Superconductivity and antiferromagnetism for an extended Hubbard Hamiltonian: Role of correlated hopping in a single-band model

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An extended Hubbard model for a single band, including Coulomb repulsion and correlated hopping between nearest neighbors, is studied using a generalized mean-field approach. Antiferromagnetism and superconductivity are probed for arbitrary occupation number, near and away from half filling. Binding of pairs in the superconducting state of this purely repulsive model is mediated by the correlated hopping in the form of a covalent-bond configuration, with partial intrasite and intersite pairings. A region of coexistence is conjectured, the superconductivity being suppressed by the saturation of the staggered magnetic moment. Singlet superconducting nonmagnetic states are obtained for the almost-empty- or full-band cases. On the other hand, antiferromagnetism induces mixed s- and p-type superconductivities in the neighborhood of half filling.

I. INTRODUCTION

The presence of superconductivity in the copper oxides has brought a convergence of several fields of interest in condensed matter physics.[1] In particular, it has been suggested that the mechanism may be of an electronic origin, and the existence of an insulating antiferromagnetic phase in most reference compounds, hints at strong correlation effects among carriers. The Hubbard model has been pointed to as a natural candidate to describe the above effects related to the metal-insulator transition. It is not clear, at the present time, whether the two-dimensional Hubbard model away from half filling may be described by the usual Fermi-liquid concepts, with the presence of a Fermi surface and long-lived quasiparticles in its vicinity. Numerical methods have been extensively used to test superconductivity and Fermi-liquid behavior. Quantum Monte Carlo simulations by Hirsch and Lin[2] show that some pair correlations are enhanced with the intrasite Coulomb repulsion U, but no tendency of condensation of pairs into a superconducting state is observed for this single-band repulsive Hubbard model. Using a different algorithm, Sorella and co-workers[3] have implemented Monte Carlo simulations for very large two-dimensional systems (up to 256 sites) and arbitrary occupation number. Their results show that the ground state retains its insulating character even for large deviations from half filling, and a Fermi surface only appears for extremely large doping. However, the above simulations are not free of finite-size effects, in spite of the large sizes are difficult to attain without numerical instabilities.[2]

At this stage, several approaches are available. Some authors argue that since holes in doped samples reside on the oxygen sites, the physics is essentially different, and two or more bands are necessary to describe the relevant degrees of freedom.[4] On the other hand, other authors claim that the two-band model can be mapped onto an effective Hamiltonian for a strongly correlated single Hubbard band.[5] In this latter case, one recovers the picture proposed by Anderson.[6]

Other treatments, within the one-band picture, obtain pairing of carriers with attractive-U parameters.[7] This attractive on-site potential may be due to coupling with a boson field (phonons or other electronic excitations), or may be of chemical origin (*disproportionation* of valence states). However, a neat physical justification of this approach is still lacking.

Low density of carriers, in the copper oxides, produces a substantial reduction of screening effects. One is then forced to revise the validity of the approximations that lead to the simple Hubbard Hamiltonian with only on-site Coulomb repulsion. From the terms neglected,[8] the first in importance is related to the repulsion V between nearest neighbors. Next come off-diagonal terms of the Coulomb interaction $V(\mathbf{r}-\mathbf{r}')$, i.e., the correlated hopping I and the exchange J. Using Hubbard's notation,[8] they are written as

$$I=\left(ii\left|\frac{1}{\mathbf{r}}\right|ij\right), \tag{1}$$

and

$$J=\left(ii\left|\frac{1}{\mathbf{r}}\right|jj\right), \tag{2}$$

where (i,j) represents Wannier orbitals centered at nearest-neighbor sites and $\frac{1}{\mathbf{r}}$ is the Coulomb potential. Both terms (1) and (2) involve bond charge density, and are a consequence of translational invariance. In fact, the electron density operator is not diagonal in the Wannier representation. For narrow-band materials, the above terms may be important, as first noted by Hubbard,[8] and also recently by several authors.[9–11] In this contribution we analyze the role of the correlated hopping I for the single-band Hamiltonian, and the interplay of antiferromagnetism and superconductivity for this extended

Hubbard model. The term correlated hopping has been coined to mean that hopping to a nearest-neighbor site may be different, whether the site is occupied or not. The importance of such a term in the copper oxides has been recently put forward, since it can give rise to extended s-wave superconductivity.[12] It appears as more fundamental than the usual exchange interactions which may lead to spurious d- or p-wave pairing, if not correctly handled. However, the superconducting solutions suggested by Hirsch[12] are limited to the almost-empty- and almost-full-band cases, and were not identified with the physics of the copper oxides. Micnas and co-workers have extensively studied the extended Hubbard model,[7] including the interaction V for nearest neighbors, and the correlated hopping and exchange terms. However, most of their solutions refer to attractive U or V parameters, and the role of the I term is somehow hidden. In our work we will show that the inclusion of the correlated hopping in the extended model leads to surprising results. In contrast to Hirsch's conjectures, pairing of carriers may be obtained in the vicinity of the half-filled band case, if partial antiferromagnetism is allowed. And finally, we do not have to resort to attractive U or V, to get superconducting solutions. In our treatment, through a *generalized* Hartree-Fock approximation, symmetry broken and correlated solutions are tested. Thus, our approach goes beyond the standard Hartree-Fock one. Moreover, it is found that the inclusion of the intersite Coulomb repulsion V (that makes the interactions less short ranged), leads to a wider range of validity of the Hartree-Fock approximation.[13]

Preliminary results of our calculation have already been published.[14] A general necessary condition to obtain pairing of carriers can be given in the form

$$4\nu I^2 > UV, \tag{3}$$

where ν is the coordination number. Condition (3) is obtained independently of the existence of antiferromagnetic ordering, and the dimensionality enters through the number of nearest neighbors. From the overlap integrals we expect the physical region for parameters to be restricted to

$$|I| < V < U. \tag{4}$$

The above conditions (3) and (4) are more likely to be fulfilled in two and three dimensions. They both restrict pairing to a limited region of the parameter space, with ranges that include realistic values of the different parameters. For instance, if we choose $U = 6$ eV (Ref. 15) in two dimensions, we get a lower bound for V equal to 0.375 eV. On the other hand, from energy-band calculations[15] one can estimate the value of V to be of the order of or less than 0.5 eV, allowing a variation of $|I|$ that ranges between the above values. We discuss this matter later in this paper. Condition (3) also shows that attractive values of U or V are not necessary for pairing of carriers, as long as the correlated hopping I is finite.

A comment concerning antiferromagnetism is in order. Pairing in the presence of antiferromagnetism is possible near the half-filled band case, but the superconducting critical temperature is drastically depressed by the presence of a magnetic moment. This picture resembles the one described by Anderson,[6] with an enhancement of the effective mass of carriers due to spin fluctuations. In our solution, superconductivity is suppressed close to saturation of the magnetic moment.

Our paper is organized as follows: in Sec. II we discuss the extended Hamiltonian and the method of solution. In Sec. III we present numerical results for several examples calculated. The last section, Sec. IV, is devoted to the final comments and discussion of our results.

II. MODEL HAMILTONIAN

We studied in detail the square lattice (two dimensions), but our approach can be extended to hypercubic d-dimensional lattices with lattice parameter a. The dimensionality enters in relation (3) through the coordination number. The above lattices are not *frustrated* to antiferromagnetic ordering, and can be partitioned into two equivalent magnetic sublattices. We model our system with an extended Hubbard Hamiltonian for a single band:

$$\mathcal{H} = \alpha\hat{N} + U\sum_i n_{i\downarrow}n_{i\uparrow} + \frac{V}{2}\sum_{\langle ij\rangle,\sigma,s} n_{i\sigma}n_{js} + \sum_{\langle ij\rangle,\sigma}[I(n_{i,-\sigma}+n_{j,-\sigma})+\lambda]\,c^\dagger_{i\sigma}c_{j\sigma}, \tag{5}$$

where $c^\dagger_{i\sigma}$ and $c_{i\sigma}$ are the usual fermion operators for a Wannier orbital with spin σ, centered at the ith site, and $\hat{N}$ is the total number operator. In writing (5) we have proceeded in a way similar as in the original formulation by Hubbard,[8] starting with a single Hartree-Fock band, and writing the corrections over the Hartree-Fock mean field. The parameters α and λ used in (5) are given by

$$\alpha = E_0 - \mu - \bar{n}(U + 2\nu V) - 2\nu I\tau,$$
$$\lambda = t - 2I\bar{n} + V\tau,$$

where E_0 is the atomic energy, t is the hopping integral related to the bandwidth, $\bar{n}$ is the average number of electrons per site and spin, τ is the average of the electronic transfer between nearest neighbors, ν is the coordination number, and μ is the chemical potential. Hamiltonian (5) shows that the I integral should be compared with the hopping t rather than with the Coulomb terms U and V, since it represents a correction to the usual hopping due to correlation effects.

The single-particle Green function

$$G^\sigma_{ij}(z) = \langle\langle c_{i\sigma}\ ;\ c^\dagger_{j\sigma}\rangle\rangle_z \tag{6}$$

allows one to calculate averages such as the site occupation and the nearest-neighbor electronic transfer. The anomalous Green function

$$S^\sigma_{ij}(z) = \langle\langle c^\dagger_{i,-\sigma}\ ;\ c^\dagger_{j\sigma}\rangle\rangle_z \tag{7}$$

is useful to compute pair correlations of electrons of opposite spins. These averages are most important to test superconductivity. If the equations of motion are calculated for both Green functions, using the formalism developed by Zubarev[16] we get the following:

$$(z-\alpha)G_{ij}^{\sigma}-\lambda\sum_{\delta}G_{i+\delta,j}^{\sigma}=\delta_{ij}/2\pi+U\langle\langle n_{i,-\sigma}c_{i\sigma}\ ;\ c_{j\sigma}^{\dagger}\rangle\rangle+I\sum_{\delta}\langle\langle n_{i+\delta,\sigma}c_{i+\delta,-\sigma}^{\dagger}\ ;\ c_{j\sigma}^{\dagger}\rangle\rangle+V\sum_{\delta,s}\langle\langle n_{i+\delta,s}c_{i\sigma}\ ;\ c_{j\sigma}^{\dagger}\rangle\rangle$$
$$+I\sum_{\delta}\langle\langle n_{i,-\sigma}c_{i+\delta,\sigma}+(c_{i,-\sigma}^{\dagger}c_{i+\delta,-\sigma}+\text{H.c.})c_{i\sigma}\ ;\ c_{j\sigma}^{\dagger}\rangle\rangle, \tag{8}$$

$$(z+\alpha)S_{ij}^{\sigma}-\lambda\sum_{\delta}S_{i+\delta,j}^{\sigma}=-U\langle\langle n_{i\sigma}c_{i,-\sigma}^{\dagger}\ ;\ c_{j\sigma}^{\dagger}\rangle\rangle-I\sum_{\delta}\langle\langle n_{i+\delta,\sigma}c_{i+\delta,-\sigma}^{\dagger}\ ;\ c_{j\sigma}^{\dagger}\rangle\rangle-V\sum_{\delta,s}\langle\langle n_{i+\delta,s}c_{i,-\sigma}^{\dagger}\ ;\ c_{j\sigma}^{\dagger}\rangle\rangle$$
$$-I\sum_{\delta}\langle\langle n_{i\sigma}c_{i+\delta,-\sigma}^{\dagger}+(c_{i\sigma}^{\dagger}c_{i+\delta,\sigma}+\text{H.c.})c_{i,-\sigma}^{\dagger}\ ;\ c_{j\sigma}^{\dagger}\rangle\rangle, \tag{9}$$

where H.c. denotes Hermitian conjugate and $i+\delta$ labels the nearest neighbors of site i.

At this step we encounter the problem of decoupling the equations of motion. As in previous works,[13,17] a generalized Hartree-Fock solution is probed. In our treatment, symmetry broken and correlated solutions are tested, thus our approach goes beyond the standard Hartree-Fock one, allowing antiferromagnetic ordering even in the presence of superconductivity. To solve (8) and (9) we replace the product of three fermion operators by

$$ABC=\langle AB\rangle C-\langle AC\rangle B+\langle BC\rangle A. \tag{10}$$

This decoupling is the simplest one that can be devised to test simultaneously the presence of antiferromagnetism and superconductivity. However, our results should be extrapolated with caution to the highly correlated regime ($U\gg t$), where one expects the Hartree-Fock approximation to fault. In this sense, our main result (3), should be considered as an upper bound. Conditions obtained through improved approximations in the highly correlated limit, may be more restrictive. Nonetheless, recent estimations of the relevant parameters for the copper oxides, point to the intermediate rather than the strong-correlation regime,[15,18] with a bandwidth comparable in magnitude with the intrasite correlation U. On the other hand, as mentioned in the Introduction, including terms that make the Coulomb potential less short ranged,[13] may widen the region of parameters where the Hartree-Fock approximation is valid. In any case, our approach yields no superconductivity in the limit $U\to\infty$, which agrees with asymptotic exact expansions for that limit.[20]

Using the above procedure, higher-order Green functions can be expressed in terms of G_{ij}^{σ} and S_{ij}^{σ}, as, for instance,

$$\langle\langle n_{i,-\sigma}c_{i\sigma}\ ;\ c_{j\sigma}^{\dagger}\rangle\rangle\simeq\langle n_{i,-\sigma}\rangle G_{ij}^{\sigma}+\langle c_{i,-\sigma}c_{i\sigma}\rangle S_{ij}^{\sigma}, \tag{11}$$
$$\langle\langle n_{i\sigma}c_{i,-\sigma}^{\dagger}\ ;\ c_{j\sigma}^{\dagger}\rangle\rangle\simeq\langle n_{i\sigma}\rangle S_{ij}^{\sigma}-\langle c_{i\sigma}^{\dagger}c_{i,-\sigma}^{\dagger}\rangle G_{ij}^{\sigma}, \tag{12}$$

where averages that do not conserve the component S_z of the total spin are neglected. The proposed decoupling (10) yields the following equations for G and S:

$$\left[z-\alpha-U\bar{n}_{i,-\sigma}-V\sum_{\delta}\bar{n}_{i+\delta,s}-2I\nu\tau_{-\sigma}\right]G_{ij}^{\sigma}-\sum_{\delta}\left[\lambda-V\tau_{\sigma}+I(\bar{n}_{i,-\sigma}+\bar{n}_{i+\delta,-\sigma})\right]G_{i+\delta,j}^{\sigma}$$
$$-\left[U\sigma\Delta_i+I\sum_{\delta}(\Gamma_{i\sigma}+\Gamma_{i+\delta,\sigma})\right]S_{ij}^{\sigma}-\sum_{\delta}\left[V\Gamma_{i\sigma}+I\sigma(\Delta_i+\Delta_{i+\delta})\right]S_{i+\delta,j}^{\sigma}=\frac{\delta_{ij}}{2\pi}, \tag{13}$$

$$\left[z+\alpha+U\bar{n}_{i\sigma}+V\sum_{\delta}\bar{n}_{i+\delta,s}+2I\nu\tau_{\sigma}\right]S_{ij}^{\sigma}-\sum_{\delta}\left[\lambda-V\tau_{-\sigma}+I(\bar{n}_{i\sigma}+\bar{n}_{i+\delta,\sigma})\right]S_{i+\delta,j}^{\sigma}$$
$$-\left[U\sigma\Delta_i^{*}+I\sum_{\delta}(\Gamma_{i\sigma}^{*}+\Gamma_{i+\delta,\sigma}^{*})\right]G_{ij}^{\sigma}-\sum_{\delta}\left[V\Gamma_{i+\delta,\sigma}^{*}+I\sigma(\Delta_i^{*}+\Delta_{i+\delta}^{*})\right]G_{i+\delta,j}^{\sigma}=0, \tag{14}$$

where

$$\Delta_i=\langle c_{i\downarrow}c_{i\uparrow}\rangle, \tag{15}$$

is the average of the destruction of a pair of electrons at the ith site,

$$\Gamma_{i\sigma}=\langle c_{i+\delta,-\sigma}c_{i\sigma}\rangle, \tag{16}$$

is the same average for a pair of electrons at neighboring sites,

$$\tau_{\sigma}=\langle c_{i+\delta,\sigma}^{\dagger}c_{i\sigma}\rangle \tag{17}$$

is the average of the electronic transfer between nearest neighbors. When considering antiferromagnetism with two identical sublattices, it is useful to define the following quantities:

$$s=\tfrac{1}{2}|\langle n_{i\sigma}\rangle-\langle n_{i,-\sigma}\rangle|, \tag{18}$$
$$\bar{n}=\tfrac{1}{2}(\langle n_{i\sigma}\rangle+\langle n_{i,-\sigma}\rangle). \tag{19}$$

Symmetry-broken states are obtained when the average $\langle n_{a\uparrow}\rangle$ is prescribed as different from $\langle n_{a\downarrow}\rangle$ for a given sublattice. We write this in compact form

$$\langle n_{a,\sigma}\rangle = \langle n_{b,-\sigma}\rangle = \bar{n} + s\sigma, \tag{20}$$

where a and b label the two sublattices.

In the presence of antiferromagnetism, the lattice parameter is doubled. Green functions in the reciprocal space are then obtained as

$$\begin{bmatrix} z-E_0+s\sigma & -t\gamma & -A & -B_{a\sigma}\gamma \\ -t\gamma & z-E_0-s\sigma & -B_{b\sigma}\gamma & -A \\ -A^* & -B^*_{b\sigma}\gamma & z+E_0+s\sigma & t\gamma \\ -B^*_{a\sigma}\gamma & -A^* & t\gamma & z+E_0-s\sigma \end{bmatrix} \begin{bmatrix} \mathcal{G}^\sigma_{ax} \\ \mathcal{G}^\sigma_{bx} \\ \mathcal{S}^\sigma_{ax} \\ \mathcal{S}^\sigma_{bx} \end{bmatrix} = \frac{1}{2\pi} \begin{bmatrix} \delta_{xa} \\ \delta_{xb} \\ 0 \\ 0 \end{bmatrix}, \tag{23}$$

where all energies are referred to μ (with $\mu = 0$) and normalized to $U = 1$, and

$$A = \sigma\Delta + I\nu(\Gamma_{a\sigma} + \Gamma_{b\sigma}),$$
$$B_{\alpha\sigma} = V\Gamma_{\alpha\sigma} + 2I\sigma\Delta,$$
$$\gamma = \sum_{\delta} \exp(i\mathbf{k}\cdot\boldsymbol{\delta}),$$

with γ being the structure factor.

The index x in (23) may be a or b, and one gets four independent Green functions for each value of the spin σ. The symmetry condition $\langle n_{a,\sigma}\rangle = \langle n_{b,-\sigma}\rangle$ implies that the order parameter Δ_i does not depend on the site index i.

III. CRITICAL TEMPERATURE AND NUMERICAL EXAMPLES

The Néel temperature T_N for the normal phase is obtained through the standard Hartree-Fock approximation, and it is only band dependent. Concerning superconductivity, we have solved our equations just at the critical point T_C (asymptotically from the low-temperature phase), where they are linear in relation to the order parameters (15) and (16). The presence of a magnetic moment at the superconducting transition temperature has been tested in a self-consistent way, but no information has been obtained at lower temperatures, where the equations are highly nonlinear. Consequently, our phase diagram is not complete, since we cannot rule out a reentrant antiferromagnetic phase. Coexistence regions for superconductivity and antiferromagnetism are then extrapolated through the magnetic state at T_C.

Keeping only linear terms in Δ and Γ, one can solve Eq. (23) for all the Green functions involved, yielding

$$2\pi\mathcal{G}^\sigma_{aa} = \frac{z-E_0-s\sigma}{(z-\varepsilon_1)(z-\varepsilon_2)}, \tag{24}$$

$$2\pi\mathcal{G}^\sigma_{ab} = \frac{t\gamma}{(z-\varepsilon_1)(z-\varepsilon_2)}, \tag{25}$$

$$\mathcal{G}^\sigma_{\alpha\beta}(\mathbf{k},z) = \sum_i G^\sigma_{ij}(z) e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}, \tag{21}$$

$$G^\sigma_{ij}(z) = \frac{2}{N_S}\sum_{\mathbf{k}} \mathcal{G}^\sigma_{\alpha\beta}(\mathbf{k},z) e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}, \tag{22}$$

where α and β refer to different sublattices, N_S is the total number of sites, and i, j belong, respectively, to sublattices a, b.

Equations (13) and (14) are actually four noting that site i may belong to any of both sublattices a or b. In matrix notation we get

$$2\pi\mathcal{S}^\sigma_{aa} = \frac{1}{\det}\{\sigma A\,([z-s\sigma]^2 - E_0^2 - t^2\gamma^2) + t\gamma^2\,(E_0[B^*_{a\sigma}+B^*_{b\sigma}] - [z-s\sigma][B^*_{a\sigma}-B^*_{b\sigma}])\}, \tag{26}$$

$$2\pi\mathcal{S}^\sigma_{ab} = \frac{\gamma}{\det}\{B^*_{b\sigma}(z^2-[E_0-s\sigma]^2) - B^*_{a\sigma}t^2\gamma^2 + 2\sigma A^* t[E_0-s\sigma]\}, \tag{27}$$

where

$$\varepsilon_1 = E_0 - R, \quad R = \sqrt{s^2+t^2\gamma^2},$$
$$\varepsilon_2 = E_0 + R, \quad \det = (z^2-\varepsilon_1^2)(z^2-\varepsilon_2^2).$$

To calculate statistical mechanics averages one must compute residues of the above Green functions. In this process, one has to evaluate sums over the Brillouin zone (two dimensional in our examples), and reliable numerical methods were necessary, specially when the critical temperature is small.[20] Typical summations encountered are in the form

$$N_n = \frac{1}{2\pi}\sum_k \gamma^n\,(\tanh\beta\varepsilon_2/2 + \tanh\beta\varepsilon_1/2), \tag{28}$$

$$J_n = \frac{1}{2\pi}\sum_k \frac{\gamma^n}{R}\,(\tanh\beta\varepsilon_2/2 - \tanh\beta\varepsilon_1/2), \tag{29}$$

$$S_n = \frac{1}{2\pi}\sum_k \frac{\gamma^n}{R}\left(\frac{\tanh\beta\varepsilon_1/2}{\varepsilon_1} - \frac{\tanh\beta\varepsilon_2/2}{\varepsilon_2}\right), \tag{30}$$

where $\beta = 1/kT_c$.

The three order parameters Δ, $\Gamma_{a\sigma}$, and $\Gamma_{b\sigma}$ are linearly related through a homogeneous system of equations. A nontrivial solution is only obtained when all of them are simultaneously nonvanishing, and when the determinant of the system is zero. This latter condition yields

$$\frac{S_2}{E_0}\left(1+\frac{VN_2}{\nu E_0}\right)\left\{(2IE_0-t)^2 - D\left[t^2J_2 + E_0^2\left(1+\frac{\bar{n}'}{E_0}\right)\right]\right\} + \left\{1+\frac{\bar{n}'}{E_0}+\frac{VJ_2}{\nu}-D\frac{\bar{n}'J_2}{E_0}\right\}\left\{1+\frac{V(N_2+s^2S_2)}{\nu E_0}\right\} = 0 \tag{31}$$

where $D = 4I^2 - \frac{V}{\nu}$ and $\bar{n}' = 1/2 - \bar{n}$. To fulfill relation (31) one gets the condition $D > 0$ for the existence of superconductivity, i.e., one recovers (3) when the parameter U is rewritten

$$4\nu I^2 > UV.$$

The above condition is obtained independently of the value of the magnetic moment s. Estimation of the single-band Hubbard parameters to make connection with the high-T_c oxides is a difficult task. Energy-band calculations have been devised to account for correlation effects and spectroscopic data simultaneously. Projections of the above calculations onto the Hubbard model (one or several bands) are however sensible to the method used, yielding a dispersion in the values quoted in the literature.[15] The situation is even worse when dealing with the extended model. The intrasite U at the copper site is estimated to be in the range 5–10 eV and the intersite repulsion $V_{p,d}$ between copper and oxygen sites is in the interval 0.6–2 eV. From the above data we crudely estimate our single-band V to be at most of the order of 0.5 eV. No estimation is available in the literature for the correlated hopping I, but some conclusions can be drawn from the above-estimated values for the other parameters. For example, to satisfy the pairing condition (3) and the inequality (4) with $U = 6$ eV in two dimensions, one gets as the lower bound the value $|I| = V = 0.375$ eV. One then sees that the pairing condition can be met in a finite region of parameter space, with reasonable values of the Hubbard parameters. Thus, our mechanism is not ruled out by recent elaborate calculations of the Coulomb-interaction parameters in the cuprate materials.

The physical situation, where the three order parameters Δ and Γ_σ are simultaneously nonvanishing, may be pictured as a covalent bond formed by holes or by electrons of opposite spins. Instead of being localized, either in one site or in nearest-neighbor sites, where the kinetic energy is high, the pair reduces the effective Coulomb repulsion and minimizes its kinetic energy by resonating between both configurations. This picture is reminiscent of Anderson's RVB idea,[6] except that in our case double occupancy is allowed. Our approach also illustrates the interplay of antiferromagnetism and superconductivity. On-site pairing is favored by the absence of antiferromagnetism. When an antiferromagnetic moment develops, intersite pairing between majority spins gets enhanced over the minority one. For a covalent bond we get an intermediate situation, where pairing coexists with itinerant antiferromagnetism. When projected using a Wannier basis, the covalent bonding yields partial on-site and intersite pairings. This picture also shows that saturation of the magnetic moment will suppress superconductivity, since no states will be available for pairing minority spin carriers. We remark that the above effects are all mediated by the correlated hopping I, and that no pairing is obtained for $I = 0$, when U and V are both repulsive.

Superconducting solutions without magnetic ordering are obtained setting $s = 0$ in (23). In this case, all sites are equivalent and $\langle c_{b\downarrow} c_{a\uparrow} \rangle = -\langle c_{b\uparrow} c_{a\downarrow} \rangle$. In the same way, magnetic solutions are obtained self-consistently for

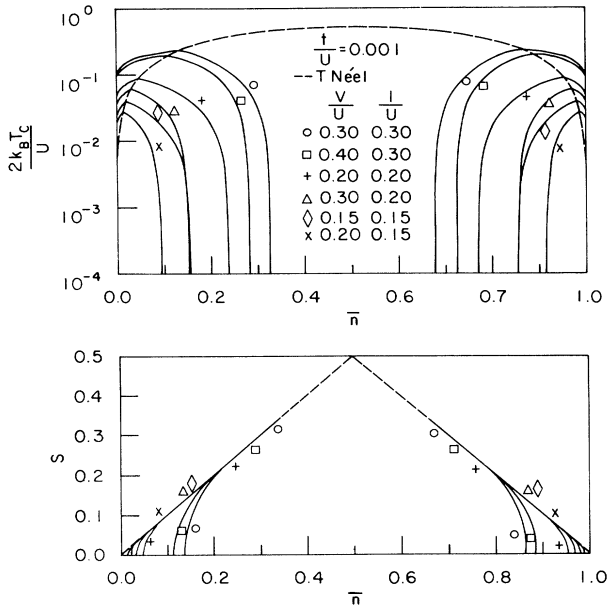

FIG. 1. Critical temperatures (upper figure) and the staggered magnetic moment (lower figure) as functions of the occupation number per spin, for $\frac{t}{U} = 0.001$ and various values of $\frac{V}{U}$ and $\frac{I}{U}$. In the upper figure the Néel temperature for the normal phase is shown with a dashed line, and the superconducting critical temperatures for the different values of parameters are displayed with continuous lines. Note that the scale of temperatures is logarithmic and that T_C and T_N go to zero for $\bar{n} \to 0$ and $\bar{n} \to 1$ (which is not apparent in the figure). Nonmagnetic and magnetic superconducting solutions are matched at the Néel temperature, but the slope is not continuous. Note also that superconductivity disappears close to saturation for electron and holelike carriers. In the lower figure the dashed line displays the saturated value of the moment as a function of the occupation number.

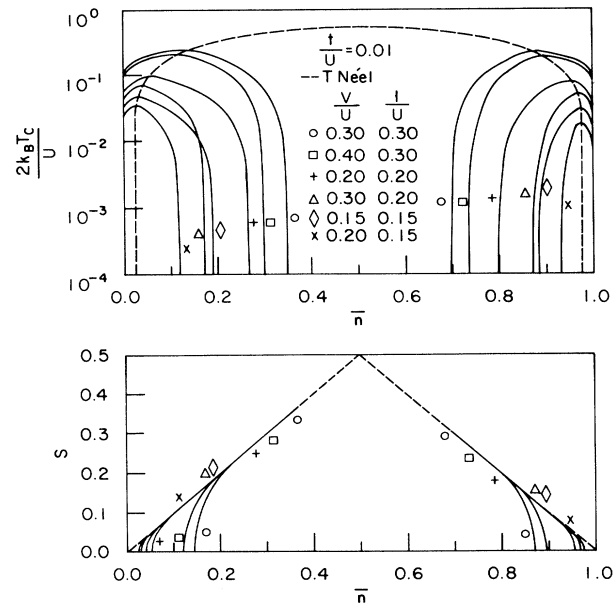

FIG. 2. Same as Fig. 1, but for $\frac{t}{U} = 0.01$. Superconducting solutions get closer to the half-filled band, $\bar{n} = 0.5$.

$s > 0$, but spin symmetry is now broken for the two sublattices.

In Figs. 1–4 we show the phase diagrams obtained in the space critical temperature vs concentration of carriers per spin, for various values of parameters. Stringent values of parameters have been adopted to test the effects described here. The Néel temperature for the normal phase is also shown as a reference, separating nonmagnetic from magnetic solutions of the superconducting critical temperature T_C. Several phases are present, namely, normal nonmagnetic, normal antiferromagnetic, superconducting nonmagnetic, and possible coexistence regions of superconductivity and antiferromagnetism. The value $\bar{n} = 0.5$ labels the half-filled band case. In the lower part of all figures we show the corresponding magnetic moment per site as a function of the concentration of carriers.

Some features are common to all cases.

(i) A nonmagnetic superconducting state is present, but restricted to the almost-empty or to the almost-full band. This result agrees with Hirsch.[12] With antiferromagnetism, the superconducting region extends itself in direction to the half-filled band, but the transition temperature is strongly depressed with the enhancement of the magnetic moment. We note that the superconducting nonmagnetic solution also exists around $\bar{n} = 0.5$, but calculation of the corresponding free energies shows that the latter is not the stable phase.[20] The eventual saturation of the magnetic moment, i.e., when $s = \bar{n}$ for electrons and $s = 1 - \bar{n}$ for holes, suppresses superconductivity. As discussed before, this latter fact is a consequence of the covalent nature of the pairing.

(ii) Electron-hole symmetry is broken by the inclusion of the correlated hopping I. This is more evident in Fig. 4, when we vary $\frac{t}{U}$ for I and V fixed, and for the biggest values of $\frac{t}{U}$. Neither the superconducting solutions nor the process of saturation of the magnetic moment are invariant under the transformation $\bar{n} \rightarrow (1 - \bar{n})$. However, our solutions still present some symmetry which can be expressed in the relation below for the critical temperature:

$$T_C(t, I, \bar{n}) = T_C(t, -I, 1 - \bar{n}) = T_C(-t, I, 1 - \bar{n}).$$

Thus, we conclude that antiferromagnetism is not a necessary condition for the onset of superconductivity in the whole parameter space. Actually, the critical temperature decreases with the appearance of a magnetic moment, but antiferromagnetism is essential in the present formulation, to stabilize pairing in a region of the phase diagram close to half filling.

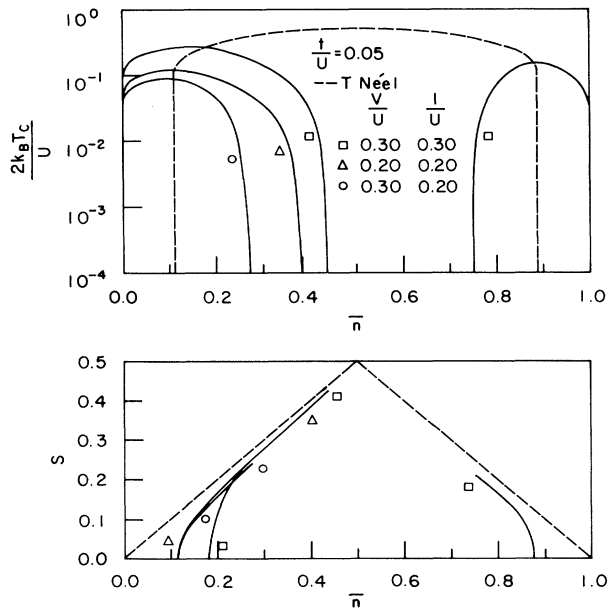

FIG. 3. Same as Figs. 1 and 2, for $\frac{t}{U} = 0.05$. In this case the asymmetry between electrons and holes is more perceptible. Note also that superconductivity disappears slightly before the saturation of the magnetic moment.

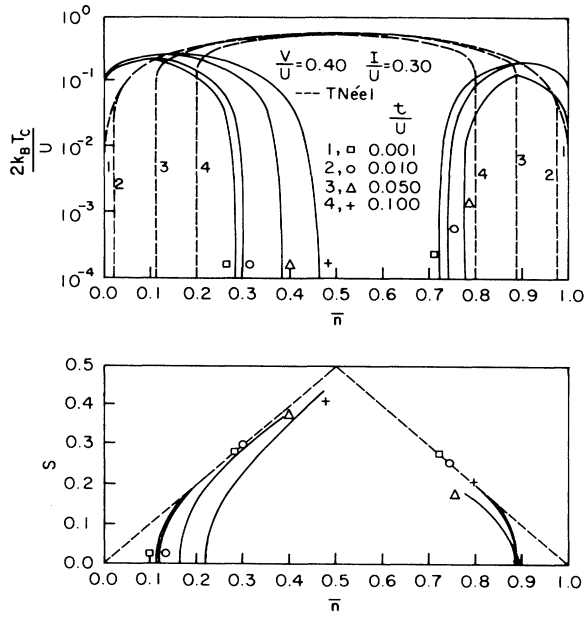

FIG. 4. We plot the same quantities as in the previous figures, but now the parameters $\frac{V}{U}$ and $\frac{I}{U}$ are fixed, while $\frac{t}{U}$ is varied. This figure is interesting, for it clearly shows superconductivity close to half filling and the breakdown of the electron-hole symmetry.

IV. CONCLUSIONS

To apply the present theory to the physics of the copper oxide superconductors, the essential point to be answered is whether the magnetic moment of the insulating antiferromagnetic phase survive the action of doping that leads to the superconducting state. Some experiments[21,22] indicate that, though the 3-d antiferromagnetism is lost in the process, a two-dimensional phase without long-range order is always present with antiferromagnetic correlations lengths ranging from 18 to 200 Å depending on the temperature and doping. These lengths are large when compared with the small super-

conducting coherence lengths that are usually measured for the copper oxide samples.[21] In formulating our theory we have assumed this to be the case, and a local pairing with a small spatial extent have been adopted, while antiferromagnetism, when present, develops long-range order.

Next, we discuss the symmetry of the order parameters (15) and (16). Pairing in a singlet state is obtained for

$$\Delta = \langle c_{i\downarrow} c_{i\uparrow} \rangle, \tag{32}$$

$$\Gamma_{a\uparrow} - \Gamma_{a\downarrow} = \langle c_{b\downarrow} c_{a\uparrow} \rangle - \langle c_{b\uparrow} c_{a\downarrow} \rangle, \tag{33}$$

while triplet symmetry appears when the combination below is not vanishing:

$$\Gamma_{a\uparrow} + \Gamma_{a\downarrow} = \langle c_{b\downarrow} c_{a\uparrow} \rangle + \langle c_{b\uparrow} c_{a\downarrow} \rangle. \tag{34}$$

Only singlets are present for the nonmagnetic solutions when all sites are equivalents. In contrast, with antiferromagnetism, the order parameter acquires a triplet admixture (34), whose magnitude in relation to the intersite singlet component (33), increases with the magnetic moment up to a maximum at saturation. Close to this point, the superconducting state extinguishes.

The inclusion of the correlated hopping breaks the electron-hole symmetry. In fact, when the sign of I is opposite to that of t, hopping to a neighboring site is inhibited when this latter is occupied. This argument is inverted for holes. Double occupancy is not forbidden completely, and depends on the delicate balance of the Coulomb parameters. This fact is essential in our approach for producing a pair binding, and also shows intuitively that the limit $U \rightarrow \infty$ displays no superconductivity.

A comment concerning the generalized Hartree-Fock approximation is in order. As it is usual in any mean-field theory, the effective fields that induce the different phase transitions, and the corresponding transition temperatures, are overestimated. Our results should be considered as upper bounds, and the phase diagram of an improved approximation may be more restrictive.

In summary, we note that an effective Hamiltonian like (5), including the correlated hopping and the intersite Coulomb repulsion, is a natural extension to account for the Coulomb interactions even for the one-band case. Translational invariance implies that the electron density operator is not diagonal in the Wannier representation. In this sense, the inclusion of off-diagonal terms *tends to restore* a fundamental symmetry. Within the present generalized mean-field approach, the role of the correlated hopping I appears as essential for binding of pairs when diagonal terms of the Coulomb potential, like U and V, are repulsive. This assertion will be tested in numerical simulations or in exact analytic studies for finite-size systems. The extension of the present calculation, to obtain the temperature dependence of the order parameters, is currently under study. Other symmetry-broken solutions, like noncommensurate charge and spin-density waves, will also be tested in the future.

As a concluding remark we mention that our pairing mechanism is of a covalent nature, as discussed in Sec. III, obviously of a different nature when compared, for instance, to the usual BCS pairing mechanism. The effective attractive interaction among any two particles, in an assembly of particles interacting solely via repulsive forces, can only have a dynamical origin. The former interaction occurs for short-time intervals, and the pairing mechanism synchronizes this attractive interaction with the appropriate resonance state, enabled by the several repulsive terms (intrasite, intersite, and correlated hoppings), the band term and a suitable relation between the magnitude of such terms.

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