Interaction of holes in a Hubbard antiferromagnet and high-temperature superconductivity

S. A. Trugman
Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545
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The CuO_2 planes in the high-temperature superconductors are described by a two-dimensional Hubbard model. The model is investigated for an infinite system with one and two electrons less than half filling. The method used is to diagonalize the Hamiltonian exactly within a retained portion of the Hilbert space. A single hole is found not to be localized by a string potential that increases linearly with distance, although it does have a large effective mass. A pair of holes, which naively should be quite mobile, is found instead to be extremely heavy due to a previously unappreciated frustration effect that impedes their motion. This lack of mobility increases the energy of the pair so that they do not bind, contrary to some recently published results using mean-field theory or intuitive arguments. The energy of one- and two-hole states is calculated as a function of wave vector **k**. The comparative energy of different angular momentum channels and magnetic polaron effects are discussed.

The discovery of high-temperature superconductivity[1] has stimulated interest in nonphonon pairing mechanisms. The high transition temperature and the small or vanishing isotope effect[2] are evidence that the superconductivity arises primarily from strongly interacting electrons. Further evidence is provided by observations of antiferromagnetic correlations and anomalous normal-state transport properties.[3,4]

A number of theoretical models have been proposed to describe nonphonon pairing mechanisms.[5-21] Takahashi[16] has independently done a calculation with some similarities to the present one, and finds that holes in the Hubbard model do not bind. Shraiman and Siggia[17] have considered this problem by a generalization of the method of nagaoka[22] and Brinkman and Rice.[23] Recent Monte Carlo calculations indicate that the two-dimensional Hubbard model does not support superconductivity.[18] There are, however, persuasive qualitative arguments why there should be pairing in the nearly half-filled Hubbard model. These arguments are given below (see also Refs. 9 and 16). It is the purpose of this paper to critically consider these qualitative arguments in the light of a quantitative calculation of the hole interaction. The present calculation is *not* a mean-field theory, and as such can assess the accuracy of recently published mean-field approximations.

The copper-oxygen plane may be described by a Hubbard model, in which the sites represent Wannier functions centered on the copper atoms. The copper $d_{x^2-y^2}$ orbitals are half filled in $La_{2-x}Ba_xCuO_4$ when $x=0$, and are less than half filled as x increases. A similar description of the copper-oxygen planes in $YBa_2Cu_3O_{6.9}$ is also possible. The Hubbard Hamiltonian is

$$H_H = -t\sum_{\langle j,k\rangle,s}(c^\dagger_{j,s}c_{k,s}+\text{H.c.})+U\sum_j n_{j,\uparrow}n_{j,\downarrow}. \tag{1}$$

The first term connects nearest-neighbor sites on a square lattice. The holes reside primarily on the copper atoms, as found by Martin and Saxe in their cluster calculation.[13] To write a model in which the holes reside on the oxygen atoms,[8] the Wannier functions would be centered on the oxygen p orbitals, which would again form a square lattice, with the only difference being that the first sum in Eq. (1) would extend over nearest and next-nearest-neighbor sites with approximately equal amplitudes. (This requires that the repulsion U now applies on oxygen sites.) The model considered here has only nearest-neighbor connections.

The Hubbard Hamiltonian may be transformed to an effective Hamiltonian by removing the doubly occupied sites using second-order perturbation theory,[24] a procedure that is valid for filling less than or equal to one electron per site and for moderate to large U. The transformed Hamiltonian is $H=PH_1P$, where P is the projection operator onto the subspace with no doubly occupied sites, and

$$H_1 = -t\sum_{\langle j,k\rangle,s}(c^\dagger_{j,s}c_{k,s}+\text{H.c.})+J\sum_{\langle j,k\rangle}(\boldsymbol{\sigma}_j\cdot\boldsymbol{\sigma}_k-n_jn_k)-t'\sum_{\langle j,k,m\rangle,s}(c^\dagger_{j,s}n_{k,-s}c_{m,s}+\text{H.c.})$$
$$+t'\sum_{\langle j,k,m\rangle,s}(c^\dagger_{j,-s}c^\dagger_{k,s}c_{k,-s}c_{m,s}+\text{H.c.}). \tag{2}$$

Both J and t' are equal to t^2/U, s is a spin label, $\langle j,k\rangle$ are nearest-neighbor sites, and $\langle j,k,m\rangle$ are three distinct adjacent sites, where both (j,k) and (k,m) are nearest neighbors. The t' terms cause a hole to hop to a next-nearest-neighbor site. The J term has the form of a Heisenberg antiferromagnet, and is the only operative term when the band is half filled (one electron per site). The ground state at half filling is assumed to be a Néel antiferromagnet with spin-wave fluctuations, which is supported by Monte Carlo simulations.[25] In this description,

it is convenient to write the spin-spin term in Eq. (2) as

$$\sigma_j \cdot \sigma_k = \sigma_j^z \sigma_k^z + 2(\sigma_j^+ \sigma_k^- + \sigma_j^- \sigma_k^+) . \quad (3)$$

The ground state in the calculations that follow is taken to be that of the $\sigma_j^z \sigma_k^z$ interaction, with the second term treated as a perturbation. (Other assumptions about the ground state have been made, such as the resonant-valence-bond model.[7])

The question being considered is whether two holes in the antiferromagnet have an attractive interaction that can give rise to superconductivity. There are two naive arguments suggesting that the holes will have an attractive interaction for large U: (1) Two separate holes lose the antiferromagnetic exchange energy of 2 J on 4 bonds each, whereas two holes on adjacent sites lose the exchange energy on only 7 bonds together, resulting in a binding energy of 2 J. (Note, however, that a *repulsive* interaction arises because a hole loses delocalization energy since it cannot hop onto the site occupied by the other hole.) (2) A mobile particle with an effective hopping matrix element of $\tilde{t}$ lowers its energy by $z\tilde{t}$ when it delocalizes (the coordination number z is 4 on a square lattice). A single hole appears to be immobile, being tied to a site by a string, whereas a pair of holes should be quite mobile. Thus, if two holes bind they can gain the delocalization energy.

The second point requires elaboration. Suppose a hole, initially at the origin, travels on a straight line by successive application of the hopping term t in the Hamiltonian [Eq. (2)]. The hole leaves in its path a line of spins with the incorrect orientation for an antiferromagnet, resulting in a string energy of 4 J per unit length binding it to the origin (see Fig. 1). In contrast a pair of holes should be able to move rather freely. One of the holes moves one space over, and the other follows it (see Fig. 2). The pair has translated to a degenerate vacuum. Hirsch[9] has given similar arguments for the one- and two-hole motion in the case where the holes are on oxygen sites (see also Ref. 16).

A more careful analysis shows that argument (2) above is incorrect, both for the single hole and for the two-hole mobility. The single hole need not travel on a straight line, trailing a string behind it. In fact, if the hole travels around a square one and a half times, it unwinds the string and finds itself translated to a next-nearest-neighbor site with the background spins undisturbed (no string energy); see Fig. 3. Thus, for large U the hole mass

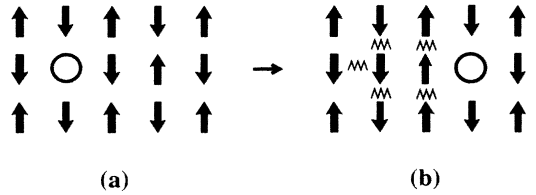

FIG. 1. The hole (a) hops right two times, leaving the spins in configuration (b). The hole leaves behind a line of spins with the incorrect orientation for an antiferromagnet. The high-energy bonds are marked.

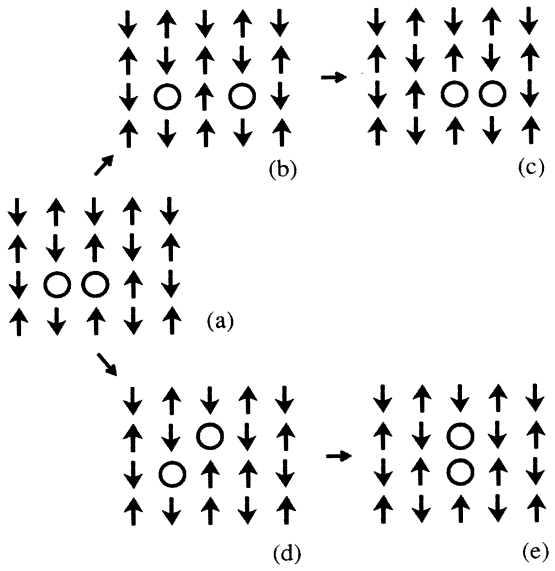

FIG. 2. The t hopping term can cause a pair of holes (a) to make a transition to an excited state (b), and then to a state (c) in which the pair is translated, but no background spins are disturbed. State (c) is degenerate in energy with state (a). The sequence (a) → (d) → (e) is also possible.

is not infinite, corresponding to a string force, but instead is rather large, corresponding to the fact that six rather than two hops are required to reach a second nearest-neighbor site, and that there is an intervening energy barrier as well. The path illustrated in Fig. 3 is the simplest of a family of paths that allow a hole to reach an inequivalent vacuum. If a hole traverses any simple closed curve two steps less than two full circuits, the net effect is to translate the hole two lattice spacings to a state with the same energy as the initial one. The hole translates either diagonally to a next-nearest-neighbor site, or along a coordinate axis to a third nearest-neighbor site. Self-

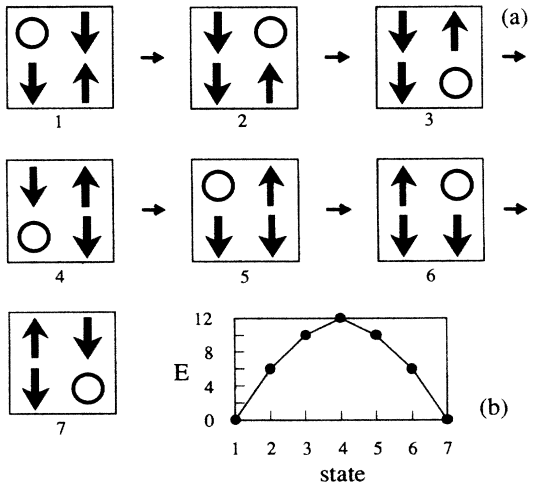

FIG. 3. (a) A hole following the sequence (1) → ··· → (7) translates to a degenerate vacuum (no string is left behind). (b) The energy of the states (1) through (7) in units of J.

intersecting paths (such as a figure 8) do not connect to a degenerate vacuum with this method. The longer paths have an effective t connecting degenerate vacua that decreases faster than exponentially with their length,[26] and will be neglected compared with the path of Fig. 3 in this work. There are, however, exponentially many long paths, and they should be taken into account to obtain quantitative results for extremely large U.

There is another effect contributing to a hole's finite mobility, which arises because the $\sigma^+\sigma^-$ term in Eq. (3) can erase a segment of the string. The t' hopping terms have the same effect. Note, however, that these effects are order t^2/U, and are of negligible importance for large U compared to the $O(t)$ effects identified above.

The argument concerning the two-hole mobility is incorrect for a more subtle reason having to do with frustration, which will be discussed later.

The energy of a single hole and that of a pair of holes is calculated quantitatively by the following method. The single-hole calculation is considered first. A Hilbert space is defined as follows: The first state included is that of a single hole at the origin will all other spins in their antiferromagnetic configuration. The Hilbert space is expanded to include all states that can be reached from the first with one application of the t term in the Hamiltonian [Eq. (2)], which causes the hole to hop to a neighboring site and also leaves the spin at the origin overturned. Also included in the Hilbert space are all states that can be reached from the initial state with either two or three t hops. States that can be reached with a single t' hop [either of the last two terms of Eq. (2)] are included as well, although they turn out to be equivalent to translations of the above states. The motivation for defining the Hilbert space in this way is that to calculate the ground state, the most important states to retain are the lowest energy states.

The Hilbert space includes the states described above, plus all translations of those states on an infinite lattice. Translations are generated as above but with the initial hole state somewhere other than the origin. See Fig. 4. One could define an even larger Hilbert space by including fourth-nearest-neighbor hops, etc., but the size of the space is ultimately limited by the computing power available. The Hamiltonian [Eq. (2)] is diagonalized exactly in the Hilbert space defined.[27] In particular, the $\sigma^+\sigma^-$ terms in Eq. (3) that were neglected in defining the ground state are included in the Hamiltonian, so that they are in a sense treated to infinite order. The problem is formally identical to that of a single particle tight-binding model in a periodic lattice,

$$H_{tb}=\sum_{j,k} t_{j,k}(b_j^\dagger b_k+\text{H.c.})+\sum_j \epsilon_j b_j^\dagger b_j\,. \tag{4}$$

A similar technique has been used by Landman and Shlesinger.[28,29] It is a rather complicated tight-binding model, in that there are 49 basis states per Wigner-Seitz cell for the Hilbert space described. Each diagonal term in the Hamiltonian [Eq. (2)] corresponds to a site energy, and each off-diagonal term to a bond that connects sites in the tight-binding model. The Wigner-Seitz cells are taken to be square. There are bonds between sites in first, second, and third-nearest-neighbor cells. Each eigenstate is indexed by a Bloch wave vector $\mathbf{k}$ in the first Brillouin zone. The tight-binding model has a band structure that has 49 bands for this example. The energy of the hole is the minimum energy over all $\mathbf{k}$ of the lowest energy band. The effective mass of the hole is given by the band width of the lowest energy band.

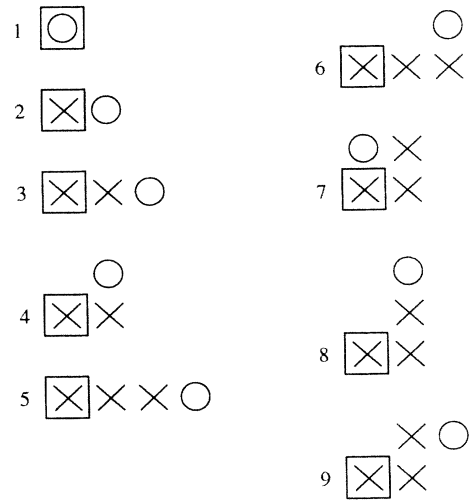

FIG. 4. The Hilbert space used for a single hole is shown. The symbol ○ denotes the hole and the symbol × denotes a spin that is overturned with respect to the antiferromagnetic reference state. All rotations, reflections, and translations of these states are included. The number of overturned spins is the same as the number of t hops required to reach the state.

The Hilbert space for two holes with antiparallel spins $S_z=0$ is similarly defined. The initial state consists of two horizontally adjacent holes, with all other spins in their antiferromagnetic configuration. Any state that can be reached from the initial state with one, two, or three t hops or with one t' hop is included. All translations and rotations (the latter corresponding to an initial state with two vertically adjacent holes) are included. This Hilbert space contains 82 states per unit cell. The holes can be separated by as many as 4 lattice spacings in this variational space. The Hilbert space for two parallel spins is defined the same way, except that the intial state consists of two diagonally adjacent holes. In principle nothing new is learned in the calculation for parallel holes ($S=1$, $S_z=1$), since the $S_z=0$ component of the $S=1$ state is already present in the calculation for antiparallel holes. In practice this is only approximately true, since the approximate Néel antiferromagnetic vacuum used is not rotationally invariant. The numerically obtained ground-state energy for parallel holes is always higher than that for antiparallel holes, and the data for parallel holes will not be presented in detail here.

The calculations are most reliable for intermediate values of U/t. For U/t sufficiently small, neglected terms in Eq. (2) that are higher order in t/U become important. To estimate the lowest reliable U, let r be the ratio of the exact energy gap (energy difference between the first excited state and the ground state) to the gap predicted by Eq. (2). For the two-site, two-electron Hubbard model,

$r=0.75$ for $U=3$ and $r=0.90$ for $U=5.7$. For U/t sufficiently large, a larger Hilbert space is desirable. When $U/t=14$, the highest energy state retained has an energy of 1 (in units of t) higher than the ground state. Results will sometimes be given for U outside this range, as they are hoped to be qualitatively correct. In particular, the large U limit is nonsingular, is simpler to understand, and is often close to the result at the upper end of the above range.

The tight-binding models on which the calculations are performed are difficult to visualize because there are so many states per Wigner-Seitz cell. To make the important ideas more apparent, a *simplified* tight-binding model describing two antiparallel holes with eight states per unit cell is considered. The simplified Hilbert space consists of the initial state with two horizontally adjacent holes and any state that can be reached with one t hop, plus translations and rotations (see Fig. 5).

The bonds marked with a slash correspond to a hopping matrix element of $+t$, in contrast to the usual bonds that represent a matrix element of $-t$. Which bonds are positive and which are negative does not have an absolute physical significance. In particular, by changing the sign defining the amplitude on site j ($|\psi_j\rangle \rightarrow -|\psi_j\rangle$), the sign changes for all bonds connected to site j. The sign change leaves all of the eigenvalues invariant, and is a type of gauge transformation. The sign convention used throughout this work is to number the lattice sites in rows beginning from the upper left, to work on a square lattice with an odd number of sites on each edge, and to order the creation operators defining a state in the order

$$c^{\dagger}_{N,\downarrow}c^{\dagger}_{N,\uparrow}\cdots c^{\dagger}_{1,\downarrow}c^{\dagger}_{1,\uparrow}|O\rangle .$$

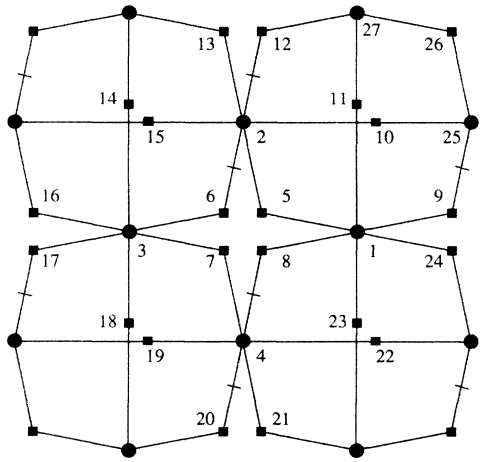

FIG. 5. The figure represents a portion of the infinite simplified tight-binding model for two antiparallel holes, in the limit $U\rightarrow\infty$. States are located near the position of the center of mass of the two holes (small displacements are made so that two sites are not on top of each other). The initial state (and its translations and rotations) are denoted by a circle, and the one t hop states by a square. A line connecting two states represents a hopping matrix element of $-t$, and a line with a slash represents a matrix element of $+t$. For finite U, additional lines would be required to represent matrix elements of strength $\pm t^2/U$.

It is not always possible to remove unwanted $+t$ bonds with a gauge transformation. In particular, whether there are an even or an odd number of $+t$ bonds in a closed loop is a gauge invariant quantity. Some of the loops in Fig. 5 in fact have an odd number of $+t$ bonds, for example the cycle (2, 12, 27, 11, 1, 5). These loops are *frustrated,* in a sense that is analogous to the use of the term in a spin glass.[30] It is straightforward to show that an isolated loop with n sites has a nondegenerate ground state with energy $-2t$ if there are an even number of $+t$ bonds, and a reduced bandwidth and *degenerate* ground state with the higher energy of

$$\epsilon=-2t\cos(\pi/n) \tag{5}$$

if it is frustrated (has an odd number of $+t$ bonds).

The physical reason that the tight-binding model representing two holes (Fig. 5) is frustrated is that the background spins are fermions, and that there are simple motions of the holes that return the entire system to its original state, with two background fermions interchanged. The extra minus sign thus arises from the interchange of two fermions (see Fig. 6). Because the tight-binding model is frustrated, one would expect that the two holes have a delocalization energy and bandwidth that are somewhat smaller than for an unfrustrated tight-binding model [see Eq. (5)].

When the effect of frustration is calculated quantitatively by exactly diagonalizing the Hamiltonian in the protion of the Hilbert space that is retained (8 states per unit cell), the results are far more dramatic. In the $U\rightarrow\infty$ limit, frustration renders the lowest energy band precisely flat [$\epsilon(\mathbf{k})$ is independent of $\mathbf{k}$]. The two-hole delocalization energy is not merely reduced by frustration, *it is reduced to zero.* The system is maximally frustrated. Since the energy is independent of $\mathbf{k}$, it is possible to write down exact localized ground states in the retained Hilbert

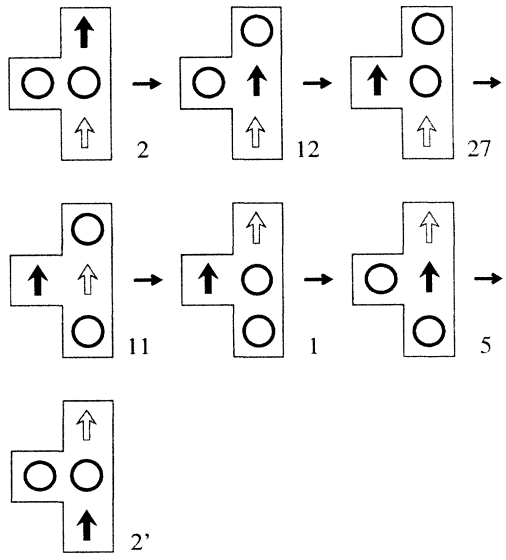

FIG. 6. The holes move so as to interchange the two spin-up electrons (one of the electrons is black). The states are numbered as in Fig. 5.

space. One may verify that the state

$$\psi_1=\psi_2=-\psi_3=-\psi_4=1/(2\sqrt{2}) ,$$
$$\psi_5=\psi_8=-\psi_6=-\psi_7=\tfrac{1}{4} ,$$
$$\psi_9=\psi_{10}=\psi_{11}=\psi_{13}=\psi_{15}=\psi_{20}=\psi_{23}=\psi_{24}=\tfrac{1}{8} , \quad (6)$$
$$\psi_{12}=\psi_{14}=\psi_{16}=\psi_{17}=\psi_{18}=\psi_{19}=\psi_{21}=\psi_{22}=-\tfrac{1}{8} ,$$

with all other $\psi_j=0$ is an exact eigenstate with $\epsilon=-\sqrt{8}$ for the tight-bonding model of Fig. 5. It is in fact a ground state. The astonishing fact that this localized state is an exact eigenstate for this translationally invariant system and does not "leak" into the rest of the infinite lattice to which it is connected can be explained as follows: Consider a zero amplitude site that borders the wave function, such as site (27). When the state [Eq. (6)] time evolves under $i\partial/\partial t\,|\psi\rangle=H\,|\psi\rangle$, the fact that there is a nonzero positive amplitude on site (11) causes site (27) to develop a nonzero positive amplitude. However, because of frustration, site (12) has a negative amplitude and contributes a negative amplitude to site (27) that exactly cancels the contribution of site (11). The net result is that the amplitude of site (27) and all other zero amplitude sites remains zero. The localization that results from frustration is similar to that caused by the magnetic field in the integral quantum Hall effect.

When the Hilbert space is expanded to include two t hops and one t' hop (32 rather than eight states per unit cell), the lowest energy band is still exactly flat. Some, but not all of the excited state bands are also dispersionless. It is only when the Hilbert space is further expanded to include three t hops and one t' hop (82 state per Wigner-Seitz cell) that the bands acquire a small nonzero dispersion.

The numerically obtained ground-state energies for a single hole and for two antiparallel holes are plotted in Fig. 7. The calculation includes three t hops and one t' hop, with 49 basis states per unit cell for the single hole, and 82 for two holes.[31] The lowest energy for a single hole lies below the energy per hole for the two-hole state, so that two holes with antiparallel spins *do not* bind together at any U. Two holes with parallel spins (not plotted) are even higher in energy than two antiparallel holes. The wave vectors $\mathbf{k}$ at which the single hole energies are plotted are chosen because the real-space unit cell is effectively expanded by $\sqrt{2}$ and rotated by 45°. This occurs because a hole in a uniform antiferromagnetic background defines a state with a different spin S_z when translated to a neighboring site. The hole must be translated to a second-nearest-neighbor site to obtain a state with the same S_z. For a single hole, the calculated energy minimum is at $\mathbf{k}a=(0,0)$ for $(U/t)>159$, at $\mathbf{k}a=(\pi/2,\pi/2)$ for $159>(U/t)>3.5$, and at $\mathbf{k}a=(\pi,0)$ for $3.5>(U/t)$. It is not clear whether the transition at $(U/t)=159$ is physical or whether it is an indication that the retained Hilbert space is too small.

The bandwidth for the two-hole state is narrow, consistent with the fact that due to frustration, high-energy states reached through three t hops are required to give the band nonzero dispersion. The effective mass may be

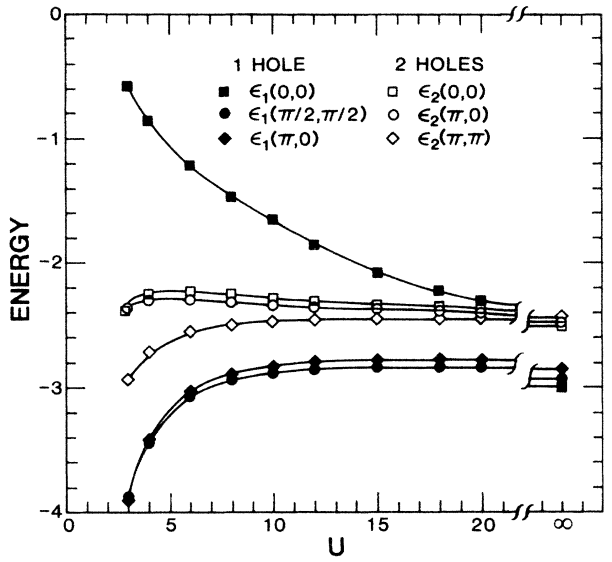

FIG. 7. The ground-state energy is plotted as a function of U for a single hole at three wave vectors $\mathbf{k}$ (filled symbols). The energy scale is chosen so that a hole localized at the origin has an energy of zero, with all energies measured in units of t. The open symbols are the energy *per hole* (with the same energy zero) for the two-hole states plotted at three wave vectors. The three wave vectors plotted in each case include the minimum and maximum energy in the band. There is a break in the U axis at $U>20$, to the right of which the energies at $U=\infty$ are plotted. The energies at different $\mathbf{k}$ cross between $U=20$ and $U=\infty$.

defined through the band width $\Delta\epsilon$ by $m^*/m_0=8/\Delta\epsilon$, which gives $m^*/m_0=1$ for a single electron on a square lattice ($z=4$). The two-hole state has a large effective mass of 78.24 at $U=\infty$ (see Table I).[32] The effective mass is so large that the two-hole state has negligible delocalization energy for large and intermediate U. If the frustration in the two hole tight-binding model were removed by replacing all of the t and t' bonds by $-|t|$ and $-|t'|$, respectively, the two-hole effective mass would

TABLE I. Effective masses for one and two holes, and the spin-spin correlation function for the one-hole ground state at the nearest and next-nearest sites to the hole, as a function of U.

U	m_1^*/m_0	m_2^*/m_0	$\langle\sigma_1\cdot\sigma_2\rangle$
∞	55.12	78.24	−0.154
100	109.42	140.25	−0.274
20	15.17	63.01	−0.399
15	10.58	39.25	−0.449
12	8.04	28.57	−0.496
10	6.53	22.54	−0.539
8	5.47	17.22	−0.597
6	4.32	12.57	−0.679
4	3.11	8.59	−0.799
3	2.41	6.87	−1.313

decrease dramatically to 6.88 at $U=\infty$, and the energy would be lowered sufficiently by delocalization that a bound state would be formed for $8.6 < U < 16.3$. This removal of frustration is, however, unphysical, and the real system does not form a bound state. The single hole also has a large effective mass for large U, reflecting the fact that it must move in a complicated path to unwind its string.

The numerical wave functions provide information about the variational bound states. One hole makes an entire orbit around the other by following the sequence of states (1, 5, 2, 6, 3, 7, 4, 8), or alternatively the sequence (1, 9, 25, 26, 27, 12, 2, 5) in Fig. 5. By examining the wave function on either of these cycles, one can determine the angular momentum of an eigenstate. It is incorrect to merely count the number of zero crossings in the eigenstate, because this number is not gauge invariant. A gauge transformation should first be performed to remove the $+t$ bonds from the cycle.[33] (For the first cycle above, the wave function should be multiplied by -1 on sites 6, 3, 7, and 4.) Over the parameter range $44.5 > U/t \geq 0.01$, the variational ground state for two holes occurs for the wave vector $\mathbf{k}a=(\pi,\pi)$, and is angular momentum zero (an s state). There are small admixtures of other even-parity states, since the square lattice is not rotationally invariant, but only invariant under 90° rotations. Over the parameter range $\infty > U/t > 44.5$, the ground state is at $\mathbf{k}a=(0,0)$, and is degenerate. This is an angular momentum 1, or p state, with small odd-parity admixtures. One can show analytically and confirm numerically that on a square lattice, even-parity eigenstates are nondegenerate, while odd-parity eigenstates are two-fold degenerate. The "bridge" states (sites 10 and 11 in Fig. 5) across the cycle (1, 9, 25, 26, 27, 12, 2, 5) lower the energy of odd-parity states relative to even-parity states, so that an odd-parity state is in fact the ground state for sufficiently large U.

For large U, as a hole travels through the lattice, it tends to leave behind a ferromagnetically ordered state. This effect has been noted by Nagaoka,[22] Nagaev,[34] and by Brinkman and Rice.[23] The effect of a hole on the local magnetic order has been measured by calculating $\langle \sigma_1 \cdot \sigma_2 \rangle$, where 1 and 2 are the hole's nearest-neighbor and second-nearest-neighbor sites (see Table I). The correlation functions are calculated for the one-hole ground state with 49 states per unit cell. The correlation function would be -1 in the antiferromagnetic ground state with no hole present. The correlation function is reduced substantially to -0.154 for $U=\infty$, although it is still negative. As U decreases, the intermediate states become energetically less favorable and the hole is less effective at creating a ferromagnetic domain. The sudden jump at $U=3$ results because the minimum energy occurs at $\mathbf{k}=(\pi/2,\pi/2)$ for $U=4$ and $\mathbf{k}=(\pi,0)$ for $U=3$.[35] The calculated correlation function does not approach $+1$ as $U \rightarrow \infty$, as required by Nagaoka's theorem.[22] This is an indication that a larger Hilbert space is required to obtain quantitative results for very large U, roughly $U > 15$, as discussed above. Other calculations are also unable to reproduce the correct $U \rightarrow \infty$ limit.[17,23]

It appears to be impossible to consistently assign a spin to each of the holes separately for a $S_z=0$ state. Consider the initial state labeled (2) in Fig. 6. The hole on the right occupies a position formerly occupied by a down spin in the Néel state, so that the hole should be assigned an up spin. Similarly, the hole on the left should be assigned a down spin. The assigned spin should travel with a hole as it moves. One may verify that the sequence portrayed in Fig. 6 exchanges the two holes, so that by the end one must assign an up spin to the left hole and a down spin to the right hole in state (2), in contradiction to the original assignment. One may, however, state that the combined S_z of the two spins is zero.

In conclusion, it is found that contrary to expectations, a hole in an antiferromagnet is not bound by a string. Furthermore, due to frustration, a pair of holes is not highly mobile. Both of these effects work against the pairing of holes, and the quantitative calculations indicate that holes do not bind in the range of U investigated. These conclusions are also likely to apply in the presence of short-range antiferromagnetic order.

The fact that a bound pair does not form suggests that Bose condensation may not occur. In two dimensions, two particles with an exclusively attractive interaction will form a bound state, and a finite density of them will Bose condense (in mean-field theory). This is to be contrasted with the situation in three dimensions, where weak attraction results in a Bose condensate but *not* a bound state between two isolated particles.

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