Theory of the spin gap in bilayer cuprates

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A model of two planes of antiferromagnetically correlated electrons coupled together by a weak antiferromagnetic interaction of strength λ has been formulated and solved. It is shown that in-plane antiferromagnetic correlations dramatically enhance the pairing effect of the interplane interaction. For the case in which the in-plane correlation length κ^{-1} is $\sim T^{-1/2}$ we find that the interaction λ leads to spin pairing at a temperature $T^* \sim \lambda$ much higher than the usual BCS result, $\exp(-J/\lambda)$. We suggest that this is a possible explanation of the spin-gap effects observed below $T^* \sim 150$ K in $YBa_2Cu_3O_{6.6}$.

It was recently argued that superconductivity and spin gaps in bilayer copper oxides such as $YBa_2Cu_3O_{6+x}$ are attributable to interplane pairing[1–3] which occurs as a result of the antiferromagnetic spin-spin interaction between the planes. Effects of this interaction have been observed in neutron scattering experiments[4] on $YBa_2Cu_3O_{6.6}$. The high-T_c materials are also believed to have strong in-plane antiferromagnetic fluctuations. An alternative mechanism for spin gap formation in copper oxide materials based on a single-plane theory of bosonic spin-waves has also been discussed.[5] In this paper we determine the effect of the in-plane fluctuations on the interplane pairing interaction which was discussed previously. We found that these fluctuations strongly enhance the interaction between the planes at wave vectors near the wave vector **Q**, where the in-plane spin susceptibility peaks. Taking into account this enhancement and the modification of the electron spectrum by the spin fluctuations,[6] we obtain an estimate for the onset temperature of the spin gap which is of the correct order of magnitude.

Several different cases which were encountered were discussed in detail elsewhere.[7] The first case is the relationship between the vector **Q** and the shape of the Fermi surface of the fermions: The vector **Q** might be a chord of the Fermi surface, its diameter, or it can be larger than $2p_F$.[2)] In this paper we will consider only the chord. The second case concerns the strength of the spin correlations. Here we assume that the spin system in each plane is very close to a $T=0$ critical point[8] which results in long-range antiferromagnetic fluctuations, whose correlation length is proportional to the power of the temperature. The third case is the nature of the fermionic excitations. We can single out the "spin-liquid" case, with a spin-charge separation and fermionic spin excitations,[9] and the "Fermi-liquid" case in which there is no spin-charge separation. Formally, the difference between these two cases stems from the presence of an additional low energy mode (gauge field) in the spin-liquid case,[10] which results in a large relaxation rate for the fermions [the electron propagator therefore is[11] $(\beta\epsilon^{2/3}-v_F|p-p_F|)^{-1}$]. We will consider both cases here. It is also believed that in underdoped high-T_c materials the electrons cannot tunnel coherently between the planes.[12] We will assume, therefore, that all low energy excitations are confined to a plane.

To model one plane of antiferromagnetically correlated fermions we write

$$H_F=\sum_p c^\dagger_{p\sigma}\epsilon(p)c_{p\sigma}+\sum_q J_q S_q S_{-q}, \tag{1}$$

where $\epsilon(p)=v_F(|p|-p_F)$ is the fermion dispersion near the Fermi surface, $S_i=c^\dagger_{i\sigma}\sigma_{\alpha\beta}c_{p\sigma}$. It is also convenient to introduce the fermion mass $m=p_F/v_F$. The interaction J_q causes antiferromagnetic correlations to peak at the wave vector $\mathbf{Q}$. For definiteness we treat the interaction in the RPA approximation and assume that the parameters are such that the spin susceptibility $\chi(k,\omega)$ is given by

$$\chi(k,\omega)=\frac{\chi_0(k,\omega)}{1-J_k\chi_0(k,\omega)} \tag{2}$$

$$=\frac{J_{\mathbf{Q}}^{-1}}{\kappa^2+(\mathbf{k}-\mathbf{Q})^2+|\omega|/\Gamma}, \tag{3}$$

where χ_0 is the susceptibility of the noninteracting fermions, κ, the inverse correlation length, is assumed to be small, and Γ is a microscopic frequency scale. Presumably $\Gamma\sim 1/m$, or $\Gamma\sim J/p_F^2$. To fit the Cu NMR relaxation rates in high-T_c materials at high temperatures, it is necessary to use $\kappa^2=MT$, where M is a constant. We emphasize that, although we have used the RPA to explain the form of (3), this form is more general than the explanation in Ref. 6, and so are the following results which depend on (3) only. The specific form of (3) holds only if the wave vector $\mathbf{Q}<2p_F$, so that at all wave vectors near $\mathbf{Q}$ a particle-hole pair is available to damp the spin excitation.

In the following analysis we choose polar coordinates on the Fermi surface, so that the points on the Fermi surface connected by $\mathbf{Q}$ correspond to angles $\pm\theta_0$. The form (1) applies to both the spin-liquid case and the Fermi-liquid case. In the $\mathbf{Q}=2p_F$ case the different functional form of χ depends on whether the fermion damping is small or large.

We assume that the only coupling between different planes is an antiferromagnetic interaction between spins:

$$H_{\text{int}}=\lambda\sum_i S_i^{(1)}S_i^{(2)}, \tag{4}$$

where the indices 1 and 2 distinguish planes in a bilayer, and λ is an interaction constant which is assumed to be small. The neutron measurements[4] imply that $\lambda\sim 200$ K, but clearly $\lambda\ll J$, where $J\sim 1500$ K is the exchange constant in one plane.

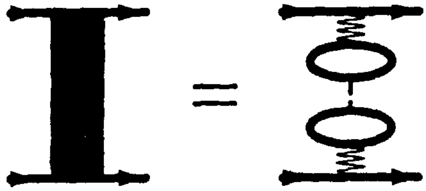

FIG. 1. Diagrammatic representation of the dominant contribution to the pairing interaction. Here the light dashed line represents the interplane interaction and the wavy line denotes the dressed spin-fluctuation interaction between electrons in one plane.

The interaction (4) leads to antiferromagnetic correlations between planes, which we assume to be weaker than the in-plane correlations. An arbitrary, weak λ was also found[1] to lead to a singlet pairing of spin excitations in different planes. In our study the antiferromagnetic correlations in each plane were disregarded and the temperature at which the spin pairing occurred was found to be very low, $T_c \sim \epsilon_F e^{-\lambda/\epsilon_F}$. We have shown that in the presence of antiferromagnetic correlations the pairing interaction becomes much stronger at the wave vectors near **Q**, the temperature at which the pairing occurs increases considerably, and the gap function becomes strongly anisotropic, opening first in a small region [about $(\theta-\theta_0) \sim \kappa/p_F$] near the points connected by the vector **Q** and then dropping at some distance from these points as $1/(\theta-\theta_0)^4$.

The physical argument is that, because the susceptibility in one plane is very large at wave vectors near **Q**, a fermion at this wave vector polarizes the electrons in the neighboring plane in a large area near it. Mathematically, we must construct the pairing vertex which connects a particle in one plane to a particle in the other plane. For small λ this vertex is linear in λ and is dressed by spin fluctuations in each plane: In the RPA approximation we have found that the dominant contribution to the dressed vertex $V(k,\omega)$ is that shown in Fig. 1, which leads to

$$H_{\text{int}}^d = \sum_{p,p',k} V(k,\omega) c_{p+k}^\dagger \sigma^\alpha c_p c_{p'+k}^\dagger \sigma^\alpha c_{p'}, \qquad V(k,\omega) = \lambda J_{\mathbf{Q}}^2 a^{-2} \chi^2(k,\omega), \tag{5}$$

where a is the lattice constant. Other contributions are negligible. To calculate the onset of the pairing from Eq. (5), we must sum the ladder diagrams shown in Fig. 2. It is important to use the complete Green's function, including the self-energy due to the spin exchange in one plane. This self energy has been studied by many authors. An approximation useful for our purpose is[13]

$$\Sigma(\omega,\theta) = \frac{\alpha_{\mathbf{Q}} |\omega| Jm}{2\pi p_F \sqrt{\omega/\Gamma + p_F^2(\theta-\theta_0)^2 + \kappa^2}}, \tag{6}$$

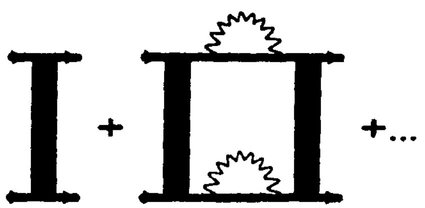

FIG. 2. Ladder sum leading to the gap equation. Here the shaded rectangle is the interaction V defined in Fig. 1. Note that the electron lines are dressed by in-plane fluctuations.

where α_Q is a function on the order of unity if $\mathbf{Q}$ is removed from $2p_F$, but which diverges as $\mathbf{Q}\to 2p_F$. We have verified that this formula applies in the spin-liquid case.

The important point here is that the gap is due to the pairing of spin excitations on different planes, so the interaction (5), although large in a certain region of momentum space, does not lead to self-energy parts or to vertex corrections. The gap equation therefore follows from the summation of the ladder series in Fig. 2. Taking the ladder sum and integrating over the momenta in the direction normal to the Fermi surface, we obtain

$$\Delta(\epsilon,\theta)$$

$$=\frac{T}{4\pi}\sum_{\omega}\int\frac{\lambda m\Delta(\epsilon+\omega,\theta')d\theta'}{[|\omega|/\Gamma+p_F^2(\theta^2+\theta'^2+2u\theta\theta')+\kappa^2]^2\sqrt{[\omega+\Sigma(\omega)]^2+\Delta(\epsilon+\omega,\theta')^2}},\tag{7}$$

where $u=1-\mathbf{Q}^2/(2p_F)^2$. We have set $\theta_0=0$. The integration over the perpendicular momenta was possible because the main contribution to this integral comes from a narrow range near the Fermi surface ($\delta p'\sim T/v_F$), where the interaction $V(\mathbf{p}-\mathbf{p}',\omega)$ does not vary significantly.

To find the onset temperature, we linearize (7) and introduce the scaled variables x and y through $\theta=\kappa x/p_F$ and $\theta'=\kappa y/p_F$. The resulting equation is

$$\Delta_n(x)=\frac{\lambda}{2\alpha_Q MTa^2J}\sum_l\int dy\frac{\Delta_{n+l}(y)\sqrt{1+y^2+\frac{2\pi}{M\Gamma}\left|n+l+\frac{1}{2}\right|}}{\left|n+l+\frac{1}{2}\right|\left(1+y^2+x^2+2uxy+\frac{2\pi}{M\Gamma}|l|\right)^2},\tag{8}$$

where l and n are integers. From (8) it is evident that Δ depends only on $1+x^2$ which is found only in the denominator of the kernel. Thus, $\Delta(\theta)$ peaks near $\theta=0$ with a width κ and decays at large θ as $1/\theta^4$, and peaks again near the lowest Matsubara frequency, $\omega_n=\pi T$, with a width $\Gamma\kappa^2\sim T$. The dimensionless kernel in (8) presumably has the largest eigenvalue, $w\sim 1$, so T^* is given by

$$T^*=\frac{w\lambda}{2\alpha_Q Ma^2J}.\tag{9}$$

Thus, apart from numerical factors, the onset temperature T^* is given by the bare interplane coupling constant λ. At $T\ll T^*$ we can replace the sum over the frequencies in (7) by an integral; this integral is dominated by the frequencies on the order of the zero temperature spin gap $\Delta(0)=\Delta^*$. Similarly, we must replace κ^2 by $M\Delta^*$, because the low-frequency spin correlations near the antiferromagnetic wave vector $\mathbf{Q}$ are eliminated by the spin gap. The result is that within numerical factors T^* in (9) is replaced by Δ^*. The gap reaches the maximum value at angles $\theta\lesssim\sqrt{M\Delta^*}$; for larger θ it is given by

$$\Delta(\theta)\sim\Delta^*\left[\frac{\kappa}{p_F\theta}\right]^4\sim\frac{(\Delta^*)^3M^2}{p_F^2\theta^4}.$$

We emphasize that due to a strongly peaked, temperature-dependent effective interaction the pairing temperature and the gap scale as the interaction constant, in contrast with the usual BCS case in which they are exponentially small. Although we have assumed a specific form of the spin susceptibility (3) with a temperature-dependent correlation length, this assumption is not essential for our results. The enhancement of the pairing between the planes is attributable to the strong temperature dependence of $\Sigma_q\chi'(q,\omega=0)^2$. This quantity was measured in the NMR T_2 experiments[14] and was found to be large and strongly temperature dependent in $YBa_2Cu_3O_{7-x}$ (Refs. 14 and 15).

The situation in the spin-liquid case is essentially identical. The square of the momentum-integrated Green's function is $[\beta|\omega|^{2/3}-\Sigma(\omega,\theta)]^{-1}$, but $\beta|\omega|^{2/3}$ is still negligible compared to $\Sigma(\omega,\theta)$ for the frequencies and angles of interest. Equations (8) and (9) therefore remain the same.

Let us now consider the experimental implications. The pairing mechanism is much weaker in $La_{2-x}Sr_xCuO_4$, because the antiferromagnetic interaction between Cu ions in different planes is frustrated, so that in tetragonal crystals Eq. (4) becomes

$$H_{\rm int}^{\rm La}=\lambda\sum_{i,\delta}\mathbf{S}_i^{(1)}\mathbf{S}_{i+\delta}^{(2)}, \tag{10}$$

where δ labels the four Cu sites in plane 2 which is equidistant from site i of plane 1. Equation (10) implies that $V(k,\omega)$ in Eq. (5) becomes

$$V^{\rm La}(k,\omega)=V(k,\omega)\cos(k_x/2)\cos(k_y/2). \tag{11}$$

Thus the singularity in the interaction is eliminated for commensurate spin fluctuations (k_x, $k_y\sim\pi$) in the tetragonal crystals. For orthorhombic crystals or for incommensurate spin fluctuations the singular part of the interaction is on the order of the square of the orthorhombicity or incommensurability, and is therefore small. This is consistent with the observation that the spin gap opens at much lower temperatures in $La_{2-x}Sr_xCuO_4$ than in $YBa_2Cu_3O_{6+x}$.

In a Fermi liquid system with no spin-charge separation the opening of the spin gap implies that the material has become superconducting. In a spin-liquid system true superconductivity occurs only at a lower temperature at which the charge carriers are a Bose condense. The former scenario is consistent with the behavior of optimally doped or overdoped $YBa_2Cu_3O_{6+x}$ and with the behavior of $La_{2-x}Sr_xCuO_4$ at all dopings, while the latter scenario is consistent with the behavior of underdoped $YBa_2Cu_3O_{6+x}$. For example, in $YBa_2Cu_3O_{6.6}$, the spin-gap effects have been observed in NMR below $T^*\sim150$ K, while the superconducting T_c is ~60 K. As previously pointed out,[1] there is also optical evidence[16] for the existence of a gap above T_c. The small value of the specific heat jump at T_c in $YBa_2Cu_3O_{6.6}$ (Ref. 17) is consistent with this scenario. However, none of these observations (except the qualitative one which shows that the spin gap opens significantly above T_c only in underdoped bilayer materials such as $YBa_2Cu_3O_{6.6}$) distinguishes the mechanism we have proposed from other possible origins of the spin gap.

There is a qualitative disagreement with the experiment. Because the gap opens first and is largest at the points on the Fermi surface connected by the wave vector where $\chi(k,\omega)$ peaks, the low-frequency antiferromagnetic spin fluctuations are suppressed more strongly than the spin fluctuations at other wave vectors. In the high-T_c materials it is believed that the antiferromagnetic fluctuations are responsible for the enhancement of the Cu relaxation rate over the relaxation rates of the other nuclei.[8] In our scenario the copper relaxation rate would therefore decrease more rapidly than the oxygen or yttrium rates as the spin gap opens, in apparent disagreement with the experimental data[18] on $YBa_2Cu_3O_{6.6}$.

Note added in proof: As this manuscript was being prepared, we learned that M. Ubbens and P. A. Lee[19] have obtained results very similar to ours.

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