Pairing in bipartite and nonbipartite repulsive Hubbard clusters: Octahedron

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Pairing instabilities found from exact studies of repulsive Hubbard clusters with different topologies provide important insights into several many-body problems in condensed-matter physics. Electron charge and spin pairing instabilities in a multiparameter phase space, defined by temperature, magnetic field, and chemical potential, lead to properties that are remarkably similar to correlated inhomogeneous bulk (perovskite) systems such as the high-temperature superconductors and colossal-magnetoresistance materials. In particular, for small to moderate values of the on-site Coulomb repulsion U, the role of square-planar geometry is borne out for weak vertex coupling in an octahedron. These conditions are favorable to forming a Bose condensate in the region of instability near one hole off half filling while strong vertex coupling has a detrimental effect on such condensation. In addition, it is shown that magnetic flux can get trapped in stable minima at half-integral units of the flux quantum in hole-rich regions. For higher values of U, Nagaoka-type ferromagnetism is examined.

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I. INTRODUCTION

Inhomogeneous materials with strong local electronic correlations are creating a new world view in condensed-matter physics. These materials with intrinsic inhomogeneities[1] have properties that are widely different from the conventional ones. Two prominent examples are the high-temperature superconductors (HTSCs) and colossal-magnetoresistance (CMR) materials. Motivated by the discovery of such materials, we have embarked on a study of finite-sized Hubbard clusters using exact-diagonalization technique and statistical mechanics. Since the discovery of the HTSCs, there has been an intense debate about a possible electron (or hole) pairing mechanism. Early on, Anderson[2] proposed that strong intra-atomic interactions contain the key to some of the perplexing physics observed in the HTSCs. The thermodynamics of doping and the stability of both charge and spin pairing are key issues in this long-standing puzzle. Pairing instabilities are clearly evident in certain regions of phase space in simple Hubbard clusters and charge pairing has been observed in previous studies (see Refs. 3 and 4). In our opinion, these regions of phase space have much more intriguing clues to offer when other variables such as the chemical potential, temperature, and magnetic field are included.

In addition, magnetic inhomogeneities seen in various transition-metal oxides at the nanoscale level, widely discussed in the literature,[5–9] can be crucial for the spin pairing instabilities, origin of ferromagnetism,[10,11] and ferroelectricity in the spin and charge subsystems. The phase separation of ferromagnetic clusters embedded in an insulating matrix is believed to be essential to the CMR effect in manganese oxides. At sufficiently low temperatures, the spin redistribution in an ensemble of clusters can produce inhomogeneities in the ground state and at finite temperatures. The nonmonotonous behavior of the electron concentration versus chemical potential found in generalized self-consistent approximation[12] also suggests possible electron instabilities and inhomogeneities near half filling. From this perspective, exact studies in the ground state and finite temperatures of electron charge and spin instabilities at various intersite couplings $U>0$ and cluster topologies can provide important clues for understanding of charge/spin inhomogeneities and local deformations for the mechanism of pairings and magnetism in "large" concentrated systems whenever correlations are local.

Important aspects of phase separation and electron instabilities that we discuss in this work are somewhat different from what is usually reported in the literature, such as in Ref. 13. The spontaneous phase separations for spin and charge degrees described in Ref. 14 strongly depend on both, the Coulomb repulsion U and cluster topology. For instance in bipartite geometries, the charge separation leads to coherent pairing at small and moderate U, while Nagaoka-type ferromagnetic instabilities for spins occurs at large U.[10] In frustrated geometries, spontaneous transitions can lead to coherent pairing and saturated ferromagnetism for all U depending on the sign of the hopping term t (energy spectrum). At finite temperature, due to the above instabilities, we predict the presence of local inhomogeneities from our cluster approach. In what follows, we identify these phenomena as instabilities in a phase space defined by suitable variables. In fact, such instabilities in a multiparameter space are found to be rather common in various topologies and they lead to phase separation. In addition, we observe such instabilities when dealing with systems having moderate to large U values where there is competition, for example, between high and low spin states. Such phenomena appear to be generic and may be applicable to spin and charge degrees providing important clues to long-standing puzzles tied to phase separation in the HTSCs and CMRs.

We note here that in our approach, any connections to bulk systems can be questioned since all of our results are for small clusters, not having focused on the thermodynamic limit. Our exact cluster studies have this limitation and the computational requirements grow exponentially with cluster size. Therefore the results must be carefully analyzed when making connections with bulk systems for which the method is rather approximate. However, it is interesting to see that certain fascinating aspects of high-temperature superconductivity and magnetism in respective bulk materials can be captured at this level whenever the correlations are local and the systems are inhomogeneous.[14] In addition, at finite temperature, the clusters form a thermal ensemble. In a later section (Sec. III E) on "size effects," we address these issues in more detail. Moreover, to our knowledge, none of the other methods, such as Monte Carlo, have been able to capture (or reproduce) some of the low-temperature critical behavior, away from half filling, for the small-sized clusters we have studied. Therefore, at this level, we believe that our exact results provide benchmarks to test the accuracy and reliability of different approximations. This work also has a direct relevance to synthesis and properties of nanoclusters of a desired topology.

In this paper, we report results for a frustrated structure without electron-hole symmetry, namely, the octahedron, which is a fundamental building block in manganites and high T_c perovskites. We will show that when the degree of frustration is somewhat weak (i.e., weak coupling to the vertices), charge and opposite spin pairing, with condensation at low temperature, are possible. A temperature-chemical-potential phase diagram for this system is calculated for doping near one hole off half filling for small U and weak vertex coupling which illustrates the above scenario. We also show that in this octahedron, magnetic flux can get trapped in stable minima at half-integral units of the flux quantum under the above conditions. In addition, when all the intersite couplings are made equal, there is no pairing as described above. However, in this case where electron-hole symmetry is absent, for large to moderate values of U, we see Nagaoka-type spin saturation for $t=-1$ appropriate for holes, while for electrons ($t=1$) there is no such maximum saturation for any U.

In a nutshell, our ongoing work clearly demonstrates that there is a general tendency in these repulsive Hubbard clusters to support charge and spin pairing away from half filling provided certain conditions are met. These conditions are tied mostly to on-site Coulomb repulsion, boundary conditions, and the sign of the hopping parameter. The exact thermal aspects, including monitoring susceptibilities in an ensemble, brings in another dimension to this work. The effects of lattice frustrations, electron-hole symmetry, and boundary conditions are some of the important lessons learned from this series of calculations, which, in our opinion, will be quite significant in the search for a mechanism of pairing in various inhomogeneous materials.

II. METHODOLOGY AND KEY IDEAS

A. Model

A key aspect of our study is that we start from the single-orbital Hubbard model (with nearest-neighbor hopping t and on-site Coulomb interaction $U>0$)

$$H=-t\sum_{\langle ij\rangle\sigma} c^{+}_{i\sigma}c_{j\sigma}+U\sum_{i} n_{i\uparrow}n_{i\downarrow} \tag{1}$$

and stay with it throughout. Focusing on this simple model gives advantages to analyze (with great accuracy) the many-body correlation effects, which are nontrivial. In order to get a handle of the basic mechanism of pairing, among others, there is *no need* to make approximations as is often done, to obtain pairing-related results. It is, of course, necessary to study the model in a thermodynamic ensemble using a grand potential of the form

$$\Omega_U=-T\ln\sum_{n} e^{-(E_n-\mu N_n-hs^z_n)/T}, \tag{2}$$

in order to obtain finite temperature (T) effects and those due to variations in a magnetic field (h) and chemical potential (μ), but the crucial physics of electron pairing and spin-charge separation seems to be intrinsic to the (Hubbard) model itself. (E_n, N_n, and s^z_n refer to the energy, the particle or charge number, and the z component of spin in the nth eigenstate of the many-electron Hamiltonian, respectively.)

In addition, the results are exact and therefore go beyond the reach of approximate schemes such as Monte Carlo that contain severe limitations. After all, once the exact eigenvalues and eigenstates are known, the statistical many-body problem can be analyzed without having to resort to any approximations. In the results reported here, the energies are measured with respect to t, the hopping parameter, which is set to 1, unless otherwise stated.

In our previous publications, we have outlined most of the details pertaining to the method (see Refs. 3, 4, and 14–17). In addition, its relationship to other small-cluster studies has also been addressed in these publications. However, for completeness, we provide here a brief description of the general methodology and the criteria for the charge and spin pairing instabilities in the canonical and grand canonical ensembles. We also note that our numerical eigenvalues and states, obtained from exact diagonalization, have been found to agree very well with analytical eigenvalues that are available for small clusters[18] and other studies.

B. Canonical gaps

Depending on the value of the Coulomb repulsion U, Hubbard model for small clusters exhibits different pairing behavior which is evident when suitable gaps are defined and their properties examined. In a particular doping region, with one hole off half filling, when the chemical potential μ lies in an interval $[\mu_+(T),\mu_-(T)]$ with $\mu_->\mu_+$, charge pairing is found. The boundaries of the interval are defined as $\mu_+(T)=E(N+1)-E(N)$ and $\mu_-(T)=E(N)-E(N-1)$, where $E(N)$ denotes the average canonical energy in an N electron state at temperature T and the charge gap is defined as

$\Delta^c(T)=\mu_+-\mu_-$. The gap at $T\geq 0$ has to be negative for a charge pairing instability to occur. Analogously, we define a spin plateau feature by flipping the spin with an applied magnetic field.[19] We calculate a canonical spin gap as the difference in the average energies between the two cluster configurations with spin S and $S+1$ states, $\Delta^s(T)=E(S+1)-E(S)$, where $E(S)$ is the average canonical energy in the spin sector at fixed N.

C. Grand canonical gaps

In addition, in the grand canonical approach, using exact analytical expressions for the grand canonical potential and partition functions as expressed in Eq. (2), we can monitor the charge $\chi_c(\mu)$ and zero field spin $\chi_s(\mu)$ susceptibilities,

$$\chi_c(\mu) = \frac{\partial\langle N\rangle}{\partial\mu}, \quad \chi_s(\mu) = \left.\frac{\partial\langle s^z\rangle}{\partial h}\right|_{h\to 0}, \tag{3}$$

as a function of the chemical potential μ and temperature. The energy difference in terms of μ between the two consecutive susceptibility peaks can also serve as a natural order parameter. The double-peak structure in the charge and spin density of states versus μ plots have a small but nonzero weight inside the gaps at infinitesimal temperature $T\to 0$. To distinguish the peak distances in zero spin susceptibility from the canonical and grand canonical gaps at finite temperature, we call it a *pseudogap* in the grand canonical approach. The presence of distinct and separated pseudogap regions for the spin and charge degrees at various μ values in the $T-\mu$ phase diagram is a characteristic feature of spin-charge separation. We locate the boundaries and corresponding critical temperatures of crossovers between various phases by monitoring maxima and minima in charge and spin susceptibilities. In equilibrium, the critical temperatures T_c and T^* are defined as the temperature at which the separation between the two consecutive charge or zero spin susceptibility peaks vanish.

D. Pairing instabilities

Based on numerous exact analytical and numerical calculations on small Hubbard clusters, it is our view that some of the correlation driven effects seen in large systems are also observed in small clusters in thermal equilibrium, especially when the correlations are spatially local. We define critical parameters for the level crossing degeneracies or corresponding quantum critical points from the condition $\Delta^{c,s}=0$. These gaps obviously depend on various parameters such as U and temperature. The sign of the gap manifests the regions for electron charge and spin instabilities, such as the electron-electron ($\Delta^c<0$) and electron-hole ($\Delta^c>0$) pairings in the charge sector or the parallel ($\Delta^s<0$) and opposite ($\Delta^s>0$) spin pairings in the spin sector. The relationship between the charge gap Δ^c and its corresponding spin counterpart Δ^s is important in identifying of various phases in frustrated cluster topologies.[14]

There is a clear distinction between the presence of a positive or negative (charge/spin) gap. A positive gap indicates phase stability and smooth crossover, while a negative gap describes spontaneous transitions from one stationary state to another. When $\Delta^{c,s}<0$ at finite temperature, instead of full phase separation, local inhomogeneities in the clusters can induce electron redistribution and quantum mixing of the various charge and spin configurations. The negative excitation gap for the many-body ground state shows an energy instability for transitions into one of these competing configurations. The fluctuations are crucial for pair redistribution even in the absence of direct electron hopping between clusters, for example, when $\Delta^c<0$.

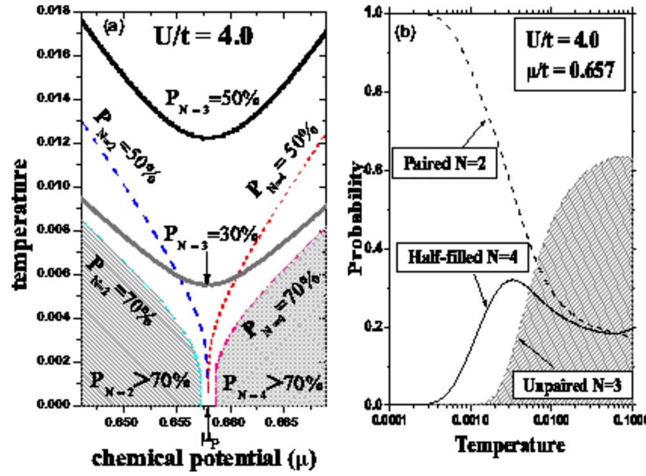

FIG. 1. (Color online) (a) Contours of probabilities in the grand canonical ensemble, associated with various (N=2, 3, and 4) electron states for the 4-site cluster as a function of temperature and chemical potential (in units of t) at U/t=4 (near one hole off half filling). μ_P identifies the critical value of the chemical potential where the transition from the charge state N=2 to N=4 happens without going through the charge state N=3. (b) The same probabilities at a fixed value of μ/t=0.657 slightly below the (zero temperature) critical value μ_P of doping at which the charge state N=3 becomes unstable.

III. RESULTS AND DISCUSSION

A. Bipartite clusters

In order to assess how properties of bipartite clusters depend on the detailed nature of the crystal lattice or topology of the primitive unit (cluster) structure, we have carried out a set of calculations involving topologically different clusters.[4,14] In the bipartite 4-site and 8-site ladder clusters, the charge and spin pairing appear to be robust. The negative charge-gap regions in the 8-site ladder (with periodic boundary conditions) for different values of coupling between the squares were reported in Ref. 4. Here, for completeness, we briefly summarize some of the published results related to the 4-site and 8-site ladder clusters. In the square clusters, for one hole off half filling at T=0, the charge gap Δ^c is negative while the spin gap Δ^s is positive when $0<U/t<U_c$=4.584 (in units of t). In this region, charge pairing instabilities are seen with the charge state N=3 (one hole off half filling) being unstable and yielding N=2 and N=4 charge states at low temperature (see Fig. 1). However, antiparallel spin pairing provides a rigid and smooth background due to the posi-

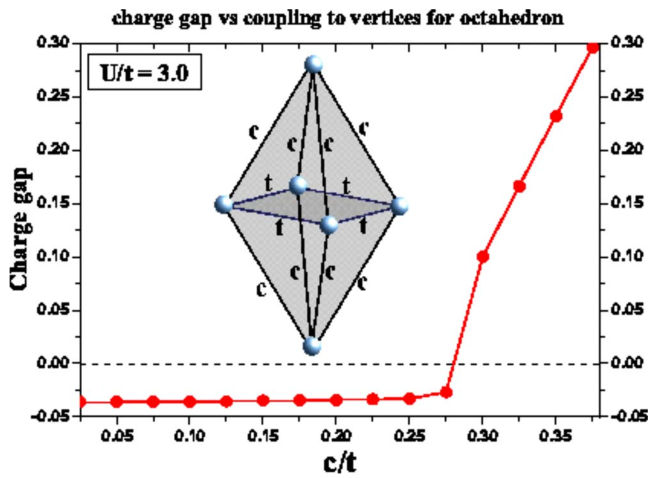

FIG. 2. (Color online) The zero-temperature charge gap at one hole off half filling in an octahedron (at $U/t=3$) as a function of the coupling strength c/t to the vertices. The negative charge gap up to $c/t=0.28$ displays a necessary condition for charge pairing instability in deformed octahedron structures. This also underlines the role of vertex coupling and the quasi-two-dimensional character of pairing which may be related to HTSC perovskites.

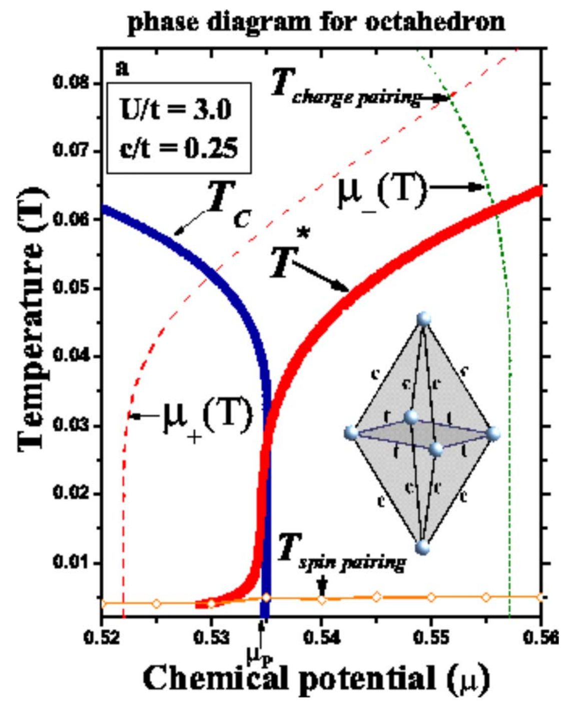

FIG. 3. (Color online) A part of the phase diagram for the octahedron ($U/t=3$) in Fig. 2 at $c/t=0.25$ showing the region of instability (one hole off half filling) in the chemical potential with charge and spin susceptibility peak positions (T_c and T^*) as well as spin and charge pairing temperatures (identified in the figure). If the hopping parameter t is set to 1 eV, the spin pairing here occurs around 40 K. For comparison, the corresponding part of the 4-site phase diagram (at $U/t=4$) can be seen in Fig. 1 of Ref. 4. The spin rigidity of the pairs in the plane is similar in both cases, although the octahedron spin susceptibilities are, of course, affected by the spins attached to the vertices.

tive spin gap at low temperatures, where $\Delta^c=-\Delta^s$ identifies a possible Bose condensation of electrons. Higher-temperature properties, including those of the pseudogaps, are also quite intriguing and discussed extensively using phase diagrams in Refs. 4 and 14.

At one hole off half filling, there is another critical value of U ($U_F=18.583$ in units of t) above which the canonical spin gap becomes negative while the corresponding charge gap stays positive. Here, parallel spin-paired ($S_z^{max}=3/2$) ground state is an indication of a Nagaoka-type (saturated) ferromagnetic instability. In the intermediate regime, $U_c<U/t<U_F$, both spin and charge gaps are positive in an unsaturated spin state ($S_z^{max}=1/2$), which can be called a spin liquid state (see Fig. 1 in Ref. 14). In passing, we note that in the 2×4 (bipartite) ladders with periodic boundary conditions, discussed in Ref. 4, similar pairing instabilities were observed.

B. Nonbipartite clusters: Octahedron

Here we discuss our results for the octahedron; it is an example of a nonbipartite cluster where particle-hole symmetry is broken. This cluster may also be regarded as a primitive block unit associated with the perovskites. The charge pairing gap for the octahedron, as a function of the coupling to the vertices c/t (Fig. 2), shows a negative value up to $c/t\leq c_0\simeq 0.28$. In addition, if the signs of the all the hopping parameters are reversed, the charge pairing phase becomes more stable showing negative charge gaps at much higher values of $|c|$. These results illustrate the relevance of two dimensionality observed in the perovskite structures and the coupling values in this region lead to charge pairing, for one hole off half filling, as seen in the bipartite clusters; spin pairing is seen to occur at a much lower temperature as evident from the phase diagram in Fig. 3.

The unpaired weak moment, induced by an infinitesimal magnetic field above T_s^P, agrees with the observation of competing dormant magnetic states in the HTSCs,[20] as discussed later. The coincidence of the charge and spin susceptibility peaks above T_s^P in Fig. 3, denoted by crossover temperatures T_c and T^*, shows full reconciliation of charge and spin degrees seen in the HTSCs above the superconducting transition temperature. As temperature decreases below the spin pairing temperature, the charge and spin gaps merge into one another and become one at zero temperature. This behavior resembles the coherent pairing in bipartite clusters obtained in phase A at weak and moderate U (see Fig. 1 in Ref. 14). The square-planar regions preserve the spin pairing that was evident in the bipartite cases which could possibly lead to Bose condensation and superconductivity in the region of instability in the chemical potential μ.

This result may be related to various detected phases in high-temperature superconductors such as $Bi_2Sr_2CaCu_2O_{8+\delta}$. When $\delta=0$, this compound is an insulator but, with additional oxygens at the apex sites (i.e., $\delta\neq 0$) which induce hole doping of the CuO_2 planes, it can become a superconductor. To understand the role of the apex electron(s) in an

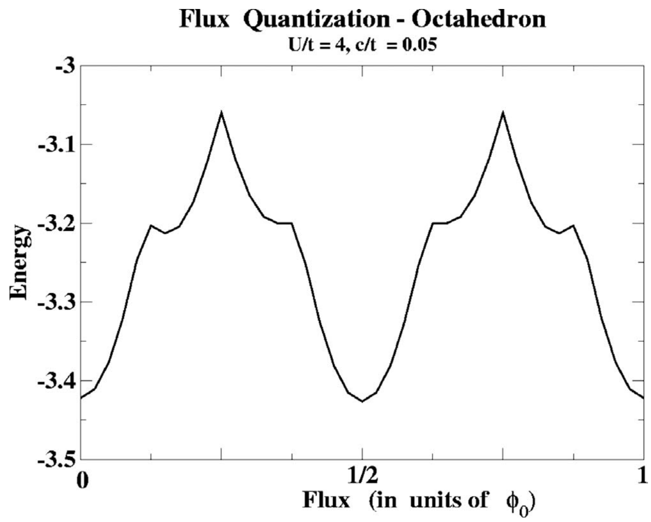

FIG. 4. Ground-state energy as a function of quantized flux at two holes off half filling for the octahedron ($U/t=4$ and $c/t=0.05$). Note the minimum at magnetic flux $\phi=\phi_0/2$, where ϕ_0 is the flux quantum, indicating the possible existence of a superconducting state (see text for more details).

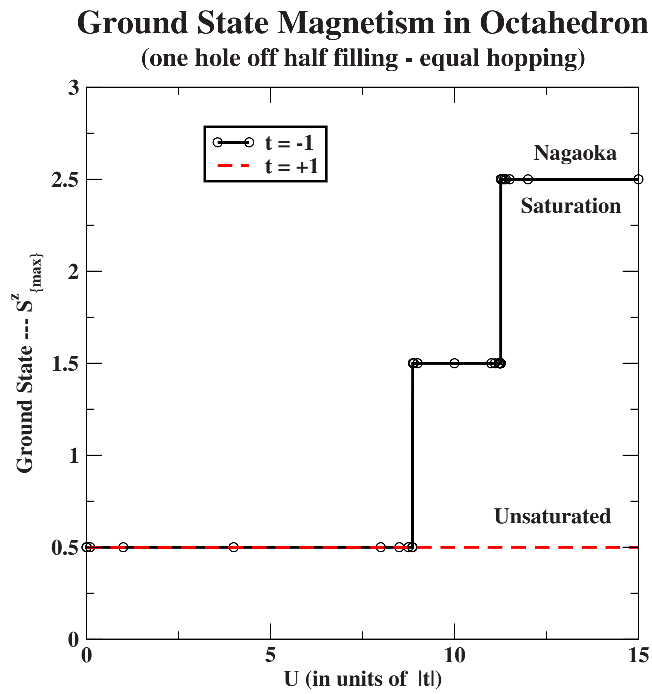

FIG. 5. (Color online) Ground-state magnetism of the octahedron for $t=\pm 1$ at one hole off half filling. Note the Nagaoka-type saturation for $t=-1$, while for $t=+1$ there is no saturation even at U/t as large as 1000.

octahedron, we have estimated the apex-electron contribution to the basal plane in the ground state. Our calculations show that when $c/t \rightarrow 0$, with no charge transfer from the apex site, the spin and charge pairings seen in the bipartite clusters are fully recovered with electron-hole symmetry. Up to $c/t \leq c_0$, the contribution from the apex site is not significant but above c_0, the electron at the apex site couples with the planar sites and the spin and charge pairings, favorable to Bose condensation, disappear.

C. Flux quantization

An interesting microscopic test that we have carried out is to examine the stability of a flux tube inside the octahedral cluster by monitoring the response of the system to a vector potential $\mathbf{A}(\mathbf{r})$. A transverse magnetic field can exist inside a type-II superconductor in the form of quantized flux tubes or vortices. By making the transformation $t_{ij} \rightarrow t_{ij} \exp[(2\pi i/\phi_0)\int_{r_i}^{r_j} \mathbf{A} \cdot d\mathbf{r}]$, where $\phi_0 = hc/e$ is the flux quantum, we have looked at the change in ground-state energy (at two holes off half filling) for a closed loop around the square base as a function of the flux $\phi = \oint \mathbf{A} \cdot d\mathbf{r}$. Superconductors show flux quantization by allowing integer and half-integer multiples of ϕ_0; clear and stable minima are visible at $\phi=\phi_0$ and $\phi=\phi_0/2$ in the octahedral cluster at the appropriate values of the parameters (U, c, and doping) discussed previously. This behavior, as a function of the magnetic flux, is shown in Fig. 4 and is periodic with period $\phi_0/2$ in the unit of $hc/2e$, which gives credence to flux quantization and the possible existence of a superconducting state with the (doubled) paired charge $2e$. Therefore, transverse magnetic fields can penetrate in quantized units of flux, creating "tubes" of normal regions in the superconducting state.

D. Nagaoka ferromagnetism

For large U in the (repulsive) Hubbard model at one hole off half filling, there is a well-known statement by Nagaoka, which claims that in higher dimensions such systems would exhibit fully saturated ferromagnetism. The exact results from our studies of the octahedron can be used to test the above statement.[10,14] At least for small clusters, such as the octahedron, frustration appears to play a significant role. As shown in Fig. 5, for hopping $t=+1$, there is no spin saturation (which has also been verified at large U). For $t=-1$, there is a saturated ferromagnetic state ($S_z^{max}=5/2$), which is insulating, at sufficiently large U (in units of $|t|$) as shown in the figure. Also, notice the unsaturated spin states having a maximum S_z value of 1/2 for $0 < U/t < 8.87$ and 3/2 for $8.87 \leq U/t \leq 11.2605$ at this filling.

Thus, it is clear that the octahedron with $c \neq 0$ (in this single-orbital Hubbard model) does not exhibit particle-hole symmetry and, accordingly, must be considered a frustrated structure. With the sign of hopping corresponding to holes ($t=-1$), it is energetically favorable to have full spin alignment (maximizing spin), reducing the Coulomb energy, at the expense of kinetic energy at large U. However, unsaturated ferromagnetism becomes stable at large U when the hopping parameter corresponds to electrons. Therefore, in these frustrated systems with spin degeneracies in the energy spectrum, (ferromagnetic) Nagaoka saturation is observed only for one type of hopping ($t=-1$), for large U beyond a critical value $U_c/|t|=11.2605$. Unsaturated ferromagnetism in the ground state becomes an alternative when $t=+1$.

E. Insights from small clusters and size effects

These exact results are valid for small clusters in a thermal ensemble and provide insights into nanoscale evolution of pairing. Understanding the effects of correlations, which are nontrivial, with a simple but exact correlated electron model has its own value. There is no consensus on whether pairing correlations must vanish in the thermodynamic limit; negative charge-gap regions are still found to exist in relatively large (30×30) clusters, pertaining to doping values of sufficient interest, in a multiband Hubbard model.[21] Our study is focused on smaller clusters but the understanding of various charge/spin crossovers and other finite-temperature aspects makes it unique. A general concern is whether a study of such clusters can shed any light on the properties of bulk materials. Starting from small clusters such as the squares and tetrahedrons, we have moved on to 2×4 ladders and octahedrons, where we still see charge and spin instabilities discussed here. As in our case, if the dominant interactions responsible for such properties are local (i.e., they do not require long-range order), then it is quite plausible that these results could provide valuable clues for bulk inhomogeneous systems.

Indeed, (in Ref. 22) we have found local charge and spin inhomogeneities for clusters similar to those seen in the high T_c cuprates, manganites, other transition-metal oxides, and rare-earth compounds.[23,24] The inhomogeneities favored by the negative gaps are essential in providing the spontaneous redistribution of the electron charge or spin. For example, a negative gap implies phase (charge) separation (i.e., *segregation*) of the clusters into hole-rich (charge neutral) and hole-poor regions. The quantum mixing of the closely degenerate hole-poor and hole-rich clusters for one hole off half filling, instead of causing global phase separation, provides a stable spatial inhomogeneous medium that allows the pair charge to fluctuate. Therefore, these studies of pairing instabilities in nanoclusters may be useful in understanding the nanoscale evolution of superconductivity and magnetism in large inhomogeneous systems. Moreover, in inhomogeneous systems such as the HTSCs and CMRs, there could very well be an optimal size[25] that is at least partly responsible for these exotic properties. If cluster-cluster interactions are weak, then we believe that these cluster studies can shed light on intrinsically inhomogeneous materials due to numerous reasons discussed above as well as experimental evidence. Below, we discuss some selected experimental evidence supporting our results reported here.

IV. EXPERIMENTAL EVIDENCE

In fact, there is remarkable support for the pairing picture from various experiments. There is qualitative agreement of our results with the dormant magnetic state,[20] T_c vs pressure,[26] specific heat vs temperature,[27] scanning tunnel microscope (STM), and other experimental results in this critical region of phase space.[28] Below, we briefly discuss two such experiments.

The STM experiments of Ref. 28, which measured the gap formation in the superconducting compound $Bi_2Sr_2CaCu_2O_{8+\delta}$, claim that the pairing gaps nucleate in *nanoscale regions* above T_c, which is the superconducting transition temperature. As temperature is lowered, these regions are said to proliferate. In the picture we have developed (see the phase diagram in Fig. 3), the charge pairing occurs at a higher temperature compared to the temperature T_s^P at which the spin pairing begins. When this is about to happen, the inhomogeneous mixed regions begin to shrink in size and, at the correct doping, $\langle N\rangle=2$ regions begin to proliferate (as shown in Fig. 1) when temperature is further lowered.

In another related experiment,[20] a magnetic state is observed in the La_2CuO_4 cuprate with hole doping (around $n_h\simeq0.125$). The resulting phase separation, into magnetic and superconducting regions, which is believed to be due to an electronic mechanism since no structural modulations were found, is determined by the total hole concentration. This corresponds well with our $\langle N\rangle\simeq3$ regions (in the square clusters as in Fig. 1) which are seen at temperatures above the spin pairing temperature. It is also mentioned that the application of a magnetic field somehow mimics doping and that the reason for this is not clear. However, we have a simple explanation as follows: In our Fig. 4 of Ref. 4, we have clearly established that the application of a magnetic field increases the percentage of $N\simeq3$ magnetic regions at the expense of $N\simeq2$ condensates since the former regions have a high magnetic susceptibility. This is quite similar to mimicking a change in the chemical potential or doping.

It may be argued that most of the essential physics can be captured at the cluster level since the materials are inhomogeneous and the correlations local. Also, working with an ensemble of clusters at finite temperature allows us to consider variations in the electron (hole) count as well as spin and other observables among the clusters. Although the issues related to superconductivity are yet to be fully addressed, we firmly believe that these results provide essential insight into pairing and the phase diagrams of the high T_c family. Similar conclusions can be drawn for Nagaoka ferromagnetism (large $U>0$) and ferroelectricity (negative U) in finite clusters.[29]

V. CONCLUSION

In conclusion, using exact techniques, we have shown that the charge and spin pairing phenomena are not uncommon in repulsive Hubbard nanoclusters with different topologies for appropriate on-site Coulomb-interaction strengths U at sufficiently low temperature. In square and ladder (bipartite) clusters, charge and spin pairing instabilities occur in the (close) vicinity of half filling at suitable interaction strengths. In frustrated clusters such as octahedrons, the coupling to the vertex, which breaks particle-hole symmetry, has a detrimental effect on charge pairing.

These results are similar to what is observed in the hole- and electron-doped high-temperature superconductors such as $La_{2-x}Sr_xCuO_{4+y}$, $Bi_2Sr_2CaCu_2O_{8+\delta}$, and $Nd_{2-x}Ce_xCuO_4$. Finite-temperature work reveals that opposite spin paring occurs at a transition temperature lower than that for charge pairing. This region of phase space is rich in physics and provides clues to understanding important concepts such as bosonic modes, coherent pairing, dormant magnetic states, and pseudogap behavior. These studies also show the range of parameters and conditions necessary for Bose condensation and possible superconductivity. At higher values of U, Nagaoka-type magnetic transitions are observed. Even at this level, our nanocluster studies provide important insights into recent experimental observations on HTSCs and CMRs. The octahedron can also be used to understand thermodynamic perplexities in other inhomogeneous, concentrated systems.

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