Cooper pairing in the Emery model

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The system energy E as a function of the gauge phase Φ has been studied in the two-dimensional Emery model, which is applied to the CuO_2 plane in high-T_c superconductors. The system energy $E(\Phi)$ has been calculated by exact diagonalization in the two-dimensional Cu_4O_8 cluster, and also by the slave boson and Monte Carlo techniques. At certain values of the Hamiltonian parameters we have observed motion of carriers with a charge of $2e$, i.e., Cooper pairs, as indicated by a characteristic maximum of $E(\Phi)$ at $\Phi \approx \Phi_0/2$, where Φ_0 is the flux quantum. We have plotted the phase diagram and determined the range of model parameters over which electron pairing takes place. The resulting Emery parameters ($U_d=(2-10)t_{pd}$, $\varepsilon=(1-4)t_{pd}$, $t_{pp}=[0-(-0.5)]t_{pd}$) are close to the values derived from experimental data. The density of states has been calculated with the phase taken into account, and we have demonstrated that the presence of the gauge phase in a small bounded system leads to effective doping, which can transform the original dielectric state into a metallic (and superconducting) phase. The effective doping parameter (0.1–0.2) is close to experimental values for high-T_c superconductors. © *1996 American Institute of Physics.*
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1. INTRODUCTION

Multiband Hubbard models (especially the Emery model[1] describing the CuO_2 plane) have been used to describe nonphonon mechanisms responsible for attraction among current carriers in high-T_c superconductors, which have recently been an active subject of discussion. In addition to the problem of Cooper pairing, the symmetry of the superconducting state has been also studied.[2] The available numerical data, however, lead to somewhat controversial conclusions. For example, the exact diagonalization[3–5] and Monte Carlo[6] techniques applied to two-dimensional Cu–O clusters with CuO_2 cell dimensions of 2×2 and 4×4 give evidence of carrier pairing, in accordance with calculations of the binding energy and pair correlations with the predominant type of symmetry (s^* in Refs. 5 and 7). On the other hand, the extrapolation of quantum Monte Carlo data on pair correlation functions towards the thermodynamic limit (to 8×8 (Ref. 8) and 16×16 (Ref. 9) CuO_2 cells) leads to a total vanishing of anomalous averages (to be exact, to the absence of divergence in the Fourier component[8,9]), hence to the absence of carrier pairing in the two-dimensional Emery model. Note that in the first case[5] the smallness of the system does not allow one to conclude ultimately whether there is long-range off-diagonal order, whereas the relatively high temperature range ($T\sim1000$ K) in which the calculation was performed in the second case[8,9] might also cause the negative result yielded by the Monte Carlo technique. Nonetheless, the Emery model is most popular with theorists attempting to describe normal and superconducting properties of HTSC. In light of these considerations, it is undoubtedly interesting to prove the possibility (or impossibility) of carrier pairing in the two-dimensional Emery model regardless of the symmetry type and without additional simplifications or assumptions concerning the nature of the ground state. The latter condition impels us to use exact numerical techniques without any approximations.

There is a criterion that makes it possible to show unequivocally that carriers with charge $2e$ (i.e., Cooper pairs) are present in the system. According to Yang,[10] when a gauge phase Φ is included in a fermion or boson system (this corresponds to introducing a magnetic flux or a circulating current in the two-dimensional toroidal geometry), the energy E of the system becomes a periodic function of the phase, so that in the presence of carriers with charge $2e$, we have the periodic condition

$$E(\Phi/\Phi_0)=E(\Phi/\Phi_0+\nu), \quad \nu=0,\pm1,\ldots, \tag{1}$$

where $\Phi_0=hc/2e$ is the magnetic flux quantum. If the carrier charge is equal to e, the period is doubled:

$$E(\Phi/\Phi_0)=E(\Phi/\Phi_0+2\nu), \quad \nu=0,\pm1,\ldots \tag{2}$$

If the system contains both superfluidity and normal Fermi liquid (quasiparticle) phases, the situations (1) and (2) can coexist, each of the phases contributing a component proportional to the respective carrier concentration. The point is that in the absence of impurities, both the supercurrent and quasiparticle current flow without dissipation, i.e., from this viewpoint, the conditions (1) and (2) are criteria of superfluidity, rather than of superconductivity. Thus, in a real situation, we expect interference of these two effects (hence two periods in the energy versus phase), and the effect in question will show up as a peak at $\Phi\approx\Phi_0/2$ in $E(\Phi)$, whereas the quasiparticle peak at $\Phi\approx\Phi_0$ should remain, indicating the emergence of a new flux quantum (and a new period) corresponding to Cooper pairs.

Moreover, if the gauge phase is considered in the calculation, one can obtain information concerning the superfluidity phase density D_s, which can be expressed as follows:[11]

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$$D_s=\frac{1}{\pi}L_xL_y\lim_{\Phi\to 0}\frac{d^2E}{d\Phi^2}, \tag{3}$$

where L is the linear size of the system in units of the cell period ($L=2$ for Cu_4O_8).

Equation (3) has the sense of the real superfluidity phase density only in the thermodynamic limit; it should therefore be considered only in the case of a sufficiently large system.

The criterion based on the gauge phase was applied to the Hubbard model,[9] and one-dimensional[12] and two-dimensional[13] Emery models. In the case of a one-dimensional Cu–O chain[12] the conditions for the existence of carriers with charge $2e$ were obtained, although the model parameters were not very realistic. But Monte Carlo calculations[13] with the phase analysis in the two-dimensional Emery model of clusters with sizes of up to 8×8 CuO_2 cells yielded a negative result, which might be due to the temperature at which the calculations were performed not being low enough. Another inherent difficulty of this calculation is that the effect is weak, which might lead to the negative result concerning superconducting pairing. A simple analysis of the two-dimensional model suggests that the energy correction due to the phase is small but finite, and does not increase with the size of the system. Hence, the effect may be undetectable by the Monte Carlo technique, since the absolute calculation accuracy degrades as the size of the system increases. Therefore, in our opinion, calculations by the exact diagonalization technique (whose calculation uncertainty is extremely small and should be suitable for detecting the desired effect) in the two-dimensional case have fundamental importance, at least in the case of a small cluster, in order to prove the existence of Cooper pairing or its impossibility.

In this paper we have applied the criterion (1) and (2) to investigate a Cu_4O_8 cluster at $T=0$ by the exact diagonalization technique. The calculations have been performed over a wide range of Hamiltonian parameters, and we have obtained clear evidence of Cooper pairing of charge carriers. Calculations based on the slave boson[14] and Monte Carlo[9] techniques in larger systems confirm the results of the exact diagonalization.

2. CALIBRATION PHASE IN THE EMERY MODEL

The Emery Hamiltonian in the hole representation[1–9] has the form

$$H=-t_{pd}\sum_{ik,\sigma}\left[d^+_{i\sigma}p_{k\sigma}\exp\left(\frac{i\pi\Phi}{2\Phi_0L}\right)+\text{H.c.}\right]+\varepsilon\sum_{k\sigma}n_{k\sigma}$$
$$+U_d\sum_i n_{i\uparrow}n_{i\downarrow}+U_p\sum_k n_{k\uparrow}n_{k\downarrow}+t_{pp}$$
$$\times\sum_{ik,\sigma}\left[p^+_{i\sigma}p_{k\sigma}\exp\left(\frac{i\pi\Phi}{2\Phi_0L}\right)+\text{H.c.}\right], \tag{4}$$

which describes the hybridization between $d_{x^2-y^2}$ and p_x, p_y orbitals in the CuO_2 plane with the overlap integral t_{pd}; the hybridization between the p_x and p_y orbitals of oxygen sites closest to each other in the diagonal direction with the overlap integral t_{pp}; the energy difference ε between the copper and oxygen sites; and Coulomb repulsion at the copper, $(U)_d$ and oxygen $(U)_p$ sites. Here Φ is the gauge phase. The vector potential $\mathbf{A}$ is introduced only in the direction of one of lattice axes (for definiteness along the x-axis, $A_x=\Phi/L$), so that the total magnetic flux integrated over the length L is Φ. After every O–O hop along the diagonal with amplitude t_{pp}, the phase $\Delta\Phi=\Phi/2L$ is added, just as in the case of a copper-to-oxygen hop in the x-direction with amplitude t_{pd} (naturally, in the opposite direction the phase difference is subtracted). Note that this way of introducing the gauge phase allows one to incorporate a toroidal magnetic flux or circulating current into the lattice geometry in the most natural manner (as in the Aharonov–Bohm effect), and is often used in boson models (Bose–Hubbard model) to study superconducting– dielectric transitions[15] to determine the superconducting component.

Let us estimate the contribution of the gauge phase Φ to the calculated energy E of the system. Without interaction the energy is a function of $\cos(k_x+\pi\Phi/2\Phi_0L)$, where $k_x=2\pi n/L$, $n=0,\ldots,L-1$. Thus the gauge phase makes an additional contribution to the energy, $E_\Phi \propto t_{pd}L^d(\Phi/\Phi_0L)^2$, where d is the dimensionality of the space. In the one-dimensional case $E_\Phi\propto 1/L$, in the two-

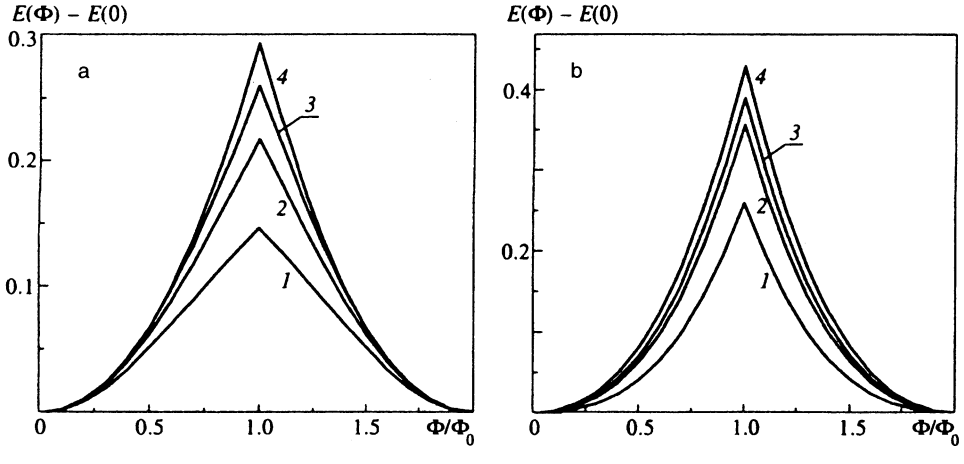

FIG. 1. Energy of the Cu_4O_8 cluster ground state (in units of t_{pd}) vs phase in the doped case at $t_{pp}=0$: (a) $N=3$, $U_d=6$, (*1*) $\varepsilon=10$, (2) 5, (*3*) 3, (*4*) 0; (b) $N=5$, $\varepsilon=1$, (*1*) $U_d=100$, (2) 10, (*3*) 6, (*4*) 2.

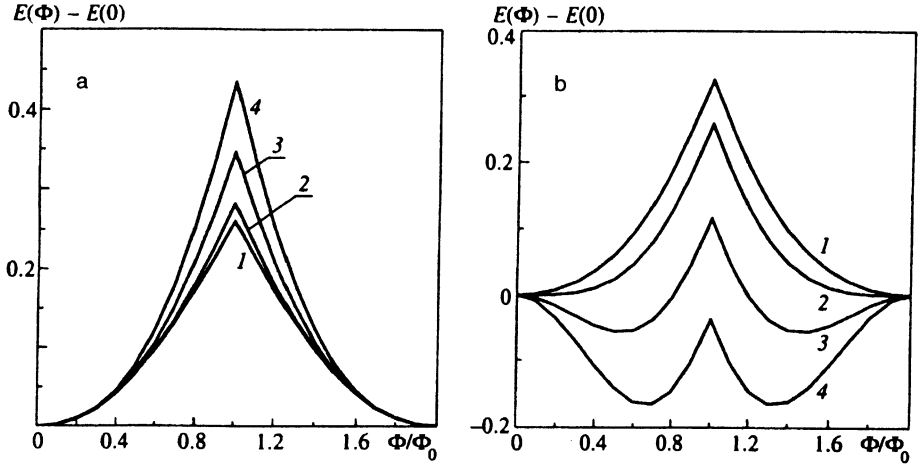

FIG. 2. Ground-state energy of the Cu_4O_8 cluster vs phase in the doped case at (a) $U_d=6$, $\varepsilon=3$, and $N=3$, and (b) $N=5$ at different values of diagonal hopping: (*1*) $t_{pp}=0$; (*2*) -0.1; (*3*) -0.3; (*4*) -0.5.

dimensional case $E_\Phi \propto \text{const}(L)$, and in the three-dimensional case $E_\Phi \propto L$. Note that although the amplitude of the effect is essentially constant with the system size at $d=2$, further calculations indicate that it is small. Given the small amplitude of the effect, the numerical precision must be high. From this viewpoint, the exact diagonalization technique has clearcut advantages over the Monte Carlo method (in addition to the fact that the ground state energy is calculated at $T=0$).

3. CALCULATION OF $E(\Phi)$ IN A Cu_4O_8 CLUSTER

In the case of a Cu_4O_8 cluster with twelve atoms and periodic boundary conditions, we have studied the following range of model parameters: $U_p=0$, $0<U_d<100$, $0<\varepsilon<10$, $-0.5\leqslant t_{pp}\leqslant 0$ (in units of t_{pd}). Most of the calculations were performed at three carrier concentrations N: $N=4$ (undoped state), $N=3$ (electron doping), and $N=5$ (hole doping). Typical calculations are plotted in Figs. 1–4, which show the ground state energy E_0 as a function of phase for various Hamiltonian parameters. Figures 1 and 2 demonstrate that in the doped state the function $E_0(\Phi)$ has a period of $2\Phi_0$, i.e., in this case the condition (2) is satisfied, which corresponds to conventional quasiparticle transport.[10,11]

On the contrary, in the "undoped" situation (as will be demonstrated below, in this case an effective doping takes place), maxima at $\Phi\approx\Phi_0, 3\Phi_0/2, \ldots$ can be seen in $E_0(\Phi)$ in Figs. 3 and 4, which indicates that condition (1) is also satisfied, i.e., Cooper pairing with charge $2e$ takes place.[10,11] Figures 3 and 4 show that the curve is exactly periodic (i.e., the contribution of quasiparticle transport is zero and the total current is due to pairs) at $U_d=2.5$, $\varepsilon=1$ (Fig. 3) and at $U_d=6$, $\varepsilon=3$, $t_{pp}=-0.3$ (Fig. 4) (in these cases $E_0(0)=E_0(\Phi_0)$). As the interaction U_d increases, the location of the maximum approaches $\Phi_0/2$. This can be explained by a decrease in the correlation lengths, and, as a consequence, an effective increase in system size. We note the importance of the oxygen–oxygen hopping amplitude t_{pp}, which significantly alters the range of the other Emery model parameters at which the effect can be observed.

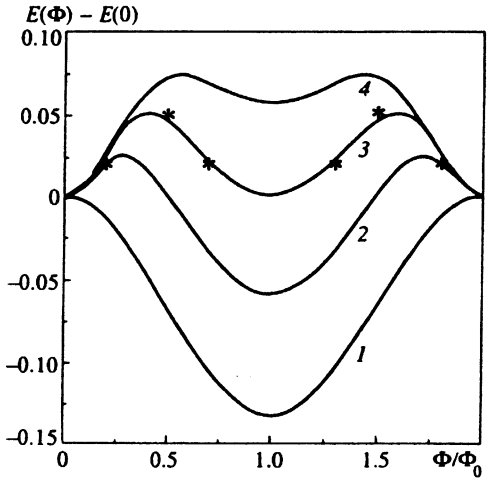

FIG. 3. Ground-state energy of a Cu_4O_8 cluster vs phase in undoped case at $N=4$, $\varepsilon=1$, and (*1*) $U_d=0$, (*2*) 1, (*3*) 2.5, (*4*) 6. Asterisks show results of the Monte Carlo trajectory method for the model parameters of curve *3*. The numerical accuracy of the Monte Carlo method $\Delta E=\pm 0.02$.

4. EFFECTIVE DOPING AND DENSITY OF STATES

At first glance, the existence of current (and supercurrent) in an initially undoped system looks like a contradiction. But it can be eliminated easily if we take into account the additional contribution of the gauge phase to the one-particle spectrum, $\Delta E_\Phi \propto t_{pd}(\Phi/\Phi_0 L)^2$. In the small system under consideration, this contribution significantly modifies the spectrum at $\Phi\sim\Phi_0$ by generating an effective hole doping, closing or blurring the bandgap, and shifting the Fermi level to the conduction band.

In order to prove this assertion, we calculated the one-particle density of states[16] using the conventional technique in the cluster after generalizing it to include the phase, i.e., a complex hermitian Hamiltonian matrix. Note that in the case of zero phase, the resulting spectra were identical to those given in Ref. 16. The results are shown in Figs. 5–7.

In the range where the Cooper peak is detected ($U_d=6$, $\varepsilon=1$, $t_{pp}=0$), the pattern corresponding to the undoped case (the Fermi level in Fig. 5a is at the middle of the band gap) changes, after including the phase, to the state with effective doping (the Fermi level in Fig. 5b is at the

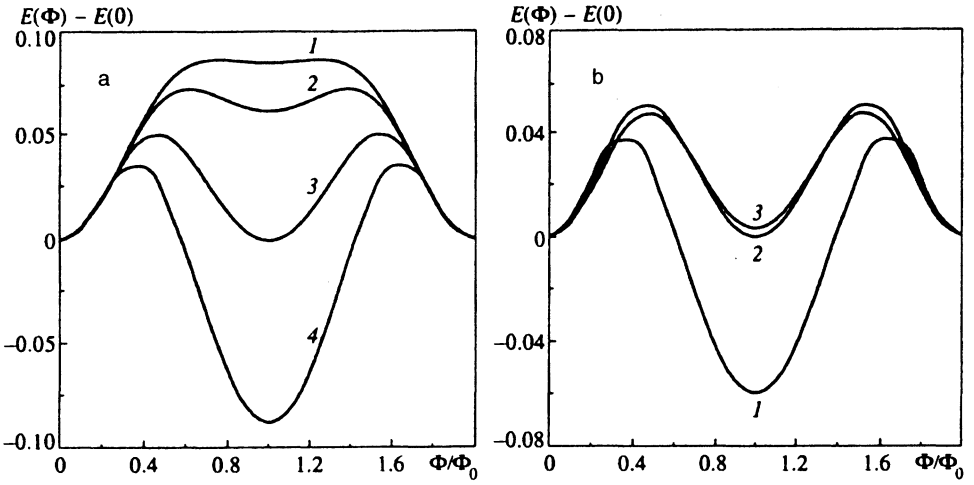

FIG. 4. Ground-state energy of a Cu_4O_8 cluster vs phase in the undoped case at different values of diagonal hopping t_{pp}: (a) $U_d=6$, $\varepsilon=3$, and (*1*) $t_{pp}=0$, (*2*) -0.1, (*3*) -0.3, (*4*) -0.5; (b) $t_{pp}=-0.3$, $\varepsilon=3$, and (*1*) $U_d=2$, (*2*) 6, (*3*) 10.

peak of the density of states, and the edges of the band gap are slightly spread). The Fermi level shift indicates that hole carriers are created in the system.

In order to demonstrate clearly that the system is doped, let us compare this situation to the case of real doping, in which additional hole is introduced ($N=5$). Figure 6a shows the density of states at this concentration. The Fermi level coincides with the peak, as in the undoped case at phase $\Phi=0.5\Phi_0$ (Fig. 5b). Moreover, the Fermi energies are essentially identical (Fig. 6b shows both these curves near the Fermi level in one plot). This means that the effective doping x^* is about 0.1–0.25 (a more accurate calculation using the density of states integral yields $x^*=0.13$).

The pattern is different in the range where the tendency to transfer to a metallic state (and, naturally, to Cooper pairing) is suppressed by an initially large dielectric gap (for example, at $U_d=10$, $\varepsilon=5$, and $t_{pp}=0$, Fig. 7a). Introduction of the gauge phase, also shifts the Fermi level, but it remains essentially within the gap and does not reach the band of correlated states (Fig. 7b). Nonetheless, weak effective doping takes place due to minor blurring of the gap edges, and a calculation yields $x^*=0.01$.

Thus, at $N=4$ the state of a Cu_4O_8 cluster is not dielectric, but metallic (phase $\Phi\approx\Phi_0/2$), with the effective carrier concentration x^* near its optimal value. The calculation of the effective carrier concentration indicates that it increases with the decreasing interaction U_d (which corresponds to a transition to a normal metallic state in the phase diagram; see below). The optimal concentrations, at which Cooper pairing takes place, range between 0.1 and 0.2. The effective doping decreases as the effect weakens in the dielectric region at large ε.

Figure 8 shows curves for x^* at various Hamiltonian parameters, derived from calculations of one-particle densities of states (the effective concentration was derived by adding densities of states between the initial Fermi level and its position shifted introduction of the phase; a Lorentzian approximation to the delta function with a smoothing parameter of about 0.1 was used). It is clear that the optimal values of x^* are obtained at Emery parameters at which the Cooper pairing is almost ideal (for example at $U_d=2$–2.5, $\varepsilon=1$).

As for the initially doped states ($N=3$ and $N=5$), in which we observe no pairing, we believe there are two basic reasons for the negative result:

a) an uncompensated spin ($S_z=\pm 1/2$), to which a small system is sensitive, and which naturally does not occur in the thermodynamic limit, makes pairing impossible;

b) effective hole doping due to the phase makes the excess carrier concentration low at $N=3$ (the Fermi level shifts towards the dielectric gap), and too high at $N=5$ (>0.5), so that the total doping is beyond the optimal range of carrier concentration for pairing.

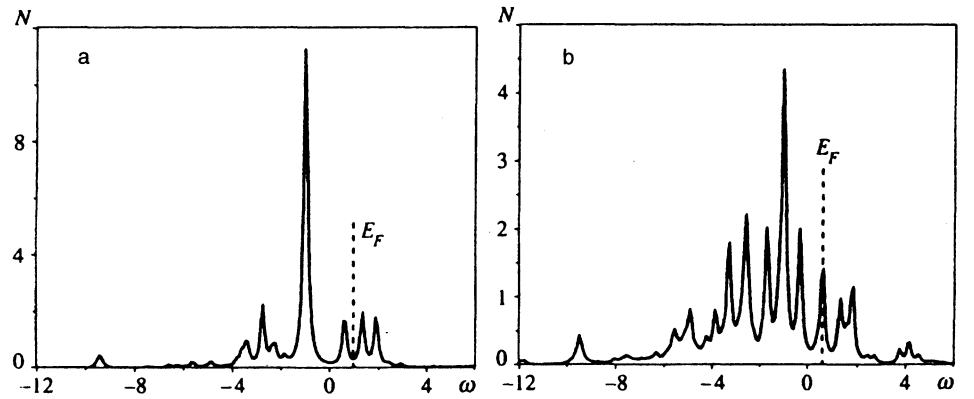

FIG. 5. Density of states of a Cu_4O_8 cluster in the undoped case at $U_d=6$, $\varepsilon=1$, $t_{pp}=0$, and (a) $\Phi=0$; (b) $\Phi=0.5\Phi_0$. When the phase is introduced (Fig. 5b), the distortion of the spectrum and shift of the Fermi level to the conduction band are evident.

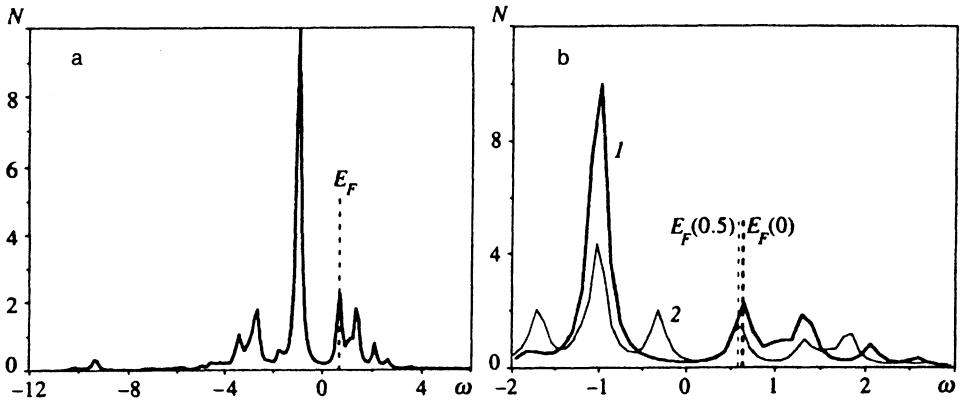

FIG. 6. (a) Density of states of a Cu_4O_8 cluster in the doped case ($N=5$) at $U_d=6$, $\varepsilon=1$, $t_{pp}=0$, and $\Phi=0$. (b) Detailed density of states near the Fermi level in comparison with the case of effective doping ($N=4$): (*1*) $N=5$, $\Phi=0$; (*2*) $N=4$, $\Phi=0.5\Phi_0$. Fermi levels of the two cases are essentially identical.

It seems to us that the more important of the two factors is the uncompensated spin.

We have also studied a system with $N=2$ and $N=6$, $S_z=0$, but have not seen any signs of pairing. The carrier concentration at $N=2$ is seemingly too low and at $N=6$ too high, so that the effect cannot be detected even when the spins cancel.

Thus, the optimal conditions for observing Cooper pairing in a Cu_4O_8 cluster obtain in the undoped state with $N=4$, since in this case $S_z=0$ and the effective carrier concentration x^* is close to the optimal value.

5. PHASE DIAGRAM OF A Cu_4O_8 CLUSTER

The results of the previous section indicate that Cooper pairing, i.e., a maximum of the function $E(\Phi)$ at $\Phi\sim\Phi_0/2$, is not observed at all values of the Emery Hamiltonian parameters. Figure 9 shows a phase diagram of superconductive, metallic, and dielectric states for a Cu_4O_8 cluster plotted against $\varepsilon-U_d$, where the region of superconducting correlations is labeled S (this region is characterized by a maximum of the function $E(\Phi)$ at $0.4<\Phi/\Phi_0<0.6$). The parameters in this region are close to those at which the binding energy for carriers in the cluster is negative.[4,5,17] Note also that when diagonal hopping t_{pp} is included, the S region shifts towards more realistic Emery parameters derived from experimental data.[18,19]

The region of the normal metallic state (Me) is characterized by a small intensity of interaction at a copper site, this interaction being too weak for Cooper pairing. The effective doping is greatest in this region (Fig. 8a). Note that the effect vanishes in our ideal system (in the sense that it does not contain impurities) because the effective correlation length increases to the system's linear size, so the transition to the normal metallic state is somewhat uncertain (it is shown as a dashed curve in Fig. 9).

The region of the insulating state (I) corresponds to large values of ε (the charge-transfer regime) and is characterized by a wide dielectric gap of the order of ε. The effective doping falls abruptly in this region (Fig. 8b) and the conditions are unfavorable for a metallic (much less a superconducting) state.

Note also that at large ε the Emery model can be treated as a two-dimensional Hubbard model for the copper sublattice. No pairing has been detected in the two-dimensional Hubbard model.[2a,20] This is in agreement with the phase diagram in Fig. 9, where the superconducting region is abruptly curtailed at large ε.

Note that the S region only approximately outlines the boundaries within which the effect takes place, and in a larger system its shape may be somewhat different. Moreover, the phase diagram depends on additional factors, since the doping level also changes with the system parameters.

6. EFFECT OF SYSTEM SIZE. PHASE DIAGRAM OF A $Cu_{16}O_{32}$ CLUSTER

We now discuss the effect of cluster size on the energy of a system as a function of phase. The thermodynamic limit

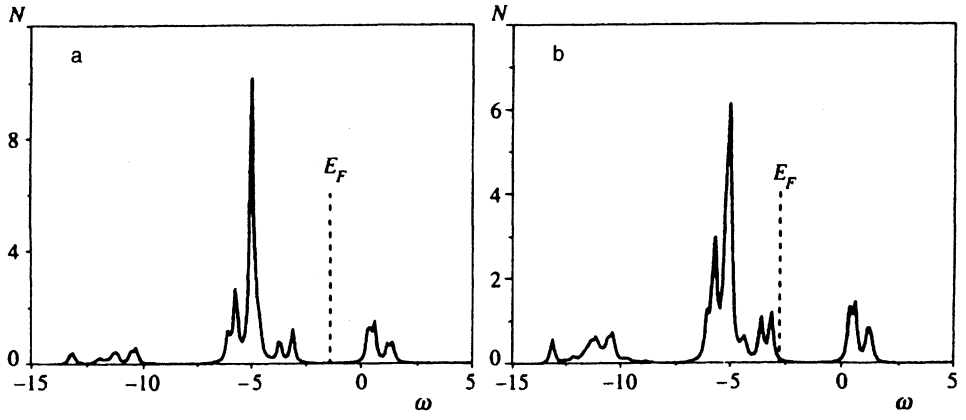

FIG. 7. Density of states of a Cu_4O_8 cluster in the dielectric case at $U_d=10$, $\varepsilon=5$, $t_{pp}=0$, and (a) $\Phi=0$; (b) $\Phi=0.5\Phi_0$. At nonzero phase (Fig. 7b) the Fermi level is shifted, but remains within the band gap.

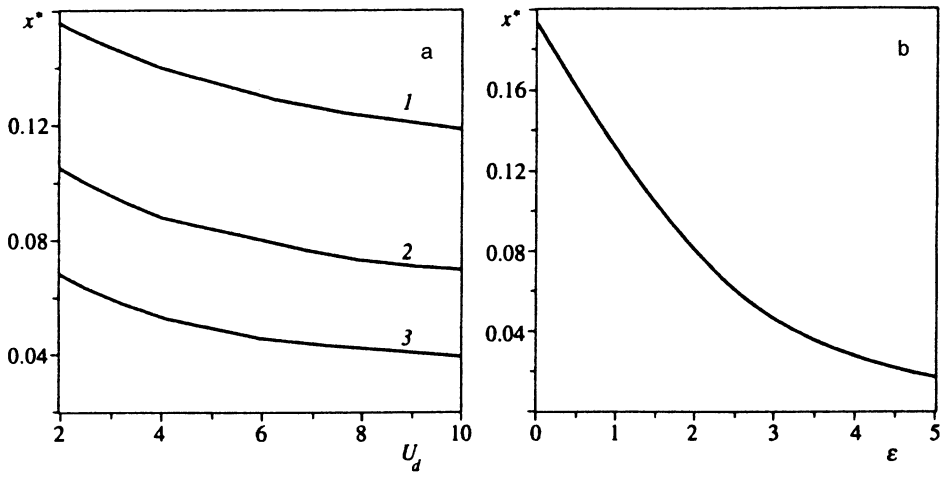

FIG. 8. Effective doping x^* derived from the density of states of Cu_4O_8 cluster in the undoped case at $t_{pp}=0$ and $\Phi=0.5\Phi_0$: (a) (*1*) $\varepsilon=1$, (*2*) 2, (*3*) 3; (b) $U_d=6$.

may be considered only when the correction to the one-particle spectrum due to the phase is small: $\Delta E_\Phi \ll t_{pd}$. Hence follows a condition on cluster linear size at $\Phi\sim\Phi_0$: $L^{-2}\ll 1$. This condition is of course hard to satisfy in a Cu_4O_8 cluster (as demonstrated by additional hole doping — the finite-size effect). Nonetheless, the absolute contribution to the (calculated) system energy due to the phase is small: $[E(\Phi)-E(0)]/E(0)\sim 10^{-2}$, and there is hope that the observed Cooper pairing is not purely a size effect.

In order to detect the effect in larger clusters, we performed calculations using the slave boson method[14] for a system with 4×4 and 8×8 CuO_2 cells. Figure 10a shows calculations for a 4×4 cluster at various doping levels (real, not effective, as in the 12-atom cluster). One can see a clear maximum at $\Phi\sim\Phi_0/2$ both electron and hole doping (hence the effect also occurs in electronic HTSC).

In the insulating phase at a carrier concentration $n=1$ the function $E(\Phi)$ is rather flat, which indicates that the effective doping is essentially negligible in such a large system (in the 8×8 cluster, the energy E is completely independent of Φ at $n=1$). Furthermore, in calculating the size of the 8×8 cluster, the position of the superconducting maximum in the $E(\Phi)$ curve is quite close to $\Phi_0/2$ for all model parameters, which must be the case in the thermodynamic limit.

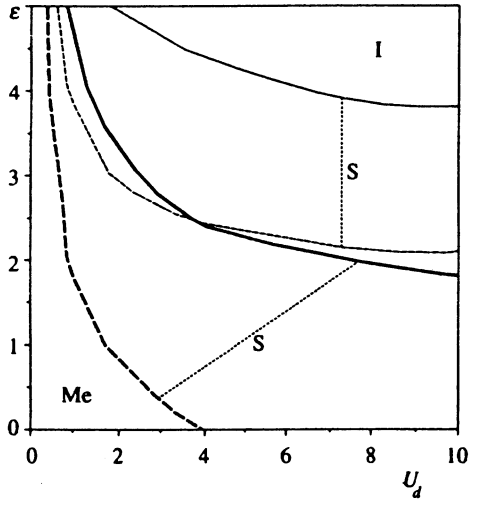

FIG. 9. Phase diagram of Cu_4O_8 cluster: S) region of Cooper pairing (the maximum of $E(\Phi)$ is in the range $0.4<\Phi/\Phi_0<0.6$); I) insulator; Me) metal; thick lines correspond to the case of $t_{pp}=0$; thin lines are for $t_{pp}=-0.3$.

Figure 10b shows the phase diagram of a $Cu_{16}O_{32}$ cluster at a doping level $x=1.25$. The boundary of the superconducting region was defined as the line where the density D_s (Eq. (3)) of the superconducting state vanishes. As might be expected, there is no upper boundary on the transition between superconducting and insulating states, which is natural when the doping is real, since initially the system is always in the metallic state.

Unfortunately, the accuracy of the slave boson approximation deteriorates as the carrier concentration deviates from being half full ($n=1$), which does not allow us to fully demonstrate the dependence of the effect on the real carrier concentration in large clusters (recall that the effect remains finite in the two-dimensional configuration, and does not grow with system size). Here we are probably facing the same problem as in the Monte Carlo calculation,[13] where the effect could not be identified (we believe) because of an inevitable increase in the statistical error with cluster size.

This problem has also significally complicated our Monte Carlo calculations. For example, we have used the effective trajectory Monte Carlo technique developed in Ref. 9 (modified for the complex Hamiltonian of Eq. (4)) in calculations of Cu_4O_8, $Cu_{16}O_{32}$, $Cu_{64}O_{128}$, and $Cu_{100}O_{200}$ clusters with parameters $U_d=6$, $\varepsilon=1-3$, and $t_{pp}=-0.3$, 0, for which, according to our data, pairing should occur.

For Cu_4O_8 and $Cu_{16}O_{32}$ clusters we have reproduced to within the numerical errors the results given by exact diagonalization and slave boson calculations, i.e., we have obtained a maximum at $\Phi\sim\Phi_0/2$ (Figs. 3, 10a). The assumed temperature was reduced to $t_{pd}/100$, i.e., about 100 K. In a small Cu_4O_8 cluster, the effect was observed at a temperature as high as $T\sim t_{pd}/10$, whereas in the 48-atom $Cu_{16}O_{32}$ cluster it could be seen only at $T\sim t_{pd}/40$, i.e., the critical temperature for this cluster is $T_c\sim 250$, K which is closer to the experimental value.

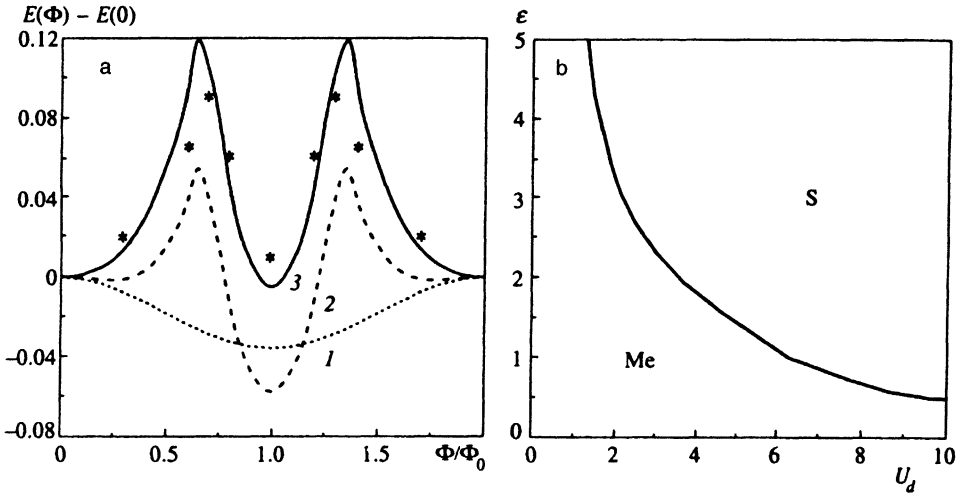

FIG. 10. (a) Ground-state energy of $Cu_{16}O_{32}$ cluster vs phase. calculated by the slave-boson technique at $\varepsilon=1$, $U_d=8$, and carrier concentration (*1*) $n=1$; (*2*) $n=0.75$; (*3*) $n=1.25$. Asterisks mark calculations by the Monte Carlo trajectory technique at $n=1.25$. The Monte Carlo numerical error is $\Delta E=\pm 0.025$. (b) Phase diagram of the $Cu_{16}O_{32}$ cluster: S) region of Cooper pairing ($D_s>0$); Me) metal.

This result for the $Cu_{16}O_{32}$ cluster is very important because it attests to superconducting pairing in a large system using a method with no approximations. Note that unlike the Monte Carlo technique, the slave boson method is a combination of variational and mean-field methods,[14] and its results might be questionable in a large system. The Monte Carlo technique, whose absolute error is directly controlled, is free of this flaw. But the necessary accuracy ($\approx 0.01 t_{pd}$ in energy absolute units) would require 5×10^6 Monte Carlo steps.

For the remaining clusters, we naturally could not perform so many steps, and therefore could not distinguished between $E(\Phi)$ and $E(0)$ to be within the numerical errors.

7. CONCLUSION

We have presented evidence for Cooper pairing and superconductivity in the two-dimensional Emery model. The values of model parameters and effective doping at which the effect can be observed are close to the experimental data, and in agreement with the values at which attraction among carriers was obtained in earlier calculations.[4,17] We stress that the exact diagonalization and slave boson techniques were applied to the ground state at $T=0$. In our opinion, regardless of the critical temperature measured in experiments, the critical temperature in these models and within the range of parameters studied may be somewhat higher than $0.01 t_{pd}\sim 100$ K, and there is hope that Monte Carlo techniques can be used to test for superconductivity. The proof of carrier pairing in the 48-atom CuO cluster obtained by the trajectory Monte Carlo technique is a clear manifestation of this. We suggest that the negative result of the search for coupling by Assaad *et al.*[13] is due both to the narrow range of Emery model parameters and too high a temperature scale, as well as difficulties in detecting the effect of a small amplitude, which is typical of two-dimensional systems.

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