Hole Dispersion and Symmetry of the Superconducting Order Parameter for Underdoped CuO$_2$ Bilayers and 3D Antiferromagnets.

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We calculate the dispersion of a hole in CuO$_2$ bilayers and 3D antiferromagnets, using the self-consistent Born approximation (SCBA) to the t – J model. Superconductivity and the symmetry of its order parameter are studied introducing a nearest-neighbor density-density attraction induced by short range antiferromagnetic (AF) fluctuations, as described in recent studies for the single layer cuprates. The well-known pairing in the $d_{x^2-y^2}$ channel observed for one plane remains robust when three dimensional interactions are turned on. In bilayers, as the exchange along the direction perpendicular to the planes grows, eventually a transition to a “s-wave” state is observed with an order parameter mixture of $d_{3z^2-r^2}$ and $s_{x^2+y^2}$ channels. For an isotropic 3D antiferromagnet the $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ channels are degenerate. Our results are compared with other predictions in the literature.

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1. INTRODUCTION

Since the discovery of high temperature superconductors, the origin of the pairing mechanism has been controversial. Numerous studies suggest that the normal state properties are anomalous and, as a consequence, above the critical temperature, $T_c$, the strongly correlated character of the conduction electrons in the cuprates should be taken into account in any realistic study. In particular, the presence of short-range antiferromagnetic fluctuations have been invoked by several groups as the origin of the deviations from a conventional Fermi liquid behavior observed in transport measurements above $T_c$. Theories based on antiferromagnetic fluctuations quite clearly predict a superconducting condensate in the $d_{x^2-y^2}$ channel. These studies are supported by experimental results for the bilayer cuprate YBa$_2$Cu$_3$O$_7$, which are compatible with a highly anisotropic pairing state, likely a $d_{x^2-y^2}$ singlet. Photoemission results for Bi-2212, which also have two CuO$_2$ layers per unit cell, support this scenario, and thus superconductivity induced by AF correlations is a strong candidate to explain the pairing mechanism of the cuprates.

The authors and collaborators have recently explored these ideas using simple models for quasiparticles (q.p.) considered as holes strongly dressed by AF fluctuations, and interacting through a nearest-neighbor (NN) density-density attraction, as suggested by the study of the two-holes bound-state of the t – J model. The presence of a large accumulation of weight in the density of states, induced by the small bandwidth of the q.p. dispersion, enhances $T_c$ beyond what would be naively expected from the strength of the hole-hole attraction. These ideas were originally referred to as the “antiferromagnetic van Hove” (AFVH) scenario, but it is important to remark that the boost in $T_c$ does not arise exclusively from a van Hove singularity but mainly from the “flat” regions observed in the q.p. dispersion, effect which is induced by AF correlations.

The purpose of this paper is (i) the study of the properties of holes and (ii) the extension of previous analysis for the symmetry of the superconducting order parameter to the case of lightly doped bilayers and 3D antiferromagnets. The effective Hamiltonian introduced in previous publications for one plane is defined on the 2D square lattice as

$$H = \sum_{k,\alpha} \epsilon_{AF}(k)c_{k\alpha}^\dagger c_{k\alpha} - V \sum_{\langle ij \rangle} n_i n_j,$$  

where $c_{k\alpha}$ denotes a destruction operator of a q.p. with dispersion extracted from accurate numerical and analytical studies of one hole in the undoped $t – J$ model given by $\epsilon_{AF}(k)/eV = 0.165 \cos k_x \cos k_y + 0.0435(\cos 2k_x + \cos 2k_y)$, where $t = 0.4eV$ and $J/t = 0.3$ are assumed.

The quasiparticles move within the same sublattice to avoid distorting the AF background ($\alpha = A, B$ denotes the sublattice). This is correct in the limit of a small number of holes in a long-range ordered AF system, and it is expected to be a good approximation even with AF short-range order, as long as the AF correlations are strong. The dispersion $\epsilon_{AF}(k)$ reflects a remarkable feature of the cuprates, observed in photoemission experiments, namely the presence of flat bands near $(0, \pi) \ (\pi, 0)$ in the standard square lattice notation.

The parameter $V$ is the intersublattice density-density attractive coupling strength between holes also discussed in previous literature, with $n_i$ the number operator. The rest of the notation is standard.

The interaction in Eq.(1) should be considered as the dominant piece of a more general and extended AF-induced effective potential between holes which in the presence of long-range order corresponds to a sharp $\delta$-function centered at $Q = (\pi, \pi)$ in momentum space, and it acquires a width as the AF correlation length $\xi_{AF}$ decreases. Even with $\xi_{AF}$ as small as a couple of lattice spacings, it has been shown that the NN interaction used in Eq.(1) remains robust. Equivalently, the NN
hole-hole attraction can be considered as arising from the “minimization of broken AF links” argument \[3\] in the large $J/t$ limit.

It is expected that Hamiltonian Eq.(1), which is certainly a very simplified version of the low energy behavior of the $t - J$ model, nevertheless captures the important features of holes moving in AF backgrounds at low doping, and temperatures smaller than $J$ where the quasiparticles are dominant. This is a regime difficult to study with numerical methods directly applied to the $t - J$ model. The analysis of Eq.(1) using standard BCS techniques, Exact Diagonalization approaches, and the Eliashberg equations, has been fairly successful in reproducing some experimental features of the cuprates. [10]

For example, in this model superconductivity appears in the $d_{x^2−y^2}$ channel, as it seems to occur in experiments, with a critical temperature $T_c \sim 100K$. In addition, the concept of “optimal doping” appears naturally due to the robust peak in the density of states (DOS) produced by the dispersion $\epsilon_{AF}$($k$), which is crossed by the chemical potential as the hole density grows. In this respect, the theory has features very similar to those discussed before in “van Hove” theories for the cuprates. [10] Indeed, the quasiparticle lifetime is linear with energy at optimal doping. However, the flat regions in the dispersion and the associated accumulation of weight in the DOS are produced by strong correlations and thus they are stable against small perturbations, like impurities and extra couplings, effects that usually destroy weak logarithmic van Hove singularities. The specific heat jump, $2\Delta/T_c$ and other important BCS ratios are in good agreement with the experimental data. [10]

Although certainly more work is needed to show that these “real-space” pairing ideas presented in previous literature are a strong candidate to describe the cuprates, its quantitative success led us here to study geometries and couplings beyond those of the single layer with some confidence. Our goal is to report the trends observed when systems different from a single layer cuprate are analyzed. Here, the hole spectrum in the bilayer and 3D antiferromagnets is calculated with the SCBA which was shown to reproduce accurately numerical results for the 2D $t-J$ model, [11] and it was successfully applied to the 2D $t'-J$ model to compare its predictions with the photoemission spectra of Sr$_2$CuO$_2$Cl$_2$. [2] Using the formalism previously described, a hole-hole attraction will be introduced producing a superconducting state. Here, the symmetry of this superconducting state will be analyzed and compare with other predictions for the same bilayer and 3D systems.

II. SELF CONSISTENT BORN APPROXIMATION.

The Hamiltonian for spins and holes used in this section is defined as,

$$H = -\sum_{\alpha} t_{\alpha} \sum_{i\sigma} (\bar{c}_{i\sigma} \bar{c}_{i+e_{\alpha},\sigma} + h.c.)$$

$$-\frac{1}{2} \sum_{\alpha\beta} t_{\alpha\beta} \sum_{i\sigma} (\bar{c}_{i\sigma} \bar{c}_{i+e_{\alpha} \pm e_{\beta},\sigma} + h.c.)$$

$$+ \sum_{\alpha} J_{\alpha} \sum_{i} [(S_{i}^{+} S_{i+e_{\alpha}}^{−} - \frac{1}{4} n_{i} n_{i+e_{\alpha}})$$

$$\pm \frac{1}{2} \theta_{\alpha}(S_{i}^{+} S_{i+e_{\alpha}}^{−} + S_{i}^{−} S_{i+e_{\alpha}}^{+}),$$

where $i$ denotes sites of a bilayer or simple 3D cubic cluster, $e_{\alpha}$ is the unit vector in the $\alpha$-direction ($\alpha = x, y, z$), $t_{\alpha}$ and $J_{\alpha}$ correspond to the NN hopping amplitude and exchange coupling, respectively, in the direction $\alpha$, $t_{\alpha\beta}$ is the next-nearest-neighbors (NNN) hopping in the directions defined by $e_{\alpha} \pm e_{\beta}$, the parameter $\theta_{\alpha}([0,1])$ represents a possible exchange anisotropy added for completeness, and the rest of the notation is standard. In the terms with NNN interactions, the summation is done with the condition $\alpha \neq \beta$, i.e. we only consider NNN hopping along the diagonals of the plaquettes. A generalization to include NNN hopping at distance of two lattice spacings along the main axes is straightforward. The constraint of no double occupancy is implemented in the kinetic energy by means of the standard definition for hole operators $c_{i\sigma} = c_{i\sigma} (1-n_{i\sigma})$, with $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$.

Let us extend the SCBA analysis which has been applied before to single planes [11] to the bilayer and 3D Hamiltonian Eq.(2). Following steps that by now are standard, first we redefine operators according to $S_{j}^{+} \rightarrow S_{j}^{+}$, $S_{j}^{−} \rightarrow -S_{j}^{−}$, $c_{j\sigma} \rightarrow c_{j\sigma}$, where $j$ denotes sites on the $B$ sublattice. Spins on the $A$ sublattice remain intact. With this procedure an AF state becomes ferromagnetic. Then, the usual linearized Holstein-Primakoff transformation is used. This transformation is defined in terms of Bose operators $a_{i}$ and $a_{i}^\dagger$, according to $S_{i}^{\pm} \approx a_{i}^\dagger \pm \sqrt{2} S_{i}^{\pm}$, $S_{i}^{\sigma} \approx a_{i}^\dagger a_{i}$, and $S_{i}^{z} = S - a_{i}^\dagger a_{i}$. To handle the hole sector, the spin-charge decomposition $c_{i\sigma} = h_{i\sigma}^\dagger$ and $c_{i\uparrow} = h_{i\uparrow}^\dagger S_{i}^{+}$ is introduced, where $h_{i\sigma}, h_{i\uparrow}^\dagger$ are operators corresponding to spinless holes. Finally, using periodic boundary conditions and after long but straightforward algebra, we can rewrite the resulting Hamiltonian in momentum space as

$$H = E_0 + \sum_{k} \epsilon_{k} h_{k}^\dagger h_{k} + \sum_{q} \omega_{q} q_{q}^\dagger q_{q}$$
where the Bose operators $b(b^\dagger)$ and $a(a^\dagger)$ are connected by a Bogoliubov transformation, \[ N \] is the number of sites in the lattice, $\epsilon_k = 4(t_{xy} \cos k_x \cos k_y + t_{xz} \cos k_x \cos k_z + t_{yz} \cos k_y \cos k_z)$ is the bare spinless hole dispersion (which cancels in the absence of an explicit NNN hopping in the Hamiltonian), and $M_{k,q} = \nu_q \beta_k - q + v_q \beta_k$ is the hole-magnon vertex. The magnon dispersion is given by $\omega_q = \omega_0 \nu_q$, where $\omega_0 = zSJ$, $J = \frac{1}{2} \sum J_a$, $S = \frac{1}{2}$ is the spin of the electrons in the original $t-J$ model language, $d$ is the number of dimensions (which will be taken equal to 3 in the rest of the paper), $z = 2d$ is the coordination number, and we have used units where $\hbar = 1$. The other quantities are defined as follows:

$$\beta_k = 2 \sum_\alpha t_\alpha \cos k_\alpha,$$

$$\nu_q = \sqrt{1 + \nu_q^2}, \quad \nu_q = -\text{sgn} \kappa_q \sqrt{1 - \nu_q^2},$$

$$\kappa_q = 2 S \sum_\alpha J_\alpha \beta_\alpha \cos q_\alpha \rho_\alpha \omega_0.$$  

The ground state energy $E_0$ has the form:

$$E_0 = -dJN[S^2 + S(1 - \frac{1}{N} \sum_q \nu_q) + \frac{1}{4}].$$  

Care must be taken in order to apply Eqs.(3) and (4) to the bilayer. The small size in the $z$-direction (one lattice spacing) does not allow us to apply periodic boundary conditions (BC) to simulate bulk effects, as we do in the $x$- and $y$-directions. The $z$-axis BC should be open. How-

the bilayer. The small size in the $z$-direction (one lattice

from their actual values. Remember also that $k_\alpha$ to 1 (spin isotropic system). We also assumed $xy$ symmetry in the planes, i.e., orthorhombic distortions are not considered here. Thus, in the rest of the paper we will use the following notations: $J$ and $t$ will refer to the in-plane exchange and hopping parameters, while $J_\perp$ and $t_\perp$ correspond to the inter-plane ones. The gener-

ity of Eqs.(2-8) would allow the interested reader to obtain SCBA results for arbitrary situations where spin or lattice anisotropies are important, or including NNN hopping amplitudes.

Regarding the numerical values of the couplings, we have introduced relations between exchange and hopping amplitudes to simplify the multiparameter analysis. In particular, we have here assumed $\frac{t}{J} = (\frac{\nu}{\nu_0})^2$, which arises from the $t-J$ model when derived from the one band Hubbard model in strong coupling. In addition, we have fixed $t = 0.4$ eV throughout the paper. Thus, as parameters we only have $J/t$ and $J_\perp/J$.

The actual value of the inter-plane exchange is controversial. The two-magnon peak in Raman spectra experiments for YBa$_2$Cu$_3$O$_{6+x}$ is consistent with an in-plane $J \sim 125$ meV, with a negligible interplane exchange. \[ 14 \] Recent measurements of the nuclear quadrupole and nuclear magnetic resonances on Cu-sites in YBa$_2$Cu$_3$O$_{15}$ (alternating 1-2-3 and 1-2-4 structures) suggest a ratio $\frac{J_\perp}{J} \sim 0.3$. \[ 15 \] However, a different value $\frac{J_\perp}{J} \sim 0.55$ was found from infrared transmission and reflection measurements, after applying linear spin wave theory. \[ 14 \] A hopping amplitude ratio $\frac{t_\perp}{t} = 0.4$ was reported on the basis of first-principles linear density approximation calculations. \[ 15 \] corresponding to $\frac{t_\perp}{t} \sim 0.16$ with our convention. In view of these discrepancies, in most of the results below the perpendicular exchange is consider a free parameter.
III. RESULTS

A. Bilayer.

Let us first discuss the one hole spectrum in the AF bilayer system using the exchange ratio $J/\Gamma = (\frac{\pi}{a})^2 = 0.16$ suggested by band structure calculations, $t = 0.4$ eV and $J = 0.125$ eV, as found in some experiments ($J/t = 0.3125$). The self-consistent calculation was performed on a $16 \times 16 \times 2$ cluster. In Fig.1 the spectrum is presented. It has two branches that correspond to the two possible momenta in the z-direction i.e. 0 and $\pi$. These branches obey the relation $\epsilon_+(\mathbf{k}) = \epsilon_-(\mathbf{k} + \mathbf{Q})$, where $\mathbf{Q} = (\pi, \pi)$ and $\mathbf{k}$ is the 2D momentum ($\epsilon_{\pm}(\mathbf{k})$ here denote the even and odd branches of the spectrum). This relation is induced by the presence of antiferromagnetic long-range order in the system, which effectively reduces the size of the Brillouin zone. The minima of the branches are close to, but not exactly at, $\mathbf{k} = (\pi/2, \pi/2)$ i.e. where the minimum of the one-layer dispersion resides. This small effect is observed from fits of the data using trigonometric functions and it is barely noticeable in Fig.1, but as we increase $J_\perp$ the splitting of the minima away from $\mathbf{k} = (\pi/2, \pi/2)$ becomes larger, and at $J_\perp = J$ it is clearly visible. The bilayer one-hole spectrum can be accurately fit by NN, NNN and next to NNN hoppings amplitudes, namely $\epsilon_+(\mathbf{k}) = \pm 0.01(\cos k_x + \cos k_y) + 0.099 \cos k_x \cos k_y + 0.033(\cos 2k_x + \cos 2k_y)$ (eV) (see Fig.1). Note that each individual branch contains a NN amplitude which is nonzero. This is necessary since individually the even and odd branches are not invariant under a momentum shift in $\mathbf{Q}$. It should also be remarked that near $(\pi, 0)$ there are “flat” dispersion regions, as observed in previous studies of the $t-J$ model. [8] It has been argued that AF correlations induce these features in models of correlated electrons even when the $\xi_{AF}$ is only a couple of lattice spacings. [8] Fig.1 shows that these features also survive the introduction of a realistic bilayer coupling.

Our SCBA calculations indicate that the antiferromagnetic bilayer has quasiparticle excitations since a large peak appears at the bottom of the hole spectral function $A(\mathbf{k},\omega)$. Typical spectral functions for the high symmetry points are presented in Fig.2. The quasiparticle peak carries a substantial percentage of the spectral weight in agreement with the calculations for a single layer. [8] Note also that the closer the momentum to the bottom of the band, the stronger the quasiparticle peak. We observed a similar behavior even for interlayer exchanges as large as $\frac{\Gamma}{\Gamma} = 3$.

The evolution of the Fermi Surface (FS) as the SCBA hole dispersion is populated in the rigid band picture is shown in Fig.3. At very low hole density it starts with hole pockets around $(\pi/2, \pi/2)$ (Fig.3(a)) for the even and odd branches. The pockets are longer along the antibonding branch, while $k_z = \pi$ to the antibonding branch.
the (0, π) – (π, 0) direction than along the main diagonal in the Brillouin zone as observed in similar studies for the single layer problem. [36] As these pockets grow in size, the Fermi level eventually hits the saddle points and the FS changes its topology (Fig.3(b) and (c)), becoming a large FS when the chemical potential is above the saddle points (Fig.3(d)). It should be remarked that after the hole pockets disappear, the FS acquire quasi-nesting features, which may lead to an enhancement of certain susceptibilities. The energy scale of the rapid change from hole pockets to a large FS is about 400K. This implies that a strong temperature dependence should be expected in transport measurements of a doped AF bilayer, similar to those observed in a single AF layer. [37] Actually the overall FS evolution obtained from the rigid band filling of the bilayer dispersion for \( t^2 = (\frac{t}{J})^2 = 0.16 \) is qualitatively similar to results found for just one CuO\(_2\) plane using the same approximations. [39,40] with the main difference being the presence of two branches. Identifying similar features in experiments could give us information about the strength of the bilayer coupling and antiferromagnetic correlations.

FIG. 3. Evolution with doping of the Fermi Surface obtained by a rigid band filling of the one hole SCBA spectrum presented in Fig.1. The density grows moving from (a) to (d). The thick (thin) line corresponds to the bonding (antibonding) branch.

**B. 3D Cubic Lattice**

In this subsection, the properties of a hole in a 3D antiferromagnetic environment will be analyzed. The SCBA quasiparticle hole dispersion for the case of an isotropic cubic lattice (i.e. \( t^2 = (\frac{t}{J})^2 = 1 \)) is shown in Fig.4. The numerical self-consistent calculation was carried out on an 8 × 8 × 8 cluster with parameters chosen as \( t = 0.4 \) eV and \( J = 0.16 \) eV, which gives \( \frac{t}{J} = 0.4 \). The minimum of the dispersion is at \( (\pi/2, \pi/2, \pi/2) \), which is natural based on the results reported for the one and two coupled planes. Our best fit of the numerical data corresponds to the following dispersion:

\[
e(k) = 0.082(\cos k_x \cos k_y + \cos k_y \cos k_z + \cos k_z \cos k_x) + 0.022(\cos 2k_x + \cos 2k_y + \cos 2k_z) \text{ (eV)}.
\]

As in the case of the one layer system, holes tend to move within the same sublattice to avoid distorting the AF background.

FIG. 4. SCBA spectrum of one hole in an isotropic 3D AF with \( J/t = 0.4 \). The momentum in the z-direction is indicated. The lines are fits to the numerical data: the solid line corresponds to \( k_z = 0 \), dashed to \( k_z = \pi/2 \), and dotted-dashed to \( k_z = \pi \). Points between \( (\pi/2, \pi/2) \) and \( (\pi, 0) \) (not shown) are related by symmetry to others presented in the figure.

It is interesting to analyze the dependence of the quasiparticle dispersion total bandwidth, \( W \), with the ratio \( \frac{J}{t} \) for the isotropic 3D AF. Here \( W \) is defined as the difference in energy between the state with the highest energy, typically at \( (0, 0, 0) \) and \( (\pi, \pi, \pi) \), and the state with the lowest energy at \( (\pi/2, \pi/2, \pi/2) \). Fig.5 shows \( W \) as the ratio \( \frac{J}{t} \) varies from 0.1 to 1. Results for a single layer on an \( 8 \times 8 \) cluster are also shown for comparison. The overall behavior of the bandwidths is qualitatively the same in both cases, with \( W \) for a 3D AF being slightly larger. In both cases \( W/t \) grows approximately linearly for small \( J/t \), and reaches saturation around \( \frac{J}{t} \sim 0.6 \). In the linear regime, we find \( W \sim 2.5J \) showing that the characteristic energy scale of the dispersion is \( J \) rather than \( t \), a well-known result obtained before in the context of holes in 2D antiferromagnets. [3] It is interesting to observe that the increase in the dimensionality of the problem does not change dramatically the bandwidth of holes.

As for planes and bilayers, the SCBA calculations show a strong quasiparticle peak in the hole spectral function \( A(k, \omega) \) of an isotropic 3D AF. In Fig.6 results are shown at particular high symmetry points. The parameters are the same as those used to calculate the dispersion of Fig.4. We checked that the relative weight of the quasiparticle peak increases with the ratio \( \frac{J}{t} \). The quasiparti-
isotropic 2D AF (evaluated on an $8 \times 8$ cluster) shown for
comparison. Lines are drawn to guide the eye.

The 3D momenta $k$ drastically distorted when a finite but small hole density

is indicated.

Bandwidth of the hole spectrum in an antiferromagnet

$W$ (eV)$A($

is similar in 2D and 3D systems, at least at the
bottom of the hole spectrum.

Particle weight $Z$ is similar in 2D and 3D systems, at least at
the bottom of the hole spectrum.

FIG. 5. Open circles represent the bandwidth $W$ vs $J/t$
obtained from the SCBA quasiparticle hole spectrum for an
isotropic 3D AF. Filled diamonds are the bandwidth of an
isotropic 2D AF (evaluated on an $8 \times 8$ cluster) shown for
comparison. Lines are drawn to guide the eye.

FIG. 6. Spectral functions of a hole in an isotropic 3D AF
at high symmetry points for the same values of parameters
used in Fig.4 with a broadening $\delta = 0.1 t$ for the $\delta$-functions.
The 3D momenta $k$ is indicated.

IV. SUPERCONDUCTIVITY.

If there is a source of attraction between the quasiparticles described in the previous sections, then the ground state of the system could become superconducting. In the underdoped regime, AF correlations are strong and, thus, it is natural to study pairing mediated by AF fluctuations assuming that the dispersion at half-filling is not drastically distorted when a finite but small hole density

is studied. Since $\xi_{AF}$ is likely of the order of only a couple
of lattice spacing at realistic dopings, a real $-$ space
approach to pairing is more suitable than a picture where
extended states (magnons) are interchanged between car-
riers ($k$ $-$ space approach). While these two variations of
AF-mediated pairing are quantitatively different, nevertheless it has been shown that they lead to the same sym-
metry for the superconducting order parameter (SCOP).

Thus, independent of the discussion of real-space vs
$k$-space approaches, we believe that it is safe to use the
real-space pairing ideas of Ref. [5] to study the symmetry of
the SCOP for the case of a bilayer and 3D AF systems.

As explained before, the simplified picture introduced
in previous literature [5] is to use the spectrum of a hole,
calculated numerically or using the SCBA, as the disper-
sion of the quasiparticles which interact through a NN
attraction regulated by a parameter $V$ (of the order of
$J$). This interaction is motivated by AF-induced pairing
since it can be shown that a potential $V(q)$ in momentum
space maximized at $q = Q$ and smeared by a finite
$\xi_{AF}$, induces a real-space potential which is dominated
by a NN attraction. Previous estimations suggest a value
$V = 0.6 J$ from the study of the two-holes bound state on
a single layer. [5] Here, the same value will be employed
for the in-plane NN interaction, while for the interaction
in the z-direction $V_\perp = 0.6 J_\perp$ will be used. In the absence
of accurate Exact Diagonalization or Monte Carlo results
for the dispersion of holes away from half-filling, a rigid-
band filling of the SCBA quasiparticle spectra obtained
at half-filling will be assumed in the BCS gap equation.

Previous studies for single layer systems have shown that
this approach provides a SCOP with a symmetry consis-
tent with other more traditional methods, and in addition
the actual values of $T_c$ and its density dependence are in
qualitative agreement with experiments. [5] Thus, it is
natural to employ the same approach to analyze the SC
properties of doped bilayers and 3D antiferromagnets.

A. Superconductivity in a bilayer.

Using the bilayer SCBA hole dispersion and the hole-
hole NN attraction described before, we have studied su-
perconductivity within the BCS formalism. To calcu-
late the SCBA hole dispersion, we fixed $t_\perp = 0.3125$
and allow for the interlayer coupling to take the values
$t_\perp = 0.16, 0.3, 0.5, 1, 2$ and $3$. Solving numerically the
gap equation on large clusters, we observed that for the
first three ratios $t_\perp$ the symmetry of the superconduct-
ing order parameter (SCOP) is $d_{x^2-y^2}$ for all the hole
densities where superconductivity exists. This is the re-

gion analytically connected to the physics of one layer,
where a similar condensate was found in previous papers.

In Fig.7, we show $T_c$ vs the quasiparticle hole density for
a bilayer with $t_\perp = 1$. This dependence is also shown for
the case of a single layer with the same $J/t$, for compar-
The group consists of 10 irreducible representations among bilayer case. In general, the tetragonal point symmetry $J/t$ plane with of the SC order parameter changes only at high densities where a bilayer changes the symmetry of the superconducting condensate into an “$s$-wave” state to be discussed below (note that a quasiparticle weight $Z$ smaller than one implies the existence of incoherent weight in the spectral function at energies larger than those of the q.p. band. Then, “high density” in this context does not imply a very small electronic density (n)). Similar conclusions were obtained in Ref. [20] where an Exact Diagonalization study of coupled layers was carried out to calculate the superconducting pairing correlations. No important enhancement of pairing correlations changing from a single $t-J$ layer to a bilayer was reported. [20]

FIG. 7. Superconducting critical temperature $T_c$ (solid line) vs quasiparticle density for an AF bilayer with $J/t = 0.3125$ and $J_{1}/J = 1$ (see text for details). The dashed line is $T_c$ vs quasiparticle density for a 2D AF plane with $J/t = 0.3125$. Both lines are calculated within the framework of the real-space pairing approach and the BCS gap equation. For bilayers, at high q.p. densities ($x \sim 55\%$) there is a transition to an “$s$-wave” state.

According to the classification of Liu, Levin and Maly [21] the $d_{x^2-y^2}$ state that we observed is labeled $(d,d)$, which means that a gap with the symmetry $d_{x^2-y^2}$ opens in both the bonding and antibonding Fermi surfaces (i.e. the Fermi surfaces corresponding to $k_{c} = 0$ and $\pi$ shown in Fig.1). This $d$-wave channel dominates up to values close to $J_{1} \sim J$. At the ratio $J_{1}/J = 1$ the symmetry of the SC order parameter changes only at high densities (i.e. around 55% filling of the quasiparticle band as shown in Fig.7) to a mixture of $d_{3z^2-r^2}$ and $s_{x^2+y^2+z^2}$, with real amplitudes of the same sign. $s_{x^2+y^2+z^2}$ is the 3D analog of the extended $s$-wave function. The relative weight of the $d_{3z^2-r^2}$ component is dominant in the bilayer case. In general, the tetragonal point symmetry group consists of 10 irreducible representations among which only five correspond to singlet pairing. The functions $3z^2 - r^2$, $x^2 + y^2 + z^2$ and also a constant function have the same transformation properties with respect to the tetragonal symmetry operations and thus belong to the same representation $\Gamma_{1}^{+}$ of the tetragonal lattice symmetry group. Then, they mix together and they form the “$s$-wave” representation with respect to rotations in the planes, while $d_{x^2-y^2}$ belongs to $\Gamma_{1}^{-}$ and $d_{xy}$ to $\Gamma_{4}^{+}$ for a tetragonal system. [22] Note that in an orthorhombic lattice $d_{3z^2-r^2}$, $s_{x^2+y^2+z^2}$ as well as $d_{x^2-y^2}$ correspond to the same representation $\Gamma_{1}$. A less trivial issue is how the symmetry evolves from a mixture of $d_{3z^2-r^2}$ and $s_{x^2+y^2+z^2}$ to the so-called $d_{z}$ state [23] (the $d_z$ state is a singlet along the link in the $z$-direction of the bilayer, i.e. it is “$s$-wave” with respect to $\pi/2$ rotations of the planes). This transition occurs as the ratio $J_{1}/J$ grows at a fixed density. The relative weight of $s_{x^2+y^2+z^2}$ in the mixture increases until both functions become equally weighted with the same signs of the weight coefficients in the limit of $J_{1} \gg J$. In this situation the mixture is exactly equivalent to the $d_z$ symmetry. In our calculations a coupling $J_{1}/J = 2$ is enough to have almost $d_z$ symmetry for all densities, with a substantial increase of $T_c$ up to 150K. The mixture of $d_{3z^2-r^2}$ and $s_{x^2+y^2+z^2}$ can also be viewed as the mixture of $d_z$ and the extended in-plane $s$-wave $s_{x^2+y^2}$, or in terms of odd-even gaps $\Delta_{\pm}(k) \propto z + \beta(\cos{k_{x}} + \cos{k_{y}})$, where $k$ is the in-plane momentum of the quasiparticle (the even and odd gaps differ by a constant corresponding to the inter-plane pairing amplitudes). In a similar fashion, as the ratio $J_{1}/J$ increases, the relative weight of the in-plane extended $s$-wave decreases.

FIG. 8. Schematic representation of the strong $V$ coupling limit of the two quasiparticle problem for the case of a bilayer. The dashed and dotted lines represent the effective hopping amplitudes contained in the SCBA dispersion that we label $t_1$ and $t_2$, respectively. For more details see text.

There is a simple intuitive way to understand the evolution with $J_{1}/J$ of the symmetry of the superconducting order parameter found here. [24] Consider the limit of Eq.(1) applied to a bilayer where the NN in-plane and inter-plane attractions dominate over the kinetic energy. In this limit, let us analyze the two quasiparticle problem and its bound state. The quasiparticles will be roughly at a distance of one lattice spacing (tight bound state).
In the reference frame of one particle, the other can occupy any of the five NN sites (four in the same plane and one in the other plane). These sites are actually linked by the dispersion in the SCBA since the five sites belong to the same sublattice. In other words, the wave function of one quasiparticle orbiting around the other can be found in this limit from a simple 5-site 1-particle problem as shown schematically in Fig.8, with the ratio of hopping amplitudes $t_1$ and $t_2$ simulating the effect of $J_\perp/J$. Solving this trivial problem we find that for $J_\perp/J < 1$ (or $t_2/t_1 < 1$) the lowest energy is obtained for a state with amplitudes $c, -c, c, -c, 0$ ($c > 0$) at sites 1, 2, 3, 4, 5, respectively, which is the $d_{x^2-y^2}$ state. On the other hand, for $J_\perp/J > 1$ (or $t_2/t_1 > 1$) the ground state amplitudes have the same value (with its sign) in-plane, and a different value and sign out of the plane, as expected from the discussion above. Note also that these simple calculations illustrate the fact that a NN attraction and on-site repulsion is not enough to have a tendency to form d-wave pairs in a dilute gas. In the present case this potential must be supplemented by a particular hole dispersion that allows for the movement of carriers within the same sublattice.

B. Comparison with other theories

In the literature, several types of interactions between quasiparticles in a bilayer have been proposed. Of particular interest for our discussion are those based on phenomenological magnetic susceptibilities in the presence of dynamical short-range AF order, both in and between the planes. Recently it has been suggested [27] that the SCOP in a bilayer can be of a particular s-wave type named $(s, -s)$ with opposite signs in the odd and even branches of the spectrum of carriers. The assumption made in Ref. [24] is that the in-plane magnetic susceptibility $\chi_\| (q)$ has the opposite sign, but the same absolute value, as the inter-plane susceptibility $\chi_\perp (q)$. In other words, $\chi_\| (q) = -\chi_\perp (q) = \chi_0 (q)$, where $\chi_0 (q)$ is the phenomenological susceptibility of a doped 2D antiferromagnet peaked at $q = Q = (\pi, \pi)$ introduced to fit NMR data [25]. This assumption needs further justification since the analysis of experimental results provides an estimation $5 \text{ meV} < J_\perp < 20 \text{ meV} [20]$ for the interplane coupling, while $J \approx 120 \text{ meV}$. Thus, it is somewhat risky to assume that the spin correlations between planes have the same strength as in the planes. Then, it seems more natural to employ the RPA approximation for the susceptibility [26] given by $\chi^{-1} (q) = \chi_0^{-1} (q) + J_\perp$, where $\chi_\pm (q)$ are the even and odd branches of the bilayer susceptibility, respectively. In this case, $\chi_\| (q)$ and $\chi_\perp (q)$ are quite different in absolute value, i.e. $|\chi_\| (q)| > |\chi_\perp (q)|$ in order to satisfy the applicability of the RPA approximation. We have checked by a direct calculation, that this approach provides $d_{x^2-y^2}$ symmetry for the SCOP on both branches of the spectrum i.e. the so-called $(d, d)$ state. This is in agreement with Ref. [21] where a similar phenomenological in-plane susceptibility derived from the neutron scattering data was used to construct the effective potential with an arbitrary relation between the in-plane and inter-plane coefficients. The above mentioned RPA model is certainly relevant to the more phenomenological approach used in this paper if one considers the expansion of $\chi_0 (q)$ in real space, assuming that the effective coupling between quasiparticles is proportional to $\chi_0$. For correlation lengths $\xi \sim 2 - 3$ lattice spacings, the expansion consists of a strong on-site repulsion $U$, and also a relatively strong NN attraction $V$ in-plane, with a ratio $U/V \sim 3$. The NNN interaction is repulsive and about one order of magnitude weaker than $U$. Other terms are negligibly small. Then, the phenomenological interaction used here and in previous literature [3] is very closely related to the RPA interaction in the realistic regime $J_\perp \ll J$. To show this result, first let us expand the susceptibility as

$$\chi_{\pm} (q) = \frac{1}{\chi_0^{-1} (q) \mp J_\perp} \approx \chi_0 (q) \mp J_\perp \chi_0^2 (q). \quad (9)$$

Using a 3D notation one can write $\chi (q, q_z) \approx \chi_0 (q) \mp \cos (q_z)J_\perp \chi_0^2 (q)$, for the case of a bilayer with $q_z = 0$ or $\pi$. The effective in-plane potential must contain an strong on-site repulsion. Consequently, $\chi_0 (q)$ can be written as $\chi_0 (q) = u + f(q)$, where $u$ is a constant proportional to the on-site repulsion $U$, and the function $f(q)$ satisfies the condition $\sum q f(q) = 0$. Hence, the susceptibility can be rewritten as $\chi (q, q_z) \approx u + f(q) \mp \cos (q_z)J_\perp [u + f(q)]^2$. Assuming that the ratio $\frac{u}{q}$ is small (i.e. the on-site repulsion is strong), we finally get:

$$\chi (q, q_z) \approx u + f(q) - J_\perp u \cos (q_z) - 2J_\perp u \cos (q_z) f(q). \quad (10)$$

The first three terms are accounted for in the calculation discussed in this paper both for a bilayer and a 3D antiferromagnet since, as it was argued above, the largest contribution to $f(q)$ comes from the NN attraction. The last term in Eq.(10) is relatively small compared to the other three, but it is assumed to have a significant contribution in the models of Refs. [21,22] explaining the difference between their results (i.e. $(s, -s)$) and ours (i.e. mixture of $d_{3z^2-r^2}$ and $s_{x^2+y^2+z^2}$). Nevertheless, both cases are “s-wave” in-plane and thus there is no qualitative difference in their transformation properties (they belong to the same representation). In addition, since $J_\perp/J \ll 1$, both are unlikely to be stable in the cuprates.

C. Superconductivity in the isotropic 3D AF.

To calculate $T_c$ and the symmetry of the SCOP in the case of a three dimensional isotropic AF, we here use the
SCBA hole dispersion obtained at $J/t = 0.4$ and again the BCS gap equation. As expected, when $\frac{J_z}{J} = 1$, the two channels $d_{z^2-r^2}$ and $d_{x^2-y^2}$ are degenerate, i.e. $T_c$ is the same for both and varies with the hole density as it is shown in Fig.9. The critical temperature in 3D is slightly smaller than for planes and bilayers. The “optimal doping” behavior is also present in 3D, but it is less pronounced than in 2D.

![Image](image-url)

**FIG. 9.** Superconducting critical temperature $T_c$ vs quasi-particle hole density for an isotropic 3D AF with $J/t = 0.4$, using the BCS gap equation and Hamiltonian Eq(1).

When $\frac{J_z}{J} \neq 1$, the system acquires tetragonal symmetry and the channels $d_{z^2-y^2}$ and $d_{x^2-r^2}$ are no longer degenerate. In fact, if $\frac{J_z}{J} < 1$, the gap possesses $d_{z^2-y^2}$ character, while if $\frac{J_z}{J} > 1$, it becomes again a mixture of $d_{x^2-r^2}$ and $s_{x^2+y^2+z^2}$, as it was mentioned in the case of a bilayer. Again, as the ratio $\frac{J_z}{J}$ increases, the symmetry of the SCOP becomes $d_z$. All these results can also be obtained following a discussion similar to that of Fig.8 but now using six sites instead of five.

**V. CONCLUSIONS**

In this paper, we have investigated the properties of bilayer and 3D antiferromagnets specially regarding the behavior of holes in such environments and the eventual formation of a superconducting state upon doping. The main assumption is that AF correlations remain of at least a few lattice spacings in range which, as a first approximation, allow us to use the dispersion of holes at half-filling and a density-density NN attraction between quasiparticles also generated by antiferromagnetism. Within the BCS gap equation superconductivity is investigated. A small coupling in the $z$-direction does not alter qualitatively the $d_{z^2-y^2}$ superconducting state found for a pure single plane layer. Only for large values of the exchange in the direction perpendicular to the planes is that a competing “s-wave” superconducting state becomes dominant.

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