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Enhancement of binding energies in linked Hubbard clusters

Richard M. Fye* and Douglas J. Scalapino
Physics Department, University of California at Santa Barbara, Santa Barbara, California 93106

Richard T. Scalettar
Physics Department, University of California at Davis, Davis, California 95616

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We calculate the binding energy of a pair of holes doped into half-filled Hubbard clusters which are linked together. For some geometries, two linked clusters exhibit binding which is monotonically reduced by intercluster hopping, as is the case between simple negative-U centers. However, for certain of the geometries, we find that binding in the linked clusters can be considerably *enhanced* over that of the individual clusters, or, in some cases, even *induced* by a relatively weak linking. In these cases, the new binding is not simply a stabilization of that for individual clusters, but instead reflects a partial sharing of the hole pair between clusters.

INTRODUCTION

A variety of numerical calculations have recently been performed of the ground-state binding energy of two holes (or electrons) in finite systems in order to determine whether Hubbard-like models might exhibit superconductivity driven by Coulomb interactions. This binding energy, denoted here by Δ, is defined by

$$\begin{aligned}\Delta_N(M)&=[E_N(M-2)+E_N(M)]-2E_N(M-1)\\&=[E_N(M-2)-E_N(M)]-2[E_N(M-1)\\&\quad-E_N(M)]\,,\end{aligned}\tag{1}$$

where $E_N(M)$ is the ground-state energy of a system of M electrons on N sites. (When the context is clear, we will henceforth suppress reference to N and M.) A negative Δ or "binding," implies that the energy of two interacting holes is lower than that of two noninteracting holes; (i.e., it is energetically more favorable to put two holes together in a single finite system than to put a single hole in each of two different systems. Although "binding" does not by itself guarantee the existence of superconductivity,[1,2] it is suggestive.

Such binding, or existence of a negative Δ, has been seen in a variety of clusters with only repulsive Coulomb or magnetic interactions.[1-3] Somewhat surprisingly, binding has also been observed in relatively large one-dimensional Hubbard rings.[4] Recent perturbative and numerical work[5] has further indicated that binding may occur in fullerene or fullerene-like Hubbard clusters, and this binding has been suggested[5] as a possible basis for the observed superconductivity in doped C_{60} materials.

Using Lanczos techniques, we consider in this paper the behavior of the ground-state binding energy when we link two Hubbard clusters together, where each cluster may individually exhibit binding. We consider this a first step in numerically exploring general binding in linked many-body clusters. Specifically, we study a simple such "prototype" system, two four-site Hubbard rings with hopping t, and on-site Coulomb interaction U coupled by inter-ring hoppings $t_\perp$. The Hamiltonian is given by

$$\begin{aligned}H=&-t\sum_{\langle ij\rangle,\sigma}(c^\dagger_{i\sigma}c_{j\sigma}+c^\dagger_{j\sigma}c_{i\sigma})\\&-t_\perp\sum_{\langle ij\rangle',\sigma}(c^\dagger_{i\sigma}c_{j\sigma}+c^\dagger_{j\sigma}c_{i\sigma})+U\sum_i n_{i\uparrow}n_{i\downarrow}\,,\end{aligned}\tag{2}$$

where σ refers to spin ($\uparrow$ or $\downarrow$), $\langle ij\rangle$ in the first sum denotes neighboring sites on the *same* ring, and $\langle ij\rangle'$ in the second sum denotes connected sites on *different* rings. We will consider both rings which exhibit binding when they are not linked and rings, which do not exhibit such binding.

We explore four different geometries, which are shown in Fig. 1. All are composed of two four-site Hubbard rings, differing only in the manner in which the rings are connected. In the first geometry, there is a single link of strength t_1. In the second geometry, the clusters are connected by two diagonal links of strength t_2. In the third, there are two adjacent links of strength t_3. Lastly, in the fourth geometry, there are four links of strength t_4; the resulting topology is that of a cube, or of two linked

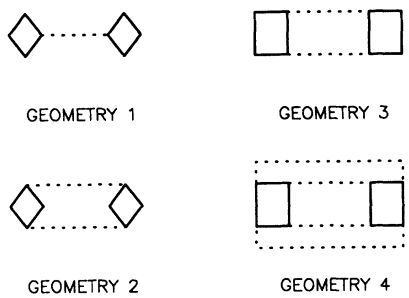

FIG. 1. The four coupled cluster geometries we will explore. All have intracluster hopping $t=1$ and on-site Coulomb repulsions U. Geometry one links the clusters with one hopping matrix element t_1, while geometry two has two diagonal links of strength t_2, geometry three has two adjacent links of strength t_3, and geometry four (cubic geometry) has four links of strength t_4.

chains with periodic boundary conditions. We always consider here the binding of two holes doped into a half-filled reference state; i.e., $M=8$ in Eq. (1) for these eight-site systems. We note that our results are independent of the signs of t and $t_\perp$ in Eq. (2). Lastly, we define an "effective hopping" t' normalized by the number of links, such that $t'=t_1/4$ for geometry 1 (one link), $t'=t_2/2$ and $t'=t_3/2$ for geometries 2 and 3 (two links), and $t'=t_4$ for geometry 4 (four links).

We begin in Fig. 2 (top) by showing the binding energy Δ versus normalized intercluster hopping t' for the single-linked geometry. We compare the behavior for $t=1$ and $U=4$ (open circles) with that for $t=0.457$ and $U=0.915$ (crosses). In both cases the binding energy for a single unlinked cluster ($t'=0$), which we will denote by Δ_0, is $\Delta_0=-0.0170$. We see that the two-cluster Δ's are very close for a range of $t'\leq|\Delta_0/2|$. This indicates that t' and Δ_0 are the only relevant energy scales in this regime, with the binding energy independent of other, higher-energy parameters. This independence does not hold, however, for $t'>|\Delta_0/2|$.

Can we easily model this behavior of the binding energy? The simplest possible modeling of such connected Hubbard clusters which individually exhibit pairing would be to replace each cluster by a single "negative-U" site with the negative-U set to Δ_0, giving the effective Hamiltonian[6]

$$H_{\rm eff}=\Delta_0\sum_{i=1}^{2}n_{i\uparrow}n_{i\downarrow}-t_1\sum_{\sigma}(c^\dagger_{1,\sigma}c_{2,\sigma}+\text{H.c.})\ . \tag{3}$$

For this two-site "negative-U" Hamiltonian, we define $\Delta_{\rm eff}=[E(0)+E(2)]-2E(1)$, giving

$$\Delta_{\rm eff}=\tfrac{1}{2}(4t_1-\Delta_0-\sqrt{\Delta_0^2+16t_1^2}\ )\ . \tag{4}$$

The magnitude of this $\Delta_{\rm eff}$ monotonically decreases with t_1 from its $t_1=0$ value of $|\Delta_0|$ to its $t_1\to\infty$ value of $|\Delta_0|/2$.

We compare in Fig. 2 (bottom) Δ versus $t'=t_1/4$ for $t=1$ and $U=4$ (single-linked geometry) with the $\Delta_{\rm eff}$ of Eq. (4). We find that there is some qualitative but little quantitative agreement between the two models. In both, the magnitude of the binding Δ is reduced steadily with hybridization, but in the negative-U system binding remains for all t' while in the linked clusters the binding energy becomes positive. This may be due to symmetry differences,[7] finite size, or more general many-body effects.[8] For example, the binding on four-site Hubbard rings appears related to degeneracies at the $U=0$ Fermi surface,[4] which may be disrupted by linking the rings. In any case, however, it is clear that some caution should be exercised in attempting to model a repulsive-U Hubbard cluster which exhibits binding by a simple negative-U center.

Another possibility for understanding the binding properties of the linked clusters is the "hole pairing" model of Hirsch,[9] given in its simplest general form by

$$H=-t\sum_{\langle ij\rangle,\sigma}(d^\dagger_{i\sigma}d_{j\sigma}+d^\dagger_{j\sigma}d_{i\sigma})$$
$$-\Delta t\sum_{\langle ij\rangle,\sigma}(d^\dagger_{i\sigma}d_{j\sigma}+d^\dagger_{j\sigma}d_{i\sigma})(n_{d,i,-\sigma}+n_{d,j,-\sigma})\ . \tag{5}$$

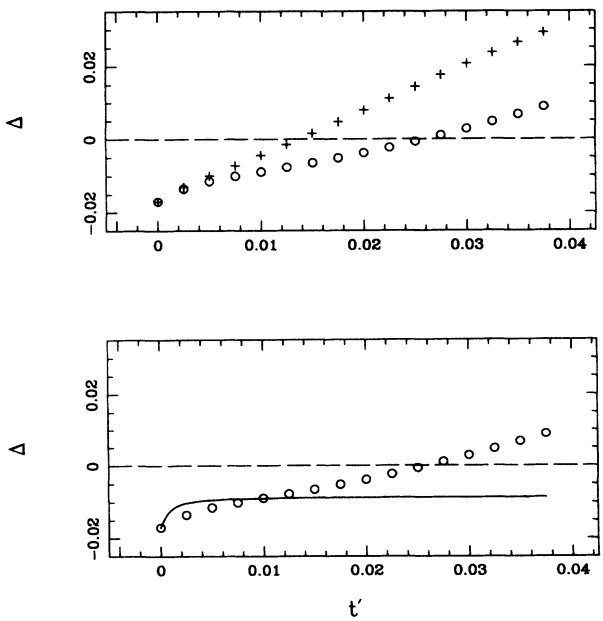

FIG. 2. Top: Δ vs t' for a single-linked cluster with $t=1$ and $U=4$ (circles) and $t=0.457$ and $U=0.915$ (crosses). Note close agreement for $t'\leq|\Delta_0/2|=0.0085$. Bottom: Δ vs t' for a single-linked cluster with $t=1$ and $U=4$ (circles) compared with two linked "negative-U" sites (solid line).

The "d" operators here refer to doped holes. In this model, the presence of an existing hole increases the overlap integral of a second hole. Binding then arises from a lowered kinetic rather than potential energy. We can test this possibility for our model by computing the quantities $S_0=\langle 0|c_{l,\sigma}|1\rangle$ and $S_1=\langle 1|c_{1,\sigma}|2\rangle$, where $|m\rangle$ here denotes the ground state with a doping of m holes off half-filling. The kinetic energy of the second doped hole is "dynamically lowered" if the quantity $1-|S_1/S_0|$ is negative.[9] We show in the top half of Fig. 3 the quantities Δ (solid line) and $1-|S_1/S_0|$ (data points) versus t' for $t=1$ and $U=4$, with the cubic geometry (see Fig. 1). We see significant correlations between a "dynamically lowered" kinetic energy and pairing in the linked clusters, particularly for small t' and for $t'>t$. This suggests that the Hamiltonian of Eq. (5) may be a more appropriate model for our system than simple linked negative-U centers in these regimes.

In the bottom half of Fig. 3, we now compare Δ versus small t' for all four different geometries with, again, $t=1$ and $U=4$. We note remarkable agreement between the single-linked and diagonal-linked geometries (squares and triangles, upper part), and also between the adjacent-linked and cubic systems (circles and crosses, lower part). In all four geometries, binding initially *weakens* when the t''s are first turned on; however, in both the adjacent-linked and cubic systems, this is followed by an *enhance-*

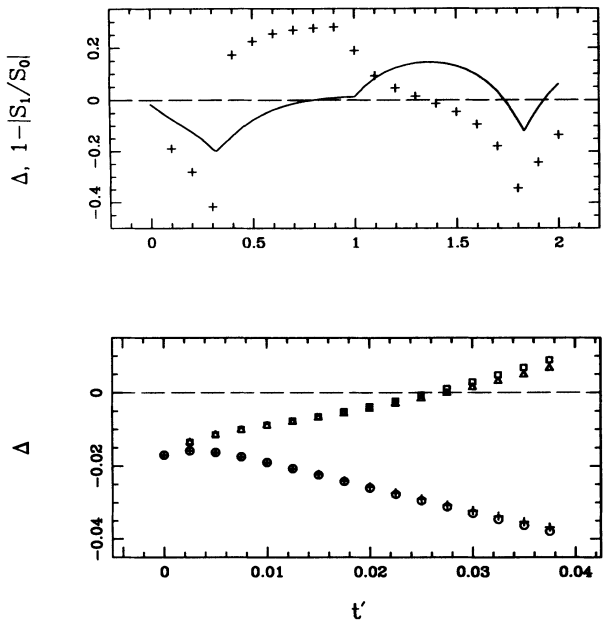

FIG. 3. Top: Δ (solid line) and $1-|S_1/S_0|$ (crosses) vs t' for cubic cluster with $t=1$ and $U=4$. Note same numerical scale for both quantities. Bottom: Δ vs t' for single-linked (squares), diagonal-linked (triangles), adjacent-linked (crosses), and cubic (circles) clusters with $t=1$ and $U=4$.

ment in binding as t' increases further.

We see this enhancement even more clearly in Fig. 4 (top) where, with again $t=1$ and $U=4$, we show Δ versus t' for both the adjacent-linked and the cubic geometries with larger t' than in Fig. 3. Δ here reaches a value of $\Delta=-0.189$ when $t'=0.3$ for the cubic geometry, significantly greater binding than seen in other clusters with comparable bandwidths.[3–5] We further note the *reentrant* binding at $t'>t$ for the cubic geometry, also seen previously in Fig. 3. In Fig. 4 (bottom) we show Δ versus t' for $t=1$ and, now, $U=8$. A single four-site cluster with $t=1$ and $U=8$ does not itself exhibit binding; i.e., $\Delta>0$ for the isolated cluster. Thus, the small-t' binding observed here is *induced* by a weak linking of the two clusters. We have not observed such induced binding for small t' in the single-linked and diagonal-linked geometries, although we have observed reentrant binding in both these geometries and induced binding for $t'>t$ in the single-linked system.

The adjacent-linked and cubic geometries can be viewed as two linked two-by-two "sheets," as seen from Fig. 1. Although our systems are very small, the inducing of binding by linking these sheets might be interpreted as suggesting that superconductivity could arise from tunneling between two-dimensional Hubbard planes which are not themselves superconducting.[10] In that case, Figs. 1, 3, and 4 indicate that the mechanism would involve adjacent links. Further, the results also suggest that superconducting correlations might dominate in chains or planes of linked clusters.

What is the nature of the binding? As a preliminary exploration we consider the expectation value of the charge disproportion operator $\Delta N=\langle(N_1-N_2)^2\rangle^{1/2}$, where $N_m=\sum_{i,\sigma}n_{i,\sigma}^{(m)}$ denotes the total charge on cluster m ($m=1,2$) when two holes are doped into a half-filled reference state. If binding occurs in a single, unlinked cluster, then $\Delta N=2$ when $t'=0$; i.e., it is energetically favorable to have both doped holes in one cluster rather than a single hole in each cluster. If binding does not occur in an unlinked cluster, then $\Delta N=0$. In Fig. 5 we

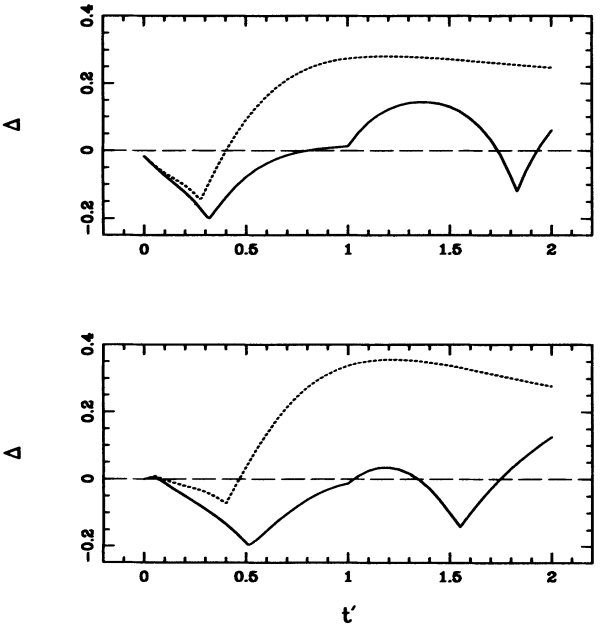

FIG. 4. Top: Δ vs t' with larger t' than Fig. 3 for adjacent-linked (dotted line) and cubic (solid line) clusters, with $t=1$ and $U=4$. Bottom: Δ vs t' with larger t' for adjacent-linked (dotted line) and cubic (solid line) clusters, with $t=1$ and $U=8$.

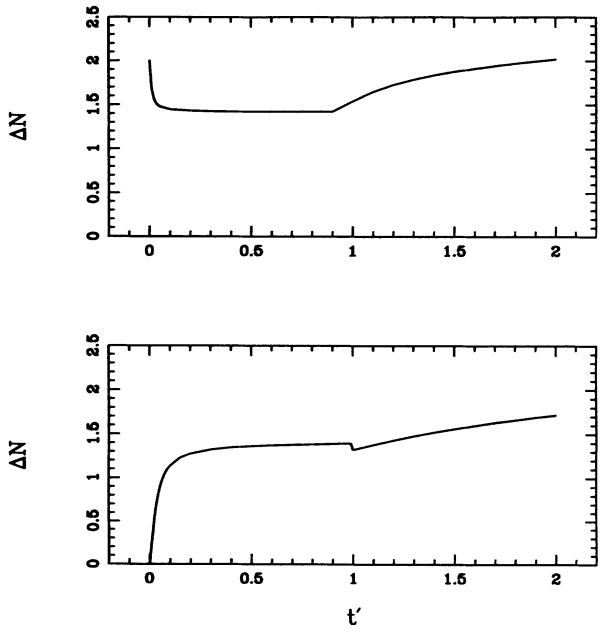

FIG. 5. Top: Charge disproportion ΔN vs t' for cubic geometry with $t=1$ and $U=4$. Bottom: Charge disproportion ΔN vs t' for cubic geometry with $t=1$ and $U=8$.

show ΔN versus t' for the cubic geometry with $t=1$ and $U=4$ (top) and $t=1$ and $U=8$ (bottom). In both cases, ΔN rapidly changes from its $t'=0$ value to achieve a plateau at small t', which approximately coincides with the existence of $t'<t$ binding. We find that this plateau corresponds to an almost constant admixture of two states; the first has exactly two doped holes on one cluster, and the second has exactly one doped hole on each cluster. Thus, the bound pairs are now partially shared between clusters.

In summary, we have considered the binding energy of two holes doped into a half-filled reference state when two Hubbard clusters are linked together. Specifically, we investigated numerically two four-site Hubbard rings connected in four different ways. We found that single clusters, which themselves exhibited binding, were not well modeled by negative-U centers when the clusters were linked, and suggested that this might be due to symmetry differences or a breaking of degeneracies. The "hole pairing" Hamiltonian of Eq. (5) appeared a better model in certain regimes. We then showed that the binding energy could be greatly enhanced for some geometries by linking the clusters, and that binding could even be *induced* by linking clusters which themselves had no binding. In these cases, even for very weak linking, bound pairs were found to have a strong intercluster as well as intracluster component.

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*Current address: Division 1422, Sandia National Laboratories, P. O. Box 5800, Albuquerque, NM 87185-5800.

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