Pairing in a tight-binding model with occupation-dependent hopping rate: Exact diagonalization study

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(Received 14 July 1995; revised manuscript received 5 September 1995)

The Hubbard model with occupation-dependent hopping rate exhibits superconductivity in a wide range of parameters within mean-field (BCS) theory. Here we study pair binding energies in this model for small clusters by exact diagonalization of the Hamiltonian. The model is defined by on-site and nearest-neighbor repulsions U and V, and occupation-dependent hopping rate $t(n)=t+n\Delta t$. We present results for one-dimensional chains and for two-dimensional square lattices of sizes 4×4, 6×6, and 8×8. As a function of carrier density n the pair binding energy first increases and then decreases, and vanishes beyond a critical density. BCS results for the pair binding energy are found to be in remarkably good agreement with the exact results. In particular, BCS theory accurately reproduces the range of interaction parameters where pair binding exists in the exact solution. The model is found to exhibit no tendency to phase separation or clustering of more than two particles even for parameters giving rise to strong pair binding, in contrast to other tight-binding models where pairing occurs.

I. INTRODUCTION

Even the simplest model to describe propagation of electrons in narrow energy bands[1] should, in principle, allow for the possibility that the probability amplitude for an electron to hop from a site to a neighboring site may depend on the occupation of the two sites involved in the hopping process.[2] In the spirit of the Hubbard model describing electrons in a single band interacting via short-ranged Coulomb repulsion, this line of reasoning leads to the Hamiltonian

$$H=-\sum_{i,j} t_{ij}^{\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.})+U\sum_{i} n_{i\uparrow}n_{i\downarrow}+V\sum_{\langle i,j\rangle} n_i n_j \tag{1a}$$

with

$$t_{ij}^{\sigma}=t_0(1-n_{i,-\sigma})(1-n_{j,-\sigma})+t_1(n_{i,-\sigma}+n_{j,-\sigma}-2n_{i,-\sigma}n_{j,-\sigma})+t_2 n_{i,-\sigma}n_{j,-\sigma} \tag{1b}$$

describing a hopping amplitude t_0, t_1, or t_2 depending on whether there are zero, one, or two additional electrons in the two sites involved in the hopping process, respectively. For the particular case where $t_0-t_1=t_1-t_2$, or in general in the low-density regime where configurations with more than two carriers at neighboring sites can be neglected due to Coulomb repulsion, the hopping amplitude Eq. (1b) takes the form

$$t_{ij}^{\sigma}=t+\Delta t(n_{i,-\sigma}+n_{j,-\sigma}) \tag{1c}$$

with $t=t_0$ or $t=t_2$ depending on whether the low-density regime of electrons or of holes is under consideration. This Hamiltonian has been proposed to describe the low-energy physics of high temperature and other superconductors (model of hole superconductivity).[3] Recent interest in this and related models [3–11] arises from the fact that even small differences in these hopping amplitudes can give rise to pairing correlations and superconductivity, without introducing explicitly attractive Coulomb interactions between electrons,[12] and without being in the neighborhood of phase separation instabilities.[13] An occupation-dependent hopping of the form Eq. (1b) or (1c) can arise in a variety of ways from elimination of other degrees of freedom in the process of obtaining a single band effective Hamiltonian from a more complicated one.[14–18] However, not in all these cases will the sign and magnitude of the parameters obtained be conducive to superconductivity.

The parameter range of interest in the model Eq. (1) for hole superconductivity is $U,V,t,\Delta t\geq 0$, with the operators in Eq. (1) describing holes, and the dilute hole concentration regime. We denote by n the average hole concentration per site. Within BCS theory, superconductivity arises in the low hole concentration regime if the condition on the parameters[3]

$$k>\sqrt{(1+u)(1+w)}-1, \tag{2a}$$

$$k=2z\Delta t g, \tag{2b}$$

$$u=Ug, \tag{2c}$$

$$w=zVg, \tag{2d}$$

$$g=\frac{1}{D}, \tag{2e}$$

is satisfied, with z being the number of nearest neighbors to a site, g is the average density of states per site, and D is the bandwidth. In a hypercubic lattice, $D=2zt$. Furthermore, in the dilute limit the exact condition for pairing of two holes in a full band is also given by Eq. (2) in one and two dimensions.[19] First-principles calculations for simple diatomic molecules have indicated that the condition on the parameters Eq. (2) may be realizable in real systems.[20]

The purpose of this paper is to study pairing in the Hamiltonian Eq. (1) by exact diagonalization, and compare the

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results with the predictions of BCS theory. Given that in the $n \to 0$ limit BCS theory becomes exact,[21,19] it is of interest to know for how wide a density range BCS theory remains accurate. As is well known, BCS theory correctly describes the binding of a single pair but does not treat exactly the interference between pairs, except for effects arising from the Pauli exclusion principle. Here we compare exact results for finite lattices with BCS results for a wide range of densities and interaction parameters. Overall, our results show that BCS theory is remarkably accurate in reproducing the exact results, for a large range of densities and interaction strengths. BCS can either over- or underestimate the pair binding depending on the parameters, but it generally becomes more accurate as the binding energy decreases. This is to be expected, as the coherence length increases with decreasing pair binding energy. We also find no tendency to clustering of more than two particles in the regime where pairing occurs. Thus our results fully confirm the expectation[3] that the mean-field solution is accurate in the regime of interest of this model for high-T_c oxides.

Other studies of the Hamiltonian Eq. (1) by exact diagonalization have recently been reported.[7,10,11] These have been mainly concerned with the one-dimensional case, although some results in two dimensions have also been reported.[11] These works also calculate other quantities that give indication of pairing in addition to pair binding energies, which generally coincide to indicate pairing in the same regime where pair binding energies are positive. No qualitative difference between one- and two-dimensional systems was found in those studies nor in the present study for this Hamiltonian. These studies as well as the present study indicate that this model is of considerable interest as the simplest tight binding model that can describe superconductivity without other competing instabilities.

II. EXACT DIAGONALIZATION

We find the ground state of the Hamiltonian Eq. (1) by using a standard Lanczos technique.[22] The largest Hilbert space studied had dimension 4 064 256, corresponding to two up-spin and two down-spin electrons on an 64-site lattice. If $E(N_h)$ is the ground-state energy for N_h holes in the system (N_h even), the pair binding energy for two additional holes at density $n = N_h/N$ is given by

$$\epsilon_b(n) = 2E(N_h+1) - E(N_h) - E(N_h+2) \tag{3}$$

and the energy per particle that is required to break a pair is

$$\Delta_0(n) = \epsilon_b(n)/2. \tag{4}$$

This is the minimum quasiparticle excitation energy that will be compared with the results of BCS theory.

A positive value of ϵ_b (or of Δ_0) implies that two particles at the Fermi surface will pair. Although this indicates a tendency to superconductivity, in principle, other things could come in the way, namely: (i) fluctuations could destroy superconductivity in low dimensions, (ii) a charge-density wave (CDW) state could develop instead of superconductivity, or (iii) there could be a tendency to clustering of more than two particles or even phase separation. Concerning (i), it is clear that an array of weakly coupled low-dimensional systems will tend to stabilize the long-range order, so that information on pairing in the low-dimensional systems is of interest even if strictly speaking superconductivity does not occur there. Concerning a CDW state, from the nature of the pairing mechanism in this model, which is kinetic, it is clear that such a state is not a realistic possibility in this case, unlike the case of the attractive Hubbard model. Furthermore, in the dilute regime a CDW state cannot occur in the absence of longer-ranged Coulomb interactions than considered here. Concerning clustering of more than two particles, it is disfavored by the kinetic hopping t as well as by the Coulomb repulsion V. The kinetic interaction Δt does not lead to clustering either as our data will show. Even though Eq. (1c) yields a larger hopping amplitude for a particle in the presence of two other particles than in the presence of one, two particles can lower their energy more effectively than three by delocalization. [With the more general kinetic energy of the form Eq. (1b) clustering of three particles could be favored if the hopping t_2 is sufficiently large, but this does not seem to correspond to a physical parameter regime.[20]] We have calculated the binding energy for three particle clusters relative to a pair and a single particle

$$\epsilon_{\rm tr} = E(2) + E(1) - E(3) \tag{5}$$

and the binding energy for four-particle clusters relative to two pairs

$$\epsilon_{qu} = 2E(2) - E(4), \tag{6}$$

and find them to be always negative, indicating no tendency to clustering of more than two particles in the parameter range of interest.

III. BCS THEORY ON FINITE CLUSTERS

The BCS equations for the model Eq. (1) at zero temperature are[3]

$$1 = K(I_1 + cI_0) - W(I_2 + cI_1), \tag{7a}$$

$$c = K(I_2 + cI_1) - U(I_1 + cI_0) \tag{7b}$$

with

$$K = 2z\Delta t, \tag{8a}$$

$$W = zV, \tag{8b}$$

$$I_l = \frac{1}{N}\sum_p \left[\frac{1}{z}\sum_\delta e^{ip\delta}\right]^l \frac{1}{2E_p}, \tag{8c}$$

$$E_p = \sqrt{(\epsilon_p - \mu)^2 + \Delta_p^2}, \tag{8d}$$

$$\epsilon_p = -(t + n\Delta t)\sum_\delta e^{ip\delta}, \tag{8e}$$

$$\Delta_p = \Delta_m\left(-\frac{\epsilon_p}{zt} + c\right), \tag{8f}$$

together with the number equation

$$n = 1 - \frac{1}{N}\sum_p \frac{\epsilon_p - \mu}{E_p}, \tag{9}$$

relating the chemical potential μ to the number of particles. In Eq. (8c), δ's are vectors connecting a site to its nearest neighbors, and E_p in Eq. (8d) is the quasiparticle excitation energy. Equations (7a) and (7b) can be combined to yield

$$1=2KI_1-WI_2-UI_0+(K^2-WU)(I_0I_2-I_1^2). \quad (10)$$

In the limit $n\rightarrow 0$ it can be shown that $\Delta_p\rightarrow 0$ (Ref. 23) and μ falls below the bottom of the band, so that

$$I_l=\frac{1}{N}\sum_p\left[\frac{1}{z}\sum_\delta e^{ip\delta}\right]^l\frac{1}{2(\epsilon_p-\mu)}, \quad (11)$$

the minimum quasiparticle excitation energy is from Eq. (8d)

$$\Delta_0=-\frac{D}{2}-\mu \quad (12)$$

and the pair binding energy is $\epsilon_b=2\Delta_0$. μ is obtained from solution of Eq. (10). This result, as well as results for the pair wave function and the pair mobility obtained from BCS theory,[23] are identical to what is obtained by solving the Schrodinger equation for two particles in the empty band.[19]

More generally, for finite n the minimum quasiparticle excitation energy is given by

$$\Delta_0=\min[\sqrt{(\epsilon_p-\mu)^2+\Delta_p^2}]. \quad (13)$$

If μ is below the bottom of the band, which occurs for small n,

$$\Delta_0=\sqrt{(-D/2-\mu)^2+\Delta_{p=0}^2}, \quad (14)$$

while if μ is in the band, the particular value of p that minimizes Eq. (13) is chosen. For an infinite lattice (continuous p), the minimum quasiparticle excitation energy is found to be

$$\Delta_0=\frac{\Delta_m}{D/2}\frac{\Delta_p(\epsilon_p=\mu)}{\sqrt{1+[\Delta_m/(D/2)]^2}}. \quad (15)$$

The BCS equations (7)–(9) can be solved on a finite lattice for comparison with the exact diagonalization results on the same size lattices. Even for a finite lattice a solution of the BCS equations usually can be found for arbitrary values of n, as the finite gap smears the structure associated with the discrete energy levels. However, as the lattice size becomes small or the gap becomes small, the BCS solution becomes discontinuous at values of n corresponding to the discrete allowed occupations of the finite system. Note that the correct value of the single-particle hopping amplitude to be used in the BCS equations includes the mean-field correction originating in Δt, as given by Eq. (8e).

IV. RESULTS

We have calculated pair binding energies for a wide range of parameters for one- and two-dimensional lattices. The results are generally consistent with expectations based on mean-field theory, as will be seen in the following.

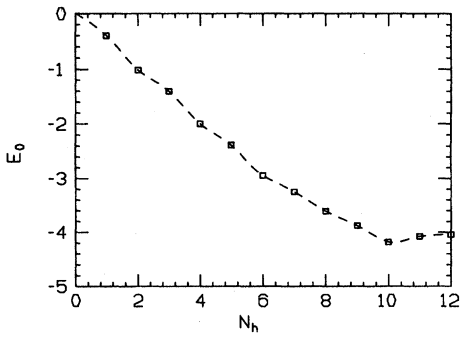

FIG. 1. Ground-state energy for a 12-site chain versus particle number. Parameters in the Hamiltonian are $U=2.5$, $V=0$, $t=0.2$, $\Delta t=0.4$.

A. Dependence on carrier concentration

Figure 1 shows an example of the behavior of the ground-state energy of the system versus number of particles, for a 12-site system. Note that the energy shows negative curvature between two subsequent even numbers of particles, indicating a positive pair binding energy. However, the overall curvature is non-negative, otherwise it would imply a tendency to phase separation. The behavior in Fig. 1 is typical of what is found in the entire parameter range where pairing occurs. The minimum quasiparticle excitation energy Δ_0 to be compared with the predictions of BCS theory is obtained from the ground-state energies for varying particle number through Eqs. (3), (4).

Figure 2 shows results for Δ_0 versus density for $N=12$ and different sets of parameters. The dashed lines drawn through the exact results are to guide the eye. We show the BCS results both for the finite lattice and for an infinite chain. In the finite lattice, discontinuities appear in the BCS solution as the couplings become weaker, nevertheless the BCS predictions for the finite and infinite lattices are qualitatively similar and in particular Δ_0 goes to zero at similar values of the density. Strictly speaking it is the finite lattice BCS solution that should be compared with the exact solution, for the allowed discrete values of n. It can be seen from these examples that the BCS results slightly overestimate the exact results for Δ_0 for small n and underestimate Δ_0 for large n. They also generally predict a smaller range where Δ_0 is nonzero than obtained from the exact solution. When a discontinuity occurs in the BCS solution it is always at a discrete value of the density allowed for the finite lattice, and it is always the limit of the BCS solution *from above* that compares favorably with the exact solution. For $n\rightarrow 0$ the BCS solution on the finite lattice and the exact solution always coincide, as expected. Other parameters studied in one dimension show similar agreement with the BCS solution to what is seen in Fig. 2.

The BCS results for Δ_0 for the infinite lattice are found to always increase first as n increases, and decrease for larger n. For the finite lattices, because only discrete values of n are available, it is sometimes found that Δ_0 decreases at the lowest nonzero n, [e.g., Figs. 2(a) and (c)]. However from results for a large set of lattices and parameter ranges we conclude that also in the exact solution the pair binding always first increases as the density increases from zero for a

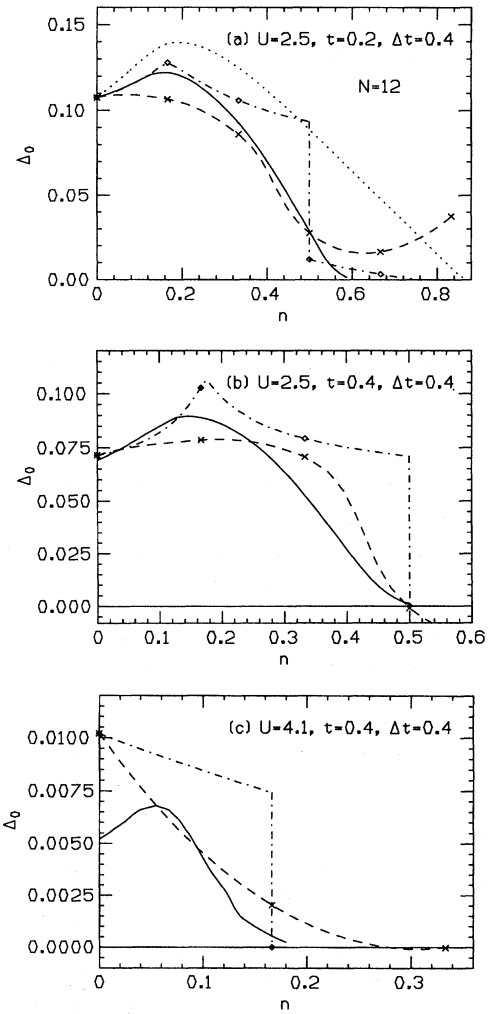

FIG. 2. Minimum quasiparticle energy Δ_0 [Eq. (4)] versus density for various sets of parameters for the $N=12$ chain. The dashed line through the exact results (crosses) are drawn to guide the eye. The BCS solution for the finite chain is given by the dash-dotted line; the values at the discrete densities allowed for the finite lattice are indicated by the diamonds. The full line gives the BCS results for the infinite chain. The dotted line in Fig. 2(a) gives the infinite chain BCS results if the single-particle hopping renormalization is not included.

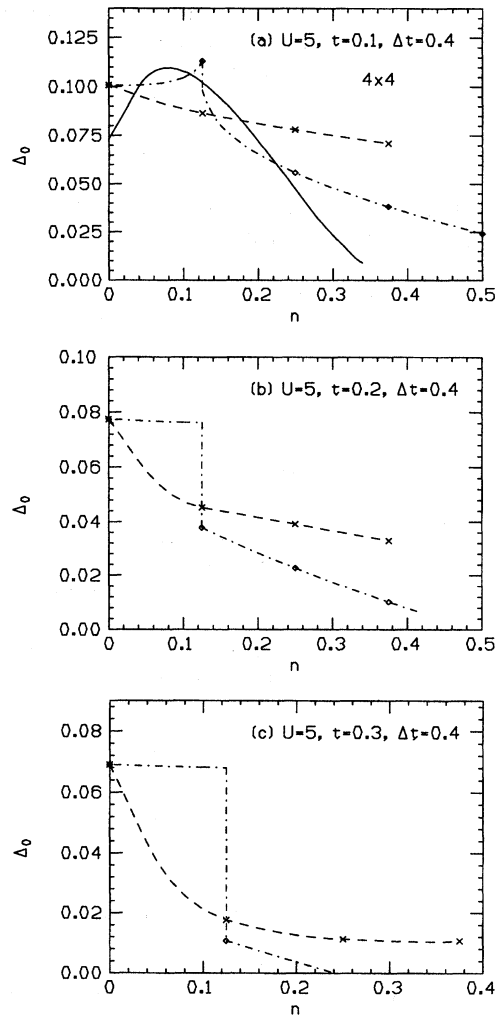

FIG. 3. Minimum quasiparticle energy Δ_0 [Eq. (4)] versus density for various sets of parameters for a two-dimensional 4×4 lattice. Line and symbol conventions are the same as in Fig 2.

sufficiently large lattice. Also it is found generally that both the exact and BCS results for the binding energy go to zero as the density becomes high. However in Fig. 2(a) we find an upturn at high density for these parameters for the exact solution. We believe that this is a finite-size effect.

We also show in Fig. 2(a) the predictions of BCS theory for the infinite chain if the single-particle renormalization of the hopping amplitude is not included [i.e., taking t rather than $(t+n\Delta t)$ as the prefactor in Eq. (8e)]. In that case BCS theory generally overestimates the binding energy as well as the density range where pairing occurs. The same is found for the corresponding finite lattice calculation. We conclude as expected that it is important to include the single-particle hopping renormalization in the BCS calculation in this model.

Within weak-coupling BCS theory one finds that superconductivity disappears beyond a maximum density $n_{\max}$, determined by the condition[3]

$$0=2k(1-n_{\max})-w(1-n_{\max})^2-u+(k^2-wu)(1-n_{\max}+n_{\max}^2/2). \tag{16}$$

For the cases of Fig. 2 this yields $n_{\max}=0.52$, $n_{\max}=0.45$, and $n_{\max}=0.12$ for the cases (a), (b), and (c), respectively. These differ somewhat from the results shown in Fig. 2 because Eq. (16) is derived assuming a constant density of states throughout the band.

Similarly, Fig. 3 shows results for various parameters for a two-dimensional 4×4 cluster. Here we have only obtained exact results up to $N_h=8$, which allows to extract $\Delta_0(n)$ up to $n=0.375$. Again it is seen that BCS generally *underestimates* the pair binding except at the lowest (nonzero) densities.

B. Dependence on parameters

As mentioned earlier, in the limit $n \to 0$ the exact and BCS results for the binding energy coincide. In that limit the binding energy increases as Δt increases, and decreases as U, V, or t increase. In this section we study the dependence of pair binding energy on the parameters in the Hamiltonian for the lowest nonzero density that can be accomodated on 4×4, 6×6, and 8×8 lattices, which correspond to densities of $n=0.125$, $n=0.0555$, and $n=0.031\,25$, respectively, and compare the results with BCS theory. It should be noted that within the model of hole superconductivity the parameters in the Hamiltonian to reproduce the observed behavior in high-T_c oxides give rise to a maximum critical temperature at a density value $n\sim0.05$, so that to study the accuracy of BCS theory at these low densities is certainly relevant.

Figure 4 shows the dependence of the pair binding energy on the single-particle hopping t for one representative set of parameters. The dashed lines give the exact solutions (the exact results obtained are densely spaced and the dashed lines smoothly connect them), and the diamonds give the BCS solutions. Note the excellent agreement between BCS and exact results, particularly for the larger lattices (smaller densities). For the 4×4 lattice the pair binding energy decreases as particles are added because it corresponds to a higher density, while in the other cases it increases, as expected. Generally it is seen that as t increases the agreement between BCS and exact results improves. This is to be expected, as increasing t corresponds to increasing coherence length. Nevertheless, even for small t the agreement is remarkably good, because of the fact that the densities are low.

For the parameters used here, the condition Eq. (2a) in the limit as $t\to\infty$

$$\Delta t > \frac{U+zV}{4z} \tag{17}$$

is satisfied. In that case, even though the pair binding energy for $n=0$ approaches zero on an infinite lattice as $t\to\infty$, it remains finite on a finite lattice. This can be seen from the exact solution determining the pair binding energy[19]

$$k=\sqrt{(1+u)(1+w)+\frac{1+u}{(\epsilon_b+D)I_0-1}}. \tag{18}$$

As $D\to\infty$ Eq. (18) becomes

$$\Delta t=\frac{U+zV}{2z}+\frac{1}{4zI_0}. \tag{19}$$

For an infinite lattice, $I_0\to0$ for any ϵ_b as $D\to\infty$ and the condition Eq. (19) cannot be satisfied. However, for a finite lattice it can be seen that I_0 approaches a constant as $D\to\infty$ [given by the $p=0$ term in the sum Eq. (8c)] and Eq. (19) yields a finite ϵ_b that approaches zero as $1/N$ as $t\to\infty$, if the parameters satisfy the condition Eq. (17).

Figure 5 shows the dependence of pair binding energy on the hopping interaction Δt for one case. For the 4×4 lattice the BCS solution considerably overestimates the binding energy ϵ_b for large Δt. However, it underestimates ϵ_b for small Δt, and in fact yields a slightly larger Δt needed for nonzero binding than the exact solution. For the larger lattices BCS is in good agreement with the exact results. Again, as a function of density it is seen that the binding energy first increases as the density increases from zero (results for the larger lattices) and decreases as the density increases further (results for the 4×4 lattice).

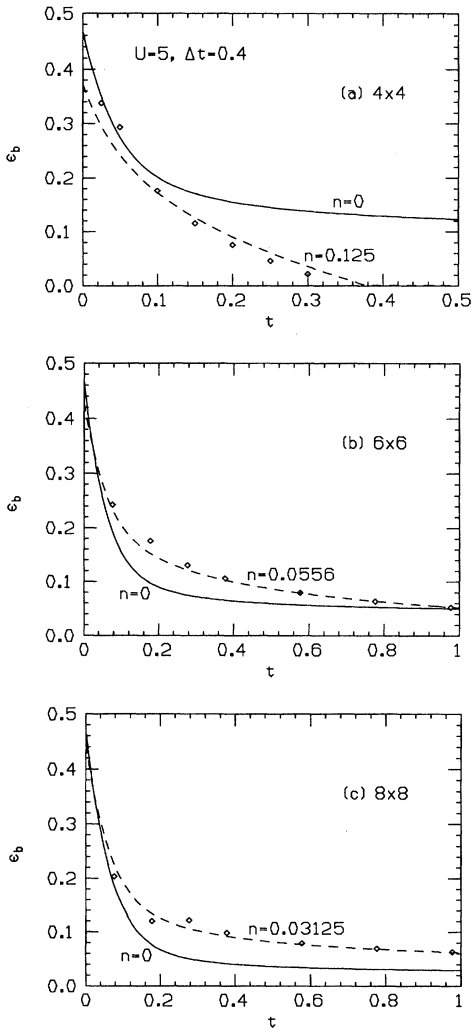

FIG. 4. Pair binding energy versus single particle hopping t for the first two particles (full lines) and the next two particles (dashed lines) from exact diagonalization of finite lattices of size 4×4, 6×6, and 8×8. The full lines correspond to density $n=0$ and the dashed lines to densities $n=0.125$, $n=0.0555$, and $n=0.031\,25$, respectively. The BCS results for $n=0$ coincide with the exact solution, and for finite n are given by the diamonds.

In Fig. 6 we show dependence on the nearest-neighbor repulsion V. Because the value of Δt used is rather large, the agreement between exact and BCS solution is not good for the 4×4 lattice, as expected from the results in Fig. 5. However, note that the agreement becomes better as V increases, and BCS theory only slightly overestimates the maximum V for which nonzero binding occurs. Again the agreement is much better on the larger lattices. Similarly, Fig. 7 shows the dependence of pair binding energy on the on-site repulsion U. Again the agreement is less good for large values of the binding energy and becomes excellent as the binding energy approaches zero.

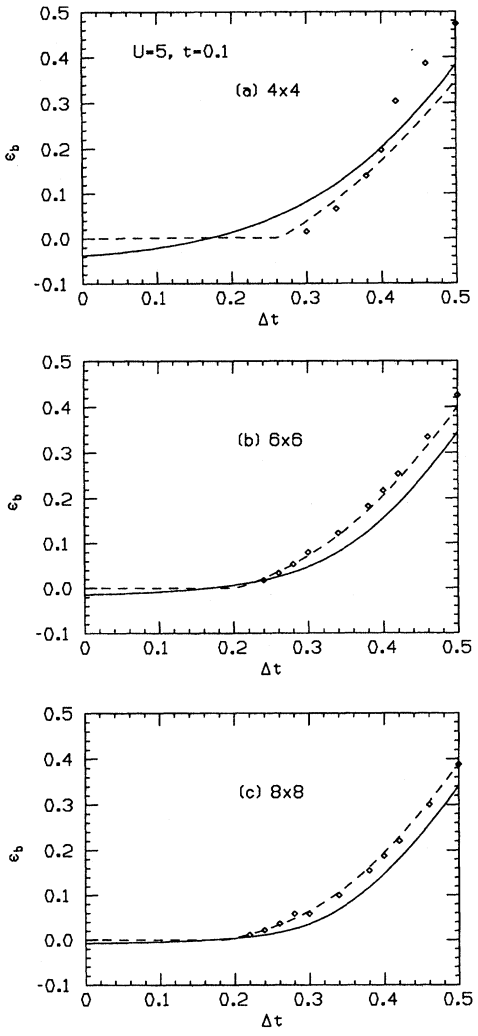

FIG. 5. Pair binding energy versus hopping interaction Δt. The line and symbol conventions are the same as in Fig. 4.

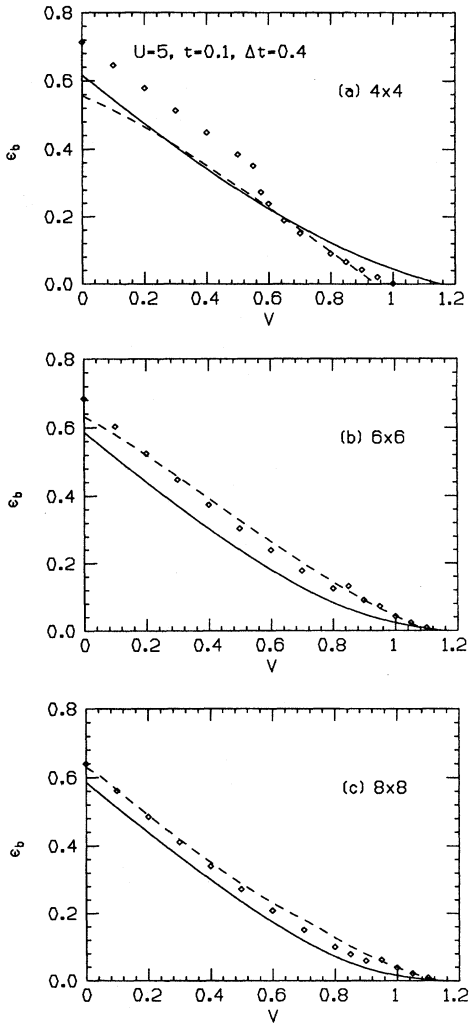

FIG. 6. Pair binding energy versus nearest-neighbor repulsion V. The line and symbol conventions are the same as in Fig 4.

For several of the cases shown, the BCS solution was found to exhibit small discontinuities as a function of Hamiltonian parameters [e.g., Fig. 5(c)]. They occur because the p values corresponding to the minimum quasiparticle energy Eq. (13) shift at that point between two different values. The discontinuities will of course disappear in the infinite lattice limit.

C. Clustering

When the binding energy for two particles is positive, indicating tendency for two particles to be bound, a natural question to be addressed is whether the system favors three, four, or more particles to be bound, leading to clustering. To investigate such possibility, we have calculated the binding energy for three- and four-particle clusters given by Eqs. (5) and (6) for all the cases we have studied and found them to be always negative, indicating no tendency to clustering. Examples for three representative cases are shown in Fig. 8. As Δt increases [Fig. 8(a)], these energies become less negative but do not approach zero even when there is strong pair binding [pair binding energies for this case are given in Fig 5(c)]. Even for zero U and V there is no tendency to clustering, as seen in Fig. 8(b), and the energies become more negative as U increases [while the pair binding is also suppressed as seen in the corresponding case in Fig. 7(b)] and as V increases (not shown). The triplet and quartet energies also become increasingly negative as the single-particle hopping t increases [Fig. 8(c)], while the pair binding is suppressed [Fig. 4(a)]. Note however that in fact for $t=0$ we do find a small positive triplet binding energy in Fig. 8(c). This is easily understood: putting the third particle away from the pair at a localized site will give an upper bound to the ground-state energy of three particles. For $t=0$ exactly, that upper bound can be slightly improved by allowing the third particle to be close to the pair. However for any small finite t the third particle lowers its energy more by delocalizing away from the pair, and the triplet pair binding is lost in the example of Fig. 8(c) already for $t=0.02$. Furthermore, as discussed below, two three-particle clusters will be unstable towards decay into three pairs.

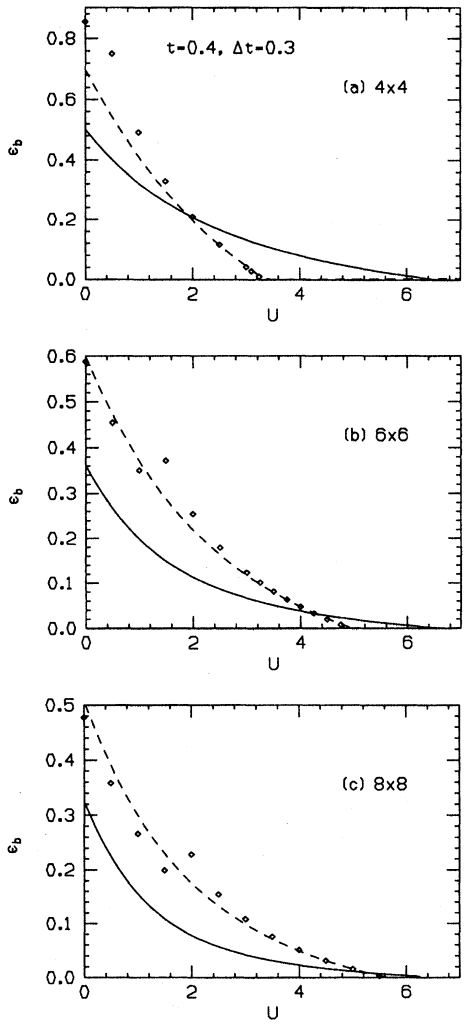

FIG. 7. Pair binding energy versus on-site repulsion U. The line and symbol conventions are the same as in Fig. 4.

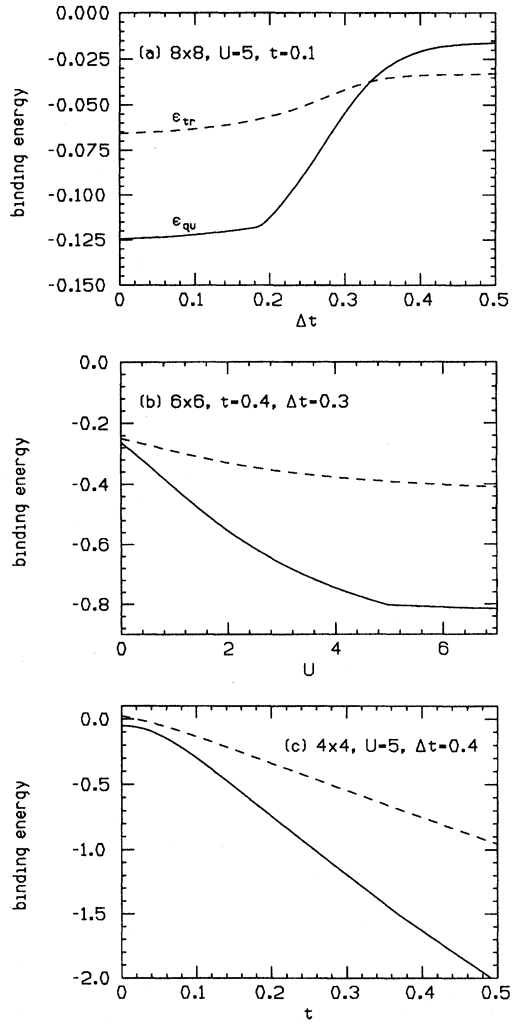

FIG. 8. Binding energy for clusters of three particles [Eq. (5), dashed lines] and four particles [Eq. (6), solid lines] as a function of (a) Δt, (b) U, and (c) t for three representative cases corresponding to the parameters of Figs. 5(c), 7(b), and 4(a), respectively.

To examine this question further, we have studied the limiting case where all parameters are zero except Δt [i.e., $t=U=V=0$, $\Delta t=1$ in Eq. (1)], which should be the most favorable case for clustering, and calculated the binding energy for three- and four-particle clusters. This is by analogy to the t-J model,[24] where one can easily show that in the limit $t=0$, clustering of particles is inevitable (regardless of dimensionality) due to the attractive potential energy of the antiferromagnet (J). For the model we studied in this work, the potential energy is repulsive ($U>0$, $V>0$) and the attraction that leads to pairing comes from the kinetic interaction Δt. For the one-dimensional case, the ground-state energies are $E(2)=-\sqrt{8}\Delta t$, $E(3)=-3.361\,714\Delta t$, and $E(4)=(-5.6570\pm 0.0001)\Delta t$ (estimated by extrapolating data from lattices up to 64 sites), respectively. We see that $E(3)<E(2)+E(1)$, which seems to indicate that it is favored to have three-particle clustering rather than to have a pair plus a single electron. However, this is an artificial effect, due to the fact that the single electron is localized because $t=0$, and it does not indicate tendency to formation of triplets for finite density of particles. If we have six particles in the system, then it is more favorable to have three pairs of paired particles $[E=3\times(-2.828\,427)\Delta t=-8.485\,281\Delta t]$ than to have two three-particle clusters $[E=2\times(-3.361\,714)\Delta t=-6.723\,428\Delta t]$. For the four-particle cluster case, $E(4)-2E(2)$ is zero within the estimated error, and a small hopping amplitude or Coulomb repulsion will certainly tilt the balance in favor of two pairs of paired particles. Thus, we conclude that there is generally no tendency to formation of clusters of more than two particles nor to phase separation in this model.

Finally one may ask whether the more general form of kinetic energy Eq. (1b) will lead to clustering, even if the particular form Eq. (1c) does not. In the hole representation used here, the relation between the parameters in Eqs. (1b) and (1c) is

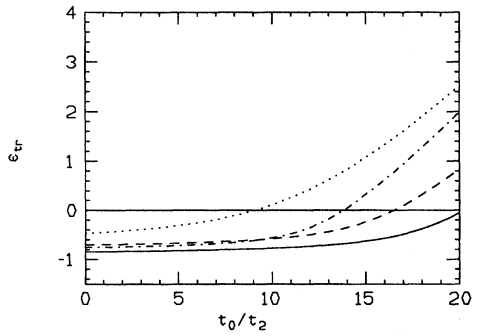

FIG. 9. Binding energy for clusters of three holes [Eq. (5)] for hopping amplitude of the general form Eq. (1b) as function of t_0, on a 4×4 lattice. Solid line: $t_2=0.4$, $t_1=1$ ($\Delta t=0.6$), $U=3.2$, $V=0.8$; the pair binding energy is $\epsilon_b=0.266$. Dashed line: $t_2=0.4$, $t_1=0.8$ ($\Delta t=0.4$), $U=3.2$, $V=0$; $\epsilon_b=0.243$. Dash-dotted line: $t_2=0.4$, $t_1=0.6$ ($\Delta t=0.2$), $U=1.6$, $V=0$; $\epsilon_b=0.110$. Dotted line: $t_2=0.4$, $t_1=1.2$ ($\Delta t=0.8$), $U=V=0$; $\epsilon_b=2.051$.

$$t_2=t, \tag{20a}$$

$$t_1=t+\Delta t, \tag{20b}$$

$$t_0=t+2\Delta t, \tag{20c}$$

and we may consider the more general situation of arbitrary t_0 instead of Eq. (20c). t_0 gives the hopping amplitude for a hole in the presence of two other holes, and it is clear that it will stabilize clusters of three holes if it is sufficiently large. In Fig. 9 we plot ϵ_{tr} [Eq. (5)] versus t_0/t_2 for various cases where pairing of two holes occurs. The most favorable situation for triplet clustering occurs for large values of t_1/t_2 (large Δt) and vanishing Coulomb repulsion U and V. Even then, rather large values of t_0/t_2 are needed to stabilize three-particle clusters, as seen in Fig. 9. These parameters are far away from the physical values of parameters estimated from the first-principles calculations of Ref. 20, where t_0 was found to be comparable or only slightly larger than t_1. Furthermore as noted above the triplet binding energy Eq. (5) being positive is a necessary but not sufficient condition for pairing to be destroyed, as two three-particle clusters may still be unstable to formation of three pairs. For the most favorable case for clustering, $t_2=U=V=0$, we find that two three-particle clusters have lower energy than three pairs only if $t_0/t_1>4.7$. Thus, we conclude that even in this "extended parameter space"[13] clustering is not a likely possibility.

D. Phase diagram

The condition on the parameters for pairing to occur in this model in the $n\to 0$ limit is given exactly by Eq. (2), both for infinite and finite lattices. For finite carrier density, BCS theory for an infinite lattice yields the condition Eq. (16) under the approximation of constant density of states. To assess the validity of BCS theory to determine the regime where pairing occurs for finite density we have calculated the phase boundaries where pairing disappears for the 4×4 lattices and 6×6 lattices with four particles. This corresponds to pairing at densities $n=0.125$ and $n=0.0556$, respectively. In Fig. 10 we show these phase boundaries obtained from exact diagonalization and from BCS theory on the same size lattice, for the case with $V=0$ and for a case with nonzero nearest-neighbor repulsion. In the BCS calculation the effective hopping $t_{\rm eff}=t+n\Delta t$ was used.

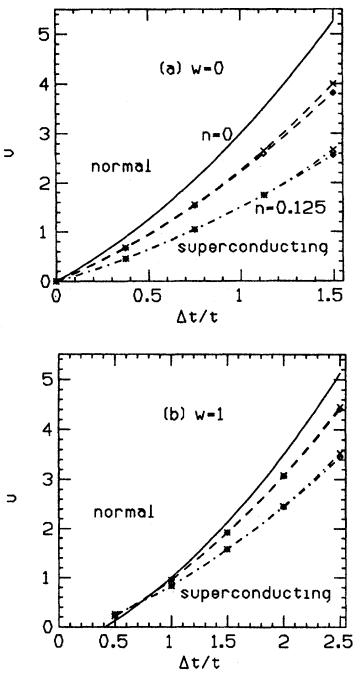

FIG. 10. Phase diagrams indicating where pairing occurs in the Hamiltonian Eq. (1). The reduced parameters $\Delta t/t$ $(=k)$, $u=U/2zt$, and $w=V/2t$ are used. The solid lines are exact (equal to BCS) results for $n=0$. The results for $n=0.0556$ and $n=0.125$ were obtained from 6×6 and 4×4 lattices, respectively, as discussed in the text. The crosses and diamonds indicate exact and BCS results, respectively. The dashed and dash-dotted lines are drawn through the results for $n=0.0556$ and $n=0.125$ to guide the eye.

It can be seen that BCS theory yields results for the phase boundaries at finite densities that are essentially indistinguishable from the exact results. Small deviations start to appear only for rather large Δt, and then BCS theory *underestimates* the parameter range where pairing occurs. It should be remembered that within the model of hole superconductivity the parameters appropriate to describe high-T_c oxides[3] give rise to a maximum T_c at approximately $n\sim 0.05$ and T_c goes to zero around $n\sim 0.15$, so that the densities considered here are relevant for that case. If the bare instead of the effective hopping amplitude is used in the BCS calculation the agreement with the exact calculation is appreciably worse, particularly for large Δt. As an example, for $w=0$, $k=1.125$ the BCS result is larger than the exact result about 5%, while with the effective hopping the difference is less than 1%. Note that in the presence of nearest-neighbor repulsion [Fig. 10(b)] the maximum U that allows pairing may increase as the density increases, contrary to the behavior for $V=0$.

V. CONCLUSIONS

The results from exact diagonalization discussed in this paper indicate that pairing occurs in the model Hamiltonian Eq. (1) for a wide range of parameters in the presence of on-site and nearest-neighbor Coulomb repulsion. Pairing exists in a finite range of densities beyond the zero density limit, and disappears for high density. In the presence of nearest-neighbor repulsion it is possible for some parameter ranges that pairing sets in at a finite carrier density rather than at $n=0$. No tendency for clustering of more than two particles is found in the parameter regime where pairing occurs.

The fact that in other tight-binding models pairing occurs in the same or nearby parameter range where clustering or phase separation occurs[13,24,25] is not accidental: pairing occurs in these models when the potential energy lowering due to two particles being nearby overcomes the cost in kinetic energy in localizing one particle near the other. Adding an extra particle to an N-particle cluster will cost unity in kinetic energy but pay N in potential energy, and thus is favored even more. However, in models such as the one considered here where pairing energy and kinetic energy do not compete but cooperate, this general trend[13] does not hold.

BCS theory was found to give good agreement with the exact results for the pair binding energy in a wide range of densities and interaction parameters. The agreement improves as the pair binding energy decreases. It was found that BCS theory sometimes over- and sometimes underestimated the pair binding energy, the former occuring for smaller carrier densities. Even for rather large carrier density (above a quarter-filled band) BCS theory was found to give reasonable estimates for the pair binding energies. Even though we have not performed any finite temperature calculations here, since in this model the transition from the superconducting to the normal state occurs through pair unbinding rather than Bose decondensation[26] these results for the pair binding energies imply that BCS theory should also yield reasonable estimates for the values of the critical temperature in this model.

For determination of the parameter range where pairing occurs in this model it was found that BCS theory yields results that are in excellent agreement with those obtained by exact diagonalization on the finite lattices. Furthermore, where small deviations between BCS and exact results occurred, BCS theory underestimated the values of the Coulomb repulsion that would destroy pairing. It is reasonable to assume that the agreement between BCS results and exact results would be similar for the same densities on infinite lattices. This implies then that BCS theory can be relied on to accurately predict the magnitude of the parameters in the Hamiltonian that will give rise to pairing and superconductivity in this model in the regime of densities appropriate to high-T_c oxides. With respect to the phase diagrams in Fig. 10, it should be noted that except for the $n=0$ case the phase boundaries will depend on lattice size, and in particular the range of parameters that gives rise to superconductivity within BCS theory in the infinite lattice is substantially larger than the corresponding range in the finite lattices.

We conclude that the predictions of BCS theory for this Hamiltonian are reliable, in the sense that any discrepancy between BCS theory and the exact results is likely to be much smaller than the uncertainty involved in determining what the size of the parameters in the Hamiltonian for a given real system should be. The question whether the Hamiltonian Eq. (1) is relevant to describe superconductivity in any real material then reduces to the question whether the parameters in the material are in the range where BCS theory predicts superconductivity. The simple first-principles calculations of Ref. 20 suggested that the optimal situation requires systems with densely packed negatively charged anions. Realistic first-principles calculations for specific materials need to be carried out.

ACKNOWLEDGMENTS

This work was supported by the Department of Physics, University of California, San Diego. Computations were performed at the National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign, and the National Energy Research Supercomputer Center, Lawrence Livermore National Laboratory. We are grateful for their support.

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