Plasmon superconductivity as a possible reason for the increase in the transition temperature in multilayer cuprate metal oxides

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A plasmon mechanism for superconductivity in a layered metal with a narrow 2D band near the Fermi level leads to an increase in the transition temperature T_c upon an increase in the number (n) of conducting layers in the primitive cell. There is a tendency toward saturation at large values of n. This behavior is in qualitative agreement with the experimental behavior of T_c as a function of n in the cuprate metal oxides $Bi_2Sr_2Ca_{n-1}Cu_nO_x$ and $Tl_mBa_2Ca_{n-1}Cu_nO_x$.

1. In the layered cuprate metal oxides, it has been found that T_c tends to increase with increasing number (n) of CuO_2 layers (Chu's rule). This increase in T_c , with a subsequent tendency toward saturation (and even some decrease, at $n \ge 4$), is seen in compounds with the general formulas $\text{Bi}_2\text{Sr}_2\text{Ca}_{n-1}\text{Cu}_n\text{O}_x$ (n=1-3; Refs. 1 and 2) and $\text{Tl}_m\text{Ba}_2\text{Ca}_{n-1}\text{Cu}_n\text{O}_x$ (n=1-5,m=1,2; Refs. 3 and 4). In these compounds, 2D CuO_2 cuprate layers alternating with monatomic layers of Ca lie in closely-packed stacks in which the CuO_2 layers are separated by a distance $d_0 \approx 3.2 \text{ Å}$. The distance between these stacks in the compounds with two BiO or TlO layers is $d \approx 12 \text{ Å}$; the corresponding distance in compounds with a TlO monolayer in the primitive cell of the crystal is $d \approx 9.6 \text{ Å}$.

In the present letter we show that this n dependence of T_c in the multilayer cuprate metal oxides might be caused by two factors. First, it might be caused by a nonuniform distribution (along the z axis) of the density of "light" current carriers (l) in a wide 2D band. These carriers would be localized in the planes of the CuO_2 conducting layers. The second possibility is a Coulomb interaction between the charges in the layers. This interaction underlies the electron-plasmon interaction with low-frequency collective excitations of the charge density of "heavy" carriers (h) in a narrow 2D band. These excitations are acoustic plasmons. This Coulomb interaction also underlies the polar electron-phonon interaction with dipole-active ion vibrations: optical phonons hybridized with acoustic plasmons.

2. We consider a layered crystal with n equivalent conducting layers in the primitive cell. These layers are gathered in $stacks^{1)}$ (Fig. 1). We take account of retardation effects due to the electron-plasmon interaction with virtual acoustic plasmons and also the electron-phonon interaction with one of the optical branches (an oxygen vibrational mode in CuO_2 layers). We adopt the generalized jellium model. We can then write the screened electron-electron interaction as^{5,6}

$$\tilde{V}_{ll}(\vec{q},\omega) = V_C(\vec{q})/\tilde{\epsilon}(\vec{q},\omega). \tag{1}$$

Here $\tilde{\epsilon}(\vec{q},\omega)$ is the effective dielectric constant of a layered metal with overlapping 2D

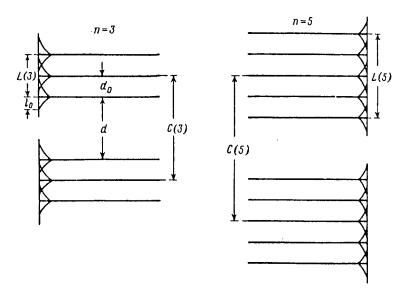


FIG. 1.

bands, one wide and one narrow, in the electron spectrum of the layers:

$$\tilde{\epsilon}(\vec{q},\omega) = \epsilon_i - V_c(\vec{q})[\Pi_l(\vec{q},\omega) + \Pi_h(\vec{q},\omega)] - \frac{\omega_{LO}^2 - \omega_{TO}^2}{\omega^2 - \omega_{TO}^2}.$$
 (2)

Here Π_l and Π_h are the polarization operators of the l and h carriers; ω_{LO} and ω_{TO} are the frequencies of longitudinal (LO) and transverse (TO) phonons; ϵ_i is the part of the dielectric constant which stems from the polarization of the ion lattice and interband transitions; and V_c is the matrix element of the unscreened Coulomb interaction. In a crystal with n equivalent layers in the primitive cell, this matrix element is given bv²⁾

$$V_{C}(q_{\parallel}, q_{z}, n) = \frac{2\pi e^{2}c(n)}{q_{\parallel}} \left\{ \frac{\operatorname{sh} q_{\parallel}c(n)}{\operatorname{ch} q_{\parallel}c(n) - \cos q_{z}c(n)} + 2\sum_{m=1}^{n-1} \cos mq_{z}d_{0} \left[e^{-mq_{\parallel}d_{0}} + e^{mq_{\parallel}d_{0}} \left(\frac{\operatorname{sh} q_{\parallel}c(n)}{\operatorname{ch} q_{\parallel}c(n) - \cos q_{z}c(n)} - 1 \right) \right] \right\},$$
(3)

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

3. The degenerate l carriers in the wide 2D band in the superconducting state have normal and anomalous eigenenergy components which are due to the electronplasmon interaction and the polar electron-phonon interaction. If we ignore Coulomb correlations ("local-field effects"), these components are determined by the system of integral equations^{5,6}

$$\Sigma_l(\vec{p}, i\omega_n) = T \sum_{\omega_m} \int \frac{d^3p'}{(2\pi)^3} \tilde{V}_{ll}(\vec{p}' - \vec{p}, i\omega_m - i\omega_n) G_l(\vec{p}', i\omega_m); \tag{4}$$

334

$$\Delta_{l}(\vec{p}, i\omega_{n}) = T \sum_{l,m} \int \frac{d^{3}p'}{(2\pi)^{3}} \tilde{V}_{ll}(\vec{p}' - \vec{p}, i\omega_{m} - i\omega_{n}) F_{l}(\vec{p}', i\omega_{m}). \tag{5}$$

Here G_l and F_l are the normal and anomalous Green's functions of the l carriers. Under the condition that the variables representing the fast longitudinal motion of the electrons (in the plane of the layers) and the adiabatically slow transverse motion of the electrons (in the direction perpendicular to the layers) can be separated, ³⁾ the pole parts of these Green's functions can be written in the following form, as $T \rightarrow T_c$:

$$G_l(p_{\parallel}, p_z, i\omega_n) = \frac{\Psi_{\perp}^2(p_z)}{i\omega_n - \xi_l(p_{\parallel}) - f_l(i\omega_n)};$$
(6)

$$F_{l}(p_{\parallel}, p_{z}, i\omega_{n}) = \frac{\Delta_{l}(p_{\parallel}, i\omega_{n})\Psi_{\perp}^{2}(p_{z})}{[i\omega_{n} - \xi_{l}(p_{\parallel}) - f_{l}(i\omega_{n})] \cdot [i\omega_{n} + \xi_{l}(p_{\parallel}) - f_{l}(i\omega_{n})]}.$$
(7)

Here $\xi_l(p_{\parallel})$ is the energy of the longitudinal motion, reckoned from the renormalized Fermi level; $f_l(i\omega_n)$ is the odd part (in terms of the sign of ω_n) of Σ_l ; and $\Psi_{\perp}^2(p_z)$ is a Fourier component of the transverse distribution of the nonuniform electron density in the layers, $|\Psi_{\perp}(z)|^2 \sim \sum \exp\{-|z-z_i|/l_0\}$. Here l_0 is the length scale of the exponential decay (Fig. 1) with distance from the planes of the layers at the points $z=z_i$.

As a result, we can distinguish a dimensionless structure factor in (4) and (5), making use of (1), (3), (6), and (7):

$$\beta(n) = c(n) \int_{-\pi/c(n)}^{\pi/c(n)} \frac{dp_z}{2\pi} \sum_{k=-\infty}^{\infty} \Psi_{\perp}^2 \left(p_z + \frac{2\pi k}{c(n)}, n \right), \tag{8}$$

The terms with $k \neq 0$ correspond to umklapp processes in terms of p_z .

Correspondingly, in a calculation of the polarization operators for the l carriers $(T \rightarrow T_c)$,

$$\Pi_l(q, i\omega_n) = 2T_c \sum_{\omega_m} \int \frac{d^3p'}{(2\pi)^3} G_l(p', i\omega_m) G_l(p' - q, i\omega_m - i\omega_n), \qquad (9)$$

we can distinguish a corresponding structure factor

$$\tilde{\beta}(n) = c(n) \int_{-\pi/c(n)}^{\pi/c(n)} \frac{dp_z}{2\pi} \sum_{k=-\infty}^{\infty} \Psi_{\perp}^4 \left(p_z + \frac{2\pi k}{c(n)}, n \right). \tag{10}$$

If umklapp processes are ignored (K=0), and if the condition $l_0 \ll d_0$ holds, the contributions of the individual layers in the stacks are nearly additive. In other words, we have $\beta(n) \approx n$ and $\widetilde{\beta}(n) \approx n^2$ (Fig. 2a). With increasing l_0 , on the other hand, $\beta(n)$ and $\widetilde{\beta}(n)$ decrease (Fig. 2b).

4. It follows that the constant of the electron-plasmon interaction and of the

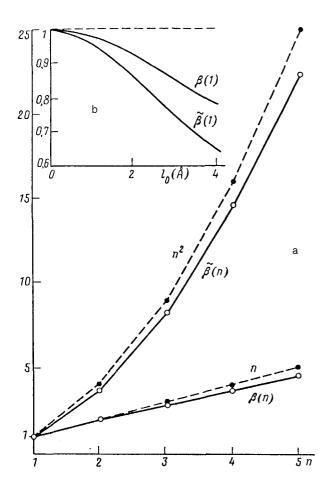


FIG. 2.

polar electron-phonon interaction,

$$\lambda_{pl}(n) = -\frac{2}{\pi} \nu_l \frac{\beta(n)}{c(n)} \int_0^\infty \frac{d\omega}{\omega} < V_c(q_{\parallel}, n) \operatorname{Im} \tilde{\epsilon}^{-1}(\vec{q}, \omega) >, \tag{11}$$

and the dimensionless constant of the Coulomb repulsion,

$$\mu_C(n) = \nu_l \frac{\beta(n)}{c(n)} < V_C(q_{\parallel}, n) \cdot \operatorname{Re}\tilde{\epsilon}^{-1}(\vec{q}, \omega_{max}) >, \tag{12}$$

increase in a nearly linear fashion with increasing number of cuprate layers in the primitive cell. Here $vl = m_i^*/2\pi$ is the density of states in the wide 2D band with an effective mass $m_l^* \sim m_0$ (m_0 is the mass of a free electron); we have $V_C(q_{\parallel},n) \approx 2\pi e^2 \cdot c(n)/q_{\parallel}$ under the conditions $q_{\parallel}c(n) \gg 1$ and $q_{\parallel}d_0 \gg 1$ [see (3)]; $\omega_{\rm max}$ is the cutoff energy of the interaction between quasiparticles, which is equal in order of magnitude of the Fermi energy of the l carriers, i.e., E_{Fl} ; and the angle

336

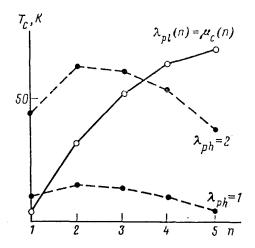


FIG. 3

brackets $\langle ... \rangle$ mean an average over the Fermi surface. Here we have $q_{\parallel} \approx 2k_{Fl}$, where $k_{Fl} = \sqrt{2\pi N_l}$ is the Fermi momentum of the l carriers, and N_l is the 2D density of these carriers in a CuO₂ layer.

We wish to stress that the constant of the nonpolar electron–phonon interaction, which differs from $V_c(q_{\parallel},n)$ in that it does not explicitly contain the lattice constant c(n), can be written in the form $\tilde{\lambda}_{\rm ph}(n) = \lambda_{\rm ph} \beta(n)/c(n)$, where $\lambda_{\rm ph}$ is the constant of the electron–phonon interaction in the n=1 case. In other words, $\tilde{\lambda}_{\rm ph}(n)$ increases far more slowly than $\lambda_{\rm pl}(n)$ or $\mu_C(n)$ with increasing n.

The solid lines with the circles in Fig. 3 show the n dependence of the maximum of T_c over the variable representing the plasma frequency of the h carriers, i.e., Ω_h . These results were calculated in the intermediate-coupling approximation^{6,8} for a "plasmon" mechanism for superconductivity, on the basis of a single-mode model of the optical phonon spectrum. The frequency of the hybrid phonon-plasma oscillations is⁵

$$\tilde{\Omega}_{+}(n) \approx \left[\frac{\Omega_{h}^{2} \tilde{\beta}(n) k_{Fl} d + \omega_{LO}^{2}}{1 + \alpha_{\infty} \tilde{\beta}(n)} \right]^{1/2}; \quad \alpha_{\infty} = \frac{e^{2} m_{l}^{*}}{\epsilon_{\infty} k_{Fl}}, \tag{13}$$

where $\lambda_{\rm pl}(n) = \mu_C(n) = \alpha_{\infty}/2\beta(n)$, and $\epsilon_l = \epsilon_{\infty}$, $\omega_{LO}^2 \gg \omega_{TO}^2$. Here we are using the following relationship between the average bulk density of l carriers, \bar{n}_l , and the 2D density of these carriers in a layer: $N_l = \bar{n}_l c(n)/n$. We thus have $k_{Fl}(n) = \sqrt{2\pi\bar{n}_l c(n)/n}$. Under the condition⁴⁾ ($\bar{n}_l \approx \text{const}$, this quantity is a decreasing function of n, while the dimensionless density parameter $\alpha_{\infty} \sim k_{Fl}^{-1}$ is an increasing function of n. We see that T_c increases with increasing n and tends toward saturation. This behavior is in agreement with experimental results. For these calculations we used the following parameter values: $\bar{n}_l = 6 \times 10^{21} \text{ cm}^{-3}$, $k_{Fl}(1) = 6 \times 10^7 \text{ cm}^{-1}$, $\epsilon_{\infty} = 4$, $m_l^* = 2m_0$, $\omega_{LO} = 320$ K, and $E_{Fl} = 0.3$ –0.6 eV in the Coulomb pseudopotential

$$\mu_C^*(n) = \mu_C(n) [1 + \mu_C(n) \ln(E_{Fl}/\tilde{\Omega}_+)]^{-1}. \tag{14}$$

In contrast, the curves of T_c versus n in the case of a nonpolar electron-phonon interaction (the dashed lines in Fig. 3, with $\lambda_{\rm ph}=1$ and $\lambda_{\rm ph}=2$), calculated with the same parameter values, have nothing in common with the experimental $T_c(n)$ dependence.

We thus see that the plasmon mechanism for high- T_c superconductivity⁵ leads to a qualitatively correct description of the behavior of T_c in the multilayer cuprate copper oxides of the BiSrCaCuO and TlBaCaCuO types. This mechanism arises from an electron–plasmon interaction and a polar electron–phonon interaction, with a hybridization of acoustic plasmons with optical phonons (oxygen vibrational modes), and a nonuniform distribution of the electron density in stacks of conducting CuO_2 layers (Fig. 1).

Translated by D. Parsons

¹⁾ We are thinking of the CuO₂ layers in the cuprate metal oxides. Insulating layers of other oxides play the role of an intermediate medium with an effective dielectric constant.

²⁾ Griffin has studied the Coulomb interaction in layered crystals with nonequivalent layers. Expression (3) was derived by Yu. M. Malozovskii.

³⁾ This case corresponds to a pronounced anisotropy of the effective mass $(m_{\parallel}^* \gg m_{\parallel}^*)$ and a slight corrugation of a cylindrical Fermi surface. A corresponding separation of variables has been proposed for the h carriers in a narrow 2D band near the Fermi level.⁶

⁴⁾ The reason for the nearly constant density of *l* carriers is the pinning of the Fermi level near the edge of the narrow band, with a high density of states.⁶

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