Antiferromagnetic Interactions and the Superconducting Gap Function

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Spin-fluctuation-mediated superconductivity is conventionally associated with \( d_{x^2-y^2} \) pairing. We show that a generalized model of antiferromagnetic spin fluctuations in three dimensions may also yield a state with formal “s-wave” \((A_1g)\) symmetry but with line nodes at \( k_z \approx \pm \pi/2c \). We study this new state within both BCS and Eliashberg theories using a realistic band structure and find that it is more stable than the \( d_{x^2-y^2} \) \((B_{1g})\) state over a wide range of parameters. Thus, models of spin-fluctuation-mediated superconductivity must consider both possibilities on an equal footing.

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One of the fundamental questions concerning the cuprate superconductors is the symmetry of the superconducting gap function \( \Delta_k \). Experiments which probe the relative sign of the Josephson currents in the \( a \) and \( b \) directions in YBa\(_2\)Cu\(_3\)O\(_7\) (YBCO) \([\dagger]\) are commonly considered proof of \( d_{x^2-y^2} \) pairing. However, recent theories which account for the CuO chains in YBCO have challenged this interpretation \([\dagger]\), and other measurements exist \([\dagger]\) which are difficult to reconcile with this pairing symmetry. Thus, current experiments do not unambiguously establish \( d_{x^2-y^2} \) pairing for all the cuprates under all conditions.

The experiments of Ref. \([\dagger]\) are consistent with theories of high-temperature superconductivity based on antiferromagnetic spin fluctuations \([\dagger]\) \([\dagger]\). Since the CuO\(_2\) planes in the cuprates are generally considered the most important structural elements for the superconductivity, most work on this subject has focussed on a single, two-dimensional (2D) band, representing the physics of an isolated CuO\(_2\) plane. Within this framework, it is now well established that antiferromagnetic spin fluctuations yield singlet pairing in a \( d_{x^2-y^2} \)-like orbital state \([\dagger]\) \([\dagger]\) \([\dagger]\). This pairing symmetry can be understood by noting that antiferromagnet spin fluctuations produce a repulsive interaction which inhibits on-site pairing but favors pairing on nearest-neighbor sites \([\dagger]\).

In materials like YBCO, though, there are two CuO\(_2\) planes per unit cell. One therefore expects that two 2D bands will be involved in the physical description, both of which may contribute to the superconductivity. Recent calculations within such bilayer systems based on either weakly \([\dagger]\) \([\dagger]\) \([\dagger]\) or strongly \([\dagger]\) \([\dagger]\) \([\dagger]\) correlated electrons concluded that an alternative to the \( d_{x^2-y^2} \) \((B_{1g})\) state may exist. In this state, there are two gap functions (one for each band) which may be strongly anisotropic in wave vector space but which do not have nodes; however, the two gap functions do have opposite signs. Hence, this state has been termed the \( s^\pm \) state \([\dagger]\). Strong-coupling Eliashberg calculations have demonstrated that the \( s^\pm \) state is actually more stable than the \( d_{x^2-y^2} \) state whenever the inter-band antiferromagnetic correlations are stronger than the intra-band ones \([\dagger]\). This pairing symmetry may also be consistent with all \([\dagger]\) of the experimental determinations of the phase of \( \Delta_k \).

The \( s^\pm \) state is restricted to the bilayer cuprates such as YBCO, and thus does not address the superconductivity in single-layer cuprates like La\(_{1-x}\)Sr\(_x\)CuO\(_4\) (LSCO). Moreover, both \( s^\pm \) and \( d_{x^2-y^2} \) states are based on a 2D picture that neglects the third dimension. In particular, increasing the bilayer separation in a three-dimensional (3D) layered system causes the two-band structure to cross-over into a single-band one. Thus, there should be a one-band analog of the \( s^\pm \) state in 3D which would compete with the \( d_{x^2-y^2} \) state.

We examine this possibility within a general model for antiferromagnetic spin fluctuations in a single 3D band. By solving both the weak-coupling BCS and strong-coupling Eliashberg gap equations at \( T_c \), we are able to compute the phase diagram for the different pairing symmetries. We find that the one-band analog of the \( s^\pm \) state exists and is stable over a large range of antiferromagnetic correlation lengths which parameterize our model. We emphasize that, even if fully oxygenated YBCO has \( d_{x^2-y^2} \) pairing, one may be able to observe a transition to this \( s^\pm \) state by changing the correlation lengths through changes in oxygen content, pressure, and chemical substitution. The possible experimental relevance of this state therefore demands that it be considered as a serious alternative to the conventional \( d_{x^2-y^2} \) state in future calculations.

To be as general as possible, we take the antiferromagnetic spin fluctuation interaction to have the form

\[
V(q, \omega) = \frac{V_0}{1 + \xi_{ab}(q|| - Q||)^2 + \xi_c^\perp(q\perp - Q\perp)^2 - i\omega/\omega_{SF}},
\]

where \( V_0 \) is the electron-spin fluctuation coupling strength; \((Q||, Q\perp) = (\pi/a, \pi/a, \pi/c)\) and \( \omega_{SF} = 7.7 \) meV are the spin fluctuation wave vector and characteristic frequency; and \( \xi_{ab} \) and \( \xi_c^\perp \) are the intra- and
inter-planar antiferromagnetic correlation lengths, respectively. [Throughout this paper, \( a \) (\( c \)) is the unit cell dimension normal to (along) the \( z \) direction.] When \( \xi \rightarrow 0 \), Eq. (1) reduces to the 2D spin fluctuation model of Mil-\[s, Monien, and Pines (14,6).\]lis, Monien, and Pines (14,6). \( \xi \) is introduced into this model in a straightforward way to account for the experimental fact that inter-planar antiferromagnetic correlations exist in YBCO (13).

This interaction [Eq. (1)] is assumed to exist between quasiparticles which have a 3D dispersion relation \( \epsilon_k \). To further relate our calculations to the cuprates, we take \( \epsilon_k \) from the single-band model developed by Andersen et al. for YBCO (14):

\[
\epsilon_k = -2t_1(\cos k_x a + \cos k_y a) - 4t_2 \cos k_x a \cos k_y a \nonumber \\
- \frac{t_3}{2}(\cos k_x a - \cos k_y a)^2 \cos k_z c - \mu. \tag{2}
\]

Here, \( t_1 = 0.25 \) eV, \( t_2 = -0.1 \) eV, and \( t_3 = 0.05 \) eV are the matrix elements for intra-planar nearest-neighbor, intra-planar next-nearest-neighbor, and inter-planar hopping, respectively; \( \mu = -0.4 \) eV is the chemical potential. Note the surprising dependence of the inter-planar hopping on the intra-planar wave vector. This behavior results from the reduction of the full local-density approximation band structure to a single-band, tight-binding dispersion; see Ref. (18) for details. Equation (2) reproduces the general features of the band structure of YBCO and yields the Fermi surface shown in Fig. 1.

With the pairing interaction and the band structure specified, we can proceed to study the superconductivity within either BCS theory or its strong-coupling counterpart, Eliashberg theory (18). For simplicity, let us first consider the BCS equation at \( T_c \),

\[
\lambda_{\text{pair}} \Delta_k = -\frac{1}{N} \sum_{k'} V_{k-k'} \frac{\tanh(\epsilon_k/2k_B T)}{2\epsilon_{k'}} \Delta_{k'}, \tag{3}
\]

where \( \Delta_k \) is the gap function, \( V_{k} = V(q,0) \) is the pairing interaction [Eq. (1)], \( \epsilon_k \) is the electronic dispersion [Eq. (2)], \( N \) is the number of sites in the lattice, \( T \) is the temperature, and \( \lambda_{\text{pair}} \) is the pairing eigenvalue. This equation is written for singlet pairing, for which \( \Delta_{-k} = \Delta_k \); for triplet pairing, \( \Delta_{-k} = -\Delta_k \), and the right-hand side of Eq. (3) is multiplied by \(-1/3\). The Eliashberg equations are similar in spirit although formally more complicated; the interested reader is referred to the literature (18).

Equation (3) is an eigenvalue equation, allowing the eigenvectors \( \Delta_k \) to be classified into different representations of the crystal point group by their transformation properties under the elements of that group (18). The “pairing symmetry” of \( \Delta_k \) refers to this representation. For example, in tetragonal systems (point group \( D_{4h} \)), “\( d_{x^2-y^2} \) pairing” corresponds to the \( B_{1g} \) representation and “\( s^\pm \) pairing” to the \( A_{1g} \) representation. To determine the most favored pairing symmetry, one can either find the representation yielding the largest \( \lambda_{\text{pair}} \) at fixed \( T \) or the largest \( T_c \) (defined by \( \lambda_{\text{pair}}(T = T_c) = 1 \)). We employ both methods to construct the phase diagram for our model and find consistent results.

We solve Eq. (3) and its strong-coupling counterpart using a fast Fourier transform technique with the wave vector integrations carried out over the entire Brillouin zone (21). The extremal eigenvalues for each one-dimensional representation of the point group are obtained by an iterative procedure with an eigenvalue shift (22). The BCS calculations are carried out on a 32 x 32 x 32 discretization of the Brillouin zone, and the strong-coupling calculations are performed on a 64 x 64 x 8 mesh with 256 Matsubara frequencies, corresponding to a frequency cut-off on the order of three times the band width. Except as noted below, our results are insensitive to these choices.

In discussing our results, we begin with an examination of the gap function symmetries associated with the dominant pairing eigenvalues. We have calculated \( \lambda_{\text{pair}} \) for all the one-dimensional representations of the
tetragonal point group over a large range of correlation lengths (see below), and we find only two representations which lead to a superconducting instability: \( B_{1g} \) and \( A_{1g} \). The \( B_{1g} \) solution is shown in Fig. 3(a) and corresponds to the \( d_{xz-zy} \)-like solution encountered in previous work on a single band in 2D. This state possesses nodal planes defined by the directions \([110]\) and \([100]\), and by \([1\overline{1}0]\) and \([001]\), and can be thought of as an intra-planar pairing of quasiparticles on nearest-neighbor sites. On the other hand, the \( A_{1g} \) solution is new. From Fig. 3(b), we see that the \( A_{1g} \) solution, while formally having “\( s^\pm \) -wave” (i.e., \( A_{1g} \)) symmetry, possesses nodal lines at \( k_z \approx \pm \pi/2c \) 2. The gap function \( \Delta_k \) thus transforms like \( \Delta_k \sim \cos k_z c \) and corresponds to the pairing of quasiparticles between different planes. This solution is the one-band analog of the \( s^\pm \) state discussed within the context of two-band, 2D models 3. We can see this analogy by mentally translating every other plane in this monolayer model to produce a bilayer; under this transformation, the regions of \( \Delta_k \) with the same sign in Fig. 3(b) would be mapped onto one of the resulting two bands, and the nodes would disappear in favor of the band gap, maximizing the superconducting condensation energy.

The one-band \( s^\pm \) state exists as a possible superconducting solution, but is it stable? When \( \xi_c \to 0 \), Eq. 3 indicates that \( \Delta_k \) can only depend on \( k_y \) and \( k_y^\prime \); we therefore expect that the only stable solution will be the \( d_{yz-zy} \)-like \( (B_{1g}) \) one. On the other hand, when \( \xi_{ab} \to 0 \), Eq. 3 must yield a \( \Delta_k \) which depends only on \( k_z \). Moreover, we require a sign change in the \( \Delta_k \) connected by wave vectors where \( V_\mathbf{q} \) is maximal (at \( \mathbf{q} = (0,0,\pi/c) \)) in order to cancel the negative sign on the right-hand side of Eq. 3. These demands are met by the \( s^\pm \) state of Fig. 3(b), and so this solution should be stable in this limit.

For intermediate values of the correlation lengths, we should see a cross-over between these states.

We have tested these expectations numerically and present our results in Figs. 2 and 3. Consider first Fig. 2, which shows \( \lambda_{\text{pair}} \) as a function of \( \xi_c \) for \( \xi_{ab} = 2.3a \) computed within strong-coupling Eliashberg theory. The largest pairing eigenvalues, and hence the most favored superconducting solutions, belong to the \( B_{1g} \) \( (d_{xz-zy}) \) or \( A_{1g} \) \( (s^\pm) \) representations. As \( \xi_c \) increases, we see that the most stable solution crosses over from the \( B_{1g} \) to the \( A_{1g} \), representation, as we expect from the preceding discussion.

To give these results a more physical interpretation, we show in Fig. 3 the critical temperature \( T_c \) of the most stable pairing symmetry as a function of the intra- and inter-planar correlation lengths determined from a BCS calculation. 2. The \( A_{1g} \) state is stable over a large region of parameter space, with the phase boundary given roughly by the line \( \xi_c/c = 2c\xi_{ab}/a \). The limiting cases discussed above are confirmed as well: the \( B_{1g} \) \( (d_{xz-zy}) \) solution dominates as \( \xi_c \to 0 \), and the reverse is true for the \( A_{1g} \) \( (s^\pm) \) state as \( \xi_{ab} \to 0 \). In addition, the critical temperatures are largest along the \( \xi_c = 0 \) and \( \xi_{ab} = 0 \) lines and increase as the antiferromagnetic correlation lengths increase.

Moving towards the phase boundary in Fig. 3, \( T_c \) decreases but does not vanish, at least for large \( \xi_{ab} \) and \( \xi_c \). At small correlation lengths, however, \( T_c \) is small near the phase boundary and very sensitive to the finite-size effects induced by our discretization of the Brillouin zone. Hence, we cannot exclude the possibility of a finger of normal phase extending between the two superconducting phases at small \( \xi_{ab} \) and \( \xi_c \). With this caveat, we believe the Fig. 3 represents the true phase diagram of our model.

It is important to note that the existence of the one-band \( s^\pm \) \( (A_{1g}) \) state depends only on the 3D interaction and not the detailed band structure. Specifically, recomputing the phase diagram with \( \lambda_3 = 0 \) in Eq. 3 gives nearly identical results. The \( s^\pm \) state may therefore be compatible with theories of the cuprate superconductors in which single-particle inter-layer hopping is suppressed but Cooper pair tunneling is not. Of course, the stability of the \( s^\pm \) state in any concrete system, as opposed to its existence, depends on microscopic details such as the band structure and must therefore be evaluated on a case-by-case basis.

To conclude, we have shown that single-band models of antiferromagnetic spin fluctuation-mediated superconductivity in 3D do not automatically give rise to \( d_{xz-zy} \) pairing. Rather, a phase which possesses formal “\( s^\pm \) -wave” \( (A_{1g}) \) symmetry with nodal lines at \( k_z \approx \pm \pi/2c \) exists.
and is stable over a wide range of parameters. Within the context of the cuprate superconductors, these results imply that this unusual s state, which is the one-band analog of the $s^\pm$ state of Ref. [4], must be considered on equal footing with the conventional $d_{x^2-y^2}$ state. This point is reinforced by the fact that the $s^\pm$ state is favored when the inter-planar antiferromagnetic correlations are stronger than the intra-planar ones, a situation which may obtain in the cuprates. Finally, the results of this paper suggest that, even in a superconductor with pure $d_{x^2-y^2}$ pairing, substitution, doping, or pressure may lead to a change in the correlations lengths and thus to a transition between different gap function symmetries. Such transitions may already have been observed in angle-resolved photoemission experiments [25].

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[22] See, for example, F. S. Acton, Numerical Methods that Work (Harper and Row, New York, 1970), Chapter 8.

[23] Numerically, the nodes are located at $k_\pm = \pm \pi/2c$ for the gap functions we have examined, but there is no group theoretic reason that they must be at those locations.

[24] The point $(\xi_{ab}, \xi_c) = (0,0)$ is exceptional in that there can be no solution for any representation when $V_0 > 0$ [cf. Eq. (3)].

[25] $T_c$ is easier to compute in BCS theory than in Eliashberg theory, but is less accurate. Nonetheless, the phase boundary from the BCS calculations is in close agreement with the Eliashberg results of Fig. 3, which supports the qualitative correctness of the BCS phase diagram.

[26] Interpreting the interaction $V_q$ as a spin fluctuation imposes a sum rule at $T = 0$, which we satisfy by adjusting $V_0$ in Eq. (1) to make the total spectral weight $\sum_q |V(q)|^2$ independent of $\xi_{ab}$ and $\xi_c$.

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