity through the formation of two mutually inducing counterflows of paired electrons.

1. Introduction. We are proposing a new mechanism for high-temperature superconductivity in crystals consisting of atomic layers with a period d, which are good conductors, alternating with atomic layers which are poor conductors. Such a structure apparently generates a high-T_c superconductivity in ceramics, leading to a Bragg reflection of conduction electron pairs and triggering the high-T_c superconductivity mechanism (discussed below) as a result screening of the Coulomb repulsion of high characteristic energy, $\hbar\omega_c \sim 1$ eV.

2. Model. We will describe the main points of the mechanism using a simplified

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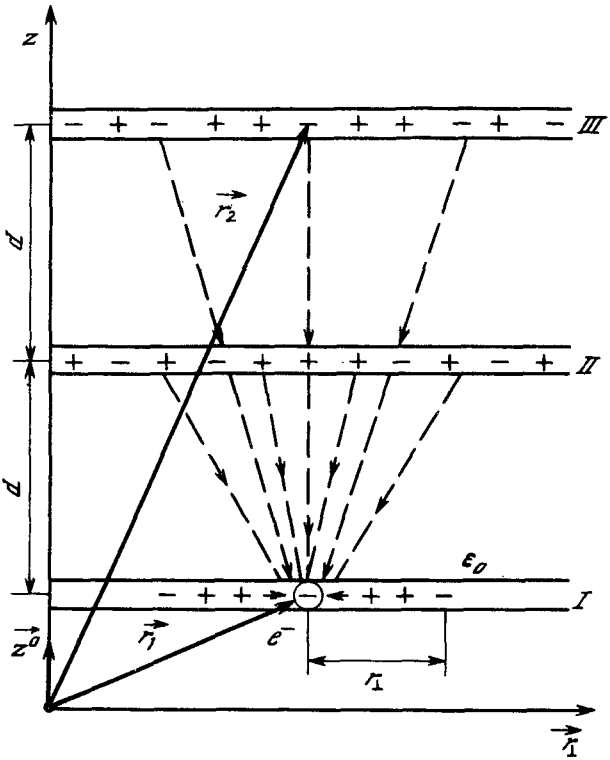
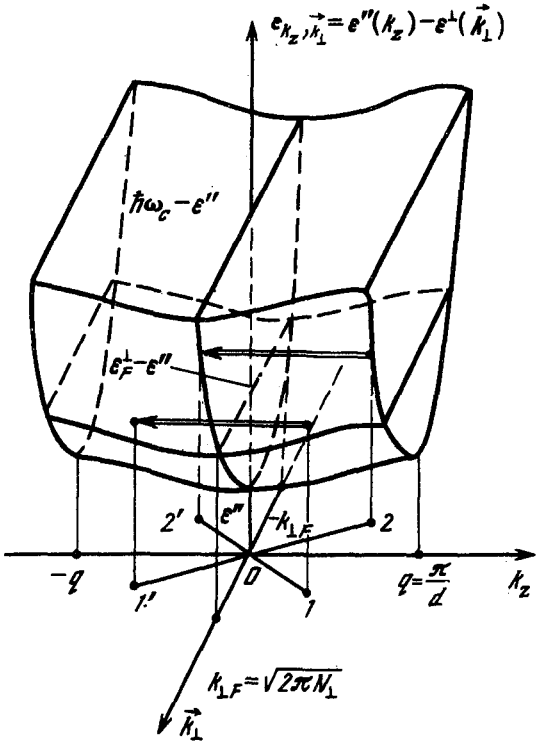


FIG. 1. Diagram of the screening of the Coulomb field of the charge e^- by the conducting layers.

plane-layered model which includes only the basic elements. We take into account the fact that the potential of the Coulomb repulsion of two electrons $v(\mathbf{r}_1,\mathbf{r}_2)$ is modulated along the z axis by the conducting layers which partially screen the potential. This potential depends not only on the relative position of the two electrons, $\mathbf{r}_1 - \mathbf{r}_2$, but also on their absolute position (Fig. 1). This situation causes a Bragg reflection, which is missing in the BCS theory, of the two electrons with the momenta $\hbar\mathbf{k}$ and $-\hbar\mathbf{k} + \hbar q\mathbf{z}^0$ from a pair of electrons with the momenta $\hbar\mathbf{k}'$ and $-\hbar\mathbf{k}' - \hbar q\mathbf{z}^0$ inside the first Brillouin zone $k_z \in (-q,q)$. This reflection is accompanied by a transfer of the momentum $2\hbar q = 2\pi\hbar/d$, but not the energy (by analogy with the Mössbauer effect), to the lattice. This high-temperature superconductivity mechanism is based on precisely a two-electron umklapp process which is characterized by the matrix element $-2\nu_1 = \langle 1'2'|v(\mathbf{r}_1,\mathbf{r}_2)|21\rangle$. The estimate of this process gives[1] $|\nu_1|V = 2\pi\alpha e^2 r_\perp r_\parallel/\epsilon_0$. Here $r_\parallel$ and $r_\perp$ are the radii of the Coulomb screening along the z axis and across it, $r_\perp \sim k_{\perp F}^{-1} = (2\pi N_\perp)^{-1/2}$, $N_\perp = Nd$ is the surface density of the electrons in the conducting layer, ϵ_0 is the "background" permittivity, α is the efficiency of Bragg reflection of the electron pair $(\mathbf{r}_1,\mathbf{r}_2)$ due to the screening by an inhomogeneous conducting layer, which depends on the structure of the lattice of the conducting layers, $\alpha \lesssim 1$; and V is the volume of the crystal.

Assuming $\nu_1 = \text{const}$ and repeating the line of reasoning similar to that which



$$A = \begin{pmatrix} \bar{\varepsilon}_1 & 0 & 0 & 0 \\ 0 & \bar{\varepsilon}_2 & 0 & 0 \\ 0 & 0 & \bar{\varepsilon}_1 & 0 \\ 0 & 0 & 0 & \bar{\varepsilon}_2 \end{pmatrix}$$

$$B = 2\nu_1 \begin{pmatrix} 0 & -\langle b_- \rangle & 0 & 0 \\ \langle b_- \rangle & 0 & 0 & 0 \\ 0 & 0 & 0 & \langle b_+ \rangle \\ 0 & 0 & -\langle b_+ \rangle & 0 \end{pmatrix}$$

FIG. 2. Bragg reflection of paired electrons 1, $2 \to 1'$, $2'$ and matrices for the electron pairing in a double-flow pairing Hamiltonian (2).

was used in the derivation of the pairing Hamiltonian in the BCS theory, we find

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \bar{\varepsilon}_{\mathbf{k}} a^{+}_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} - 2\nu_1 (b^{+}_{-} b_{+} + b^{+}_{+} b_{-});$$

$$b_{+} = \sum_{\mathbf{k}_\perp} \sum_{0 < k_z < q} a_{-k_z+q,\,-\mathbf{k}_\perp,\downarrow} a_{k_z,\mathbf{k}_\perp,\uparrow},$$

$$b_{-} = \sum_{\mathbf{k}_\perp} \sum_{-q < k_z < 0} a_{k_z,-\mathbf{k}_\perp,\downarrow} a_{-k_z-q,\mathbf{k}_\perp,\uparrow}. \qquad (1)$$

In this model Hamiltonian $a_{k_z,\mathbf{k}_\perp,\uparrow}$ is the operator which annihilates the electron with the momentum $\hbar\mathbf{k} = \hbar(k_z\mathbf{z}^0 + \mathbf{k}_\perp)$, the spin $\sigma = \uparrow$, and the energy $\bar{\varepsilon}_{k_z,\mathbf{k}_\perp} = \epsilon^{\perp}(\mathbf{k}_\perp) + \epsilon^{\parallel}(k_z) - \mu$, which is reckoned from the chemical potential μ (Fig. 2). The summation in $b_{\pm}$ is carried out over the region $D_{\pm}$, where $|\bar{\varepsilon}_{k_z,\mathbf{k}_\perp}|$, $|\bar{\varepsilon}_{-k_z \pm q,\mathbf{k}_\perp}| < \hbar\omega_c$. For simplicity we write $\epsilon^{\perp} = (\hbar\mathbf{k}_\perp)^2/2m$.

3. In the self-consistent-field approximation the solution of model (1) is

$$\mathcal{H} \to \widetilde{\mathcal{H}} = \sum_{\mathbf{k}_\perp} \sum_{0<k_z<q} \sum_{i,j=1}^{4} \{A_{ij} c_i^+ c_j + \frac{1}{2}(B_{ij} c_i^+ c_j^+ + B_{ji}^* c_i c_j)\} \; ;$$

$$c_1 = a_{k_z, \mathbf{k}_\perp, \uparrow}, \quad c_2 = a_{-k_z+q, -\mathbf{k}_\perp, \downarrow}, \quad c_3 = a_{-k_z, -\mathbf{k}_\perp, \downarrow}, \quad c_4 = a_{k_z-q, \mathbf{k}_\perp, \uparrow}. \tag{2}$$

Diagonalizing the 4×4 matrix by the canonical-transformation method, we obtain two order parameters for the mutually inducing, paired-electron counterflows $\langle b_+\rangle = \gamma\langle b_-\rangle$, $\langle b_-\rangle = \gamma\langle b_+\rangle$ and a self-consistency equation at an arbitrary temperature T

$$\gamma^2 = 1; \quad \gamma \equiv \frac{\lambda}{2q} \int_{D_\pm} \int_0^{q/2} \frac{\tanh(\Lambda_2/2\kappa T) - \tanh(\Lambda_1/2\kappa T)}{\sqrt{(\bar{\epsilon}_1 + \bar{\epsilon}_2)^2/4 + \tilde{\Delta}^2}} \, dk_z d\epsilon^\perp,$$

$$\lambda = \frac{\nu_1 V m q}{2\pi^2 \hbar^2}, \quad \bar{\epsilon}_1 = \bar{\epsilon}_{k_z, \mathbf{k}_\perp}, \quad \bar{\epsilon}_2 = \bar{\epsilon}_{q-k_z, \mathbf{k}_\perp} \tag{3}$$

This equation determines T_c and the gaps in the quasiparticle spectrum $E_{1,2} = |\Lambda_{1,2}|$, $\Lambda_{1,2} = [\bar{\epsilon}_2 - \bar{\epsilon}_1 \mp \sqrt{(\bar{\epsilon}_2 + \bar{\epsilon}_1)^2 + 4\tilde{\Delta}^2}]/2$, where $\tilde{\Delta} = |2\nu_1\langle b_+\rangle| = |2\nu_1\langle b_-\rangle|$ (Fig.

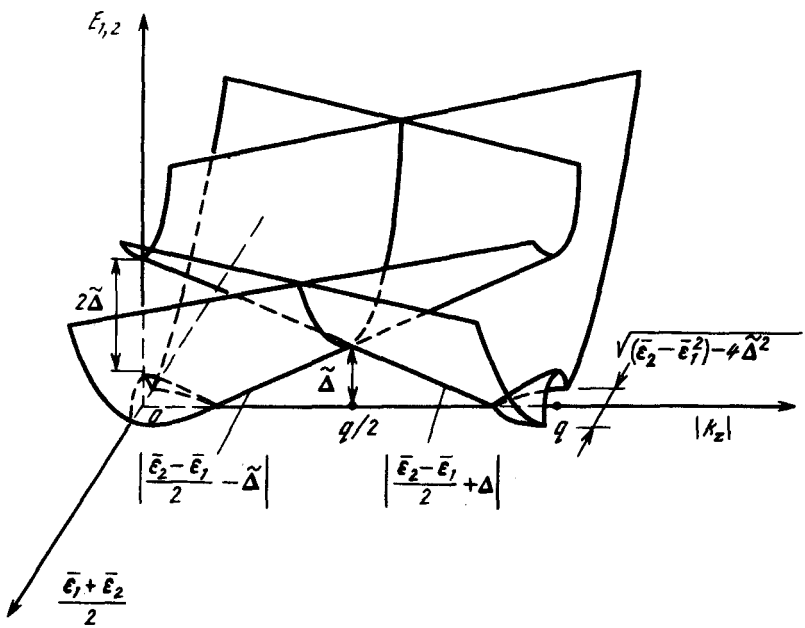


FIG. 3. Spectrum of high-T_c superconductivity quasiparticles which takes the dispersion $\epsilon^{\parallel}(k_z)$ into account. At $2\tilde{\Delta} > |\bar{\epsilon}_2 - \bar{\epsilon}_1| \equiv |\epsilon^{\parallel}(q-k_z) - \epsilon^{\parallel}(k_z)|$ there are no gap-free excitation regions.

3). Result (3) means that high-T_c superconductivity in model (1) occurs at any sign of the ν_1 coupling and as a result of Coulomb repulsion, rather than only as a result of the BCS phonon attraction. In contrast with the BCS model, the electron momenta of an electron pair are directed in the same direction, rather than in the opposite direction, along the z axis.

An estimate of T_c and $\tilde{\Delta}(T=0)$ for a narrow Brillouin zone lying along the k_z axis is $\epsilon^{\parallel}(k_z) \approx \text{const}$ (for high-T_c ceramics its width is $\lesssim 0.2$ eV). If the bond is weak $|\lambda| \ll 1$, and if $2\kappa T_c \ll \mu - \epsilon^{\parallel} \approx \epsilon_F^{\perp} < \hbar\omega_c$, we derive from Eq. (3) the equations

$$\kappa T_c \approx 1{,}14\sqrt{\hbar\omega_c \epsilon_F^{\perp}} \exp\left(-\frac{1}{|\lambda|}\right), \quad 2\tilde{\Delta}(T=0) \approx 3{,}5\,\kappa T_c;$$

$$\epsilon_F^{\perp} = \frac{\hbar^2 k_{\perp F}^2}{2m} = \frac{\pi\hbar^2 N_{\perp}}{m}. \tag{4}$$

Here $\hbar\omega_c = \min\{e^2/r_{\perp}\epsilon_0,\ \Delta\epsilon^{\perp} - \epsilon_F^{\perp}\} \sim 1$ eV is determined either by the Coulomb repulsion energy, $\sim e^2/r_{\perp}\epsilon_0$, or by the width of the energy gap, $\Delta\epsilon^{\perp} > \epsilon_F^{\perp}$, if the band gap is above it, $\Delta\epsilon_g > e^2/r_{\perp}\epsilon_0$.

4. High-temperature superconductivity of layered ceramics ($T_c \sim 100$ K) can be explained by the double-flow Bragg-Coulomb mechanism proposed by us and it corresponds to the actual parameters $N_{\perp} \sim 5\times 10^{14}$ cm^{-2}, $r_{\perp} \sim 2$ Å, $r_{\parallel} \sim d/2$, $m \sim 10m_e$, $\epsilon_0 \sim 5$, $\alpha \sim 0.6$, and $|\lambda| \sim 1/4$. To raise T_c, it is necessary first of all to increase the coupling constant $|\lambda| \propto \alpha r_{\perp} r_{\parallel}/\epsilon_0 d$. High-temperature superconductivity can therefore be achieved at room temperature by fabricating layered materials, in which the conducting layer differs from the CuO layer of the yttrium ceramic and for which the relation between the Bragg reflection parameters and the longitudinal and transverse screening parameters has been improved. The foregoing remarks are consistent with the increase of T_c as the number of CuO layers in the cell for bismuth and thallium ceramics is increased. These remarks are also consistent with the fact that T_c depends slightly on the atomic species of the insulating layers and on the pressure. The last dependence is also characteristic of other layered intercalation superconductors[1]: chalcogenide, graphite, organic, and niobium superconductors in which a double-flow Bragg-Coulomb mechanism operates.

In the case of high-T_c superconductivity the electron (hole) density $N_{\perp}$ should be at a certain maximum value, but not too large. If a ceramic has CuO layers, the electron density is determined by the fractional valence of copper and by the oxygen deficiency. A slight change in the oxygen concentration causes $N_{\perp}$ to fall off from the peak value, reduces the coupling constant, and causes high-T_c superconductivity to vanish. This situation occurs in $YBa_2Cu_3O_{7-\delta}$ at $\delta \gtrsim 0.5$. The paired electrons are found primarily in the near conducting layers, which accounts for the small coherence length ($\sim d \sim 12$ Å), for its anisotropy ($\xi_{\parallel} \sim 10$ Å, $\xi_{\perp} \sim 30$ Å), and for the very strong critical magnetic fields, $H_{c2} \sim 10^6$ G. The observable positive curvature of the $H_{c2}(T)$ curve, which is absent in the BCS theory, may also be attributable to the stratification of the structure.[2]

A jump in the electron specific heat at $T = T_c$, calculated on the basis of the approximations in (4), is $\Delta C_e = 1.43\ (2\pi^2/3)N(0)\kappa^2 T_c \sim 4\times 10^5$ erg/(K·cm^3),

where the state density at the Fermi level is $N(0) = mq/\pi^2\hbar^2 \sim 2\times 10^{34}$ erg^{-1} cm^{-3}. The relative jump $\Delta C_e/C_{en} = 1.43$ is the same as the well-known jump in the BCS model. The indicated values are in agreement with the experimental values, for example, for $YBa_2Cu_3O_7$.

Analysis has shown that Coulomb repulsion inside each of the two electron-pair counterflows [the auxiliary term $-2\nu_0(b_+^+ b_+ + b_-^+ b_-)$ in (1)] weakens high-T_c superconductivity but does not suppress it if the matrix element of the Bragg reflection of the pairs is larger than that of the forward scattering: $|\nu_1| > -\nu_0$. In crude terms, the first harmonic (with respect to the variable $z_1 + z_2$) of the potential $v(\mathbf{r}_1,\mathbf{r}_2)$ must predominate over the zeroth harmonic. The satisfaction of this condition depends on the lattice structure; the optimal ratio of the screening lengths to the layer thicknesses is on the order of 1. Whether v, ν_1, and ν_0 can be calculated for ceramics or whether the condition $|\nu_1| > -\nu_0$ can be satisfied, if only for certain momenta $k_z - k_z'$, remains an open question. A slight BCS phonon attraction affects the high-T_c superconductivity only slightly, consistent with the absence (small value) of the isotope effect in ceramics.

The scatter of the high-T_c superconductivity gap, $2\Delta(0)/\varkappa T_c$, measured in the range from 0.6 to 17, may stem from its anisotropy (which is due to the interaction anisotropy[3]), from the dispersion $\epsilon^{\parallel}(k_z)$, and from the presence of two types of quasiparticles, $E_{1,2}$ (Fig. 3.).

5. The high-temperature superconductivity mechanism proposed by us differs substantially from the mechanisms which were discussed previously. The origin of high-T_c superconductivity can usually be found in the 2D conducting layers. The interaction of electrons in the adjacent layers of the lattice was considered only in several studies, e.g., Refs. 4–6. In those studies and in most of the other studies, as in the BCS theory, the underlying cause, however, is assumed to be the superconductivity due to some sort of attraction (through phonons, excitons, etc.) and the high-T_c superconductivity is explained by a mechanism through which it becomes intensified.[1]

Mathematically, model (1) is similar to a two-zone model[7] and a model which describes the superconductivity better and which takes into account the structural phase transition.[1] Our mechanism for high-T_c superconductivity is, however, of a fundamentally different physical nature which is governed by Coulomb scattering of conduction electron pairs involving an umklapp process inside an energy band.

A Bragg-Coulomb double-flow mechanism can be used to explain the high-T_c superconductivity of ceramics and to show how layered atomic structures with a higher critical temperature can be fabricated. In addition, it offers a positive, constructive solution of an old problem addressing the question of whether a Coulomb high-T_c superconductivity is possible.

[1)] The calculation of v and ν_1 and allowance for the jump-free scattering, whose matrix element ν_0 usually is appreciable compared with ν_1, are outside the scope of this model.

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