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ON THE THEORY OF THE SPIN GAP IN BILAYER CUPRATES

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We formulate and solve a model of two planes of antiferromagnetically correlated electrons coupled together by a weak antiferromagnetic interaction of strength λ. We show that in-plane antiferromagnetic correlations dramatically enhance the pairing effect of the interplane interaction. For the case where the in-plane correlation length $\kappa^{-1} \sim T^{-1/2}$, 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 $YBa_2Cu_3O_{6+x}$ may be due to interplane pairing [1, 2, 3] caused by the antiferromagnetic spin-spin interaction between the planes. Effects of this interaction have been observed in neutron scattering experiments on $YBa_2Cu_3O_{6.6}$ [4]. 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 discussed previously. We find that they strongly enhance the between-planes interaction at wave vectors near the wave vector Q where the in-plane spin susceptibility is peaked. 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 for the spin gap which is of the correct order of magnitude.

Several different cases arise which we discuss in detail elsewhere [7]. One issue is the relation between 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 and be larger than $2p_F$. [2)] In this paper we consider only the chord case. Another issue 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] resulting in long range antiferromagnetic fluctuations with a correlation length proportional to a power of temperature. A third issue is the nature of the fermionic excitations. One may distinguish the "spin liquid" case with spin-charge separation and fermionic spin excitations [9] and the "Fermi liquid" case, where there is no spin-charge separation. Formally, the difference between these two pictures originates from the presence of an additional low energy mode (gauge field) in the spin liquid case

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[2)] All these conditions have trivial generalization for a non-spherical Fermi surface, for brevity we discuss only the circular case here.

[10], which results in a large relaxation rate for the fermions (so the electron propagator is $(\beta\epsilon^{2/3} - v_F|p - p_F|)^{-1}$ [11]). We treat both cases here. It is also believed that in underdoped high-T_c materials electrons cannot tunnel coherently between planes [12], so we shall assume that all low energy excitations are confined to a plane.

To model one plane of antiferromagnetically correlated fermions we write

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

where $\epsilon(p) = v_F(|p| - p_F)$ is the fermion dispersion near the Fermi surface, $\mathbf{S}_i = c^\dagger_{i\sigma}\sigma_{\alpha\beta}c_{p\sigma}$. It is also convenient to introduce the fermion mass $m = p_F/v_F$. The interaction J_q causes antiferromagnetic correlations peaked at wave vector 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

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

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

where χ_0 is the susceptibility of the non-interacting 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 take $\kappa^2 = MT$ 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 [6] and so are the following results which depend on (3) only. The specific form of (3) holds only if the wave vector $Q < 2p_F$, so that at all wave vectors near Q a particle hole pair is available to damp the spin excitation.

In the following we choose polar coordinates on the Fermi surface so that the points on the Fermi surface connected by Q correspond to angles $\pm\theta_0$. The form (1) applies to both the 'spin liquid' and Fermi liquid cases. In $Q = 2p_F$ case the functional form of χ is different and 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:

$$H_{int} = \lambda \sum_i \mathbf{S}_i^{(1)}\mathbf{S}_i^{(2)}, \tag{4}$$

where indices 1 and 2 distinguish planes in a bilayer and λ is an interaction constant, assumed small. Neutron measurements [4] imply that $\lambda \sim 200K$, but certainly $\lambda \ll J$ where $J \sim 1500\,\mathrm{K}$ is the exchange constant 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 has also been shown [1] to lead to a singlet pairing of spin excitations in different planes. In this work the antiferromagnetic correlations within each plane were not taken into and the temperature at which the spin pairing occurred was found to be very low ($T_c \sim \epsilon_F e^{-\lambda/\epsilon_F}$). Here we show that in the presence of antiferromagnetic

correlations the pairing interaction becomes much stronger at wave vectors near Q, the temperature at which the pairing occurs is greatly enhanced and the gap function becomes very anisotropic, opening first in a small region (about $(\theta - \theta_0) \sim \kappa/p_F$) around the points connected by the vector Q and dropping rapidly away 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 wavevector polarizes the electrons in the neighboring plane in a large area around itself. Mathematically, we must construct the pairing vertex connecting a particle in one plane to a particle in the other. For small λ this vertex will be linear in λ and will be dressed by spin fluctuations in each plane: within RPA we have found that the dominant contribution to the dressed vertex $V(k,\omega)$ is that shown on Fig.1 which leads to

$$H^d_{int} = \sum_{p,p',k} V(k,\omega) c^\dagger_{p+k} \sigma^\alpha c_p c^\dagger_{p'+k} \sigma^\alpha c_{p'},$$
$$V(k,\omega) = \lambda J_Q^2 a^{-2} \chi^2(k,\omega), \tag{5}$$

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 full Green's function, including the self energy due to spin exchange within one plane. This self energy has been studied by many authors. An approximation convenient for our purposes is [13]:

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

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

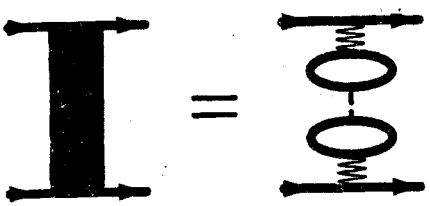

Fig.1.

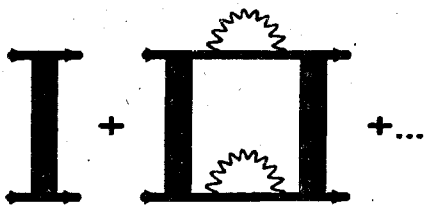

Fig.2.

Fig.1. Diagrammatic representation of dominant contribution to pairing interaction. Here the light dashed line represents the interplane interaction and the wavy line represents the dressed spin-fluctuation interaction between electrons in one plane
Fig.2. Ladder sum leading to gap equation. Here the shaded rectangle is the interaction V defined in Fig 1. Note that electron lines are dressed by in-plane fluctuations.

It is important that the gap is due to the pairing of spin excitations on different planes, so the interaction (5), although large in some region of momentum space, does not lead to self energy parts or vertex corrections. The gap equation, thus, follows from the summation of the ladder series in Fig.2. By performing the

ladder sum and integrating over the momenta in the direction normal to the Fermi surface we get

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

where $u=1-Q^2/(2p_F)^2$ and 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 $V(\mathrm{p}-\mathrm{p}',\omega)$ does not vary significantly.

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

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

where l and n are integers. From (8) it is evident that Δ depends only on $1+x^2$ which enters only in the denominator of the kernel. Thus, $\Delta(\theta)$ is peaked about $\theta=0$ with a width κ and decays for large θ as $1/\theta^4$, and is similarly peaked about the lowest Matsubara frequency $\omega_n=\pi T$ with the width $\Gamma\kappa^2\sim T$. The dimensionless kernel in (8) presumably has a 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. For $T\ll T^*$ we may replace the sum over frequencies in (7) by an integral; this integral is dominated by frequencies of the order of the zero temperature spin gap $\Delta(0)=\Delta^*$; similarly, we must replace κ^2 by $M\Delta^*$ because low frequency spin correlations near the antiferromagnetic wavevector Q are eliminated by the spin gap. The result is that up to numerical factors T^* in (9) is replaced by Δ^*. The gap takes its maximum value for angles $\theta\lesssim\sqrt{M\Delta^*}$; for larger θ it 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 and temperature dependent effective interaction, the pairing temperature and the gap scale as the interaction constant, unlike the usual BCS case where they are exponentially small. Although we have assumed specific form for the spin susceptibility (3) with a temperature dependent correlation length, this assumption is not essential to our results. The enhancement of the between-planes pairing is due to the strong temperature dependence of $\sum_q\chi'(q,\omega=0)^2$. This quantity is measurable via NMR T_2 experiments [14] and has been found to be large and strongly temperature dependent in $YBa_2Cu_3O_{7-x}$ [14, 15].

The development in the spin liquid case is essentially identical. The momentum integrated Green's function square 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, so Eqs. (8), (9) are not changed.

We 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

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

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

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

Thus the singularity in the interaction is eliminated for commensurate spin fluctuations ($k_x, k_y \sim \pi$) in tetragonal crystals. For orthorhombic crystals or for incommensurate spin fluctuations the singular part of the interaction is of order 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 will only occur at a lower temperature where the charge carriers bose condense. The former scenario is consistent with the behavior of optimally doped or overdoped $YBa_2Cu_3O_{6+x}$ and with $La_{2-x}Sr_xCuO_4$ at all dopings, while the latter scenario is consistent with the behavior of underdoped $YBa_2Cu_3O_{6+x}$. For example, in $YBa_2Cu_3O_{6.6}$, spin gap effects are observed in NMR below $T^* \sim 150\,\mathrm{K}$ while the superconducting $T_c \sim 60\,\mathrm{K}$. 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 $YBa_2Cu_3O_{6.6}$ [17] is also consistent with this scenario. However, none of these observations (except the qualitative one 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 one qualitative disagreement with experiment. Because the gap opens first and is largest at the points on the Fermi surface connected by the wavevector where $\chi(k,\omega)$ is peaked, the low frequency antiferromagnetic spin fluctuations are suppressed more strongly than spin fluctuations at other wavevectors. 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]; therefore in our scenario the copper relaxation rate would drop more rapidly than the oxygen or yttrium rates as the spin gap opened, in apparent disagreement with experimental data on $YBa_2Cu_3O_{6.6}$ [18].

Note added: 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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