Mechanism for high-T_c superconductivity in $(Ca_{1-x}Sr_x)_{1-y}CuO_2$ with an "infinite" number of cuprate layers

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A plasmon mechanism for superconductivity is discussed. In this mechanism the superconductivity results from a Cooper pairing of light carriers as a result of their interaction with collective excitations of the charge density of heavy carriers (acoustic plasmons). This occurs in layered crystals with closely packed superconducting layers, as the result of a proximity effect and local-field corrections. For this mechanism, the electron–plasmon interaction constant increases faster than linearly with an increase in the number (n) of interacting layers which are in a common, coherent superconducting state. The increase in the transition temperature T_c with increasing n then quickly reaches saturation because of strong-coupling effects. This circumstance explains the high value $T_c > 110$ K in the compound $(Ca_{1-x}Sr_x)_{1-y}CuO_2$ as $n \to \infty$.

1. The new metal oxide compound $(Ca_{1-x}Sx_x)_{1-y}CuO_2$, with an "infinite" number of cuprate (CuO_2) layers, was recently synthesized. This compound does not contain intermediate layers of BiO and SrO or TlO and BaO, but it nevertheless exhibits a high superconducting transition temperature,[1] $T_c \approx 110$ K.

This result is evidence that the 2D CuO_2 layers play a key role in the superconductivity of these cuprate metal–oxide compounds, while the insulating oxide layers (BiO, SrO, TlO, BaO, or LaO) play a secondary, auxiliary role. On the other hand, intermediate layers of Ca^{2+} ions are important structural elements. They lead to a strong ionic bonding between the cuprate (CuO_2) layers (in $YBa_2Cu_3O_{7-\delta}$, this role is played by layers of Y^{3+} ions). The stoichiometric compound $CaCuO_2$ is a simple layered crystal with a single CuO_2 layer in the primitive cell. It would seen that a single crystal of this sort should have a relatively low transition temperature $T_c < (20–30)$ K, as in the case of cuprates such as $La_{2-x}(Ba,Sr)_xCuO_4$ and $Bi_2Sr_2CuO_x$ (the Michel–Raveau phase).

In the present letter we show that the high-T_c superconductivity of $(Ca_{1-x}Sr)_{1-y}CuO_2$ with $n \to \infty$ may be due to a proximity effect involving the superconducting CuO_2 layers, which are separated by a distance $d_0 \approx 3$ Å, which is comparable to the transverse coherence length $\xi_\perp \ll \xi_\parallel$. Here $\xi_\parallel$ ($\xi_\parallel > 10$ Å) is the longitudinal coherence length in the plane of the layers. The situation is similar to that involving the CuO_2 layers in the cuprates $Bi_2Sr_2Ca_{n-1}Cu_nO_x$ ($n \geqslant 2$; Refs. 2 and 3) and $Tl_mBa_2Ca_{n-1}Cu_nO_x$ ($m = 1,2$; Refs. 4–7) with a packet structure (Fig. 1). High values $T_c > 100$ K are reached by virtue of a plasmon superconductivity mechanism.[8]

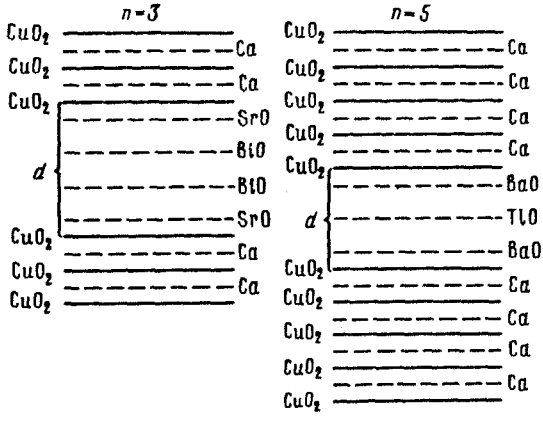

FIG. 1.

2. The presence of groups of insulating layers, BiO and SrO or TlO and BaO, in the cuprates BiSrCaCuO or TlBaCaCuO, has the consequence that the distance ($d > 10$ Å) between packets of n conducting CuO_2 layers separated by $(n-1)$ layers of Ca^{2+} ions is considerably larger than the distance ($d_0 \approx 3$ Å) between the CuO_2 layers in a packet. Furthermore, the condition $d \gg \xi_\perp = \xi_\parallel \sqrt{m_\parallel^*/m_\perp^*}$ holds, where $\xi_\perp$ and $m_\perp^*$ are the transverse (with respect to the plane of the layers) coherence length and effective mass, and $\xi_\parallel$ and $m_\parallel^*$ are the corresponding longitudinal values.[9] On the other hand, we have $d_0 \sim \xi_\perp$. Consequently, a proximity effect occurs between the superconducting CuO_2 layers in the packet, and the coupling between packets is weak (it is a Josephson coupling).

In a study of the superconducting state in these metal oxides we can accordingly restrict the analysis, in a first approximation, to an individual packet of n CuO_2 layers, ignoring the periodicity along the z axis and associated Umklapp processes.[10] This periodicity is automatically disrupted in thin films and in fine-grain ceramic cuprates. Nevertheless, the values of T_c in these cases are essentially the same as in single crystals. This result is evidence in favor of the model proposed here.

Because of the pronounced anisotropy of the effective masses of the quasiparticles in the 2D conducting layers ($m_\perp^*/m_\parallel^* \gtrsim 10^2$–$10^3$), we can separate the "fast" longitudinal variables from the "slow" transverse variables corresponding to the motion of electrons (holes) in the one-particle normal and anomalous Green's functions:

$$G(x-x', \quad y-y';z) = i\langle \Psi_\parallel(x,y)\Psi_\parallel^+(x',y')\rangle |\Psi_\perp(z)|^2, \tag{1}$$

$$F(x-x', \quad y-y';z) = i\langle \Psi_\parallel(x,y)\Psi_\parallel(x',y')\rangle \Psi_\perp^2(z), \tag{2}$$

where

$$|\Psi_\perp(z)|^2 \sim \sum_{j=1}^{n} \exp\{-|z-z_j|/l_0\}, \tag{3}$$

and l_0 is a scale length of the decay of the electron (hole) density with distance from the plane of the layer, along the coordinate z_j.

A Fourier component of the transverse density distribution (3) in a packet of n conducting layers is

$$\Psi_\perp^2(p_z,n)=\begin{cases}\dfrac{1}{1+(p_z l_0)^2}\left[1+2\sum\limits_{m=1}^{k-1}\cos mp_z d_0\right], & n=2k-1;\quad (k=1,2,3\ldots)\\ \dfrac{2}{1+(p_z l_0)^2}\sum\limits_{m=1}^{k}\cos\dfrac{(2m-1)}{2}p_z d_0, & n=2k.\end{cases} \tag{4}$$

The structure factor of the electron density of the packet, which appears in the equations for the normal self-energy part (Σ, the mass operator) and the anomalous one (Δ, the gap parameter),[10] takes the following form in the limit $l_0\to 0$:

$$\beta(n)\equiv c(n)\int_{-\pi/c(n)}^{\pi/c(n)}\frac{dp_z}{2\pi}\Psi_\perp^2(p_z,n)$$
$$=\begin{cases}1+\dfrac{2c(n)}{\pi d_0}\sum\limits_{m=1}^{k-1}\dfrac{1}{m}\sin\dfrac{m\pi d_0}{c(n)}, & n=2k-1\\ \dfrac{4c(n)}{\pi d_0}\sum\limits_{m=1}^{k}\dfrac{1}{(2m-1)}\sin\dfrac{(2m-1)\pi d_0}{2c(n)}, & n=2k\end{cases}, \tag{5}$$

where $c(n)=d+(n-1)d_0$ is the lattice constant along the z axis.

On the other hand, the structure factor which figures in the electron polarization operator II (Ref. 10) is given by ($l_0=0$)

$$\tilde{\beta}(n)\equiv c(n)\int_{-\pi/c(n)}^{\pi/c(n)}\frac{dp_z}{2\pi}\Psi_\perp^4(p_z,n)=n+\frac{2c(n)}{\pi d_0}\sum_{m=1}^{n-1}\frac{n-m}{m}\sin\frac{m\pi d_0}{c(n)}. \tag{6}$$

It is easy to see that under the conditions $n\gg 1$ and $c(n)\gg\pi d_0$ the following equations hold quite accurately:

$$\beta(n)=n;\quad \tilde{\beta}(n)=n+2\sum_{m=1}^{n-1}(n-m)=n^2. \tag{7}$$

3. As in Ref. 10, we assume at this point that the primary mechanism for the high-T_c superconductivity in the layered cuprates is a plasmon mechanism.[8]

In this case the electron–plasmon interaction constant is given by

$$\lambda_{pl}(n)=-\frac{2}{\pi}\nu_l\beta(n)\int_0^\infty\frac{d\omega}{\omega}\langle V_C(\mathbf{q})\mathrm{Im}\tilde{\varepsilon}^{-1}(\mathbf{q},\omega)\Gamma_C(\mathbf{q},\omega)\rangle, \tag{8}$$

where $\nu_l=m_l^*/2\pi$ is the density of states of the l carriers, with an effective mass $m_l^*\sim m_0$ (m_0 is the mass of a free electron); $\tilde{\varepsilon}(\mathbf{q},\omega)$ is the generalized dielectric constant of the crystal; Γ_C is the Coulomb vertex, which satisfies the Ward (–Pitaevskiĭ) identity[11,12] as $q\to 0$ and $\omega\to 0$; and V_C is the matrix element of the

unscreened Coulomb interaction in a layered crystal with a packet structure. This matrix element is given for arbitrary $q_\parallel$ and q_z by

$$V_C(q_\parallel, q_z, n) = \frac{2\pi e^2}{q_\parallel}\left\{\frac{\sinh q_\parallel c(n)}{\cosh q_\parallel c(n) - \cos q_z c(n)}\left[1 + 2\sum_{m=1}^{n-1} \cos mq_z d_0 e^{-mq_\parallel d_0}\right]\right.$$
$$\left. + 2\sum_{m=1}^{n-1} \cos mq_z d_0 e^{mq_\parallel d_0}\left[\frac{\sinh q_\parallel c(n)}{\cosh q_\parallel c(n) - \cos q_z c(n)} - 1\right]\right\}. \quad (9)$$

The angle brackets in (8) mean an average over the cylindrical Fermi surface of the l carriers. When this average is taken, the value of λ_{pl} is dominated by large values $q_\parallel \approx 2k_{Fl} \gg 1/c(n)$, where k_{Fl} is the Fermi momentum of the l carriers, so we have $V_C(q) \approx 2\pi e^2/q_\parallel$.

For $n=1$ and $n \to \infty$, expression (9) becomes the known[13,14] expression for $V_c(q_\parallel, q_z)$ in a simple layered crystal with distances d and d_0 between layers.[1)]

4. According to Ref. 8, in an ionic crystal, with a static dielectric constant satisfying $\epsilon_0 \gg \epsilon_\infty$, where ϵ_∞ is the optical dielectric constant of the lattice, the electron–plasmon interaction constant λ_{pl} is essentially the same as the Coulomb-repulsion constant μ_C at high energies ($\omega \gtrsim E_{Fl}$ is the Fermi energy of the l carriers). It is given approximately by

$$\lambda_{pl}(n) \approx \mu_C(n) \approx \frac{\alpha_l}{2} n; \quad \alpha_l = 1/k_{Fl} a_l^*, \quad (10)$$

where $a_l^* = \epsilon_\infty/m_l^* e^2$ is the effective first Bohr radius of the l carriers.

However, the effective electron–plasmon interaction constant which is directly responsible for the Cooper pairing of the l carriers can be estimated from the following expression, where we are incorporating a renormalization of the "extra" Coulomb vertex $\Gamma_C \approx 1 + \lambda_{pl}$ in the equation for the gap due to local-field effects:[15,16]

$$\tilde{\lambda}_{pl} = -\frac{2}{\pi} \nu_l \beta(n) \int_0^\infty \frac{d\omega}{\omega} \langle V_C(\mathbf{q}) \operatorname{Im} \tilde{\varepsilon}^{-1}(q,\omega) \Gamma_C^2(\mathbf{q},\omega) \rangle \approx \lambda_{pl}(1+\lambda_{pl}). \quad (11)$$

As a result, for a spectrum with a single vibrational mode at the frequency of hybrid phonon–plasma oscillations with $q_\parallel \approx 2k_{Fl}$ (Ref. 8), we have

$$\tilde{\Omega}_+(n) \approx \left[\frac{n^2 \Omega_h^2 k_{Fl} d + \omega_{LO}^2}{1 + \alpha_l n^2}\right]^{1/2}. \quad (12)$$

Here $\Omega_h = \sqrt{4\pi e^2 N_h/\epsilon_\infty m_h^* d}$ is the plasma frequency of the h carriers in a narrow 2D band with a 2D density N_h and an effective mass $m_h^* = 4/a^2 W_h \gg m_l^*$ (W_h is the width of the narrow band, and a is the lattice constant in the plane of the layers), and ω_{LO} is the frequency of the dipole-active longitudinal optical vibrations of the O^{2-} oxygen ions in the CuO_2 layers. The exponential expression derived from T_c in Ref. 17 becomes

$$T_C(n) = \tilde{\Omega}_+(n) \exp\{-1/\Lambda(n)\}, \quad (13)$$

where

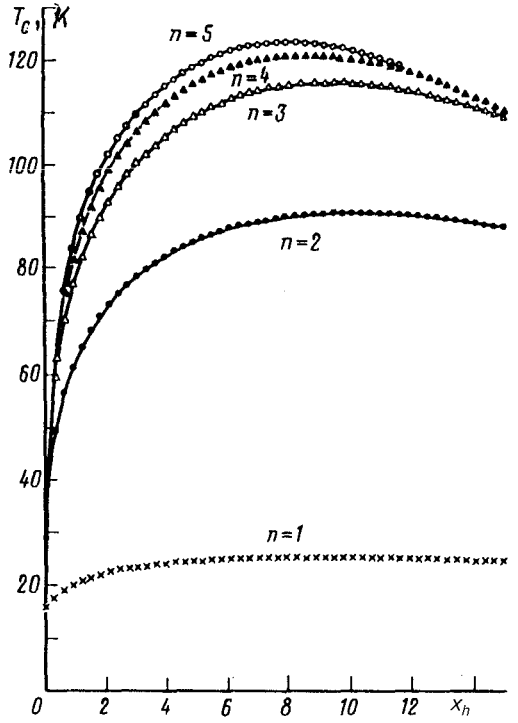

FIG. 2.

$$\Lambda(n)=\frac{\tilde{\lambda}_{pl}(n)-\tilde{\mu}_C^*(n)[1+\tilde{\lambda}_{pl}(n)\ln 2]}{1+\lambda_{pl}(n)+\tilde{\lambda}_{pl}(n)\ln 2}; \tag{14}$$

$$\tilde{\mu}_C^*(n)=\tilde{\mu}_C(n)[1+\tilde{\mu}_C(n)\ln(\tilde{E}_{Fl}/\tilde{\Omega}_+)]^{-1}; \quad \tilde{\mu}_C(n)\approx\tilde{\lambda}_{pl}(n); \tag{15}$$

and $\tilde{E}_{Fl}$ is the Fermi energy of the l carriers, renormalized because of the Fermi–liquid (Coulomb) interaction.

It follows from (11), (14), and (15) that the local-field corrections to the Coulomb vertex completely cancel out the nonadiabatic renormalization $(1+\lambda_{pl})$ of the effective electron–plasmon interaction constant which is characteristic of strong-coupling superconductors.[16] This circumstance was pointed out in Ref. 15. Consequently, Λ increases substantially, promoting high T_c's.

Figure 2 shows plots of $T_c(n)$ versus the parameter $x_h=\Omega_h^2/\omega_{LO}^2$, for various values $n=1$–5. In other words, this is essentially a plot against the dopant or oxygen concentration, since the "pinning" of the Fermi level in the narrow 2D band with the high density of states ($\nu_h\gg\nu_l$), which arises in the course of the doping, raises the density of h carriers, while the density of the l carriers, $\bar{n}_l$, remains nearly constant (if $\nu_l=$const). In a numerical calculation based on (13)–(15), we selected the following

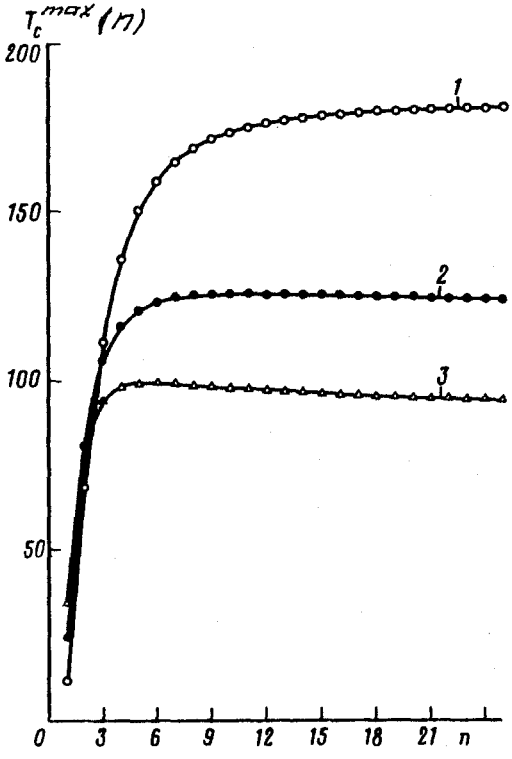

FIG. 3.

parameter values, which are typical of the cuprates: $a=4$ Å, $m_l^*=1.8\,m_0$, $\epsilon_\infty=4$, $\omega_{LO}=300$ K, and $\bar{n}_l=4\times10^{21}$ cm^{-3}. We see that the theoretical curves agree completely satisfactorily, both qualitatively and quantitatively, with the experimental plots of T_c versus the dopant concentration, i.e., versus the number of holes in the primitive cell per CuO_2 layer.[18,19]

5. According to (11), (12), (14), and (15), in the limit $n\to\infty$ the coupling constant $\Lambda(n)$ and the frequency $\tilde{\Omega}_+(n)$ tend toward constant limiting values:

$$\Lambda_\infty=\frac{1}{\ln 2}-\frac{1}{\ln(\tilde{E}_{Fl}/\tilde{\Omega}_+^\infty)};\quad \tilde{\Omega}_+^\infty=\Omega_h\sqrt{k_F d/\alpha_l}. \tag{16}$$

Under the condition $\tilde{E}_{Fl}>2\tilde{\Omega}_+^\infty$, according to (13), these values correspond to the asymptotic value

$$T_c^\infty=\tilde{\Omega}_+^\infty\exp\{-1/\Lambda_\infty\}. \tag{17}$$

Figure 3 shows plots of the maximum value of T_c with respect to $x_h\sim N_h$ versus n for the same parameter values as in Fig. 2; curve 1 corresponds to $m_l^*=m_0$, curve 2 to $m_l^*=1.5m_0$, and curve 3 to $m_l^*=2m_0$. We see that the last of these curves agrees

most accurately with the experimental data on the cuprates $TlBa_2Ca_{n-1}Cu_nO_x$ with a single TlO layer ($n=1$) (Refs. 6 and 7), while at $n \geqslant 4$ we see a slight decrease in T_c.

On the other hand, it follows from this model for a plasmon mechanism for superconductivity in a system of closely packed cuprate layers[8,10] that with increasing number (n) of interacting superconducting layers, dependence of T_c quickly reaches saturation at $T_c > 100$ K, because of a proximity effect and because of renormalizations of the electron–plasmon interaction constant due to local-field and strong-coupling effects. This conclusion agrees with experimental data on the compound $(Ca_{1-x}Sr_x)_{1-y}CuO_2$ with an "infinite" number of CuO_2 layers.[1]

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[1)]An incorrect expression was written for $V_C(q_\parallel, q_z n)$ in Ref. 10. That expression does not satisfy the limits in the cases $n=1$ and $n \to \infty$, but it does give the correct result for $q_\parallel c(n) \gg 1$.

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