s-Wave Superconductivity from an Antiferromagnetic Spin-Fluctuation Model for Bilayer Materials

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It is usually believed that the spin-fluctuation mechanism for high-temperature superconductivity results in d-wave pairing, and that it is destructive for the conventional phonon-mediated pairing. We show that in bilayer materials, due to nearly perfect antiferromagnetic spin correlations between the planes, the stronger instability is with respect to a superconducting state whose order parameters in the even and odd plane bands have opposite signs, while having both two-dimensional s symmetry. The interaction of electrons with Raman- (infrared-) active phonons enhances (suppresses) the instability.

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Currently the most exciting discussion about high-T_c superconductivity deals with the symmetry of the pairing state [1]. Intimately related to this is the question of whether the superconductivity is due to antiferromagnetic spin fluctuations [see, e.g., Monthoux and Pines (MP) Ref. [2], and also Refs. [3,4]], to electron-phonon (EP) interaction enhanced by interlayer pair tunneling [5], or to neither of the two. In this discussion, it is indirectly assumed that the antiferromagnetic spin-fluctuation (AFSF) mechanism necessarily leads to d-wave pairing, and that the AFSF and EP mechanisms cannot coexist.

In this Letter we point out that whereas the AFSF mechanism leads to d pairing for one layer it may lead to (two-dimensional) s symmetry for a bilayer. The condition for that is the existence of strong antiferromagnetic correlations between the two layers in a bilayer, as found experimentally in $YBa_2Cu_3O_7$ [6–8]. We find that, for a given coupling strength, $T_c(s)$ is about twice as high as $T_c(d)$, thus making it easier to achieve the observed values of $T_c \sim 100$ K. Essential for the positive influence of layer doubling is the *single-particle* tunneling which splits the one-electron plane bands into even and odd with respect to the mirror plane between the layers. In this aspect our mechanism is very different from the interlayer *pair-tunneling* (IPT) mechanism discussed by Anderson and co-workers [5]. Nevertheless, similar to the IPT model, any attractive interaction between electrons in the same band, such as the one mediated by even (Raman-active) phonons, enhances T_c. This is opposite to the previously considered single-layer AFSF models in which such interactions are mutually destructive.

Support for such an enhancement mechanism may be found in the experimental fact (e.g., Refs. [9,10]) that some members of the cuprate family ($Nd_{2-x}Ce_xCuO_4$, $HgBa_2CuO_4$) behave as conventional s-wave EP superconductors. MP AFSF theory, on the other hand, would have to imply principally different mechanisms for this compound and for those with high T_c's. Another experimental fact which suggests a constructive interplay between phonon and nonphonon mechanisms is that in $YBa_2Cu_3O_7$ the isotope effect increases smoothly when the superconductivity is suppressed [11]. Finally, the most impressive argument is that in all high-T_c materials T_c is *anticorrelated* with the in-plane antiferromagnetic correlation length ξ. In particular, in $YBa_2Cu_3O_{7.0}$, ξ is about one lattice parameter, which would make the single-layer AFSF superconductivity virtually inoperative. To the contrary, as we shall argue below, the proposed bilayer model is barely sensitive to the in-plane AF correlation length ξ at all.

In the following we shall assume a conventional picture in the sense that the one-electron tunneling between the planes is allowed both in the normal and in the superconducting states. This is in contradiction with the IPT scenario [5], but in agreement with some photoemission experiments [12]. In this case, the single-particle eigenstates for a bilayer are the even $|+,\mathbf{k}\rangle$ and odd $|-,\mathbf{k}\rangle$ combinations of the individual plane states and $\mathbf{k}$ is the 2D Bloch vector. The properties of the even and odd bands are discussed in detail in Ref. [13], but, for the purpose of comparison with the MP model, we use the same band model as they did. We neglect completely the k_z dispersion due to small intercell c hopping, which can lead to interesting effects (see, e.g., Ref. [14]) but which are, however, beyond the scope of this Letter. Accordingly, in the following the term "bands" always means "two-dimensional bands." As regards the interplane hopping inside the unit cell $t_\perp(\mathbf{k})$, we assume that it is sufficiently large to set even and odd symmetry of the two-dimensional bands, but we neglect, for simplicity, in the following numerical calculations the even-odd splitting $\epsilon_-(\mathbf{k}) - \epsilon_+(\mathbf{k}) = 2t_\perp(\mathbf{k})$.

The generalization of the MP AFSF model to two bands is straightforward; one has only to take into account that the effective vertex for scattering of an electron from band i to band j by a spin fluctuation depends on i,j, while the spectrum of the fluctuations χ is the same as in

MP. Then, Eqs. (6)–(8) of MP become

$$\Sigma_{ij}(\mathbf{k}, i\omega_n) = T\sum_{\mathbf{q}m}\sum_{kl} V_{ik,lj}(\mathbf{k}-\mathbf{q}, i\omega_n - i\omega_m) \times G_{kl}(\mathbf{q}, i\omega_m),$$

$$G_{ij}^{-1}(\mathbf{k}, i\omega_n) = [i\omega_n - \epsilon(\mathbf{k}) + \mu]\delta_{ij} - \Sigma_{ij}(\mathbf{k}, i\omega_n), \quad (1)$$

$$\Phi_{ij}(\mathbf{k}, i\omega_n) = -T\sum_{\mathbf{q}m}\sum_{klst} V_{ik,tj}(\mathbf{k}-\mathbf{q}, i\omega_n - i\omega_m) \times G_{kl}(-\mathbf{q}, -i\omega_m)\Phi_{ls}(\mathbf{q}, i\omega_m)G_{st}(\mathbf{q}, i\omega_m),$$

where Σ and Φ are, respectively, the normal and anomalous self-energies, G is the single-particle Green's function, ϵ is the bare electron energy, and $\sum_{\mathbf{q}m}$ denotes the *average* over the Brillouin zone plus the sum over the Matsubara frequencies. V is the AFSF pairing interaction determined by the exchange interaction of electrons with the AFSF's, $V_{ij,kl} = \int d\mathbf{R}\, d\mathbf{R}' \sum_{\alpha\beta\gamma\delta} \langle i\alpha|J(\mathbf{r}-\mathbf{R})\sigma_{\alpha\beta}|j\beta\rangle \tilde{\chi}(\mathbf{R}-\mathbf{R}')\langle k\gamma|J(\mathbf{r}-\mathbf{R})\sigma_{\gamma\delta}|l\delta\rangle$, where J is the exchange interaction and $\tilde{\chi} = \langle \mathbf{S}(\mathbf{R})\mathbf{S}(\mathbf{R}')\rangle$ is the spin-spin correlation function. For a bilayer, one can let $\mathbf{R}$ be a two-dimensional vector and introduce $\tilde{\chi} = \chi(\mathbf{R}-\mathbf{R}')I_{uv}$, where $u, v = 1, 2$ label layers, and I accounts for interplane correlations, if any. Then the function χ is the same as in MP.

The key to our bilayer AFSF model is the experimental fact that the spin fluctuations in the bilayer of $YBa_2Cu_3O_{7-x}$ are always antiferromagnetically correlated between the planes [6–8]. Even fully oxygenated samples, where the in-plane correlation length is already of the order of the lattice parameter, show nearly perfect interlayer correlation [8]. The exchange potential setup by such a spin fluctuation is therefore *odd* with respect to the midlayer mirror plane and, correspondingly, couples exclusively *even and odd* electron states (but neither odd to odd nor even to even). In other words, $I_{u\neq v} = -I_{uu} = -1$. In this case, after summation over u, v in the expression for $V_{ij,kl}$ and defining the appropriate coupling constant g, Eqs. (1) become

$$\Sigma_-(\mathbf{k}, i\omega_n) = Tg^2\sum_{\mathbf{q}m}\chi(\mathbf{k}-\mathbf{q}, i\omega_n - i\omega_m)G_+(\mathbf{q}, i\omega_m),$$

$$G_+^{-1}(\mathbf{k}, i\omega_n) = i\omega_n - \epsilon(\mathbf{k}) + \mu - \Sigma_+(\mathbf{k}, i\omega_n), \quad (2)$$

$$\Phi_+(\mathbf{k}, i\omega_n) = -Tg^2\sum_{\mathbf{q}m}\chi(\mathbf{k}-\mathbf{q}, i\omega_n - i\omega_m) \times G_-(-\mathbf{q}, -i\omega_m)\Phi_-(\mathbf{q}, i\omega_m)G_-(\mathbf{q}, i\omega_m),$$

and the same with + and − subscripts interchanged, and g and χ are the same as in MP.

For reasons of symmetry, the solution of these equations must have the form $G_+ = G_-$, $\Phi_+ = \pm\Phi_-$. For the upper choice of the sign, Eqs. (2) reduce precisely to the original MP pairing state. For the lower choice, Eqs. (2) again reduce to the one-plane case, *but now the interaction in the equation for Φ is effectively attractive.* In other words, now the order parameter has the opposite sign in the two bands, and therefore the last equation in (2) can be rewritten in terms of $|\Phi|$, and with plus instead of minus on the right-hand side.

The concept of a superconducting state where two distinctive bands had the order parameters of the opposite signs was first discussed in 1973 in connection with semimetals [15]. More recently, in a two-layer Hubbard model, such a solution was found by Bulut, Scalapino, and Scalettar [16] (which they labeled as the "d_z" state) and in the conventional superconductivity theory [17], where it appears in the case of strongly anisotropic electron-phonon and/or Coulomb interaction, or because of a strong interband scattering by magnetic impurities. In all cases, order parameter has s symmetry inside each band and changes sign between the bands.

From Eqs. (2) it is quite plausible that such an instability is stronger than the $d_{x^2-y^2}$ one, and will occur at a higher T_c. Below we shall prove this numerically, but before going to numerical results, it is instructive to get a conceptual understanding about these two different solutions. The physical reason for having d symmetry in the one-plane case is that the AFSF interaction makes pairing energetically favorable only when it couples parts of the Fermi surface which have opposite signs of the order parameter [18]. In Y123 the AFSF interaction is peaked at $\mathbf{Q} = (\pi/a, \pi/a)$. The shape of the Fermi surface is such that the condition is satisfied only for $d_{x^2-y^2}$ symmetry. On the other hand, the small-$\mathbf{q}$ interaction couples parts of the Fermi surface where the order parameter has the same sign. This makes pairing unfavorable. Since $\chi(\mathbf{q}\approx\mathbf{Q}) \gg \chi(\mathbf{q}\approx 0)$, nevertheless, more is lost by making an s state than by making a d state (which has been found numerically by MP), because the latter loss is the difference between the small-q loss and the large-q gain, while in an s state one loses over the whole Fermi surface [19].

Now, coming to the bilayer case, we observe that there is no conflict between the small and large q's anymore. The AFSF interaction spans two different sheets of the Fermi surface, which always have order parameters of the opposite signs. Thus the AFSF interaction is as attractive for s pairing in a bilayer as it is repulsive in a single plane, and consequently more attractive than d pairing in a single plane. Of course, the resulting s state is likely to be highly anisotropic, to take better advantage of the large $\chi(\mathbf{q})$ at $\mathbf{q}\approx\mathbf{Q}$. This is similar to the model of Anderson and co-workers [5]. To demonstrate this effect numerically, we have solved Eqs. (2) with the parameters from MP paper, and using the same numerical technique. As expected, the maximal eigenvalue of the last equation in (2) is larger than that for the MP d pairing (about 1.5 compared to 1). Figure 1 shows the plot of T_c as a

function of the interaction constant g for both cases. To test the numerics, we have also solved the original MP equations and obtained the similar results as MP.

From Fig. 1, one immediately observes that the value (0.69 eV) of the coupling constant g, which yields $T_c \approx$ 90 K for two planes and s symmetry, is much smaller than the corresponding value (1.24 eV) for one plane and d symmetry. Actually, $T_c(s) \sim 2T_c(d)$ for g up to about 1 eV. At stronger couplings, $T_c(d)$ saturates faster than $T_c(s)$ due to stronger effect of mass renormalization. Similarly, as we shall see below, the ratio of the maximal gap to T_c tends to be larger for the one-plane model, for the same T_c.

One can also obtain the self-consistent solution for Φ at $T \ll T_c$. To do that, one has to include higher-order terms (see, e.g., Ref. [3]). In this case one of the Green's functions in the Eq. (2) for Φ should be replaced by

$$\tilde{G}_-^{-1}(\mathbf{k}, i\omega_n) = i\omega_n - (\epsilon_{\mathbf{k}} - \mu) - \Sigma_-(\mathbf{k}, i\omega_n),$$
$$G_-^{-1}(\mathbf{k}, i\omega_n) = \tilde{G}_-^{-1}(\mathbf{k}, i\omega_n) - \Phi_-(\mathbf{k}, i\omega_n)\tilde{G}_-(-\mathbf{k}, -i\omega_n)\Phi_-(-\mathbf{q}, -i\omega_n). \quad (3)$$

This new set of equations can be solved iteratively, starting with $G = \tilde{G}$ (which is correct to first order in Φ). The actual solution for $T = T_c/2$, shown in Fig. 2, was achieved by making two iterations of Eqs. (3). The frequency-dependent superconducting gap is related to Φ as

$$\Delta(\mathbf{p}, i\omega_n) = \frac{\Phi(\mathbf{p}, i\omega_n)}{Z(\mathbf{p}, i\omega_n)} = \frac{\Phi(\mathbf{p}, i\omega_n)}{1 - \mathrm{Im}\Sigma(\mathbf{p}, i\omega_n)/\omega_n}.$$

From Fig. 2 we observe that the *absolute value* of Δ behaves similarly in both cases, having a minimum along (11) directions and a maximum along (10) directions. Furthermore, $|\Delta|$'s in both cases differ by less than 10% on two-thirds of the whole Fermi surface, thus making it extremely difficult to distinguish between the two in an experiment which does not probe the relative phases of Δ. In other words, the order parameter, formally having s symmetry, is still strongly anisotropic, but nodeless.

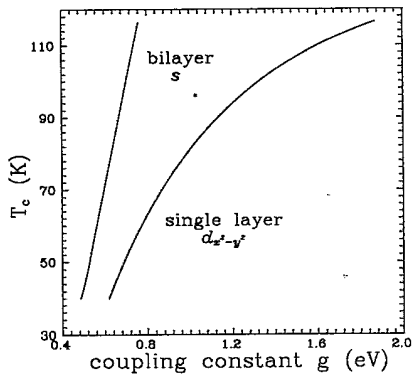

FIG. 1. Critical temperature as a function of the coupling strength g for a single plane ($d_{x^2-y^2}$ symmetry) and for two planes (p_z symmetry). Parameters are as in Ref. [2].

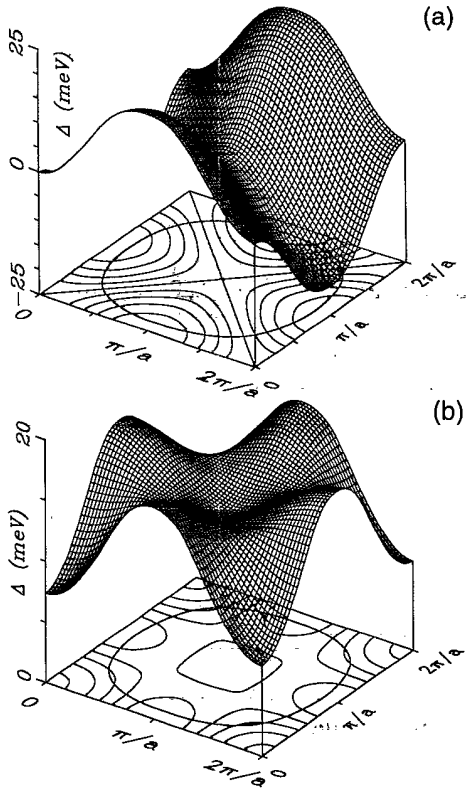

FIG. 2. Superconducting gap Δ for the lowest Matsubara frequency $\omega_n = \pi k_B T$ in the 2D Brillouin zone at $T = 0.5T_c$ for a single plane (a) and for two planes (b). The Fermi-surface contour shown at the base of the plots corresponds to $E_F = -0.37$ eV (0.25 hole/plane).

Now we shall briefly discuss some experimental consequences of the bilayer AFSF superconductivity model. It turns out that many difficulties associated with the original AFSF superconductivity model disappear in the present version.

(1) In-plane vs perpendicular-to-the-planes Josephson tunneling. Recent searches for the d pairing in $YBa_2Cu_3O_7$ (Refs. [20,21] and others) still do not give a definite answer. Experiments probing the angular dependence of the order parameter, as well the existence of the so-called "paramagnetic Meissner effect" [22], indicate the existence of order parameters of opposite signs: Many experiments were interpreted in terms of $d_{x^2-y^2}$, but such interpretations can be questioned because of the presence of the chain band [17]. On the other hand, the existence of the finite tunneling current perpendicular to the planes [21] is incompatible with d pairing, but compatible with our model once the simplifying assumption $\epsilon_-(\mathbf{k}) = \epsilon_+(\mathbf{k})$ is removed [23].

(2) The original MP model is very sensitive to the in-plane correlation length ξ: According to Ref. [2], T_c drops from 90 to 35 K when ξ is reduced from $2.3a$ to a. Experimentally, in fully oxygenated samples ($O_{6.9-7.0}$) ξ

is small and still decreases closer to the O_7 composition where it becomes less than a. T_c is, however, not sensitive to the oxygen content in this regime. In our model and contrary to MP, T_c is hardly sensitive to the sharpness of $\chi(q)$, which predominantly influences the gap anisotropy.

(3) One of the arguments in favor of the AFSF mechanism has been the strong T_c suppression upon Zn doping. However, it has remained unclear why chain disorder hardly affects T_c. (One could argue that the chains are completely decoupled from the planes, but this is inconsistent with the strong effect on the Ba A_{1g} phonon mode of the onset of superconductivity.) This finds natural explanation in our AFSF model: The chain impurity potential is even with respect to the midplane reflection and does therefore not produce scattering between the even and odd bands.

(4) The MP model has difficulty in explaining the continuous change of the isotope effect with oxygen content, as well as in reconciling the apparent phonon s-wave superconductivity in Nd cuprate with the assumed AFSF superconductivity in $YBa_2Cu_3O_7$. The basics of this conflict is as follows: The AFSF interaction is pairing when a pair changes the sign of its order parameter upon scattering; this is the case MP model for $\mathbf{q} \approx (1,1)\pi/a$. It is *depairing* if there is no sign change. The opposite is true for the electron-phonon interaction. Obviously, the only way to reconcile the MP model with the known facts about the role of phonons in superconductivity is to assume that the electron-phonon interaction, contrary to the AFSF interaction, is strong for $\mathbf{q} \to 0$ and weak for large q's; this is opposite to common wisdom. In our model the corresponding assumption is much less painful: One has to assume that the *even* phonons, like, for instance, A_{1g} Raman-active phonons, interact with electrons stronger than the *odd* ones. This seems quite plausible and some indirect arguments can be given in support of this assumption (e.g., the even phonons strongly influence the extended van Hove singularities [13]).

In conclusion, we have shown that from the observed strong antiferromagnetic correlations between the Cu-O planes in bilayer materials the strongest superconducting instability due to antiferromagnetic spin fluctuations appears in the anisotropic s channel, but so that the order parameters in the bonding (symmetric) and antibonding (antisymmetric) bands have opposite signs. This helps to reconcile the magnetic-induced superconductivity model with many experiments which previously seemed to contradict the magnetic scenario. In particular, the interrelation between the doping dependences of the magnetic and superconducting properties can be much easier understood.

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