Pairing interaction in CuO clusters

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We examine the tendency to pairing of holes added on CuO clusters with one hole per Cu as the reference state, for a variety of cluster geometries. The model Hamiltonian considered contains on-site and short-range Coulomb repulsion terms. Confirming and extending our previous results, we find a tendency to pairing for a wide range of parameters in the model Hamiltonian. The tendency to pairing arises from a disruption of the local order in the insulating system (with one hole per Cu) by addition of the extra holes. We discuss to what extent it is possible to identify the pairing mechanism as "charge mediated" or "spin mediated" as a function of the parameters. We examine the stability of the system with respect to real condensation (phase separation) in the regime where the pair interaction is attractive. Finally, we discuss the possible connection of our results to the superconductivity mechanism in high-T_c oxides.

I. INTRODUCTION

Two years after the discovery of high-T_c oxide superconductors, a broad consensus exists that the explanation of the phenomenon does not lie within the traditional Bardeen-Cooper-Schrieffer (BCS) phonon-mediated mechanism. A variety of experimental as well as theoretical evidence supports this perception.[1] However, there is no consensus on what the actual mechanism is, except for the fact that it must be somehow related to the Coulomb interactions between electrons or holes in the system. Two classes of mechanisms can be broadly identified, one involving predominantly spin degrees of freedom,[2-7] and the other charge degrees of freedom.[8-13] Within these groups, various specific mechanisms have been proposed. However, it is not even obvious that one can make a clear distinction between these two classes of mechanisms, and the actual phenomenon may well involve both charge and spin degrees of freedom in an essential way.

What seems to be clear is that the mechanism is a strong-coupling phenomenon, and that the coherence length of the Cooper pairs is short, of the order of a few unit-cell lattice spacings.[14] Under those circumstances, we believe a theoretical approach based on exact studies of model Hamiltonians on small clusters offers a better possibility of yielding useful information than approximate approaches based on weak-coupling perturbation theory, mean-field, or variational calculations. Once the essential mechanism is identified from the small cluster studies, it may suggest a reasonable approximate analytic approach to the problem.

We have studied a variety of small clusters modeling pieces of CuO planes by exact diagonalization.[12] We start from a reference state containing one hole per Cu atom, which is expected to be antiferromagnetic and insulating. We then consider the properties of the system under doping, i.e., addition of extra holes. The reference state exhibits both spin order (antiferromagnetism) and charge order (charge is mostly localized on Cu atoms). An extra hole will disrupt both the spin and the charge order to some extent. Pairing can arise if a second hole added to the region described by our clusters causes *less* additional disruption than the first one, so that it is preferable to add it in the same region as the first rather than elsewhere. This will happen if the first hole caused a large disruption where the second one can "fit in" without significantly changing the background further.

We define the quantity

$$\Delta_N(n) = [E_0(n+2) - E_0(n+1)] - [E_0(n+1) - E_0(n)] , \tag{1.1}$$

where $E_0(n)$ is the ground-state energy of n holes on a given N-site cluster. $\Delta_N(n)$ is a measure of the pairing interaction between two particles added to the n-particle background of an N-site cluster. A negative value for Δ (we will drop the indices N and/or n when not needed) indicates that the two add particles want to bind; as the size of the cluster goes to infinity, $-\Delta$ becomes the binding energy of a Cooper pair. In that limit, a negative Δ indicates a superconducting ground state with gap $|\Delta|$ (unless a charged-ordered state of pairs exists, which could happen

for high particle concentration). For a small cluster, $\Delta < 0$ indicates an attractive interaction in that region, which is likely to lead to superconductivity on the infinite system, while $\Delta > 0$ does not rule out superconductivity; in fact, we find that as the size of the cluster becomes larger the conditions on the parameters to give $\Delta < 0$ become less stringent.

Note that for thermodynamic stability one needs $\partial^2 E_0/\partial n^2 = \Delta > 0$ *on the average*. This can be ensured by requiring $\Delta(n) + \Delta(n+1) > 0$ for all n. Thus, we compute also

$$\Delta'_N(n) = \Delta_N(n) + \Delta_N(n+1) = E_0(n+3) - E_0(n+2) - [E_0(n+1) - E_0(n)] , \tag{1.2}$$

which compares the energy of adding a third particle in the same cluster with the energy of adding it in a different cluster. If Δ' is negative in a small cluster our results suggest it will remain negative in a larger cluster, and lead to an unstable situation. On the other hand, a positive Δ' on a small cluster may still turn into a negative Δ' in a large cluster.

Let us summarize the point of view we are taking. We compute $\Delta_N(n)$ and $\Delta'_N(n)$ in a given cluster of size N, where n is the number of particles corresponding to one hole per Cu atom. We look for the region in parameter space for which

$$\Delta_N(n) < 0 , \tag{1.3a}$$

indicating an attractive pairing interaction, and

$$\Delta'_N(n) > 0 , \tag{1.3b}$$

indicating stability. The phase boundaries that define this region are clearly a function of N. In the limit $N \to \infty$, the region of parameter space where $\Delta < 0$, $\Delta' > 0$ corresponds to a stable superconducting ground state of the system. Here, we obtain some information about the trends with increasing N by looking at different clusters.

In the next section, we define the model Hamiltonian and discuss some of its qualitative features. Section III presents our numerical results, and we conclude in Sec. IV with a discussion of the possible relevance of our results to high-T_c superconductivity.

II. MODEL AND CLUSTERS STUDIED

We consider the following model Hamiltonian for Cu-O planes:

$$H = -t \sum_{\langle i,l\rangle,\sigma} (d^\dagger_{i\sigma} c_{l0} + \text{H.c.}) + \varepsilon \sum_{l,\sigma} c^\dagger_{l\sigma} c_{l\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + U_p \sum_l n_{l\uparrow} n_{l\downarrow} + V \sum_{\langle i,l\rangle} n_i n_l + V_{00} \sum_{\langle l,l'\rangle} n_l n_{l'} , \tag{2.1}$$

where $d^\dagger_{i\sigma}$ creates a $d_{x^2-y^2}$ Cu hole at site i, and $c^\dagger_{l\sigma}$ creates a $p-\sigma$ oxygen hole at site l. The orbitals and interactions involved are shown in Fig. 1. We have included in H on-site repulsions for holes on Cu and O atoms (U and U_p), a nearest-neighbor Cu-O repulsion V, and a near-neighbor O-O repulsion V_{00}. ε is the site-energy difference between Cu and O levels.

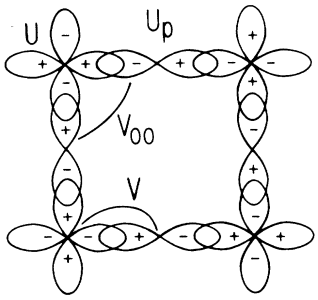

FIG. 1. Orbitals and interactions involved in the Hamiltonian [Eq. (2.1)]. + and − denote the phase convention used for the atomic orbitals.

We first discuss qualitatively the effect of the different interaction terms. The U on Cu, as is well known, induces magnetic moments on the Cu sites that interact antiferromagnetically. In the case of a band filling corresponding to one hole per Cu atom, this interaction will lead to an antiferromagnetic ground state, just as in the single-band Hubbard model. This is easy to see, for example, within random-phase approximation (RPA), as the spin susceptibility is strongly divergent (as $\ln^2 T$) for $\mathbf{q} = (\pi,\pi)$ for that band filling. In strong coupling, the superexchange interaction between two Cu moments is given by

$$J \sim \frac{t^4}{(\varepsilon+V)^2}\left(\frac{1}{U} + \frac{2}{2\varepsilon+U_p}\right) , \tag{2.2}$$

which is valid for $\varepsilon+V, U, 2\varepsilon+U_p \gg t$. This expression suggests that increasing U_p and V weakens the superexchange between Cu ions, and that their effect can be compensated by a corresponding change in ε. However, particularly in the doped system, these interactions also have other effects that cannot be represented by an effective ε.

As the system is doped, additional holes go predominantly onto the O sites if $U > \varepsilon + 2V$. As previously discussed,[11–13] in the doped state the interaction V can have the effect of significantly distorting the Cu−O bond charge distribution by pushing charge away from Cu onto neighboring O. This distortion of the charge-ordered background can lead to an effective attractive interaction between two added O holes in the same region. At the same time, added O holes will significantly disrupt the spin order: An O hole between two Cu spins tends to align the neighboring Cu spin ferromagnetically, creating frustrated bonds nearby.[3,7,15] An extra added O hole can fit into this distorted spin background more easily than elsewhere, thus leading to an effective attractive interaction. While these mechanisms appear to be very different, our numerical results suggest that they can also act simultaneously in a substantial region of parameter space.

The interactions U_p and U_{00} do not have any obvious favorable effect on pairing, and in fact our numerical results show that they usually destroy pairing to varying de-

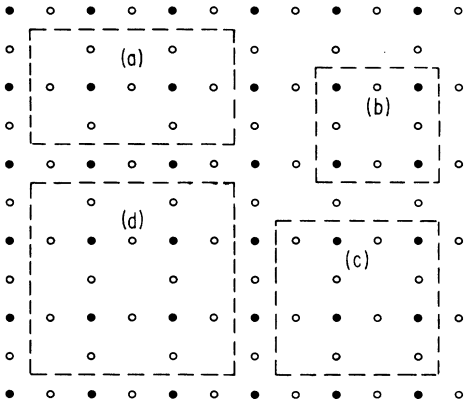

FIG. 2. Clusters studied by exact diagonalization. The open circles denote O atoms, the closed circles Cu atoms. The undoped state ($Cu^{2+}O^{2-}$) has one hole per Cu atom.

grees. For large V the effect of U_p becomes small, but the effect of V_{00} is still appreciable. On the other hand, these interactions tend to prevent condensation of the added O holes. It is not *a priori* obvious from these simple considerations that a parameter regime exists where two added O holes pair while additional ones do not condense in the same region. The results presented in the next section show that this is, in fact, possible. Thus, our results suggest that the model discussed here can indeed give a rise to high-temperature superconductivity. Whether it is the correct model for the high-T_c oxides, and which region of parameter space they belong to, remains to be established. We discuss this question in our concluding remarks.

Figure 2 shows the clusters that we have studied by exact diagonalization of the Hamiltonian of (a) 9 sites, (b) 8 sites, (c) 12 sites, and (d) 16 sites. For the 12-site cluster we have used periodic boundary conditions; for the 9- and 16-site clusters we used free end boundary conditions, but included the effect of the average charge occupation of Cu outside the cluster in a mean-field way, by renormalizing the O level energy for the sites of the cluster next to the boundary to $\varepsilon' = \varepsilon + V\langle n_{Cu}\rangle$. The 8-site cluster is equivalent to a one-dimensional 8-site Cu-O chain with periodic boundary conditions. We used a Lanczos algorithm to perform the matrix diagonalizations. The largest matrix diagonalized, for six particles in the 16-site cluster, was 313 600×313 600.

III. RESULTS

A. Binding energy of two added particles

We define our unit of energy so that $t=1$. We start by discussing results in the absence of intersite repulsion. Figure 3 shows the dependence of Δ on U for the various clusters, for $U_p=0$ and $U_p\neq 0$. Note that for $U_p=0$ the effective interaction is *attractive* in clusters (b), (c), and (d) when U is turned on. This was recently emphasized by Ogata and Shiba,[15] who studied the $U_p=0$ case. The attraction can be interpreted as due to a disruption of the antiferromagnetic spin order in the cluster. It is, however,

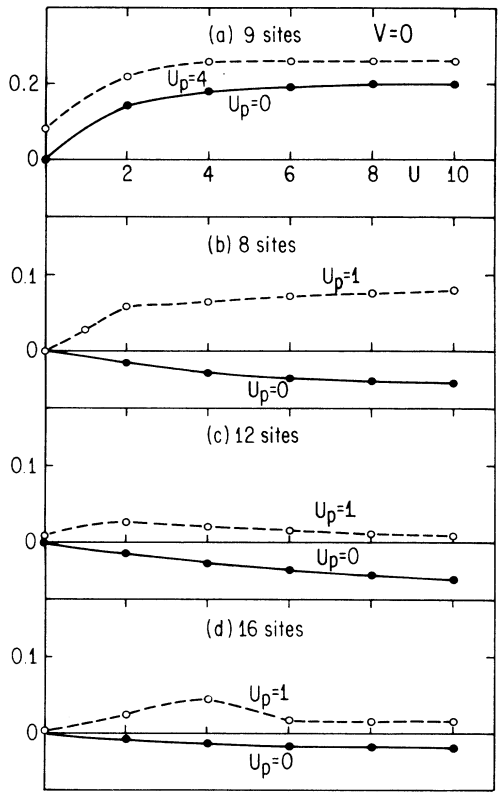

FIG. 3. Effective interaction Δ [Eq. (1.1)] vs U for various cases for the four clusters studied. $\varepsilon=0$ in (a) and (d), $\varepsilon=1$ in (b) and (c). $V=V_{00}=0$ in all cases.

small and rapidly suppressed in the presence of an on-site O repulsion U_p. Note that the attraction is largest for the 12-site cluster, where antiferromagnetic interactions are strongest due to the periodic boundary conditions (in the 16-site cluster there is no superexchange coupling mediated by the outer O atoms). In the 9-site cluster the effective interaction is repulsive because there are only two Cu atoms.

In Fig. 3 the O level energy was taken to be $\varepsilon=0$ and $\varepsilon=1$ in different cases. The best value of ε depends on the size of the cluster, and for all cases studied tends to be somewhere between 0 and 1.5. These small values of ε lead to a hole occupation on the Cu sites of about 0.45 to 0.65 in the undoped case. Figure 4 shows the ε dependence of Δ for the case $U=8$ and $U_p=0$.

As seen in Fig. 3, a small on-site repulsion on the O sites suppresses the attractive pairing interaction. Figure 5 shows the dependence on U_p in more detail for various cases. As a hole is doped onto an O site, the presence of holes on the two neighboring Cu sites inhibits the doped hole's delocalization due to the large U. To regain this energy, these neighboring Cu holes move off, influencing the surrounding spins on nearby Cu atoms more strongly than one would imagine *a priori*. Indeed, on the 16-site cluster—for which Cu holes may move to O sites that do not connect to any other spin-polarizable Cu sites—the binding energies at $U_p=0$ are noticeably smaller than for

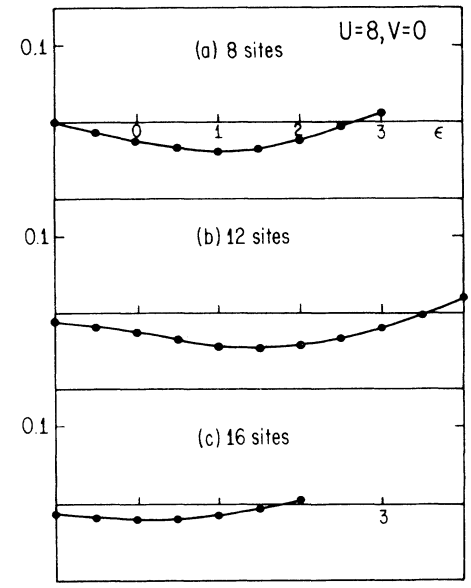

FIG. 4. Δ vs ε for $U=8$, $U_p=V=V_{00}=0$. The best values are ε and $\varepsilon\sim 1$, 1.5, and 0 for the 8-, 12-, and 16-site clusters, respectively.

the 8- and 12-site clusters. Meanwhile, the U_p dependence of the energies at different doping levels, and hence of the binding energy, is given to lowest order by $U_P\langle\sum_l n_{l\uparrow}n_{l\downarrow}\rangle$, summed over O sites. As we see from Fig. 5, as the number of O sites for the four Cu atoms increases from Fig. 5(a) to Fig. 5(b), to Fig. 5(c), the amount of room for the holes to spread out also becomes larger and the dependence on U_p falls off. For the 16-site cluster, each outside O atom shares valence fluctuations with only one Cu atom—these sites, therefore, are particularly immune to the effects of U_p, leading to the small U_p dependence of Fig. 5(c). It is conceivable that for a much larger cluster an attractive interaction could coexist with larger values of U_p. This could come about because the substantially spatial extent of the disruption of the antiferromagnetic order. In effect, there are more sites where the second hole can fit in than are contained in the clusters we have studied. As the pair function is extended, the effect of U_p will be reduced. Still, it appears difficult in the present model to obtain an effective attraction with realistic values for U and U_p and no other interactions.

We now consider the effect of the nearest-neighbor interaction V. For the 9-site cluster, only in the presence of V do we get an attractive interaction, as shown in Fig. 6(a). For the other clusters, V enhances the attractive in-

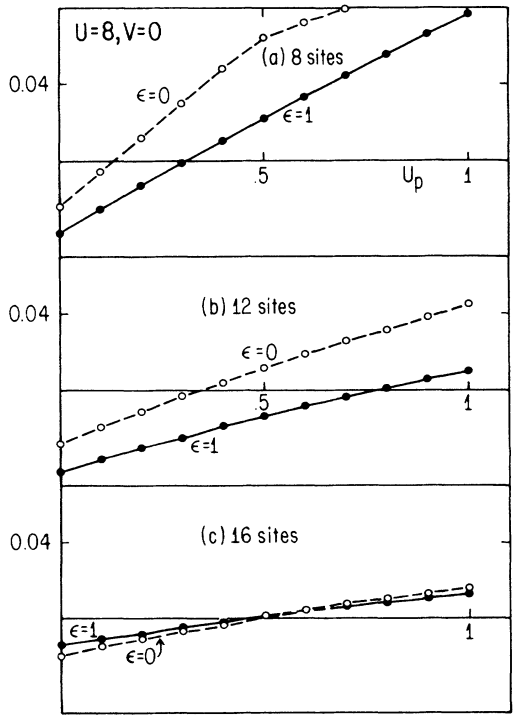

FIG. 5. Δ vs U_p for $U=8$, $V=0$, and two values of ε. Note that the behavior is approximately linear.

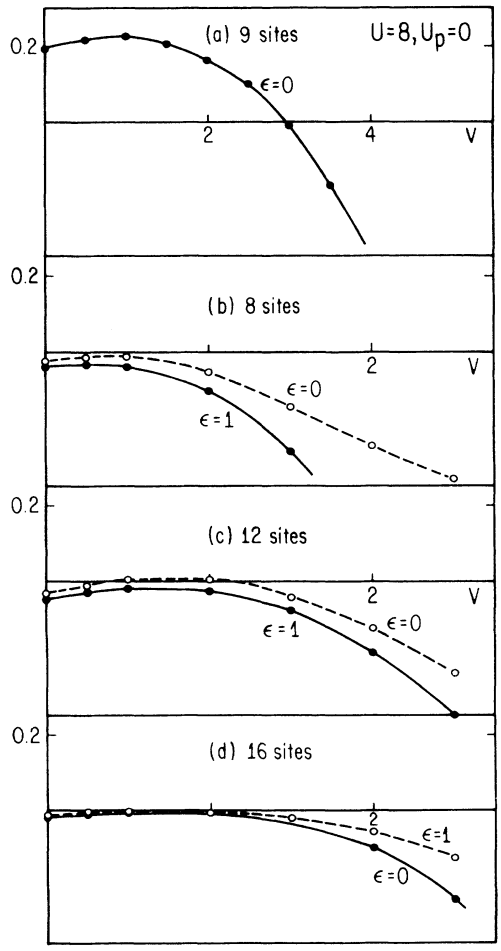

FIG. 6. Δ vs nearest-neighbor repulsion V for $U=8$, $U_p=0$. Note the different horizontal scale in (a). Results obtained for $\varepsilon=1$ for the 9-site cluster were almost indistinguishable from those shown in (a). Note that $\varepsilon=1$ is more favorable than $\varepsilon=0$ for the 12-site cluster, and the situation is reversed for the 16-site cluster.

teraction substantially. In some regions of parameter space, turning on V first makes the interaction repulsive, as seen in Fig. 6(c). Mostly it appears, however, that V and U act together: the first added hole causes a disruption in both the charge and spin order, where the second added hole can fit in more easily. A large U is always necessary for V to be effective for pairing. This is shown in Fig. 7 for various cases. Note that in the presence of V the effective interaction can become very large. However, this will also lead to an instability of the system, as discussed in the next subsection.

In the presence of the nearest-neighbor repulsion V, the on-site O repulsion U_p does not have as damaging an effect on pairing as for $V=0$. This is illustrated in Figs. 8 and 9. For sufficiently large V, U_p has essentially no effect or is even slightly favorable to pairing.

B. Binding of a third added particle

As discussed in Sec. II, to avoid real-space condensation the energy of a third added particle should be higher than that of the first added particle, i.e., Δ' defined in Eq. (1.2) should be positive. We have examined the dependence of

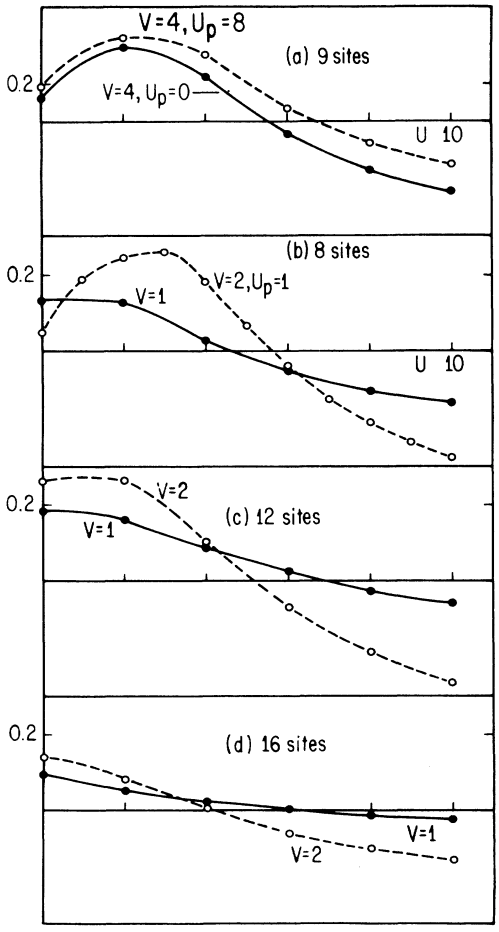

FIG. 7. Δ vs U in the presence of nearest-neighbor repulsion V. $\varepsilon=0$ in (a) and (d), $\varepsilon=1$ in (b) and (c).

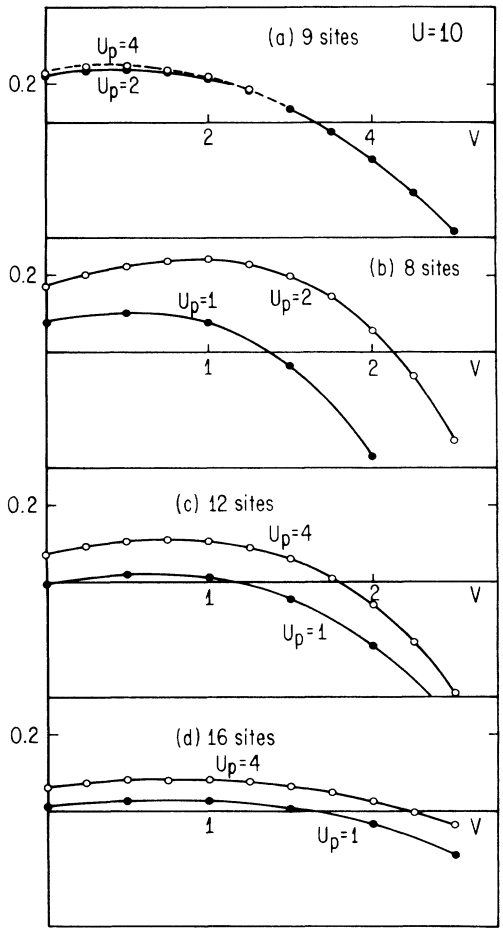

FIG. 8. Dependence of Δ on V for $U_p \neq 0$. $U=10$, $\varepsilon=0$ in (a) and (d); $\varepsilon=1$ in (b); $\varepsilon=1.5$ in (c).

Δ' on the parameters for a variety of cases in the 8-, 9-, and 12-site clusters. In the 16-site cluster, the Hamiltonian matrix for the case of a third added particle becomes too large and we are unable to diagonalize it exactly.

For the 9-site cluster, we find that including a nearest-neighbor O-O repulsion V_{00} is necessary to have stability in the region where $\Delta<0$. V_{00} weakens the attraction, but there is still a parameter range where $\Delta<0$, $\Delta'>0$. This is illustrated in Fig. 10. In the 8-site cluster there is a large region of parameter space where $\Delta<0$, $\Delta'>0$, in the absence of V_{00}, as illustrated in Fig. 11. This region starts at $V=0$ and extends out to values of V, where $|\Delta|$ has increased by a factor of 15 from the case $V=0$ for $U_p=0$. For $U_p\neq 0$, the parameter region for $\Delta<0$, $\Delta'>0$ becomes smaller. Similar results are obtained for the 12-site cluster, as shown in Fig. 12.

Figures 13 and 14 show the region in parameter space that can give rise to a stable superconducting ground state for the clusters of 8 and 12 sites. For $U_p=0$, the attractive region extends down to $V=0$, although Δ is always very small in that case ($\lesssim 0.05$). For small U, increasing V first turns the effective interaction repulsive and then again attractive for larger V (except for very small U). As

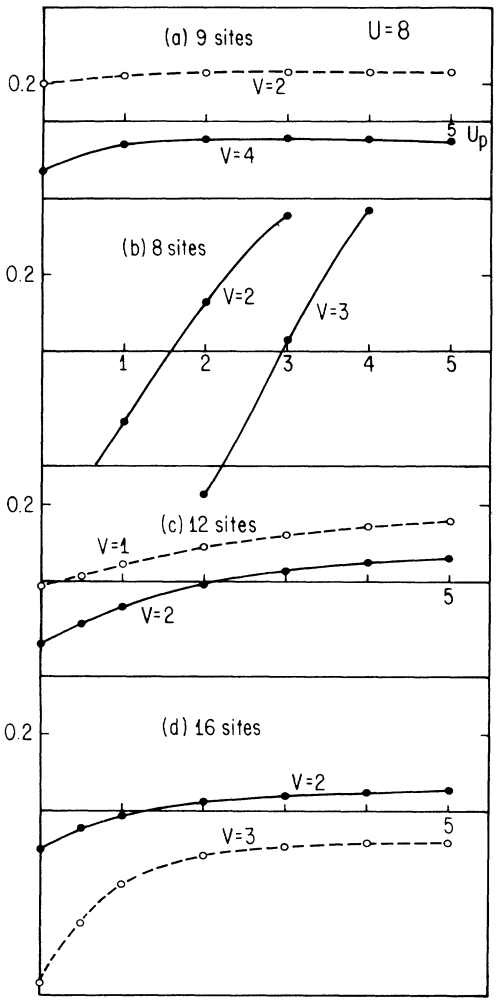

FIG. 9. Dependence of Δ on U_p for $V \neq 0$. $U=8$, $\varepsilon=0$ in (a) and (d); $\varepsilon=1$ in (b), $\varepsilon=1.5$ in (c).

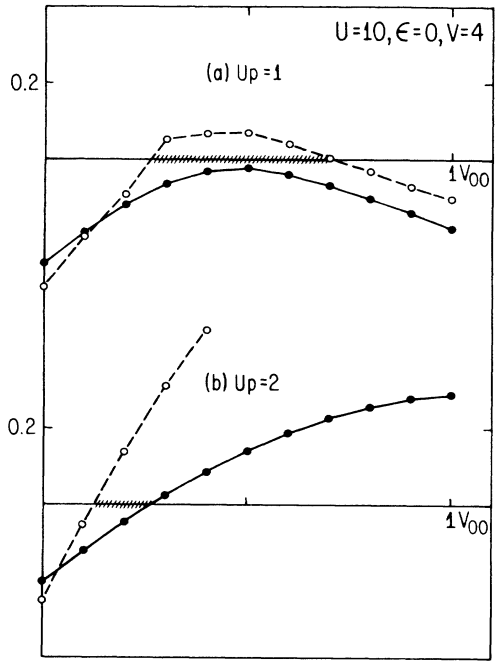

FIG. 10. Effective interaction Δ (solid line) and energy for adding a third particle Δ' [Eq. (1.2)] for the 9-site cluster vs nearest-neighbor O repulsion V_{00}. $U=10$, $\varepsilon=0$, $V=4$. The region $\Delta<0$, $\Delta'>0$ (hatched on the horizontal axis) corresponds to a stable superconducting state.

U becomes large, the effective interaction remains attractive and increases as V increases. For larger V the system becomes unstable to real-space condensation. As U_p is turned on, the repulsive region grows at the expense of the attractive region that does not extend to $V=0$ any longer. It can be seen that the effect of U_p is less severe in the 12-site than in the 8-site cluster; this is easy to understand, as in the 12-site cluster, pairing can occur on nearest-neighbor oxygens as U_p becomes large. As discussed earlier, we expect these phase boundaries to change with the size of the cluster, and we have not attempted a quantitative extrapolation.

C. Effects of kinetic energy

In general, the effect of kinetic energy is to compete against the attraction mechanism. In particular, as individual holes become more mobile, it becomes increasingly difficult for larger numbers of holes to bind. Here, we investigate the effect of the kinetic energy on the stable su-

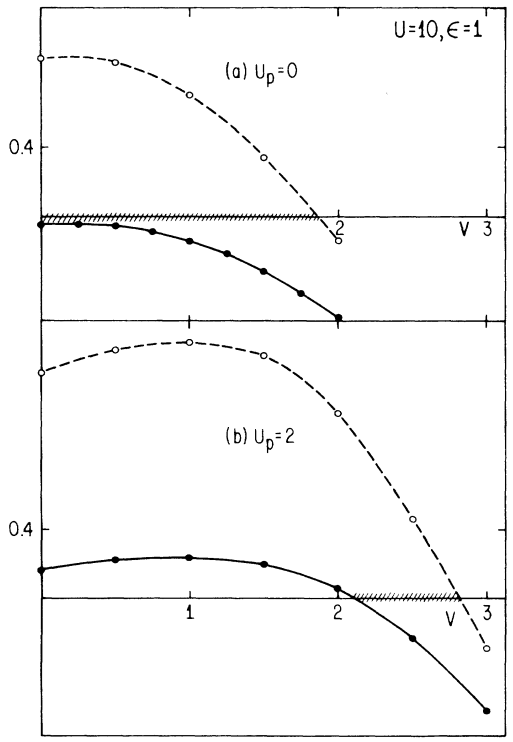

FIG. 11. Δ and Δ' vs V for the 8-site cluster. $U=10$, $\varepsilon=1$.

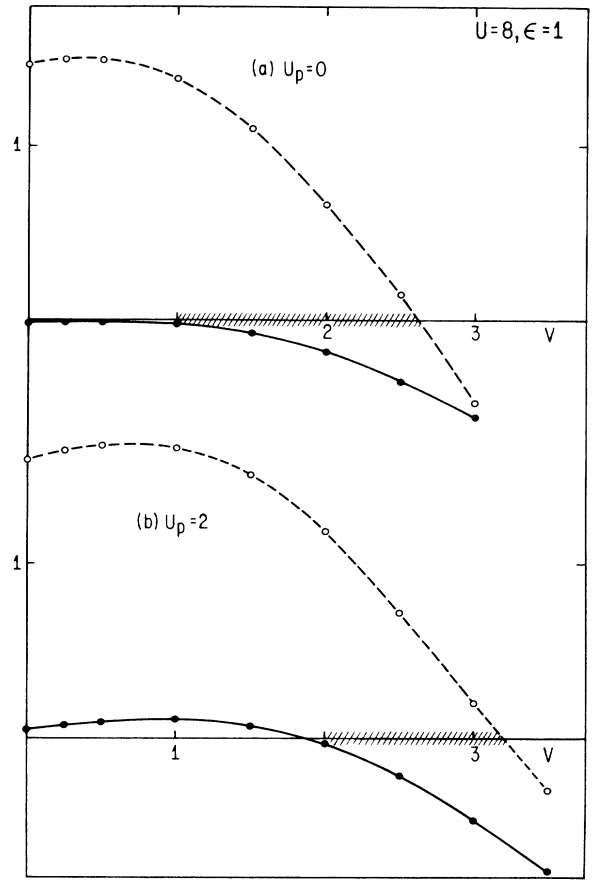

FIG. 12. Δ and Δ′ vs V for the 12-site cluster. $U=8$, $\varepsilon=1$.

perconducting ground state of Fig. 13(a) along the line $U=5$.

In Fig. 15 the energies of a second and of a third added hole are plotted as functions of the hopping parameter t at $V=2$. In the absence of hopping, $t=0$, the energies go to easily deduced strong-coupling values for which the system is unstable. In general, in the strong-coupling limit, doped holes will phase separate from the reference background. As the holes are allowed to hop, Δ and Δ′ both increase, with the effect of t on Δ′ more dramatic than on Δ. For this set of parameters, there is a regime for which holes will bind and yet remain stable against phase separation.

The same measurements are reported in Fig. 16 for $V=0$. Again, turning on a hopping t increases Δ and, especially, Δ′. In this case, however, the fourth-order superexchange interaction J, from (2.2), causes holes to bind in pairs as it wins out over the kinetic energy at moderate values of t. Hence, in this case, holes may bind in intermediate coupling.

Finally, we may also add a nearest-neighbor O-O hopping

$$-t'\sum_{\langle l,l'\rangle}(c_l^{\dagger}c_{l'}+\text{H.c.}) \tag{3.1}$$

to the Hamiltonian (2.1). While overlapping lobes of orbitals conventionally share the same sign in electron models, for our hole model we have chosen overlapping lobes to have opposite signs, as in Fig. 1. Now both t and t' are positive and so cooperate. (Of course, other choices for the orbital phases would not change the physics. On the other hand, a different choice of orbitals—say the $p-\pi$ instead of $p-\sigma$ orbitals on the O sites—could lead to a competition between direct O-O and indirect O-Cu-O

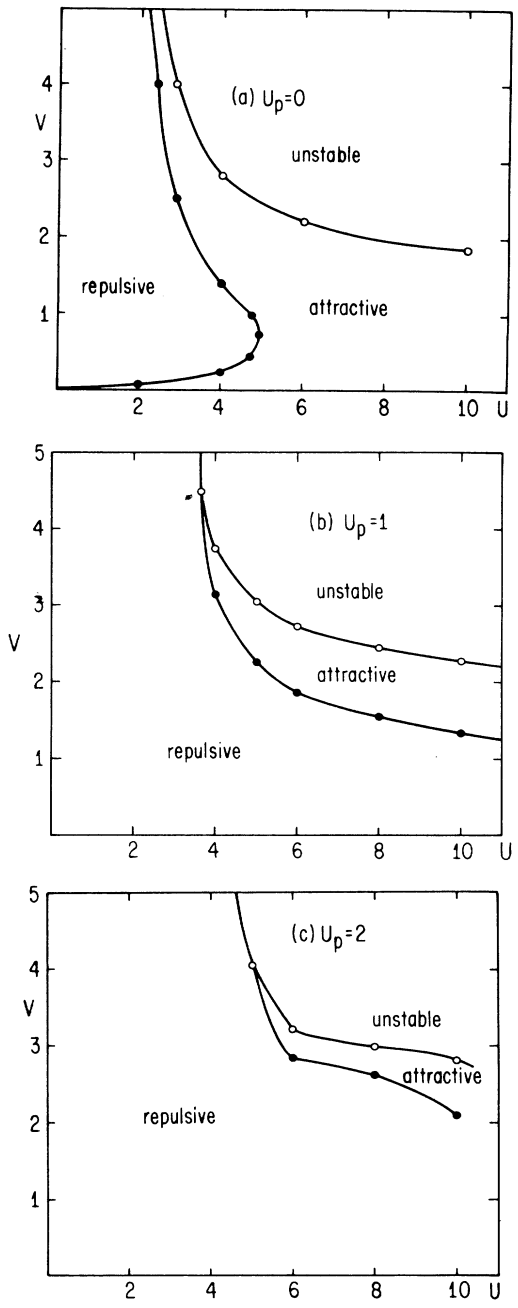

FIG. 13. Phase diagram for the 8-site cluster. $\varepsilon=1$. The different regions are characterized by the signs of Δ and Δ′ [Eqs. (1.1) and (1.2)]. Repulsive: Δ,Δ′ > 0; attractive: Δ < 0, Δ′ > 0; unstable: Δ,Δ′ < 0.

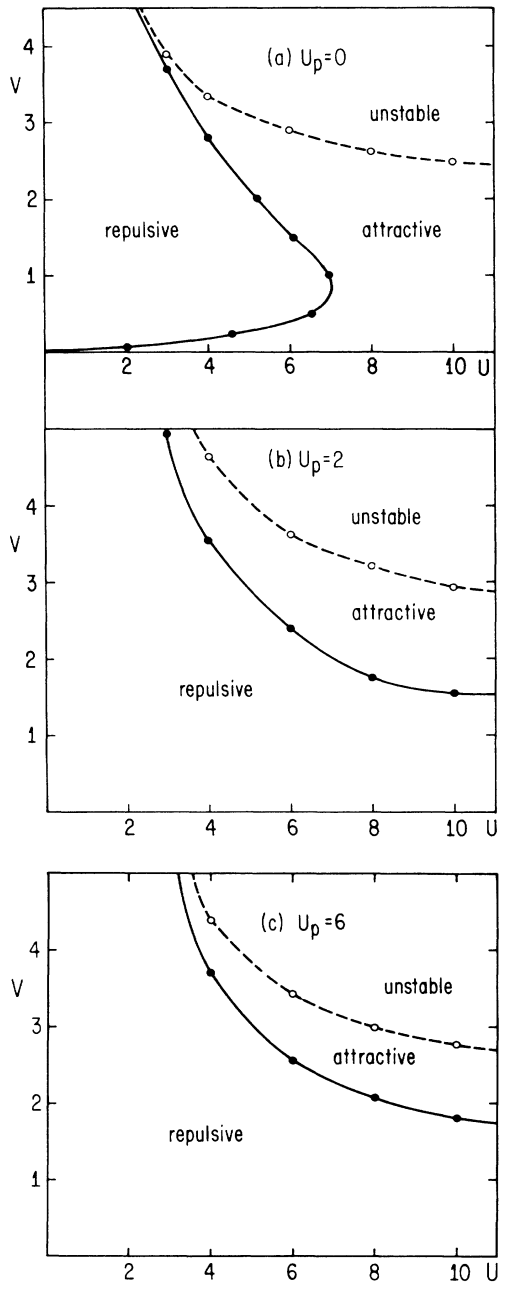

FIG. 14. Phase diagram for the 12-site cluster. $\varepsilon=1$.

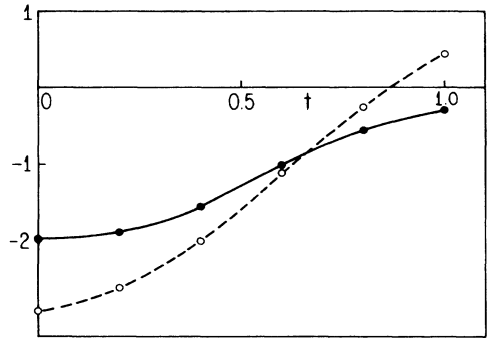

FIG. 15. Δ and Δ' vs Cu-O hopping t for the 8-site cluster. $U=8$, $V=2$, $U_p=0$, $\varepsilon=1$.

IV. CONCLUSIONS

These cluster calculations provide a strong-coupling view of possible pairing mechanisms. As we have seen, it would appear that both charge and spin degrees of freedom can give rise to pairing and may act together. For the CuO system, the nominally undoped state with one hole per Cu exhibits both local charge and spin order. In this insulating state the holes tend to be localized on the Cu sites, and through superexchange develop strong antiferromagnetic correlations. This local order is disrupted by the addition of more holes. Figure 20 shows the changes in the staggered magnetic order,

$$\langle M_s^2\rangle=\left\langle\left[\sum_i^4(-1)^i(n_{i\uparrow}-n_{i\downarrow})\right]^2\right\rangle, \tag{4.1a}$$

and the Cu charge "order parameter," defined as

$$\langle C^2\rangle=\left\langle\left[\sum_i^4(n_{i\uparrow}+n_{i\downarrow})\right]^2\right\rangle \tag{4.1b}$$

as a function of the addition of holes to the 12-site cluster for two sets of parameters which give $\Delta<0$: (a) $V=0$ and (b) $V=2$, with $U=8$ and $\varepsilon=1$ in both cases. The spin order is substantially reduced by doping in both cases. The *charge order* is reduced only in the second case, as doping causes the Cu occupation to be reduced due to the strong Cu-O repulsion. In both cases, the second hole fits into the distorted background with less cost in energy than it would require to distort a separate region, thus yielding $\Delta<0$.

hopping.) In Fig. 17 we plot Δ and Δ' along the line $U=5$ for $t'=0.3$. We see that in the presence of a t' there is attraction over a more restricted range of V. Again, however, the dominant effect of hopping is to make binding of a third hole more difficult. The effect of t' is to increase the O bandwidth, delocalizing the doped holes and making it more difficult for doped holes to bind. To lowest order, t' does not increase the Cu-Cu superexchange. The dependence of Δ and Δ' on t' is shown in Figs. 18 and 19 for the cases $\varepsilon=1$, $U=8$, $V=0$, and $\varepsilon=1$, $U=8$, $V=1$.

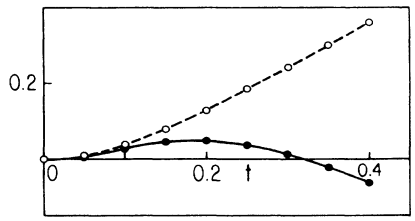

FIG. 16. Δ and Δ' vs t for the 8-site cluster. $U=8$, $V=0$, $U_p=0$, $\varepsilon=1$.

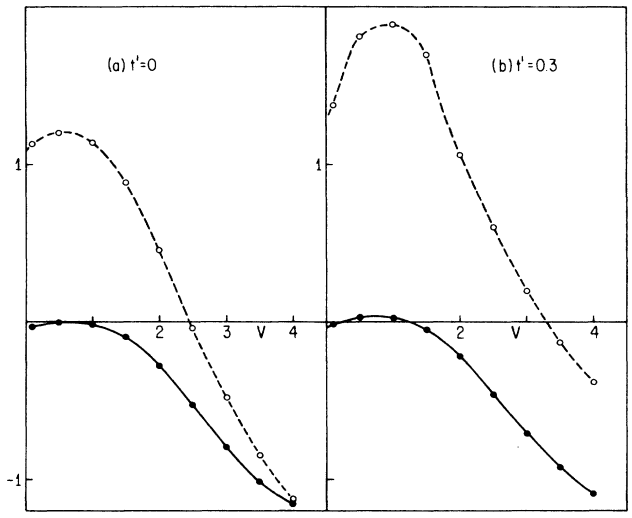

FIG. 17. Δ and Δ′ vs V for two values of nearest-neighbor O-O hopping t'. For the 8-site cluster, $U=5$, $U_p=0$, $\varepsilon=1$.

While it is difficult to limit the effects of pressure in the layered oxides to changing in-plane parameters only, we would expect that the dominant effect would be to change the orbital overlaps t (and t') rather than the Coulomb terms U, U_p, V, and V_{00}. In such a case, we have seen that at large V the binding energy—and so presumably T_c—decreases with increasing t for pairing which is dominated by charge fluctuations. The situation for small

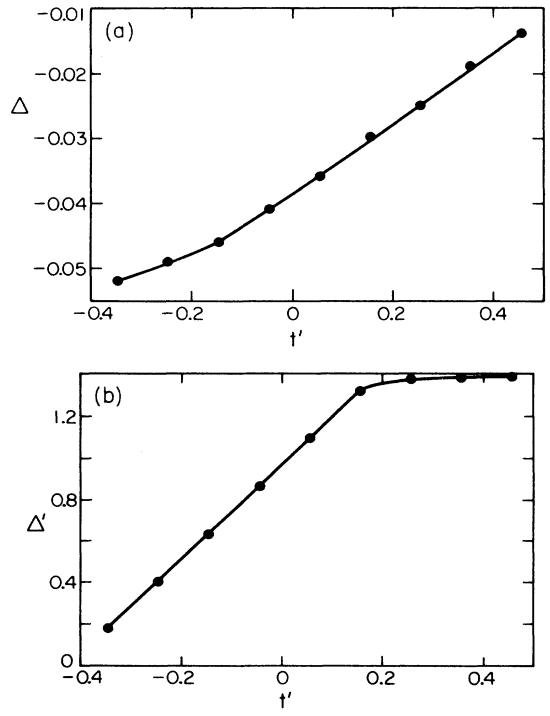

FIG. 18. (a) Δ and (b) Δ′ vs nearest-neighbor O-O hopping t' for the 8-site cluster. $U=8$, $\varepsilon=1$, $V=0$.

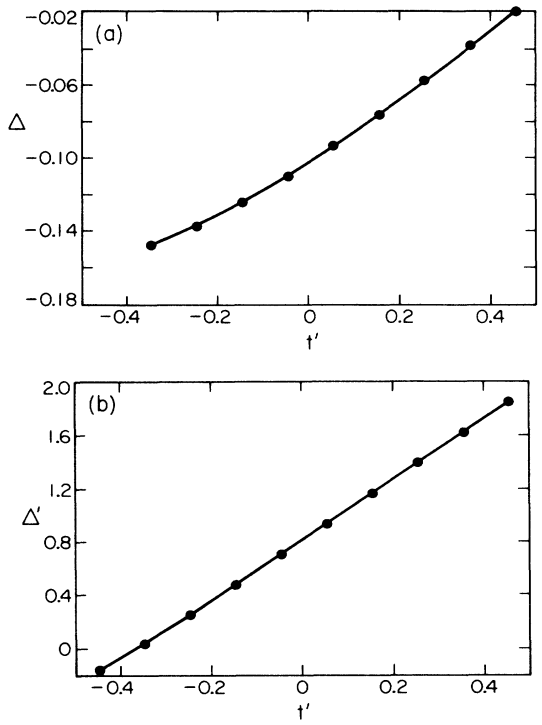

FIG. 19. (a) Δ and (b) Δ′ vs t' for the 8-site cluster. $U=8$, $\varepsilon=1$, $V=1$.

Coulomb repulsions U_p and V is somewhat ambiguous. In that regime, while increasing t' increases the effects of kinetic energy and so tends to break pairs apart, increasing t increases the Cu-Cu superexchange and so binds pairs more strongly.

In this paper we have treated a model in which the additional holes go onto the O in an antibonding state, as proposed by Emery.[3] For the parameters of Fig. 20(a), pairing originates in the disruption of the antiferromagnetic correlations. This is related to the recent spin-frustration ideas of Aharony *et al.*,[7] as well as to the original suggestions.[2,3] The recent work on clusters by Ogata and Shiba[15] also suggests a mechanism of this type. Our calculations suggest that this phase is sensitive to a direct O-O hopping t' and especially to Coulomb repulsions V and U_p. For the parameters of Fig. 20(b), the pairing originates dominantly from a charge-density disruption. Here, following the addition of one hole, there are low-lying Cu^{2+}-$O^{2-} \rightarrow Cu^{1+}$-$O^{1-}$ charge distortions which favor the addition of another hole to this region. This is related to the original suggestion of Varma, Schmitt-Rink, and Abrahams of a charge transfer excitation mechanism,[8] with the added recognition that a large U on the Cu is essential.[11–13] While there are parameter regions in which these mechanisms can be viewed separately, we find that they may also act simultaneously. This could be the situation in the Cu oxide materials. Recently discovered high-T_c superconducting oxides without Cu,[16] as well as the "old" oxide superconductors,[17] would also fit well into this generalized picture, with the charge

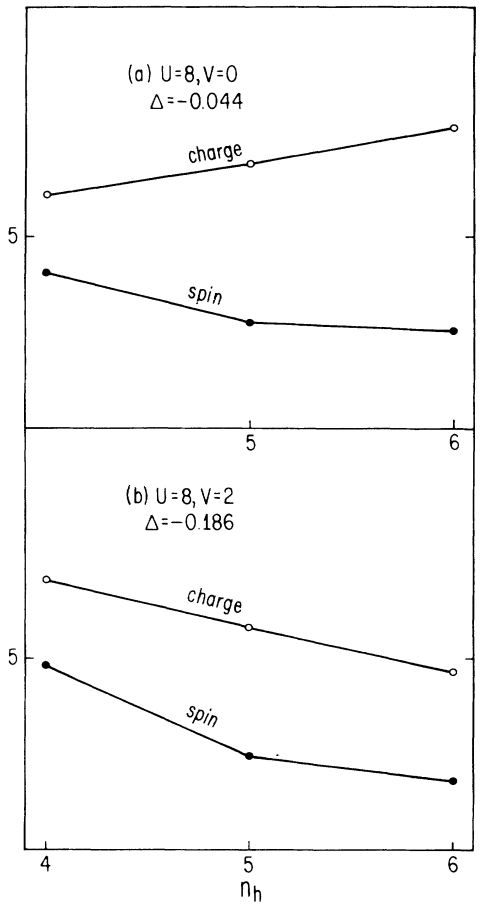

FIG. 20. Spin and charge order parameters [Eq. (3.1)] vs number of holes for the 12-site cluster. $U=8$, $\varepsilon=1$. (a) $V=0$, (b) $V=2$.

transfer aspect dominating. It will be important to understand how these strong-coupling results are related to the weak-coupling limit. One view is that the local spin or charge distortion becomes an amplitude distortion of spin-density-wave (SDW) or charge-density wave (CDW) correlations, giving rise to a bag.[6] An alternative possibility is that the weak-coupling limit is characterized by pairing due to the exchange of SDW or CDW fluctuations.[5]

The generalized notion of a defect-induced attraction is that doped holes locally disrupt the order—charge, spin, or perhaps other—of the reference state, making it energetically favorable for two holes to occupy the same disrupted region as opposed to disturbing two distinct regions of space. The resultant effective attraction between holes does not ensure superconductivity, however, since the disrupted region could grow indefinitely, accommodating more and more holes. Several effects compete with such a local nucleation. As we have seen in the last section, longer-range Coulomb repulsions can prevent the clumping of three or more doped holes. While V_{00} decreases the attractive interaction between holes and so reduces the chances of binding, it also improves the stability of the system. This still fairly short-ranged Coulomb repulsion, on the other hand, cannot act alone. Indeed, our extended-Hubbard model cannot produce stable pairing for $t=0$. Rather, in strong coupling, added holes nucleate pockets of the undoped phase. As a hopping t is turned on, the bandwidths for bound states of holes grow. Since the bandwidths grow fastest for bound states of fewer particles, the kinetic energy breaks apart the largest nucleation pockets first. For suitable values of the parameters, holes will bind in pairs only. Monte Carlo results on the one-dimensional single-band extended-Hubbard model[18] and a two-dimensional single-band model for spinless fermions[19] show that in these models one also requires a minimum value of the hopping t to achieve superconductivity in the ground state over real-space condensation in the region of bare attractive interactions. Finally, for limited magnitudes of U and U_p, Pauli exclusion will also tend to pairing of two holes while excluding a third.

A clear limitation of the present approach is the size of the clusters that can be studied. As shown in Ref. 12, if the range of an instantaneous attractive interaction is small compared to the cluster size, increasing the cluster size will lead to a smaller value of $|\Delta|$. However, if the attractive interaction is retarded and opposed by an instantaneous short-range repulsion, the magnitude of the binding energy can initially increase with cluster size. Similarly, if there is a short-range screened repulsion (U_p, V_{00}) and the spatial range of the attractive interaction is larger than the cluster, then the cluster will clearly have a reduced binding energy. For the CuO system, the scales of energy are such that the effects of retardation, which enter only logarithmically, are unlikely to change things qualitatively. However, the range of the effective attraction is likely to extend beyond the present cluster sizes and thus reducing the repulsive effects associated with U_p and V_{00}.

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