Exact two-particle effective interaction and superconductivity in the two-level Hubbard model

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(Received 19 September 1988)

A two dimensional two-level Hubbard model with on-site repulsions only, is studied. By solving the two-particle problem, the effective interaction in the lower band is calculated exactly in the empty band limit. This interaction is found to consist of two terms: an on-site repulsion and a nearest-neighbor resonant superexchange. Within the Hartree-Fock approximation it is found that high-T_c s-wave superconductivity develops in a variety of situations. The validity of this model for the high-T_c Cu-O superconductors is discussed.

I. INTRODUCTION

The high critical temperatures of the new copper oxide superconductors[1-8] have stimulated the search for a pairing mechanism of purely electronic origin. The common feature of the different families of superconducting cuprates is the presence of $(CuO_2)_n$ layers in which the Cu atoms occupy a square lattice and are linked by the oxygen atoms. A simple analysis of the chemistry of this problem, supported by band calculations,[9-15] shows that the partially filled band is essentially made of the hybridization of x^2-y^2 d orbitals of Cu and p orbitals of the O in the layers. Small composition changes in these substances lead to metal-insulator transitions and to the appearance of antiferromagnetic phases. This fact shows the importance of electron correlations and the necessity of considering the electron-electron Coulomb repulsion. In this work we will describe the $(CuO_2)_n$ layers by means of a Hubbard Hamiltonian with two kinds of sites. The states under consideration are those that correspond to the introduction of holes into a background lattice made of Cu^+ ions (full $3d$ shell) and O^{2-} ions (full $2p$ shell). In the systems La-(Ba,Sr)-Cu-O and Y-Ba-Cu-O there are between 1 and 2 holes per Cu atom. We restrict the accessible states for the holes to the x^2-y^2 d-orbital of each Cu atom and the p-orbital of each oxygen directed towards the neighboring Cu atoms. We call Δ the energy difference between p and d orbitals, U_d and U_p the on-site Coulomb repulsions and t the hopping matrix element between Cu and O sites. The O-O and Cu-Cu direct hopping and the Cu-O Coulomb repulsion are neglected. The one-particle solutions of this model, when $\Delta > 0$, consist of a lower band of mainly Cu character and upper bands of mainly O character. The lower band is partially filled with holes.

Many theories that have been proposed are based on this same physical background. Some of them neglect the effect of the oxygen and reduce the problem to a single-band Hubbard model.[16-20] Pairing interactions are then looked for in the limit of large U. However, recent analytical[21] and numerical[22,23] calculations indicate that the 2D one-band Hubbard model does not exhibit superconductivity. Other theories[24-27] include the effect of oxygen but still consider the system in the large U limit, so that at least part of the system is a magnetic insulator. On the contrary our aim is a simpler one: We look for superconductivity in the *metallic* phase. The problem reduces therefore to finding the effective interaction between holes in the lower band. In addition to a reduced on-site repulsion the effective interaction is expected to have a superexchange via the oxygen term even in the metallic phase, in contrast to the dynamical superexchange that appears only in the limit $U \to \infty$. Pairing will be possible when the attractive interactions overcome the repulsive ones.

Although we are not the first ones to indicate superexchange via oxygen as a possible pairing mechanism,[28,29] in this paper we find an expression for the effective interaction valid within the Hartree-Fock (HF) approximation and show that in some conditions such a mechanism indeed leads to superconductivity.

The superexchange via oxygen can be obtained by perturbative methods[30] (e.g., canonical transformations), but as it is a fourth-order term it becomes negligible in the limit in which the perturbation expansion is valid ($t/\Delta \ll 1$). Instead, we approach the problem by means of a nonperturbative method, which consists of comparing the states of an effective Hamiltonian with the corresponding states of the true one. In this way we are able to find the effective interaction in the strong hybridization regime ($\Delta \sim t$). In Sec. II we study the one- and two-dimensional systems. By solving the two-hole problem we obtain the exact analytic expressions of the effective interactions in an empty band. In Sec. III we use those expressions, which are valid within HF approximation, to show that indeed pairing is possible in a variety of situations. Finally, in Sec. IV we show that this model agrees qualitatively with many properties of copper oxide superconductors.

II. THE EFFECTIVE INTERACTION

We obtain the effective interaction between holes in the lower band by comparing the states of one and two holes of a single-band effective Hamiltonian with those of the true two-level Hamiltonian. As the lower band has mainly a Cu character we propose an effective Hamiltonian in which only Cu sites appear

$$H_{\rm eff}=E_0\sum_i n_i - t'\sum_{\langle i,j\rangle;\sigma} d_{i\sigma}^\dagger d_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow} - \tfrac{1}{2}J\sum_{\langle i,j\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4}n_in_j)\,. \tag{1}$$

It is a Hubbard Hamiltonian plus an explicit nearest-neighbor exchange interaction. The form of the exchange term is determined by two requirements: (i) it is a two-body interaction, and (ii) it vanishes for pairs of holes in triplet states, which do not feel the on-site repulsions. As we shall see, it is possible to reproduce the exact results if the effective parameters are considered to be functions of the energy. Only in the limit $\Delta\gg t$ the effective Hamiltonian becomes energy independent. We will also see that the energy dependence of J is essential for obtaining superconductivity.

A generic one-particle state of the effective system may be written as

$$\psi=\sum_i \phi_i d_{i\sigma}^\dagger|0\rangle\,. \tag{2}$$

From the Schrödinger equation $(H_{\rm eff}-E)\psi=0$ one obtains

$$(E_0-E)\phi_i - t'\sum_{\langle l\rangle}\phi_{i+l}=0\,. \tag{3}$$

We need also the states of two holes. As two holes in the triplet states do not interact we consider only $S=0$ states. We will restrict ourselves to hole pairs without center-of-mass (c.m.) motion. A generic pair with $S_z=0$ and $q_{\rm c.m.}=0$ is of the form

$$\psi=\sum_n \alpha_n|n\rangle\,, \tag{4}$$

where $|n\rangle$ is

$$|n\rangle=N^{-1/2}\sum_i d_{n+i\uparrow}^\dagger d_{i\downarrow}^\dagger|0\rangle\,. \tag{5}$$

The singlet states fulfill the additional condition $\alpha_n=\alpha_{-n}$. From the Schrödinger equation we get

$$\left(2E_0-E+U\delta_{n0}+J\sum_{\langle l\rangle}\delta_{nl}\right)\alpha_n - 2t'\sum_{\langle l\rangle}\alpha_{n+l}=0\,. \tag{6}$$

Equations (3) and (6) are all that is needed for comparison with the complete systems.

A general Hubbard Hamiltonian with on-site repulsion is of the form

$$H=\sum_{i,\alpha}\varepsilon_\alpha n_{ai}+\sum_{i,\alpha}U_\alpha n_{ai\uparrow}n_{ai\downarrow} - \sum_{i,j,\alpha,\beta,\sigma} t_{\alpha\beta}(j-i)c_{\alpha j\sigma}^\dagger c_{\beta i\sigma}\,, \tag{7}$$

with $t_{\alpha\beta}(m)=t_{\beta\alpha}^*(-m)$. For our model in one dimension α may take the values d and p. Besides, $\varepsilon_d=0$, $\varepsilon_p=\Delta$, $t_{dd}=t_{pp}=0$, and

$$t_{dp}(m)=t(\delta_{m1}-\delta_{m0})\,. \tag{8}$$

The one-particle states are

$$\psi=\sum_i(\phi_i c_{di\sigma}^\dagger+\xi_i c_{pi\sigma}^\dagger)|0\rangle \tag{9}$$

and the equation $(H-E)\psi=0$ reduces to

$$-E\phi_i+t(\xi_i-\xi_{i-1})=0\,, \tag{10}$$

$$(\Delta-E)\xi_i+t(\phi_i-\phi_{i+1})=0\,. \tag{11}$$

From Eq. (11) one can express ξ as a function of ϕ. Therefore, given an energy E the whole wave function is determined by its projection on the subspace of d orbitals. Replacing ξ into Eq. (10) one gets

$$\left(\frac{-2t^2}{\Delta-E}-E\right)\phi_i+\frac{t^2}{\Delta-E}(\phi_{i+1}+\phi_{i-1})=0\,. \tag{12}$$

The comparison between Eq. (12) and Eq. (3) yields

$$E_0(E)=-\frac{2t^2}{\Delta-E} \tag{13}$$

and

$$t'(E)=-\frac{t^2}{\Delta-E}\,. \tag{14}$$

So the d-orbital component of the wave function fulfills a Schrödinger equation with an energy-dependent effective Hamiltonian.

Consider now the hole pairs with $q_{\rm c.m.}=0$. Defining

$$|\alpha\beta;n\rangle=N^{-1/2}\sum_i c_{ai+n\uparrow}^\dagger c_{\beta i\downarrow}^\dagger|0\rangle\,, \tag{15}$$

the wave function of a generic pair is

$$\psi=\sum_{\alpha,\beta,n}A_n^{\alpha\beta}|\alpha\beta;n\rangle\,, \tag{16}$$

with the condition $A_n^{\alpha\beta}=A_{-n}^{\beta\alpha}$ required for singlet states. The Schrödinger equation reduces to the following set of equations:

$$\begin{aligned}
&(U_d\delta_{n0}-E)\alpha_n+t(\xi_n+\eta_n-\xi_{n-1}-\eta_{n+1})=0\,,\\
&(2\Delta+U_p\delta_{n0}-E)\beta_n+t(\xi_n+\eta_n-\xi_{n-1}-\eta_{n+1})=0\,,\\
&(\Delta-E)\xi_n+t(\alpha_n+\beta_n-\alpha_{n+1}-\beta_{n+1})=0\,,\\
&(\Delta-E)\eta_n+t(\alpha_n+\beta_n-\alpha_{n-1}-\beta_{n-1})=0\,,
\end{aligned} \tag{17}$$

where for simplicity of notation we have set $A^{dd}=\alpha$, $A^{pp}=\beta$, $A^{dp}=\eta$, and $A^{pd}=\xi$. Also in this case it is easy to express β, ξ, and η in terms of α in order to obtain the following equation:

$$(U_d\delta_{n0}-E)\alpha_n+\frac{4t^2}{2\Delta-E}(\alpha_{n+1}+\alpha_{n-1}-2\alpha_n)=-\frac{2t^2}{(\Delta-E)(2\Delta-E)}\left[U_d-\frac{U_p(U_d-E)}{2\Delta+U_p-E}\right](\delta_{n+1,0}+\delta_{n-1,0}-2\delta_{n0})\alpha_0\,. \tag{18}$$

We can obtain the effective parameters by matching this equation with Eq. (6). For $|n| \geq 2$, Eq. (18) reduces to the form of Eq. (6) when the values $E_0(E/2)$ and $t'(E/2)$ are used. That should be expected as $E/2$ is the energy of each hole in the pair. For $n=0$ one obtains

$$[2E_0(E/2)+U(E)-E]\alpha_0-2t'(E/2)(\alpha_1+\alpha_{-1})=0\,, \tag{19}$$

where

$$U(E)=U_d+\frac{2t'(E/2)}{\Delta-E}\left[U_d-\frac{U_p(U_d-E)}{2\Delta+U_p-E}\right]. \tag{20}$$

Finally, setting $n=1$, using Eq. (19) and the relation $\alpha_1=\alpha_{-1}$ one obtains

$$J(E)=\frac{2t'(E/2)[U_d-U(E)]}{2E_0(E/2)+U(E)-E}\,. \tag{21}$$

When the single-particle energy $E/2$ is within the lower-energy band Eqs. (20) and (21) represent, respectively, an on-site effective repulsion and a nearest-neighbor attraction between the holes of the band. The Cu-O hybridization on one hand reduces the U_d on-site repulsion, on the other hand it also allows U_p to contribute to the effective repulsion. J is a fourth-order effect that vanishes when both U_d and U_p are zero. Note that U_p gives a repulsive contribution to J.

The possibility of describing a pair in the lower band with the effective Hamiltonian of Eq. (1), in which only Cu sites appear, is based on the fact that the oxygen behaves as a link between the Cu atoms, since only the Cu-O hopping has been included.

Very similar results are obtained with a much lengthier calculation for the two-dimensional (2D) lattice. In that case there are two different oxygen sites in the x and y directions. In Eq. (7) now we have $\alpha=d,x,y$; $\varepsilon_d=0$, $\varepsilon_x=\varepsilon_y=\Delta$, $t_{dd}=t_{xx}=t_{yy}=t_{xy}=0$, and

$$t_{dx}(m)=t(\delta_{ma}-\delta_{m0})\,,$$
$$t_{dy}(m)=-t(\delta_{mb}-\delta_{m0})\,, \tag{22}$$

where a and b are the unit vectors of the lattice. For the one-hole states the 2D calculation is essentially equal to the 1D case. The result is

$$t'(E)=-\frac{t^2}{\Delta-E} \tag{23}$$

and

$$E_0(E)=4t'(E)\,. \tag{24}$$

The generic two-hole state is still given by Eq. (16) and the coefficients are determined by solving $(H-E)\psi=0$. The difficulty is that in 2D there is no obvious way in real space of expressing the other eight $A^{\alpha\beta}$ coefficients in terms of A^{dd}. However, it can be done by Fourier transforming the equations. One ends with the following equation:

$$(E-2E_0-U_d\delta_{n0})A_n^{dd}+2t'\sum_{\langle l\rangle}A_{n+l}^{dd}=\frac{t'}{\Delta-E}\{2\delta_{n0}[2U_dA_0^{dd}-U_p(A_0^{xx}+A_0^{yy})]-(\delta_{an}+\delta_{-an})(U_dA_0^{dd}-U_pA_0^{xx})$$
$$-(\delta_{bn}+\delta_{-bn})(U_dA_0^{dd}-U_pA_0^{yy})\}\,. \tag{25}$$

One needs also the relationship

$$(U_d-E)A_0^{dd}=(2\Delta+U_p-E)(A_0^{xx}+A_0^{yy})\,. \tag{26}$$

Like in the 1D case, comparison of Eqs. (6) and (25) yields the effective interaction. For $|n|>|a|$ Eq. (25) has the same form of Eq. (6). For $n=0$, using Eq. (26) one obtains

$$U(E)=U_d+\frac{2t'(E/2)}{\Delta-E}\left[2U_d-\frac{U_p(U_d-E)}{2\Delta+U_p-E}\right]. \tag{27}$$

But for $n=a$, b there is a difference with the 1D case. In Eq. (6) the nearest-neighbor interaction term has the form $J\alpha_1$ while in Eq. (18) it is proportional to α_0. This is not a problem in 1D because the wave function α_n is completely determined by its value at any point, as only even solutions are allowed. On the contrary, in 2D, A_a^{dd} and A_b^{dd} can be chosen independently. In Eq. (25) the interaction term for $n=a$ is not proportional to A_a^{dd}, because $A_0^{xx}\propto A_a^{dd}$ but $A_0^{dd}\propto(A_a^{dd}+A_b^{dd})$. All this amounts to a symmetry-dependent interaction. For a wave function with s-wave symmetry ($A_a^{dd}=A_b^{dd}$) one has the same 1D result

$$J_{s\,\mathrm{wave}}(E)=\frac{2t'(E/2)[U_d-U(E)]}{2E_0(E/2)+U(E)-E}\,, \tag{28}$$

which is attractive at least at the bottom of the band if U_p is not too large. Instead, for d waves J vanishes when $U_p=0$ and is repulsive if $U_p>0$.

For some values of the parameters, U and J change sign. For example, if the hybridization is large enough U may become negative. On the other hand, the denominator $(2E_0+U-E)$ of J may vanish for some particular E if U is not too large. It is this resonant behavior that is the key for superconductivity in this system.

The interaction J is due to the virtual transitions to doubly occupied levels that contribute to the energy of a singlet pair when the holes are on neighboring copper sites. The resonance of J appears when such transitions change from virtual to real. When Δ is small enough such a resonance may happen at energies inside the lower band, even for large U_d, since in such a case E_0 acquires a large negative value in the upper part of the band.

III. SUPERCONDUCTIVITY

Although the expressions for the effective interactions found in the previous section are exact results only in the empty band limit, it should be expected that similar interactions persist when the bands are partially filled. In

particular, J could have an essential role in determining the magnetic behavior of the system. This superexchange, in contrast with the dynamical one that appears in the Hubbard model in the large U limit, is present for any nonvanishing value of U_d, so also for delocalized conduction electrons. In this section, we explore the possibility that attraction due to J may overcome the on-site repulsion U leading to pairing of holes in the metallic regime. Within the Hartree-Fock approximation the only effect of on-site repulsion is to shift the Cu and O levels. The modified separation is then

$$\Delta' = \Delta + U_p\langle n_p\rangle - U_d\langle n_d\rangle , \tag{29}$$

where $\langle n_p\rangle$ is the occupation of each oxygen level. This approximation is good as long as $\langle n_{i\uparrow}n_{i\downarrow}\rangle \simeq \langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle$, that is, as long as the system remains a metal without local moments. Within the above approximation, the effective interactions are still given by the same formulas, provided one uses the parameters of the self-consistent energy band. We have now all that is needed in order to determine the transition to superconductivity.

The finite temperature gap equation is

$$\Delta_q = -\frac{1}{N}\sum_k \frac{1-2f}{2E_k}\Delta_k V(q-k) , \tag{30}$$

where $E_k = [(\varepsilon_k-\mu)^2+\Delta_k^2]^{1/2}$, f is the fermionic occupation factor and for $V(q-k)$ one must use

$$V(q-k) = U(2\varepsilon_k) + J(2\varepsilon_k)\sum_{\langle l\rangle} e^{i(\mathbf{q}-\mathbf{k})\cdot l} . \tag{31}$$

In two dimensions and for s waves U is given by Eq. (27) and J by Eq. (28). By replacing V into Eq. (30) one finds that for s-wave pairing Δ_k has the form

$$\Delta_q = \Delta_0 + \Delta_1\sum_{\langle l\rangle} e^{i\mathbf{q}\cdot l} . \tag{32}$$

Then the gap equation reduces to a pair of coupled equations for Δ_0 and Δ_1

$$\begin{aligned} &(1+f_{00})\Delta_0 + f_{01}\Delta_1 = 0 , \\ &f_{10}\Delta_0 + (1+f_{11})\Delta_1 = 0 , \end{aligned} \tag{33}$$

where

$$f_{00} = \frac{1}{N}\sum_k \frac{1-2f}{2E_k}U(2\varepsilon_k) , \tag{34}$$

$$f_{01} = \frac{1}{N}\sum_k \frac{1-2f}{2E_k}U(2\varepsilon_k)\xi_k , \tag{35}$$

$$f_{10} = \frac{1}{4N}\sum_k \frac{1-2f}{2E_k}J(2\varepsilon_k)\xi_k , \tag{36}$$

$$f_{11} = \frac{1}{4N}\sum_k \frac{1-2f}{2E_k}J(2\varepsilon_k)\xi_k^2 , \tag{37}$$

with $\xi_k = \sum_{\langle l\rangle} e^{i\mathbf{k}\cdot l}$. The order parameters Δ_0 and Δ_1 are determined self-consistently from Eqs. (33).

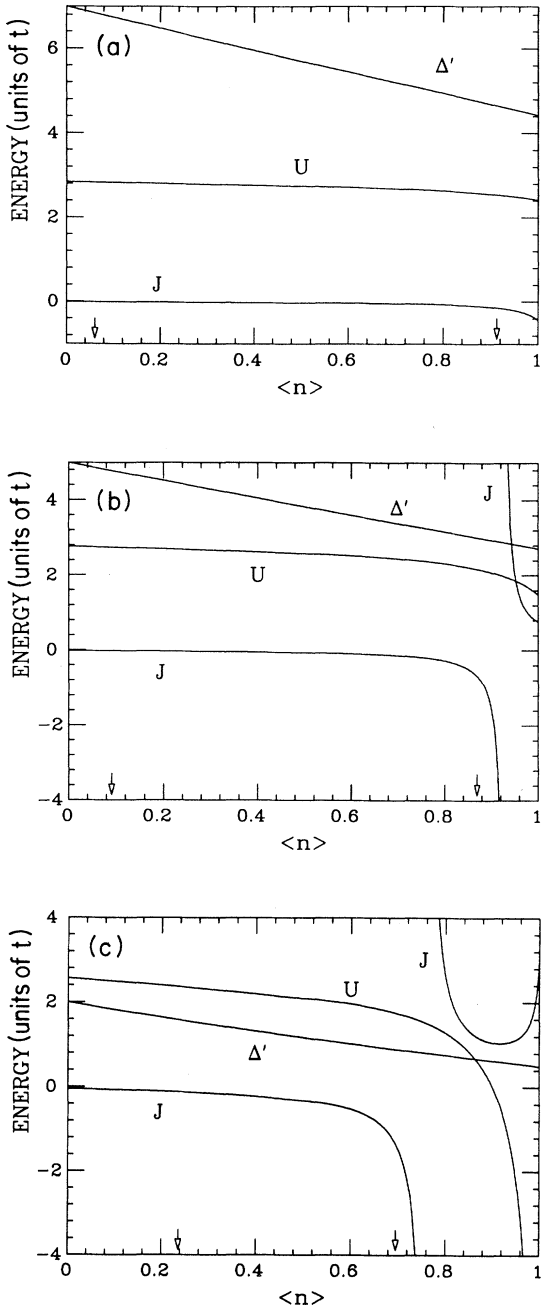

FIG. 1. Δ', $J(2\mu)$, $U(2\mu)$ vs $\langle n\rangle$. $U_d=3$, $U_p=1$, $t=1$; (a) $\Delta=7$, (b) $\Delta=5$, (c) $\Delta=2$. The arrows indicate the limits of the region in which a local moment develops.

The onset of superconductivity is dominated by the value of the interactions at the Fermi energy μ. In the Figs. 1–3 we show Δ', $U(2\mu)$, and $J(2\mu)$ as functions of the band occupation number $\langle n\rangle$ for different values of the parameters. For large values of Δ and for any value of the filling, U is positive and J is negative but very small [see Fig. 1(a)]. No superconductivity is to be expected in such

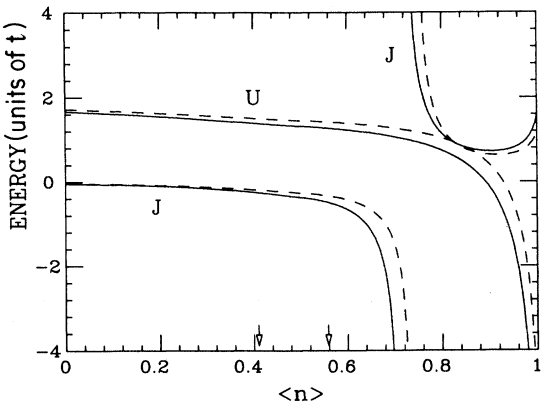

FIG. 2. $J(2\mu)$, $U(2\mu)$ vs $\langle n\rangle$. $U_d=2$, $\Delta=2$, $t=1$. Solid line: $U_p=0$; dashed line: $U_p=1$. The arrows indicate the limits of the region in which a local moment develops.

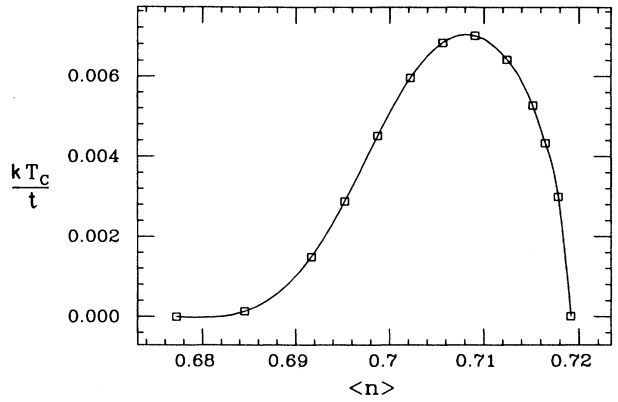

FIG. 4. T_c vs $\langle n\rangle$. $U_d=3$, $U_p=1$, $\Delta=1$, $t=1$. The squares correspond to the points actually calculated. The solid line is an interpolation.

a case. As the value of Δ decreases, the resonance of J moves inside the band approaching the half-filling point [see Fig. 1(b)]. Superconductivity is expected for $\langle n\rangle$ slightly smaller than the resonance value, so that the attractive J may overcome the repulsive U. For values of Δ even smaller a region of negative U appears near the top of the band [see Fig. 1(c)]. Note that in this region J is positive and large, so there is competition with U; nevertheless, hole-pairing will be possible also in this region if the negative values of U are large enough. The effect of U_p is to reduce the absolute value of J and to increase U (see Fig. 2). A different situation appears when $U_d=0$ and $U_p>0$, as it is shown in Fig. 3. In this case, J is repulsive at the bottom of the band and has a resonance near the half-filling point, while U is positive and very small for all values of $\langle n\rangle$. Superconductivity will be present on the right-hand side of the resonance.

Note that as the energy of half-filling is the value at which $E_0(E)=E$, the resonance of J will always be in the upper half of the band. No pairing is therefore possible for $\langle n\rangle<0.5$.

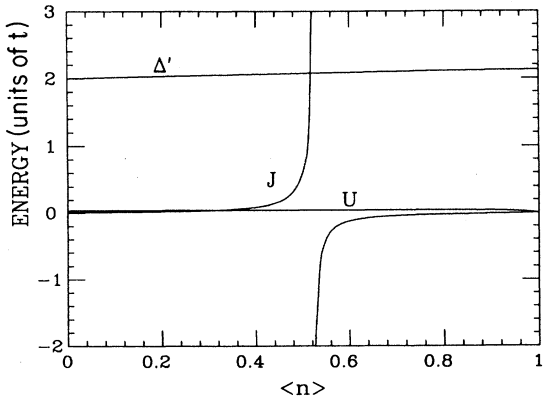

FIG. 3. Δ', $J(2\mu)$, $U(2\mu)$ vs $\langle n\rangle$. $U_d=0$, $U_p=1$, $\Delta=2$, $t=1$.

The arrows in the figures indicate the limits of the region in which a local moment develops on the copper. These points were obtained by using the theory of Wolff[31] (i.e., the condition $U_d\chi_{00}=1$, where χ_{00} is the local susceptibility of copper sites). In the cases shown in the figures the resonance of J remains outside the region of local moments, but for higher values of U_d it may lie inside. In such a case the HF approximation we have employed would not be applicable.

In Fig. 4 a T_c vs $\langle n\rangle$ curve is presented for a typical set of parameters. The $\langle n\rangle$ values are close to the resonance of $J(2\mu)$. Critical temperatures of the order of $10^{-2}t$ are obtained. Finally, the Δ_1 and Δ_0/Δ_1 vs T plots are given in Fig. 5 for the same set of parameters at a particular occupation. As it should be expected, Δ_0 is a small fraction (9%) of Δ_1 because of the repulsion U.

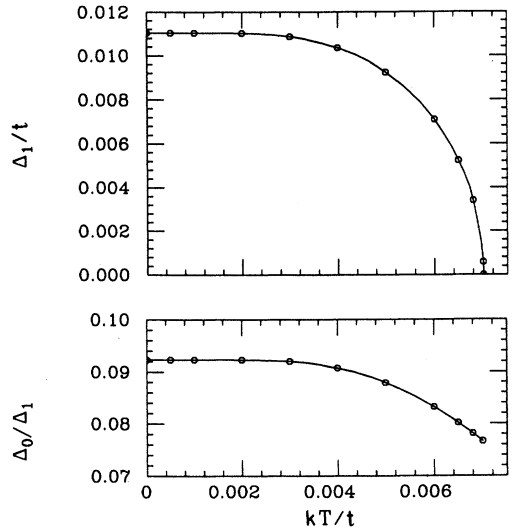

FIG. 5. Order parameters vs T. $U_d=3$, $U_p=1$, $\Delta=1$, $t=1$, $\langle n\rangle=0.709$. The circles correspond to the points actually calculated. The solid lines are interpolations.

IV. COPPER OXIDE SUPERCONDUCTORS

Many theories that have been proposed for the copper oxide superconductors are based on the same Hamiltonian we use, but most of them assume the large U limit (Mott insulator), in contrast with our approach which is valid for the nonmagnetic metal. Which one of those two positions is favored by the experimental evidence? Although it is still difficult to give a definitive answer to this question, we can list some properties of the superconducting cuprates that are in accord with our model.

Superconductivity is confined to a range of $\langle n \rangle$. For $(La_{1-x}Sr_x)_2CuO_4$ T_c grows from zero at $x \simeq 0.03$, goes through a maximum, and vanishes at $x \simeq 0.16$.[32,33] If one assumes rigid band doping such a behavior is in qualitative agreement with the predictions of our model (see Fig. 4). In the system $YBa_2Cu_3O_{7-y}$ oxygen deficiency reduces the number of holes; superconductivity is suppressed at $y \sim 0.5$.[34]

Metallic conduction. It is observed above T_c at the superconducting compositions in all of the substances.[1-8,32-36] For La-Cu-O it is also observed for $x > 0.16$ at low temperatures,[33] contrary to what happens at the lower concentration bound that seems to be related or to be very close to a metal-insulator transition. For the Y-Ba-Cu-O system there is evidence for a region of nonsuperconducting metallic behavior between the insulating and the superconducting phases.[35]

Lack of superconductivity for $\langle n \rangle < 0.5$. No superconductivity has been found for $\langle n \rangle < 0.5$. This is a consequence of our model, as explained in the previous section.

Positive carriers. Hall effect measurements[32,37] indicate hole-type conduction in La-Cu-O Y-Ba-Cu-O. For the lower Cu-O band the points at which the effective mass changes sign are located near the top. Therefore, it is possible to have simultaneously $\langle n \rangle > 0.5$ and a positive effective mass.

T_c of the right order. The model yields critical temperatures of the right order of magnitude, for example, in the case of Fig. 4 at the maximum $T_c \sim 0.007t$, which for $t \sim 2$ eV corresponds to $T_c \sim 150$ K.

Existence of an energy gap. Many experiments show the existence of an energy gap[38-44] which varies, depending on the experimental method and the sample, from $1T_c$ to $8T_c$. Our model, because of the predicted s-wave pairing, also gives a gap. For example, in the case of Fig. 5 the gap can be estimated to be $E_g \simeq 2[\Delta_0 + \Delta_1 \xi(\mu)] \simeq 3.8T_c$.

Lack of local moments at superconducting compositions. In the limit $U \to \infty$ local magnetic moments are expected even at the *superconducting compositions* above T_c. Although oxygen deficiency induces antiferromagnetism in both La-Cu-O and Y-Ba-Cu-O, the experimental evidence is against the coexistence of superconductivity and magnetism in the Cu sites. Let us consider the La-Cu-O case in detail. The undoped material is antiferromagnetic.[45,46] Above T_N it is an unusual paramagnet: no moment is found by ESR and susceptibility measurements give a very small moment value;[45] instead, strong instantaneous 2D antiferromagnetic correlations exist up to very high temperatures.[47] At low temperatures the moment saturates to a fractional value[46] ($\sim 0.4\mu_B$). T_N decreases with increasing impurity content up to the complete suppression of long-range order ($x \sim 0.008$). The low-temperature moment as measured by nuclear quadrupole resonance (NQR)[48] remains constant. This situation is consistent with the hypothesis of the system being a Mott insulator with fully developed moment, both below and above T_N. The fractional moment found can probably be understood in terms of quantum fluctuations of the 2D, $S = \frac{1}{2}$ Heisenberg model. At higher concentrations a region of short-range spin correlations is found at low temperatures by NQR.[48] The moment value decreases continuously vanishing at $x \simeq 0.025$, more or less the same concentration at which superconductivity appears. This intermediate region could be described as a region of progressive hole delocalization and moment destruction. This interpretation is consistent with the measurements[49] of γ, the coefficient of the linear term of the specific heat. It has a very low value in the antiferromagnetic (AF) region, increases continuously in the intermediate region, and saturates in the superconducting region. So in La-Cu-O, superconductivity develops after the local moments have essentially disappeared. While some overlap of magnetism and superconductivity cannot be ruled out at the lower concentration bound, such a doubt does not exist for the upper one: Measurements[45,50] of normal and superconducting samples near $x \sim 0.16$ show enhanced Pauli susceptibilities. All this is perfectly consistent with our model (see, for example, Fig. 2). Magnetic ordering and localization are expected within the local moment region. Strong spin correlations induced by J in the metal are also to be expected. In the $YBa_2Cu_3O_{7-y}$ case a similar situation arises by varying the oxygen content. The data seem to indicate that superconductivity appears only when AF order has disappeared.[51-54] For the undoped compound ($y = 0$) no moment is found either by ESR (Ref. 55) or by susceptibility measurements,[56] or by muon spin relaxation.[52]

Theoretical estimation of the parameters. Finally, we want to mention some theoretical estimates of the parameters that agree with our model. For instance, Mattheiss[10] has estimated $\Delta' \sim 0$ and $t \sim 1.85$ eV from his band calculation of La-Cu-O. Zaanen *et al.*[57] have also calculated the parameters using the local density approximation to the density functional theory; they obtain $\Delta \sim 0$–1 eV and $U_d \sim 8$ eV and concluded that the system is probably delocalized in spite of such a large U_d because of the smallness of Δ.

V. CONCLUSIONS

As the hole-pairing mechanism induced into the metallic phase by the resonant superexchange descends directly from the Hamiltonian that is commonly assumed to describe the essential features of Cu-O layers, and as it is in accord qualitatively with many relevant properties of the superconducting copper oxides, we believe that such a mechanism should be considered as a possible origin of the high-T_c superconductivity in those substances.

Additional work has to be pursued in order to determine the validity of the present model. We are now trying

to fit the model to specific substances. In this respect it is worth mentioning that a realistic and quantitative description will probably require the interlayer coupling and additional Cu and O states. From the theoretical point of view additional work should be done in order to go beyond the HF approximation for determining how band filling affects the effective interactions. Numerical studies, such as Monte Carlo simulations for example, could provide very useful information about this model. Work is in progress in this direction.

ACKNOWLEDGMENTS

We thank Dr. L. Pietronero, Dr. W. Geerstma, and Miss M. Di Stasio for many useful discussions. We also wish to thank the Istituto Nazionale di Fisica Nucleare and in particular Dr. E. Marinari, Dr. G. Parisi, and Dr. N. Cabibbo for their kind hospitality in the APE group. This work was partially supported by the Consejo Nacional de Investigaciones Científicas y Técnicas of Argentina, and Istituto Nazionale di Fisica Nucleare of Italy.

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