Mechanism for high-temperature superconductivity

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An explanation of the mechanism for high-temperature superconductivity is given, based upon a strong-coupling analysis of the extended Hubbard model previously introduced by one of us. The basic carriers are oxygen-hole quasiparticles in $p\sigma$ orbitals, whose spin is strongly correlated with that of adjacent copper holes. These quasiparticles interact through the enhanced superexchange of the associated spins on the Cu sites, and an enhanced zero-point motion of the surrounding Cu holes. These are nonretarded attractive interactions whose strength increases as the oxygen-copper Coulomb repulsion increases and can be strong enough, for realistic parameters, to overcome the direct oxygen-oxygen Coulomb repulsion. The superconducting transition temperature that results is proportional to the Fermi energy of the oxygen holes.

I. INTRODUCTION

There is a great deal of experimental evidence to support the view that the essential feature of high-temperature superconductors[1] is the quasi-two-dimensional motion of holes in CuO_2 planes.[2] Some time ago, it was proposed[3] that an appropriate description of this system is provided by a suitably extended Hubbard model that allows for motion of holes in both Cu $3d$ and O $2p$ states. It was shown that, for one hole per unit cell, the holes are largely on the Cu sites and the system is an antiferromagnetic insulator. Added holes go onto oxygen sites and are superconducting in virtue of a magnetic coupling mediated by Cu spins. This general picture is consistent with much of the available experimental evidence.[2,3] Originally,[3] the properties of the model were worked out for intermediate coupling, as required by the experimental information which was available at the time. Since then, the interpretation of some of the early experiments has been modified and it has become increasingly clear that a strong-coupling description is more relevant.[4] The purpose of this paper is to consider the properties of the model and the mechanism for superconductivity in that limit. It will be shown that a hole added to an oxygen site forms a quasiparticle state with the neighboring Cu holes, organizing their spins into a small polaron configuration and enhancing their zero-point motion. The attractive interactions responsible for superconductivity are (a) a superexchange between a Cu spin from each quasiparticle, enhanced by the presence of the oxygen hole, and (b) a lowering of the zero-point energy of motion of the hole at the copper site common to the two quasiparticles when the oxygens are nearest neighbors. Several brief accounts of this work have been presented previously.[5]

The original motive for studying intermediate coupling[3] came from the observation[6] that the plasma frequency ω_p in $La_{2-x}M_xCuO_4$ (where M is Ba, Sr, or Ca) was independent of x. However, it now seems that the feature of the optical data from which ω_p was inferred was not a plasma edge; it was subsequently identified as part of a narrow, possibly excitonic, peak.[7] Moreover, measurements of the penetration depth λ_L (which is related to ω_p by $\lambda_L = c/\omega_p$ in the London limit) clearly show that ω_p^2 is proportional to the carrier concentration.[8] Following the arguments of Ref. 3, this implies that the holes on the Cu sites are quite well localized, as in the strong coupling limit of the Hubbard model. This conclusion is supported by the values of the parameters of the model inferred from spectroscopic measurements and cluster calculations.[9] It also follows from the magnitude of the antiferromagnetic order parameter,[10] which is consistent with zero-point motion of localized rather than itinerant spins.[11]

As in Ref.3, an extended Hubbard model will be used to describe the motion of holes in the oxygen $2p$ and copper $3d$ levels. In the strong coupling region, it is possible to regard the system as a set of mobile O $2p$ holes moving through a system of spins localized mainly in Cu $3d$ states. The effective Hamiltonian, given in Sec. II, has two parts: (a) a term containing the hopping motion of the oxygen holes and their coupling to the Cu spins, and (b) a superexchange interaction between Cu spins. In the perturbation theory in the p-d hopping parameter t, these terms are of order t^2 and t^4, respectively: For realistic values of the parameters it is necessary to include contributions from higher orders. In any case, the Cu-Cu superexchange is the weaker part of the Hamiltonian.

An O $2p$ hole does not move freely through the background but forms a quasiparticle state in which the spins of nearby Cu holes are polarized and their zero-point motion increased. The quasiparticle carries spin and charge. A detailed description of this state will be given elsewhere[12] but the main features are summarized in Sec. III.

The quasiparticles do not have a very large spatial extent and do not leave behind then a "wake" of reversed Cu spins. Also, the members of a singlet pair of quasiparticles have average spin zero and hence, in lowest order, do not interact with their environment via the Cu-Cu su-

perexchange. It follows that the pairing force is of short range. As described in Sec. III, the major contribution comes from superexchange when the spins of Cu holes in different quasiparticles are near neighbors. The essential features are (a) the superexchange and Cu-hole zero-point energy are enhanced by the Coulomb interaction with the oxygen hole, (b) the interaction is independent of the state of the background Cu spins (range of antiferromagnetic correlations, etc.). The only requirement is that there is a well-defined local moment associated with a Cu site, and (c) because the intermediate state energies for near-neighbor superexchange are electronic, the effective interaction between quasiparticles is nonretarded. The enhancement of the superexchange is crucial—without it, it is impossible to overcome the Coulomb repulsion and obtain a net attractive pairing force.

In Sec. IV, it is shown that the model leads to superconductivity in a Bardeen-Cooper-Schreiffer (BCS) theory. For the low carrier concentrations n_c found in $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_{7-x}$, s-state pairing dominates because the d-state scattering amplitude is proportional to n_c^2 and is very weak. As a result of the nonretarded nature of the effective interaction between quasiparticles, the transition temperature T_c is proportional to the Fermi temperature T_F. Both of these conclusions are consistent with the behavior of the penetration depth, as measured by muon-spin relaxation. From this point of view, high T_c occurs because the scale is set by T_F (which is a few thousand degrees) rather than by the Debye temperature, which is much smaller. Also, the difference in T_c from one material to another is a consequence of the change in n_c. Finally, it will be pointed out in Sec. IV that there is the interesting possibility of a crossover from s-state to d-state pairing, as the carrier concentration is increased.

II. EFFECTIVE HAMILTONIAN

As in Ref. 3, the Hamiltonian for the extended Hubbard model is given by

$$H=\sum_{\mathbf{i},\mathbf{j},\sigma}\varepsilon_{\mathbf{ij}}a^{\dagger}_{\mathbf{i}\sigma}a_{\mathbf{i}\sigma}+\tfrac{1}{2}\sum_{\substack{\mathbf{i},\mathbf{j}\\ \sigma,\sigma'}}U_{\mathbf{ij}}a^{\dagger}_{\mathbf{i}\sigma}a_{\mathbf{i}\sigma}a^{\dagger}_{\mathbf{j}\sigma'}a_{\mathbf{j}\sigma'}, \tag{2.1}$$

where $\mathbf{i}$ is (m,n) for a copper site and $(m+\frac{1}{2},n)$ or $(m,n+\frac{1}{2})$ for an oxygen site. The vacuum consists of Cu^+ (all $3d$ states occupied) and O^{2-} (all $2p$ states occupied), and the $a^{\dagger}_{i\sigma}$ creates holes of spin σ in copper $3d_{x^2-y^2}$ orbitals or oxygen $2p_x$ or $2p_y$ orbitals. It is assumed that a factor $(-1)^{m+n}$ is absorbed into the $a^{\dagger}_{i\sigma}$ for copper and oxygen creation operators in cell $\mathbf{m}\equiv(m,n)$ to take account of signs in hopping integrals. The site-diagonal terms $(\varepsilon_{\mathbf{ii}},U_{\mathbf{ii}})$ are (ε_p,U_p) and (ε_d,U_d) for O $2p$ and Cu $3d$ states, respectively. There is an interaction $U_{\mathbf{ij}}=V$ between holes on neighboring Cu, O sites and it will be important later to include the effects of the longer-range Coulomb interaction. It is assumed that there is a hopping integral $\varepsilon_{\mathbf{ij}}=t$ between Cu-O neighbors. In principle there is also a direct oxygen-oxygen hopping t_p but, to simplify the presentation, this will be ignored since an excellent tight-binding fit[13(a)] to the band structure may be obtained with a negligible value of t_p. We shall take $t\simeq 1$ eV as before[3] but use the more recent and somewhat larger values[9] $U_p\simeq 5$–7 eV and $U_d\approx 8$–10 eV, which together imply[3] $\varepsilon\equiv\varepsilon_p-\varepsilon_d=1$–$2$ eV. The magnitude of V will be considered later. It has been pointed out[9] that the Hamiltonian should also include a direct ferromagnetic exchange $J_D\approx 0.2$ to 0.5 eV between holes on neighboring Cu and O sites and this will be incorporated into an effective Hamiltonian to be derived later in this section.

Consider first the case of one hole per cell and $t=0$, for which there is exactly one hole on each of the N Cu sites and a 2^N-fold spin degeneracy. As is well known, the spin degeneracy is lifted by superexchange to give an effective Hamiltonian

$$H_s=J_C\sum_{\langle\mathbf{i},\mathbf{j}\rangle}(\vec{S}_{\mathbf{i}}\cdot\vec{S}_{\mathbf{j}}-\tfrac{1}{4}), \tag{2.2}$$

where $\langle\mathbf{i},\mathbf{j}\rangle$ denotes near-neighbor *copper* sites and $\vec{S}_{\mathbf{i}}$ are spin-$\frac{1}{2}$ operators. Because the superexchange goes via an oxygen site J_c is $O(t^4)$ and is given by

$$J_c=\frac{4t^4}{(\varepsilon+V)^2}\left(\frac{1}{U_d}+\frac{2}{U_p+2\varepsilon}\right). \tag{2.3}$$

This could also have been obtained as the strong-coupling limit of the effective Hubbard model for Cu holes, previously derived,[3] although Eq. (2.3) contains all terms of fourth order. Note that the Coulomb interactions U_p and V, which are often omitted from models of this kind, both serve to diminish the value of J_c. We have estimated $J_c=0.12$ eV from the measured[13(b)] spin-wave velocity $v_s=0.7$ eV Å, using the spin-wave theory result $v_s=\sqrt{2}J_ca$ where a is the in-plane lattice constant. The error in this estimate should be less than 20% and it gives a quite sensitive constraint on the parameters of the model. It is in agreement with the value obtained from light scattering measurements.[13(b)]

As discussed in Ref. 3, since $U_d>\varepsilon+2V$, any addition holes, produced by doping or changing the oxygen content, will go onto oxygen sites. By now there is considerable spectroscopic evidence to support this picture for the high-T_c oxides, following the initial experiments of Tranquada and co-workers.[14] It should be noted that V cannot be too large, otherwise the added holes will cause a local rearrangement of the charge configurations and lead to clustering, as will be discussed later.

For $t=0$, the ground state is degenerate because the energy is independent of spin configurations and the location of the oxygen holes. The degeneracy is resolved by using second-order degenerate perturbation theory in t. Although J_c is a weaker interaction, it is not negligible since it is responsible for antiferromagnetic correlations and for the suppression of ferromagnetic bubbles which might otherwise have been generated by the motion of oxygen holes. However, the conditions are quite different from those considered previously,[3] where for intermediate coupling the $O(t^2)$ terms did not dominate.[15]

Let the position index $\mathbf{i}$ be denoted by $\mathbf{m}$ for a Cu site at the corner of a cell and $\mathbf{m}+\boldsymbol{\Delta}$ for an oxygen site displaced by distance $\Delta[(\pm\frac{1}{2},0),(0,\pm\frac{1}{2})]$ in one of the four directions. Then the effective Hamiltonian for a single

added hole is

$$H_2 = (t_1+t_2)\sum_{\substack{\Delta\neq\Delta'\\ \mathbf{m},\sigma,\sigma'}} a^\dagger_{\mathbf{m}\sigma'}a_{\mathbf{m}\sigma}a^\dagger_{\mathbf{m}+\Delta,\sigma}a_{\mathbf{m}+\Delta',\sigma'} + t_2\sum_{\substack{\Delta\neq\Delta'\\ \mathbf{m},\sigma}} a^\dagger_{\mathbf{m}+\Delta,\sigma}a_{\mathbf{m}+\Delta',\sigma} + J\sum_{\mathbf{m}\Delta}(\vec{S}_{\mathbf{m}}\cdot\vec{S}_{\mathbf{m}+\Delta}-\tfrac{1}{4})n_{\mathbf{m}+\Delta} - 2\Delta E_c\,, \tag{2.4}$$

where $n_{\mathbf{m}+\Delta}$ is the occupation number at the site $\mathbf{m}+\Delta$. Also, ΔE_c is the change in the self-energy of a single Cu hole due to the presence of the oxygen hole. To second order in t

$$t_1 = t^2/\varepsilon\,, \tag{2.5}$$

$$t_2 = t^2/(U_d-2V-\varepsilon)\,, \tag{2.6}$$

$$J = \frac{2t^2}{\varepsilon+U_p-V}+\frac{2t^2}{U_d-2V-\varepsilon}-J_D\,. \tag{2.7}$$

These expressions illustrate the dependence of H_2 on the parameters of the original Hamiltonian. Evidently Eqs. (2.5)–(2.7) are not accurate when the energy denominators are comparable to t, but it is straightforward to obtain more accurate values by using a modified form of Wigner-Brillouin perturbation theory or by studying small clusters, as described in the Appendix.

An effective Hamiltonian[16] similar to H_2 was used for intermediate coupling in Ref. 3 where it was assumed that the motion of the added hole did not disturb the background which was taken into account by using the Green's function of the Cu holes. In the strong-coupling limit, however, the terms included in Eq. (2.4) are dominant and the quasiparticle states involve the correlated motion of copper and oxygen holes.

The parameters of H_2 will be modified when two oxygen holes are close together. This is one of the effects to be included in the interaction of oxygen holes, discussed in detail in the next section.

III. QUASIPARTICLE DYNAMICS AND INTERACTIONS

A. Kinetic energy of a single quasiparticle

1. *Stationary single oxygen hole*

Let us, for the moment, neglect the fourth-order terms that lead to Cu-Cu exchange and consider only the second-order processes. The parameters of the Hamiltonian have been chosen so that the background of Cu holes is stable when an additional hole is added, which will reside primarily on the oxygen sites. Its energy is clearly degenerate with respect to the location of the oxygen site, and it will hop from site to site, becoming the carrier of the supercurrent. It does not hop as a bare carrier, however, but as a dressed object, polarizing the surrounding spins. The physics may be understood by dividing the Hamiltonian into two parts, a site diagonal term and a hopping term as in Eq. (2.4). The site diagonal term, for a single hole located in either the x or y bonds of the unit cell is

$$h_3 = J\vec{s}\cdot(\vec{S}_1+\vec{S}_2)\,, \tag{3.1}$$

where $\vec{s}$ is the spin of the oxygen hole and $\vec{S}_1$ and $\vec{S}_2$ the spins on the neighboring copper holes. We have suppressed a constant self-energy term of $-\frac{1}{2}J$.

For a single hole, the ground-state spin configuration of the oxygen hole and its surrounding copper spins is

$$|\psi\uparrow\rangle = [2\uparrow\downarrow\uparrow-(\downarrow\uparrow\uparrow+\uparrow\uparrow\downarrow)]/\sqrt{6} \tag{3.2}$$

or its degenerate, spin-reversed partner, with an energy of $-J$. This is clearly a spin-$\frac{1}{2}$ state. An alternative way of writing $|\psi\uparrow\rangle$ is as a linear superposition of singlets

$$|\psi\uparrow\rangle = [(\uparrow\downarrow-\downarrow\uparrow)\uparrow-\uparrow(\uparrow\downarrow-\downarrow\uparrow)]/\sqrt{6}\,, \tag{3.3}$$

which is useful in considering the hopping motion of the quasiparticle. Note that the two singlet components in Eq. (3.3) are not orthogonal and, as a result, there is an average spin of $-\frac{1}{3}$ on the oxygen site. The first excited state of the Hamiltonian defined in Eq. (3.1) has energy zero and corresponds to the two Cu spins in a singlet that does not interact with the oxygen hole. The degeneracy of the energy with respect to the location of the oxygen is lifted by the hopping term in Eq. (2.4).

2. *Moving oxygen hole*

When the hopping terms are included, the oxygen hole is free to move through the lattice. The basis of our physical picture is that it hops from site to site as the entity described in Sec. III A 1, so that the spin configuration of its neighboring copper spins as described in Eq. (3.2). Zhang and Rice[17] have proposed an alternative picture, in which an oxygen hole in a Wannier state forms a singlet with a copper spin in the same cell, and this singlet is to be thought of as hopping through the lattice. On the basis of this picture, they claim that the extended Hubbard model we have been considering is "equivalent" to the one-band Hubbard model, the singlet being equivalent to a vacancy. This is not correct. We have solved exactly the problem of an oxygen hole hopping on a ferromagnetic background,[12] starting from their second-order Hamiltonian. Although the bandwidth that results is very close to the value one would obtain by making their approximation, the states differ in important details. At the bottom of the band, the lowest energy state is described slightly better by a superposition of states of the form (3.2) with equal amplitude to be at each site, than it is by a superposition of singlets. More important, the average value of the spin on an oxygen site is not zero, as it would have to be if their picture were strictly correct. In as much as the spinless nature of a vacancy in the one-band model is an essential feature, the extended and one-band models cannot be "equivalent." This will be discussed in more detail in a separate paper.[12]

There are, however, significant differences in the spin configuration around the oxygen hole as the quasiparticle energy increases towards the middle of the band. The spin deviations on surrounding copper spins become more delocalized, the average value of the spin on adjacent coppers

is reduced, and the average spin at the oxygen site decreases, vanishing near the center of the band. It is also the case that the zero-point motion of the adjacent copper holes is enhanced by the presence of the oxygen hole, as a result of the Coulomb repulsion. These effects play a role in the mechanism for superconductivity, and will be discussed in the next section. For the moment, we will treat the quasiparticle as having the spin configuration of Eq. (3.2).

An accurate calculation of the hopping of the quasiparticle on the antiferromagnetic background has not been done, but one can get some idea of the effective mass from the following argument. For many purposes, the motion of the quasiparticle state is well approximated by the hopping of the singlet component[12] shown in Eq. (3.3). That is, motion to the left (right) is produced by the component in which the singlet stands to the left (right) of the isolated spin. This follows because a singlet is quite mobile since all hopping processes in H_2 add up coherently to give an effective hopping amplitude of (t_1+2t_2). (For an oxygen hole, the hopping amplitude is t_1, t_2, or t_2-t_1, according to the state of the Cu spin.) Hopping of the quasiparticle is reduced by a factor of two to take account of overlap between one singlet component and the full quasiparticle wave function. Finally, allowing for zero-point spin fluctuations in the ground state of the Heisenberg model, it may be shown[12] that long- or short-range antiferromagnetic correlations reduce the hopping by a further factor of $\frac{2}{3}$ to give

$$\bar{t} \approx (t_1+2t_2)/3 . \tag{3.4}$$

Using the values of t_1 and t_2 obtained in the Appendix, Eq. (3.4) gives $\bar{t} \approx 0.3$ eV. This may be compared with the experimental value of 0.15 eV inferred from muon measurement of the penetration depth which is probably a lower limit.[8] Equation (3.4) also does not take account of the zero-point motion of the Cu hole. We note that this estimate does not depend on the existence of long-range order; it is sufficient to have local antiferromagnetic correlations in the neighborhood of the quasiparticle.

The dispersion relation of the quasiparticle is then

$$t_k = -2\bar{t}(\cos k_x + \cos k_y) + \text{const} . \tag{3.5}$$

So far, the discussion omitted the fourth-order coupling J_c between Cu spins, and it might be imagined that this is unjustified if the direct exchange J_D in Eq. (3.7) is so large that J is not much larger than J_C. However, all terms of order t^2 must be taken into account and it is important to recognize that, in general, a singlet hops much more readily than a free oxygen hole. The kinetic energy ensures that terms of order t^2 dominate J_C and that the spin configurations of Eq. (3.2) and of Eq. (3.3) are good representations of the mobile quasiparticle.

B. Effective potential between quasiparticles

Having obtained an expression for the kinetic energy of the quasiparticles, we now determine their effective interaction potential. We will consider only the effective potential in a singlet state of two quasiparticles. This potential arises from several distinct sources, depending upon the distance between the oxygen holes.

1. *Holes on the same site*

When the oxygen holes are on the same site, we have the direct Coulomb repulsion U_p, and in addition, since they no longer polarize their surroundings, an energy of $2J$ above the energy of two well-separated quasiparticles, which we will use as a reference. Thus, the total repulsive energy is U_p+2J.

2. *Holes on adjacent oxygen sites*

When the two oxygen holes are on adjacent sites, that is, they both have bonds to the same copper site, their Hamiltonian is

$$h_5 = J[\vec{S}_1+\vec{S}_2)\cdot\vec{s}_1+(\vec{S}_2+\vec{S}_3)\cdot\vec{s}_2] . \tag{3.6}$$

We have not indicated any indices on the sites since the energy of this configuration does not depend upon them. The ground-state spin configuration of these five spins has an energy of $-1.95J$, that is, $0.05J$ higher than two separated quasiparticles. The dominant spin configuration is $\uparrow\downarrow\uparrow\downarrow\uparrow$ or the reverse, and we will denote it this way in subsequent figures. The complete configuration is given in Table I. The five-spin state can also be represented by the combination of Cu-O singlets shown in Table II.

The five-spin state has spin $\frac{1}{2}$ and the total state that we need to consider must be the singlet combination of the five-spin state and a copper hole adjacent to one or the other ends. A configuration as shown in Fig. 1(a) can then hop onto the one shown in Fig. 1(b). The $\leftrightarrow$ symbol is to be understood as indicating the singlet combination of the right and left states. To second order in t, the extra spin does not interact with the remaining five, so the energy is the same, $-1.95J$.

Thus, the Cu-O exchange leads only to a slight $(0.05J)$ repulsive energy when the two oxygen holes are on adjacent sites. There is an additional mechanism, however, that can play a role in providing an effective attraction. We will call this enhanced zero-point motion. It involves the charge rather than the spin degrees of freedom, and lowers the energy of the five-spin state. Consider the

TABLE I. Nearest-neighbor wave function.

Configuration	Amplitude
$\uparrow\downarrow\uparrow\downarrow\uparrow$	−0.665
$\downarrow\uparrow\uparrow\downarrow\uparrow$	0.384
$\uparrow\downarrow\uparrow\uparrow\downarrow$	0.384
$\uparrow\uparrow\downarrow\downarrow\uparrow$	0.233
$\uparrow\downarrow\downarrow\uparrow\uparrow$	0.233
$\downarrow\uparrow\downarrow\uparrow\uparrow$	−0.233
$\uparrow\uparrow\downarrow\uparrow\downarrow$	−0.233
$\uparrow\uparrow\uparrow\downarrow\downarrow$	0.048
$\downarrow\downarrow\uparrow\uparrow\uparrow$	0.048
$\downarrow\uparrow\uparrow\uparrow\downarrow$	0.199

TABLE II. Nearest-neighbor wave-function, singlet representation.

Configuration	Amplitude
$\uparrow\leftrightarrow\downarrow\uparrow\uparrow\leftrightarrow\downarrow$	−0.199
$\uparrow\leftrightarrow\downarrow\uparrow\leftrightarrow\downarrow\uparrow$	+0.233
$\uparrow\uparrow\leftrightarrow\downarrow\downarrow\leftrightarrow\downarrow$	+0.233
$\uparrow\uparrow\uparrow\downarrow\downarrow$ $\leftrightarrow$ $\downarrow\uparrow\uparrow\uparrow\uparrow$	+0.048

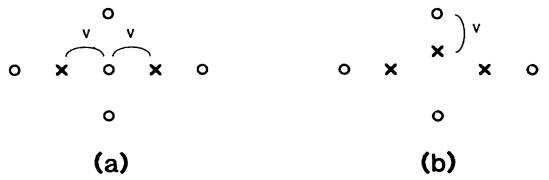

FIG. 2. (a) The hole configuration when $V \ll \varepsilon$. (b) The hole configuration when $V \gg \varepsilon$. The copper sites occupied by a hole are denoted by O, the occupied oxygen sites by ×, and the empty sites not shown. The central Cu hole delocalizes readily onto the two unoccupied oxygen sites, lowering the zero-point energy of the state when two oxygen holes are adjacent.

copper hole that is adjacent to two oxygen holes in Fig. 2(a), in the limit of very weak hopping. The energy of the configuration of Fig. 2(b) is then lower than that of Fig. 2(a) if $V > \varepsilon$. When this condition is met, Fig. 2(b) becomes the stable configuration. With finite values of t, the wave function will continuously go from one in which the hole is localized on the copper site to one in which it is delocalized on the surrounding oxygen sites. Delocalizing it lowers its zero-point energy, providing an additional attraction. This energy increases as V increases. It is calculated in the Appendix and shown in Fig. 3 for $U_D = 9$, $U_p = 6$, $t = 1$ (in eV). There is also a fourth-order attractive energy arising from the spin degrees of freedom described in the next section.

3. *Two holes separated by one vacant oxygen site: enhanced superexchange*

When there is an empty oxygen site between the copper spins of the quasiparticles, as in Fig. 1(a), one must go to fourth order to obtain the effective potential.

When the two quasiparticles are as in Fig. 1(a), the two interior copper spins have an average exchange energy of $-J_c/3$ as a result of the quasiparticles being in the singlet state. [This can be thought of as $-\frac{3}{4}J_c$ for two spins in a singlet reduced by $(\frac{2}{3})^2$ as a result of the reduction of the average spin on the copper.] This would not be a very large energy if it were not for the fact that the value of J_c that is appropriate is significantly enhanced by the presence of the oxygen holes, whose Coulomb repulsion increases the zero-point motion of the copper hole and hence the effective exchange. The value of J_c for the two interior copper spins, to fourth order in t, is

$$\tilde{J}_c = 4t^2(t/\varepsilon)^2[1/U_d + 2/(U_p + 2\varepsilon - 2V)] . \tag{3.7}$$

This is increased over the value when the oxygen holes are not present both by an overall factor of $[(\varepsilon+V)/\varepsilon]^2$, and the reduction in the denominator of the second term. With $U_p = 6$, $U_d = 9$, $\varepsilon = 1.5$, $t = 1$, and $V = 2$ (in eV) we find $\tilde{J}_c/J_c = 8.3$ while with $V = 1$, the ratio is only 3.3. The former set of values leads to a value of J_C of about 0.1 eV, close to the measured value of 0.12, while the second is too large by a factor of 2. The extreme sensitivity to t and ε makes it difficult to use the measured value of J_c to draw any firm conclusions about the denominators in (3.7). It is also the case that the straightforward second-order perturbation theory is not accurate, since t/ε is not small. A better calculation is given in the Appendix, and the results are shown in Fig. 5. Enhancement factors between 2 and 4 seem plausible. Adopting a value of the middle of this range for further discussion, we see that there is an attractive energy of 0.12 eV whenever two copper spins associated with quasiparticles are on adjacent copper sites. This would still not be a very large energy were it not for the fact that there are 16 such sites and a total of 18 attractive bonds. This is shown in Fig. 4. There is also an enhanced superexchange between the five-spin state and the additional spin with which it forms a singlet [see Fig. 1(b)]. Taking account of the effective spin on the end site

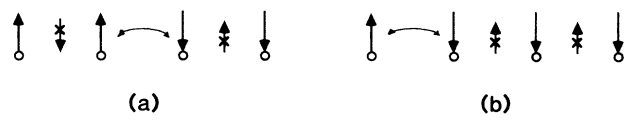

FIG. 1. (a) Two quasiparticles in a singlet state. (b) The five-spin state formed when two oxygen holes are adjacent forms a singlet with the remaining copper spin. Only the major component of the spin configuration is shown. The ⌒ symbol indicates the singlet combination of the entire configuration, given by Eq. (3.2) or Table I, of the states to the right and the left. The states shown in (a) hop easily onto those shown in (b).

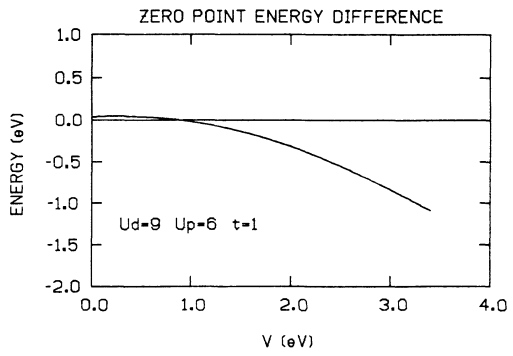

FIG. 3. The difference of the zero-point energies of surrounding copper holes when two oxygen holes are and are not adjacent, as a function of V. [$U_D = 9$, $U_P = 6$, $t = 1$ (in eV)].

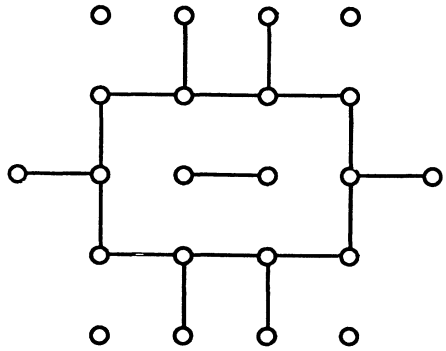

FIG. 4. The location of oxygen quasiparticles that participate in enhanced superexchange with the central quasiparticle. The copper sites are denoted by O.

of Table I, this is approximately $\frac{3}{8}\tilde{J}'$, where $\tilde{J}'$ is enhanced by only one factor of $(\varepsilon+V)/\varepsilon$ since there is only one oxygen hole near a copper. With the correction given in the Appendix, this would be a factor of between 1.4 and 2.0. Again taking a value in the middle of the range, we will assign an attractive energy of 0.08 eV/site to this spin configuration. There are six different sites for the pair of oxygen holes that correspond to the five-spin state of Sec. III B 2, with one oxygen hole fixed at a given site. The net attractive energy is $\simeq$0.04 eV, assuming $J\simeq$0.8 eV and subtracting the repulsive energy of $0.05J$. The attraction due to enhanced zero-point motion will typically be much larger than this.

For larger separations, there will be some interaction, both because the quasiparticle distorts the polarization of surrounding copper spins out to more than just the neighbors of the oxygen hole, and because the copper holes have some probability of being displaced onto the surrounding oxygen sites. Both effects fall off exponentially with distance and give a momentum cutoff in the potential, discussed in Sec. IV. They do not contribute significantly to the forward scattering amplitude, and hence do not strongly affect T_c. In addition, there will be a retarded interaction at a longer distance that may be thought of as multiple magnon exchange. Although this may provide some additional attractive energy, the dependence of the critical temperature on the density of oxygen holes indicates that it cannot be the dominant effect, as discussed in the next section, and it will be neglected.

We now have a complete description of the model potential. The dominant magnetic attraction comes from the enhanced superexchange when the oxygen holes are separated by an intervening oxygen site, as in Fig. 4, and is on the order of 0.12 eV/site. There is a smaller attractive energy of 0.04 eV for each of the six sites in which the oxygens are adjacent to the same copper, and there is a large ($\simeq$8 eV) repulsion when the two oxygen holes are on the same site. Left out of the model we have started with, but certainly present in the real system, is the Coulomb repulsion of the oxygen holes when they are on different sites. This subtracts directly from the attraction counted above, and must be included. There is, in addition, an enhanced zero-point fluctuation contribution when two oxygen holes are adjacent, depending strongly on V, and on the order of 0.5 eV (see Fig. 3).

The potential together with the kinetic energy of a single quasiparticle obtained in Sec. III A 2, allows for a description of the Fermi surface instability that leads to superconductivity, to which we now turn.

IV. SUPERCONDUCTIVITY

In this section, it will be shown that the effective interaction between the quasiparticles leads to s-state superconductivity with T_c proportional to $T_F=\bar{t}k_F^2a^2$. Although T_F is relatively small (we estimate $k_BT_F=0.15$ eV for $La_{1.83}Sr_{0.15}CuO_4$ and 0.4 eV for $YBa_2Cu_3O_7$) it is much higher than the typical Debye energies that set the scale for most metallic superconductors, and this allows high-temperature superconductivity without a particularly strong pairing force. Furthermore, it can be seen that the variation in T_c from one material to another is a consequence of the change in carrier concentration in the CuO_2 planes: $n_c=k_F^2/2\pi$.

To bring out those points, we shall use the Bardeen-Cooper-Schrieffer (BCS) equation for T_c in the form[18]

$$\chi_{\mathbf{k}}=(1/N)G_k\sum_{k'}V_{\mathbf{k}-\mathbf{k}'}\chi_{\mathbf{k}'} \tag{4.1}$$

where

$$G_k=\frac{\tanh(\frac{1}{2}\beta_c\varepsilon_k)}{2\varepsilon_k} \tag{4.2}$$

with $\beta_c\equiv(k_BT_c)^{-1}$, $\varepsilon_k=\bar{t}(k^2-k_F^2)a^2$, and N the number of cells in the CuO_2 lattice. Equation (4.1) is the condition for an instability of the Fermi surface of the lower of the two bands of oxygen quasiparticle states—the one that is partially occupied. The spectrum $-2\bar{t}[\cos(k_xa)+\cos(k_ya)]$ has been expanded to second order in k_x and k_y, which is a good approximation for low carrier densities. Equation (4.1) neglects fluctuation effects which are more significant than usual because of the short coherence length and the two-dimensional band structure. However, it should be sufficient for a discussion of the main features of the pairing and the systematics of superconductivity.

An essential feature of Eq. (4.1) is the use of an instantaneous interaction $v_{k-k'}$ between the quasiparticles. There are three energy scales involved—quasiparticle kinetic energy, intermediate states for superexchange, and Coulomb excitations. For the *near-neighbor* superexchange discussed in Sec. III, all intermediate states are *electronic* excitations with energies greater than the bandwidth $W\simeq$1.2 eV. But the Coulomb interaction is able to excite states of even higher energy and they must be summed into an effective interaction to be used in the lower oxygen band. The renormalization is somewhat smaller than for μ^* in the usual theory of superconductivity because the lower limit of intermediate state energies is much higher than typical phonon energies. Nevertheless, the enhanced superexchange is sufficiently retarded relative to the Coulomb force to have a net attraction that can account for the observed transition temperatures. The energy scale of the resultant interaction is larger than

typical quasiparticle energies so it is effectively instantaneous in the equation (4.1) which determines T_c.

This classification of energies is not appropriate for the usual spin-fluctuation exchange for which the least upper bound of intermediate state energies $2J \propto 0.24$ eV is smaller than the Fermi energy in $YBa_2Cu_3O_7$, and therefore the effective interaction is retarded.

Equation (4.1) may be solved by the method used previously[19] in the theory of superfluid He^3 and helium mixtures to obtain

$$T_c = 4.52\bar{t}k_F^2a^2e^{4\pi\bar{t}/\lambda_l(k_F)}, \tag{4.3}$$

where $\lambda_l(k_F)$ is an effective scattering amplitude for angular momentum l and relative momentum k_F. The result is appropriate when the interactions provide a momentum-transfer cutoff, otherwise $\bar{t}k_F^2a^2$ should be replaced by $(\bar{t}k_F^2a^2W)^{1/2}$ where W is the bandwidth. The cutoff at large momentum transfer occurs because Coulomb and superexchange are not, in reality, point interactions but fall off gradually with distance.[20]

It is instructive to consider the lowest-order perturbation theory expression for $\lambda_l(k_F)$ at low density:

$$\lambda_l(k_F) = \sum_{\mathbf{R}_n} \cos^2(l\theta_n) v(\mathbf{R}_n) J_l^2(k_F R_n), \tag{4.4}$$

where $J_l(k_F R)$ is a Bessel function of order l and $v(R)$ the potential in real space. The sum is carried out over lattice vectors $\mathbf{R}_n \equiv (R_n, \theta_n)$ and the axis for polar coordinates is chosen to maximize T_c. From Eq. (4.4), $\lambda_l(k_F) \sim k_F^{2l}$ at low densities and hence s-state pairing will dominate. In that limit, the entire density dependence of T_c is in the prefactor in Eq. (4.3) and $T_c \sim k_F^2$. This conclusion is confirmed by two features of the penetration depth λ_L, measured by muon-spin relaxation in a range of samples of doped La_2CuO_4 and $YBa_2Cu_3O_{7-x}$. Comparison of T_c with the value of λ_L at $T=0$ shows that $T_c \sim k_F^2$ (Ref. 8) whereas the temperature dependence of λ_L implies that there are no zeros of the energy gap, as in s-state pairing.[8,21] Deviations from the predicted density dependence of T_c in $La_{2-x}Sr_xCuO_4$ may be attributed to a crossover associated with the metal-insulator transition at $x \approx 0.05$ and to inhomogeneity of the materials.

The experiments do not seem to be consistent with d-state pairing, for which there would be zeros of the energy gap and a strong additional variation of T_c with carrier concentrations because $\lambda_2(k_F) \sim k_F^4$ appears in the exponent in Eq. (4.3). There have been suggestions of d-state pairing because of the temperature-dependence of λ_L obtained from inductive measurements.[22] However, the values of λ_L obtained in this way are an order of magnitude larger than given by the muon experiments, apparently because the measurement is dominated by Josephson coupling between grains.[23] Anisotropic pairing was also proposed as an explanation of an anomaly[24] in the orthorhombic strain at T_c, but experiments with better characterized samples and higher resolution[25] have failed to reproduce this effect. It should be noted that the situation for intermediate coupling is quite different.[3] In that case, the Fermi surface approached the square $\cos(k_x a) + \cos(k_y a) = 0$ as the carrier concentration decreased, and d-state pairing may dominate.[3] As pointed out in the Introduction, other experiments show that the materials studied so far are not in this region. However, as in helium mixtures,[19] there can be a crossover to d-state pairing as the carrier concentration is increased and, although it is difficult to estimate precisely where this will occur, it is a possibility to be kept in mind for the higher-T_c materials based on Bi and Tl.[26]

At lower carrier concentrations, T_c is determined by the forward scattering amplitude $\lambda_0(0)$. Following the discussion of the preceding section, the balance of forces is most easily discussed in real space. But it is necessary to recognize that, just as for intermediate coupling,[3] the Fourier transform of $v_{\mathbf{k}-\mathbf{k}'}$ is the interaction between holes occupying the Wannier states of the lower quasiparticle band, rather than individual oxygen sites. Since the bare interaction is not diagonal in this representation, there are interband transitions which have been summed to obtain the effective v. The most significant effect is on the energy $\bar{U}$ required to put two particles into the same Wannier state, since it is possible to avoid U_p by mixing in the upper band. The actual value of $\bar{U}$ depends on V but is typically 1 to 2 eV.[27] In order to get a simple estimate for $\lambda_0(k_F)$ we evaluate the t matrix for $\bar{U}=\infty$ and use the Born approximation for the contribution of first and higher neighbors to the forward scattering amplitude. The repulsive contributions are about $4\bar{t} \simeq 0.6$ eV for $\bar{U}=\infty$ (using the experimental value of $\bar{t}$) and 2.4 eV from the Coulomb interaction (allowing a dielectric constant of 10 and a factor of 2 for the renormalization discussed earlier). The attractive contribution from enhanced superexchange and reduction in zero-point energy may be obtained by transforming from the oxygen site representation to the Wannier representation. A balance of $\lambda_0(k_F) = -0.35$ eV which is required to fit the experimental values of T_c is obtained for V between 2 and 2.5 eV. We have verified these estimates by carrying out a numerical solution of the two-body problem on a lattice, and it is straightforward to extend the study to the full t-matrix equation for $\lambda_l(k_F)$, once our knowledge of the parameters is sufficiently accurate to warrant it.

V. CONCLUSION

In the preceding sections we have studied the strong-coupling limit of a model of the copper oxide planes in the high-temperature superconductors. The major consequences of the model are as follows.

(i) For one hole per unit cell, the system is an antiferromagnetic insulator with holes localized on or in the neighborhood of Cu sites.

(ii) When charge carriers are added by doping or by changing oxygen content, they move mainly on oxygen sites and form quasiparticle states involving the spin and zero-point motion of holes on nearby Cu sites. The quasiparticles are fermions which carry both spin and charge.

(iii) s-state pairing with T_c proportional to the Fermi temperature is produced by an enhancement of superexchange interactions and zero-point kinetic energy and is characterized by a time scale which is short compared to that of the electronic motion.

The enhancement of the interactions is a consequence

of the inclusion of extended range interactions in a Hubbard model. It is known that such interactions play an important role in the theory of the one-dimensional electron gas.[28] The Coulomb interaction between holes on neighboring copper and oxygen sites was also a central feature of an excitonic pairing mechanism proposed by Varma, Schmitt-Rink, and Abrahams.[29]

It is desirable to check our picture by carrying out numerical calculations—Monte Carlo or direct diagonalization of the Hamiltonian. Unfortunately, at present it is quite impractical to work with a lattice that is large enough to accommodate even two quasiparticles in all of the relative positions at which there is an attractive interaction. Recent studies of small clusters have found that two oxygen holes bind if V is large enough.[30] However, it appears that the binding comes about because the Cu holes are destabilized and that if two particles bind, so do three or more.[31] This clustering is not a physical property of high-temperature superconductors and we regard these calculations as providing an upper stability limit for V. However, we believe that if such calculations were carried on a sufficiently large lattice it would be possible to have both stability and binding via the mechanism we have described.[32]

After this work was completed, we received a copy of the work of Stechel and Jennison,[33] who also considered the strong-coupling limit of the model proposed in Ref. 3. They gave a detailed discussion of the parameters involved and proposed that there is a significant Cu-O ferromagnetic direct exchange and oxygen-oxygen hopping. They gave a discussion of oxygen quasiparticle states which we believe to be less complete and consistent than ours. Their estimate of the energy to be gained from relieving the frustration of the antiferromagnetic background when two quasiparticles are next neighbors is too large by a factor of 2. They do not include significant enhancement of the exchange, however, so their attractive energy for the states is comparable to ours, although the mechanism is quite different. They also underestimate the effect of the Coulomb repulsion between oxygen holes by subtracting the average one-particle Coulomb energy from the two-particle potential, which is incorrect. With our estimates of the energies involved, we do not believe their mechanism would lead to a superconducting state.

We also became aware of the work of Birgeneau, Kastner, and Aharony,[34] which also considers holes on oxygen sites and a magnetic pairing force for $La_{2-x}Sr_xCuO_4$. Their model is totally different from ours. The holes move on oxygen $p\pi$ orbitals and form d-state pairs of spin-$\frac{3}{2}$ complexes interacting via an oscillating retarded "spin-frustration" interaction characterized by the magnetic correlation length and wave vector $(\pi/a,\pi/a)$ that does not span the Fermi surface. This interaction is not enhanced and, according to our estimates, it is not strong enough to overcome the Coulomb and other repulsive interactions stemming from the overlap of the spin-$\frac{3}{2}$ complexes. We also believe that the spin-$\frac{3}{2}$ complexes are not very mobile, since one must take into account the strong coupling to the copper spins in calculating their hopping, and that kinetic energy favors the oxygen $p\sigma$ orbitals assumed in our work. The arguments against d-state pairing were given in Sec. IV.

We emphasize again that the enhanced superexchange between quasiparticle singlets is independent of the background and is distinct from the spin-frustration mechanism of these two papers.

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APPENDIX

The values of the parameters that seem to fit the experiments are such that the ratio of the hopping amplitude to some of the energy denominators is not small enough to enable perturbation theory to be used with confidence. This is particularly true of the enhanced superexchange, where the presence of an oxygen hole lowers the energy difference in the intermediate state to ε, and $t/\varepsilon \simeq 0.7$. This difficulty can be handled systematically by using Wigner-Brillouin perturbation theory, instead by Rayleigh-Ritz. For second-order calculations, this is equivalent to diagonalizing the small matrices that include all the states that are connected by one hop to the original state.

For a fourth-order calculation, such as the superexchange we will simply diagonalize numerically the small matrices that result from including all the states that appear as the intermediate states in the perturbation calculation. This is simplified by the fact that the energy difference between the singlet and the triplet state of two Cu spins is just J_c, and the triplet state is affected by the hopping only by the lowering of its energy due to zero-point motion, a second-order effect. Thus J_c is the difference between the energy of the singlet and the zero-point energy of two Cu spins. The latter may be calculated in the same fashion by diagonalizing a small matrix. The four states that enter into the energy of the singlet, if we use the right-left symmetry about the central oxygen site, are symbolically, $\uparrow\!\times\!\downarrow, \circ\uparrow\downarrow\circ$, $(1/\sqrt{2})(\uparrow\downarrow\times\circ+\circ\times\downarrow\uparrow)$, $(1/\sqrt{2})(\uparrow\leftrightarrow\uparrow\circ+\circ\downarrow\leftrightarrow\circ)$. The $\times$ and $\circ$ denote oxygen and copper sites, respectively, without holes. The energies of these state with and without neighboring oxygens are easily worked out and the exchange energies obtained by subtracting the zero-point energy, which is the result one obtains by allowing transitions only between the first and last of these states. The results are shown in Fig. 5, for $U_D = 9$, $U_p = 6$, $t = 1$ (in eV) as V is varied.

Another place in which a small energy denominator appears is in the calculation of the hopping parameter t_1 in Eq. (2.5). This parameter can be estimated by diagonalizing the Hamiltonian of Eq. (2.1) in the subspace given by the three states $\uparrow\uparrow\times$, $\uparrow\times\uparrow$, $\times\uparrow\uparrow$. Its value can be shown to be half the lowest energy obtained in this way, which is

$$t_1 = \tfrac{1}{2}\,|\,\varepsilon/2 - [(\varepsilon/2)^2 + 2t^2]^{1/2}\,|\,. \tag{A1}$$

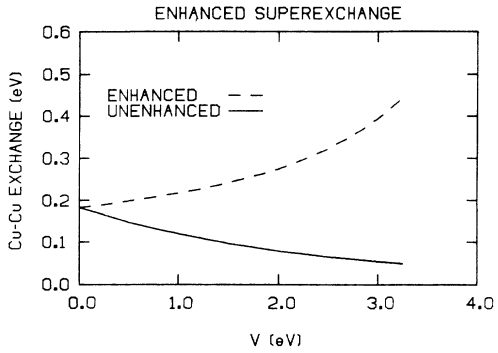

FIG. 5. The exchange parameter between two copper spins when both are next to oxygen holes as in Fig. 1(a) (enhanced), and when neither is (unenhanced). $U_D=9$, $U_P=6$, $t=1$ (in eV). The results are very sensitive to the value of t, so that the unenhanced measured value of 0.12 cannot be used to determine V. The ratio of enhanced to unenhanced exchange is, however, insensitive to t.

Using $\varepsilon=1.5$ and $t=1$ yields $t_1=0.43$ eV. t_2, with the same choice of U_D, U_P, and t as made previously, and $V=1.5$ is given accurately enough by (2.6) as $t_2=0.22$ eV.

Finally, we consider in detail the lowering of the energy of the state of Fig. 1(b) with respect to that of Fig. 1(a) as a result of the enhanced zero-point motion of the central copper spin, as shown in Fig. 2. In addition to the energy of the spin configuration already discussed in the text, there is an energy difference between the states as a result of the difference in zero-point motion of the copper spins in the two configurations. In Fig. 1(a), the energy would be $-12t_1$, whereas in Fig. 1(b), it is $-6t_1$ plus the zero-point energy of the individual spin in Fig. 1(b) and the zero-point energy of the central copper spin in Fig. 1(b). The former would be $-4t^2/(\varepsilon+V)$ in Rayleigh-Ritz perturbation theory, and is more accurately, using Wigner-Brillouin theory,

$$(\varepsilon+V)/2-\{[(\varepsilon+V)/2]^2+4t^2\}^{1/2}. \tag{A2}$$

The zero-point energy of the central copper, by the same sort of estimate, is

$$(\varepsilon-V)/2-\{[(\varepsilon-V)/2]^2+2t^2\}^{1/2}. \tag{A3}$$

The zero-point energy of the copper spins in Fig. 1(a) is $3t_1$ for small t, but is more accurately given as

$$\varepsilon/2-[(\varepsilon/2)^2+3t^2]^{1/2}. \tag{A4}$$

The value of the difference in zero-point energies of the configurations of Fig. 1(a) and Fig. 1(b) is (A2)+(A3)−2(A4) and is shown in Fig. 5. The minimum energy of the spin degrees of freedom is essentially the same, whether the central copper is as in Fig. 1(b) or has moved as in Fig. 3(b), so that this difference in zero-point energy appears as an attractive contribution to the potential of two oxygen holes separated on adjacent sites.

We note that within the present model, the zero-point enhancement is the same for five-spin states involving one oxygen hole on the x axis and one on the y, as it is for those in Fig. 1(b). A more realistic treatment of the Coulomb repulsion would find that such "corner" states were lower in energy than "straight" states, due to a greater zero-point enhancement.

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