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Role of interlayer coupling in oxide superconductors

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The role of interlayer coupling in high-T_c oxide superconductors is considered. Within the assumption that the direct hopping between layers is vanishingly small, we find that the interlayer coupling in the particle-particle channel caused by interactions plays a very important role in the enhancement of T_c and stabilizes the superconducting order with respect to fluctuations. The interlayer coupling in the particle-hole channel plays a relatively minor role. The introduction of a small interlayer hopping matrix element reduces T_c in the lowest-order approximation.

The recent discovery of high-T_c superconductivity in Cu-based oxide superconductors[1-6] has generated enormous interest in the origin of pairing in these materials. Several theories have appeared proposing that a new mechanism for superconductivity may be responsible for $T_c \sim 100$ K. The mechanisms invoked include the resonating valence-bond state,[7-11] antiferromagnetic spin fluctuations,[12] excitons,[13] and plasmon-mediated pairing,[14,15] as well as the bipolarons.[16] The anomalously strong electron-phonon interaction has also been pointed to as a possible source of high T_c.[17-19] Most of the above models, although not all of them, emphasize a two-dimensional character of the electronic states in oxide superconductors, with "nesting" of the Fermi surface in a square lattice playing a prominent role in the enhancement of T_c. The band-structure calculations for the layered perovskites $La_{2-x}Ba_xCuO_4$,[17,18] and $YBa_2Cu_3O_{6.9}$,[19] reveal the antibonding Cu $d_{x^2-y^2}$ and oxygen p orbital-derived bands at the Fermi level with very little dispersion along the z axis, supporting the picture of a quasi-two-dimensional layered character of these compounds.

In this context the question arises as to why the superconducting transition is so sharp, at least in the resistivity,[20] and what is the nature of fluctuations in these systems? In ordinary layered superconducting structures, the phase fluctuations of the order parameter in different layers are stabilized by the hopping matrix element describing electron tunneling between the layers.[21] If the direct hopping between layers is vanishingly small in the conduction band of oxide superconductors, as suggested by band-structure calculations, we have to think of other mechanisms which can prevent phase fluctuations from destroying the long-range order.

I propose in this paper that the interlayer coupling due to *interactions* plays an important role *both* in stabilizing the long-range order in oxide superconductors and providing a mechanism for *further enhancement* of T_c. The "Josephson-like" coupling between the layers which arises through interaction of electrons in the neighboring CuO_2 planes enhances the transition temperature within the layer, *irrespective* of its sign. This situation is quite different from that encountered in most ordinary layered compounds.[22] There the layer coupling is due to direct interlayer hopping found in the single-electron band structure. We propose that such direct hopping is only a higher-order effect in oxide superconductors, and that their conduction band is basically two dimensional. The electron transport arises only via scattering to the three-dimensional bands, above and below the Fermi level, arising through Coulomb interactions. This makes oxide superconductors a very special, novel class of layered materials.

The Hamiltonian of our model can be written as follows:

$$H = \sum_i H_i^{\text{intra}} + \sum_{\langle i,j \rangle} H_{\langle ij \rangle}^{\text{inter}} , \tag{1}$$

where H_i^{intra} is the layer BCS-type Hamiltonian given by

$$H_i^{\text{intra}} = -2D \sum_{\mathbf{k},\sigma} \gamma_{\mathbf{k}} c_{\mathbf{k}\sigma,i}^{\dagger} c_{\mathbf{k}\sigma,i} + V \sum_{\mathbf{k},\mathbf{k}'} c_{\mathbf{k}\uparrow,i}^{\dagger} c_{-\mathbf{k}\downarrow,i}^{\dagger} c_{\mathbf{k}'\downarrow,i} c_{-\mathbf{k}',\uparrow,i} . \tag{2}$$

In (2) $c_{\mathbf{k}\sigma,i}^{\dagger}$ is the creation operator for electrons in the ith CuO_2 layer, with the linear momentum $\mathbf{k}$ within the layer and spin σ, $\gamma = \cos(k_x a) + \cos(k_y a)$, $2D$ is the bandwidth, and $\langle i,j \rangle$ indicates that i and j are neighboring layers. The attractive interlayer interaction $V = -|V|$ is assumed, originating from some of the proposed mechanisms, which we *do not specify* here. The interlayer coupling is contained in $H_{\langle ij \rangle}^{\text{inter}}$, given by

$$H_{\langle i,j \rangle}^{\text{inter}} = -t \sum_{\mathbf{k},\sigma} c_{\mathbf{k}\sigma,i}^{\dagger} c_{\mathbf{k}\sigma,j} + Y \sum_{\mathbf{k},\mathbf{k}',\alpha,\beta} c_{\mathbf{k}\alpha,i}^{\dagger} c_{-\mathbf{k}\beta,j}^{\dagger} c_{\mathbf{k}'\beta,j} c_{-\mathbf{k}',\alpha,i} + W \sum_{\mathbf{k},\mathbf{k}',\alpha,\beta} c_{\mathbf{k}\alpha,i}^{\dagger} c_{-\mathbf{k}\beta,i}^{\dagger} c_{\mathbf{k}'\beta,j} c_{-\mathbf{k}',\alpha,j} . \tag{3}$$

The first term in (3) is the direct hopping between the layers, while the second and the third terms describe the interlayer coupling due to interactions. This is a very general form of the interlayer coupling. As already emphasized, t is very small in oxide superconductors. Y denotes the interlayer coupling constant in the particle-hole channel and may contain contributions from plasmon-, exciton-, and phonon-assisted transitions, as well as direct Coulomb interaction between charged layers. W is the coupling constant in the particle-particle channel, which is not due to any density fluctuations, but can arise through Coulomb interaction causing transitions

from the band at the Fermi surface to some of the fully occupied or empty bands away from the Fermi level, with finite dispersion along the z axis. From the calculations of Refs. 17 and 18, it follows that there is a number of such bands within a few eV of the Fermi level. This is a peculiarity of the band structure which we suggest is very important for superconductivity in these materials. Figure 1 depicts the type of processes contributing to W.

We now assume that the Hamiltonian (1) can be treated within the weak coupling BCS theory. This seems a sensible starting point to obtain some qualitative results, particularly if the pairing interaction is of the electronic origin. We first set $t=0$. Then the BCS expression for the free energy can be written as

$$F=-\sum_{i,j}\Theta_{ij}\Delta_i^*\Delta_j-\frac{1}{Y}\sum_{i,\gamma}\Gamma_{i\gamma}^*\Gamma_{i\gamma}-T\sum_{\mathbf{k},\omega_n}\sum_{i,j}\ln\det G_{ij}(\mathbf{k},\omega_n), \tag{4}$$

where Δ_i and $\Gamma_{i,\gamma=\pm1}$ are, respectively, the intralayer and interlayer order parameters, arising from the anomalous expectation values of the type $\langle c_{\mathbf{k}\uparrow,i}c_{-\mathbf{k}\downarrow,i}\rangle$ and $\langle c_{\mathbf{k}\uparrow,i}c_{-\mathbf{k}\downarrow,i+\gamma}\rangle$, and ω_n's are the Matsubara frequencies. We have assumed that order parameters are uniform within a layer. The matrix $G_{ij}(\mathbf{k},\omega_n)$ is given by

$$G_{ij}(\mathbf{k},\omega_n)=\frac{1}{(\omega_n^2+\xi_{\mathbf{k}}^2)^{1/2}}\left[\begin{pmatrix} i\omega_n-\xi_{\mathbf{k}} & \Delta_i \\ \Delta_i^* & -i\omega_n-\xi_{\mathbf{k}}\end{pmatrix}\delta_{i,j}+\begin{pmatrix}0 & \Gamma_{i\gamma}\\ \Gamma_{i\gamma}^* & 0\end{pmatrix}\delta_{i,j-\gamma}\right], \tag{5}$$

where $\xi_{\mathbf{k}}\equiv-2D\gamma_{\mathbf{k}}-\mu$, μ being the chemical potential. The coupling of the order parameters Δ_i's on different layers is determined by

$$\Theta_{ij}=\frac{1}{N}\sum_{k_z}\frac{e^{ik_z(z_i-z_j)}}{V+2W\cos(k_zd)},$$

where N is the number of layers, d is the separation between them, and $z_i\equiv id$.

Note that expanding the last term in (4) to second order in Δ_i and $\Gamma_{i\gamma}$ *does not* generate any interlayer coupling. To this order, the interlayer coupling is solely due to Θ_{ij}, and it is nonzero only for *finite* (i.e., nonzero) W. Therefore, the finite coupling constant for interlayer interactions in the particle-particle channel generates the "Josephson-like" coupling between order parameters on different layers. If $W=0$ the order parameters of different layers are uncoupled, and phase fluctuations will prevent the establishment of a true long-range order. The wealth of available experimental information suggests that oxide superconductors behave in a way indicative of a long-range superconducting order.[23] We propose here that in these materials, where t seems to be very small (i.e., $t<0.1$ eV), it is the above mechanism of the interlayer coupling that is primarily responsible for stabilizing the superconducting state. An objection can be raised here that the very type of interband transitions that contribute to W could result in the effective hopping matrix element of a similar magnitude. We can show,[24] assuming short-ranged interactions acting only within a layer, that the contributions to t of interband processes in Fig. 1 either vanish by symmetry or are negligible in comparison with W. This ensures that our model, in which t is initially set to zero, has an internal consistency. Similarly, we do not expect any phonon or low-energy plasmon processes to be effective in the interband scattering; the characteristic energies for these processes are way below the 1-eV scale.

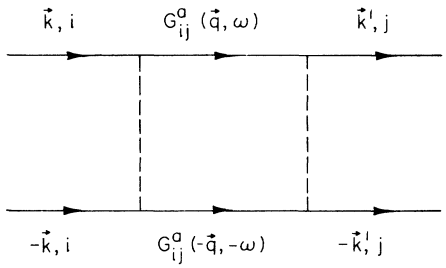

FIG. 1. Type of interband scattering processes contributing to W. Two electrons in layer i are scattered by the Coulomb interaction into the bands away from the Fermi level. If these bands have a finite dispersion along the z axis, the electrons propagate to a neighboring layer j where they are scattered back to the original band at the Fermi level. $G_{ij}^a(\mathbf{q},\omega)$ are the propagators of the intermediate band states. The dotted lines represent Coulomb interactions.

Let us now search for the self-consistent solution of this BCS-like theory by minimizing the free energy in Eq. (4) with respect to Δ_i and $\Gamma_{i\gamma}$. It is easy to convince oneself that the values of the order parameters at the minima of (4) satisfy $\Delta_i\Gamma_{i\gamma}=0$ $\forall i,\gamma$. This is the consequence of $t=0$. If $Y>0$, $\Gamma_{i\gamma}=0$ at any temperature. For $Y<0$, the phase with nonzero Γ is possible only if $|V|+2|W|<|Y|$. In view of the above discussion, and the fact that most of the proposed theories emphasize the intralayer coupling as a source of high T_c, this possibility appears unlikely. Therefore we limit ourselves to the case when $|V|+2|W|>|Y|$. Then there is a single second-order phase transition, to a state with $\Delta_i\neq0$. Let us first assume that W is negative. Then the minimum of the free energy is obtained for $\Delta_n=|\Delta|\exp(i\phi)$, with the magnitude and the phase of the order parameter identical in all layers. If W is positive, the favored state is $\Delta_n=|\Delta|\exp(i\phi+in\pi)$, with the constant magnitude, but with the phase which changes by $\pm\pi$ as one crosses from one layer to the next. We denote these two states as favored (F) and antifavored (AF), respectively. The transition temperature depends *only* on $|W|$ and can be written as

$$T_c=1.14\omega_0\exp\left[-\frac{1}{\lambda_V+2\lambda_W^*}\right], \tag{6}$$

with $\lambda_V\equiv N(0)|V|$, $\lambda_W\equiv N(0)|W|$, $N(0)$ being the

density of states at the Fermi level, and

$$\lambda_W^* = \frac{\lambda_W}{1+2\lambda_W \ln(\Omega_0/\omega_0)} .$$

It is assumed here that ω_0 is the frequency cutoff of the pairing mechanism responsible for intralayer attraction, while Ω_0 is the energy scale characteristic of processes contributing to W.

The fact that W enhances the transition temperature regardless of its sign has a formal resemblance to the two-band model proposed by Lee and Ihm.[25] In our case it is the interlayer coupling arising through interactions that plays a role similar to the interband scattering mechanism of Ref. 25. It is conceivable that the "excitonic" type of processes shown in Fig. 1 could lead to sizable W. One can very roughly estimate $W \sim n_b \tilde{N}(0) V_c^2 (\tilde{t}^2/K^2)$, where $\tilde{N}(0)$ is the typical density of states for bands near the Fermi level, n_b is the number of bands which contribute to the process, and $\tilde{t}$ and K are characteristic dispersion and the distance from the Fermi level for these bands. V_c measures the strength of the interband Coulomb interactions. While $\tilde{t}$ appears to be small in these materials, there is some evidence that V_c may be quite large, of the order of few eV.[26] If we take as typical values $\tilde{t} \sim 0.3$ eV, $N(0) \sim \tilde{N}(0) \sim 1.0$ eV^{-1}, $V_c \sim 3.0$ eV, and $K \sim 3.0$ eV we find $W \sim 0.1 n_b$. As there are several bands near the Fermi surface that could contribute to this scattering, it appears likely that the value of W due to such "excitonic" processes could give a significant contribution to the enhancement of T_c.

What would be the experimental manifestations of the F and AF states? One clearly expects some interesting behavior in the upper critical magnetic field, in the direction parallel to the layers. This upper critical field is the subject of our current work,[24] and one would hope that H_{c2} measurements on a single-crystal sample could be used to differentiate between F and AF types of superconducting states. There should be no Josephson effect (to the lowest order) between the AF superconductors and the ordinary superconductors if the junction is manufactured in such a way that the plane of contact is perpendicular to the layers of oxide superconductor. But for a careful determination of the stable state in oxide superconductors, it will be first necessary to produce single crystals of sufficient size.

Finally we discuss the effect of small but finite t, in the interlayer Hamiltonian given by Eq. (3). Such matrix elements can arise through phonon- or plasmon-assisted hopping, for example. To evaluate T_c in this case, we assume that coupling constants V and W do not change significantly with the introduction of small dispersion along the z axis. To justify this assumption it would be necessary to invoke a specific assumption about the nature of the interaction leading to superconductivity, and to calculate V and W within a given model. Clearly, this is beyond the scope of this paper. Therefore we proceed, keeping V and W fixed. The calculation of the lowest-order correction in T_c involves expanding the logarithm of the determinant in Eq. (4) in power series in t and finding the first contributing term. In the F state, after some algebra, we find

$$T_c \cong T_{c0} \exp\left(-\frac{t^2}{2\pi^2 T_{c0} D}\right) , \tag{7}$$

while, for the AF state one obtains

$$T_c \cong T_{c0} \exp\left(-\frac{7\zeta(3) t^2}{2\pi^2 T_{c0}^2}\right) . \tag{8}$$

In the above T_{c0} is the transition temperature for $t=0$. Therefore, within the limits of our assumption, introducing the small hopping matrix element between layers reduces T_c in both types of superconducting states. This reduction is much more pronounced for the AF superconductor, as $T_{c0} \ll D$. One should add that the effect of t on the F state is very dependent on assumptions about density of states in the conduction band.

If the intralayer coupling owes its strength to a quasi-two-dimensional nature of electronic states, as is now claimed by a number of authors, we expect that the coupling constants will either not change or will decrease if the hopping between layers is allowed. The results of Eqs. (7) and (8) are consistent with such behavior, and one would generally expect that in such a case an increased direct hopping between layers would be unfavorable for high-T_c superconductivity. One should mention, however, that in Ref. 12 it is proposed that, if the electron-electron attraction is induced by spin fluctuations, making a system more three dimensional would increase the pairing interaction and would also decrease a depairing effect arising from very strong inelastic electron-electron scattering. In such a situation, we cannot make any firm conclusions, since the reduction predicted by (7) and (8) may be offset by an increase of the coupling constants.

Finite t may also lead to an additional second-order phase transition, to the state with $\Gamma \neq 0$. Such a state would be characterized with two different excitation gaps, and would have a very anisotropic excitation spectrum. The anisotropy of the spectrum has been recently used by Maekawa, Ebisawa, and Isawa[27] to explain the discrepancy between the infrared and the tunneling data for the gap parameter.

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[1]J. G. Bednorz and K. A. Müller, Z. Phys. B **64**, 189 (1986).
[2]C. W. Chu *et al.*, Phys. Rev. Lett. **58**, 405 (1987).
[3]R. J. Cava, R. B. van Dover, B. Batlogg, and E. P. Rietman, Phys. Rev. Lett. **58**, 408 (1987).
[4]M. K. Wu *et al.*, Phys. Rev. Lett. **58**, 908 (1987).
[5]P. H. Hor *et al.*, Phys. Rev. Lett. **58**, 911 (1987).
[6]J. M. Tarascon, L. H. Greene, W. R. McKinnon, and G. W. Hull, Phys. Rev. B **35**, 7115 (1987).
[7]P. W. Anderson, Science **235**, 1196 (1987).
[8]G. Baskaran, Z. Zhou, and P. W. Anderson (unpublished).
[9]S. Kivelson, D. Rokhsar, and J. Sethna, Phys. Rev. B **35**, 8865 (1987).
[10]M. Cohen and D. H. Douglass, Phys. Rev. B **35**, 8720 (1987).
[11]H. Fukuyama and K. Yosida, Jpn. J. Appl. Phys. (to be published).
[12]P. A. Lee and N. Read, Phys. Rev. Lett. **58**, 2691 (1987).
[13]C. M. Varma, S. Schmitt-Rink, and E. Abrahams (unpublished).
[14]V. Kresin, Phys. Rev. B **35**, 8716 (1987).
[15]J. Ruvalds, Phys. Rev. B **35**, 8869 (1987).
[16]P. Prelovšek, T. M. Rice, and F. C. Zhang, J. Phys. C (to be published)
[17]L. F. Mattheiss, Phys. Rev. Lett. **58**, 1028 (1987).
[18]J. Yu, A. J. Freeman, and J.-H. Xu, Phys. Rev. Lett. **58**, 1035 (1987).
[19]L. F. Mattheiss (unpublished).
[20]Many groups now have samples exhibiting the width of a resistivity transition of the order of 1% or less.
[21]R. A. Klemm and K. Scharnberg, Phys. Rev. B **24**, 6361 (1981).
[22]A good early review can be found in R. A. Klemm, Ph.D. thesis, Harvard University, 1974 (unpublished).
[23]I find it impossible to do justice to the enormous amount of experimental information already available on oxide superconductors by listing only a few references. Most of the conventional experimental techniques have been applied to these materials and they seem to indicate that the long-range order is well established in the superconducting state.
[24]Z. Tešanović (unpublished).
[25]D. H. Lee and J. Ihm (unpublished).
[26]G. Baskaran (private communication).
[27]S. Maekawa, H. Ebisawa, and Y. Isawa, Jpn. J. Appl. Phys. (to be published).