Hubbard model with one hole: Ground-state properties

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The ground state of the two-dimensional Hubbard model on a square lattice is studied in the large-U limit in a half-filled band with a dynamical hole. For a 4×4 lattice with hopping $t=1$ and coupling $J<J_c\approx0.075$, the ground state has zero momentum (**k**) and spin 15/2 (ferromagnetic background). For $J\geq J_c$ the ground state is degenerate with nonzero **k** and spin 1/2, in agreement with recent variational calculations. The nonzero **k** of the ground state comes from a nontrivial phase in the overlap of the spin states before and after a hole move. For small lattices we show that the effective Hamiltonian of the hole is that of a particle moving in a magnetic field. We also find that many of the features of the weak-coupling region carry over continuously to the strong-coupling region.

The understanding of the mechanism underlying high-temperature superconductivity[1] is one of the most challenging problems in condensed-matter physics at present. It is evident that strongly correlated electrons are involved in the phenomenon. Following the observation of antiferromagnetic order in La_2CuO_4 and in $YBa_2Cu_3O_{6+x}$,[2] it was proposed that the quasiparticle excitations in the normal and superconducting phases of these materials are strongly influenced by the spin correlations. Anderson suggested[3] that the spins are in a "resonating-valence-bond (RVB) state" of resonating spin pairs, with each pair coupled to total spin zero. This is suggested to occur for large Hubbard interaction U in an antiferromagnet when doping is included. In the small-U limit, antiferromagnetism occurs through spin-density-wave (SDW) order. In this case the quasiparticles are holes with an associated region of decreased antiferromagnetic order. This spin bag is a spin-$\frac{1}{2}$ charged fermion and leads to a pairing attraction which may account for high-T_c superconductivity in a natural way based on the standard pairing theory.[4]

An important issue is whether similar spin-bag effects occur in the large-U limit as well. In particular, we are interested in whether the antiferromagnetic spin correlations $\langle \mathbf{S}_i\cdot\mathbf{S}_{i+n}\rangle$ at sites near an added hole are reduced in magnitude, by how much and over what range. Also, what is the nature of the ground state of the system in the presence of the hole? Do two such dressed holes, or bags, attract each other? If so, what is the depth and range of the potential? In other words, does a spin-bag picture describe the physics of dynamical holes in the strong-coupling regime as well as in the weak-coupling regime for which it was introduced? In this paper we address the questions related to the physics of a single hole through a numerical study of the strong-coupling limit of the Hubbard model on a two-dimensional square lattice. Note that although many of our conclusions are in qualitative agreement with the spin-bag ideas, our results are independent of them and should be reproduced by any approach to the physics of one hole in the Hubbard model in strong coupling.

The model we study is described by the Hamiltonian

$$H=J\sum_{\mathrm{i},\hat{\mathrm{e}}}(\mathbf{S}_{\mathrm{i}}\cdot\mathbf{S}_{\mathrm{i}+\hat{\mathrm{e}}}-\tfrac{1}{4}n_{\mathrm{i}}n_{\mathrm{i}+\hat{\mathrm{e}}})-t\sum_{\mathrm{i},\hat{\mathrm{e}},\sigma}(\bar{c}^{\dagger}_{\mathrm{i},\sigma}\bar{c}_{\mathrm{i}+\hat{\mathrm{e}},\sigma}+\mathrm{H.c.})\ . \tag{1}$$

Thus, we consider a Heisenberg interaction for the spins and an electron hopping term acting with the constraint of no double occupancy with $J=4t^2/U$ and $t=1$ in the standard notation of the Hubbard model:

$$\mathbf{S}_{\mathrm{i}}=\tfrac{1}{2}\sum_{\alpha\beta}c^{\dagger}_{\mathrm{i}\alpha}\boldsymbol{\sigma}_{\alpha,\beta}c_{\mathrm{i}\beta}$$

is a spin-$\frac{1}{2}$ operator at site **i** of a two-dimensional square lattice with periodic boundary conditions. $\hat{\mathbf{e}}$ denotes unit vectors in the two directions. The operator $\bar{c}^{\dagger}_{i\sigma}$ is defined as $\bar{c}^{\dagger}_{i\sigma}=c^{\dagger}_{i\sigma}(1-n_{i-\sigma})$, where $c^{\dagger}_{i\sigma}$ is the electron creation operator and $n_{i-\sigma}=c^{\dagger}_{i-\sigma}c_{i-\sigma}$ with $n_i=\sum_\sigma n_{i\sigma}$.

As a numerical technique, we use a modification of the Lanczos method.[5,6] The algorithm starts with some initial trial state having a nonzero projection on the exact ground state. Applying H to the trial state we can construct a vector orthogonal to it and by diagonalizing the 2×2 Hamiltonian matrix in that subspace we improve the initial values of the energy and ground state. This process can be iterated. After the starting vector is selected the method spontaneously generates the corrections in a systematic way. It converges to an excellent approximation to the exact result after some number of iterations, depending on the required accuracy in the ground-state energy and wave function.[7]

Due to memory constraints we have worked with a 4×4 lattice[8] in the subspace with $\sum_i S_i^z=\frac{1}{2}$. Since many of the interesting properties of the model are short range in space, we expect these observables to be relatively well represented with this lattice size. We use translation invariance to reduce the dimensionality of the Hilbert space by requiring that our states have a definited momentum. In practice this involves using a basis where each vector represents a linear combination with appropriate phases of the 16 translational copies of a state having a given hole location and spin configuration (both spins and the hole are translated together). Details will be presented elsewhere. After this reduction the number of states is 6435, which presents no computational difficulties, as the present method requires the storage of only a few vectors of this size.

Our results are summarized in Fig. 1. The ground-state energy per site of the Hamiltonian Eq. (1) in the one-hole sector is given in Table I, and the lowest levels in the six independent momentum sectors for various J are given in Table II. We find the remarkable result that the ground state has a finite total momentum $\mathbf{k}=(\pm\pi/2,\pm\pi/2)$, $(0,\pi)$ or $(\pi,0)$ for $J>J_c$ with $J_c\approx0.075$. Thus the ground state is degenerate above J_c. Note that the finite momentum of the ground state was also found in a spin-wave and variational calculation by Shraiman and Siggia.[9] Our numerical results confirm the validity of those approximate calculations [also on previous numerical work on 10-site lattices[10] it was observed that the ground state of one hole had $\mathbf{k}=(3\pi/5,\pi/5)$]. For $J<J_c$ the ground state is ferromagnetic as will be shown (in fact, in a narrow region around J_c, other states with intermediate values of spin become the ground state). By replacing the Heisenberg term in Eq. (1) with an Ising interaction we find that this effect disappears and the ground state has $\mathbf{k}=(0,0)$ for all J. Therefore quantum fluctuations from the transverse spin-spin interaction play an essential role in this result. Exact results on a 3×3 lattice also show this unusual behavior.[11] We have also numerically studied "square" lattices of 8, 10, and 18 sites (the last one for only a few values of the coupling). The aforementioned values of $\mathbf{k}$ already appear in the ground state for the 8-site lattice. In the 10-site lattice those values of $\mathbf{k}$ are not allowed but the ground state has the closest momentum to them. For the 18-site lattice and $J=0.1$ we found that the ground state has a momentum closer to $\mathbf{k}=(\pm\pi/2,\pm\pi/2)$ than to $\mathbf{k}=(0,\pi)$ or $(\pi,0)$, but that may depend on J. From the analysis of different lattice sizes plus the good agreement obtained with spin-wave calculations[9] we believe that our results will survive the bulk limit.

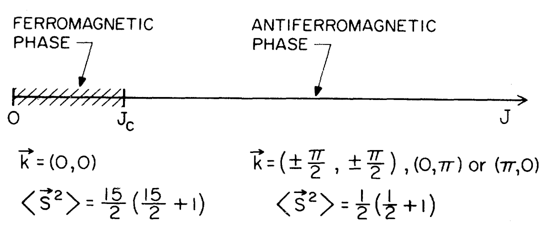

FIG. 1. Schematic phase diagram of the Heisenberg model with a dynamical hole in a 4×4 lattice. $\mathbf{k}$ is the total momentum of the system.

TABLE I. Ground-state energy per site E_1 of the 2D Heisenberg model with one hole on a 4×4 lattice (at $t=1$). For completeness we also include the energy E_0 in the absence of holes. The error is in the last digit.

J	E_1	E_0
0.0	−0.250 000	−0.000 000
0.1	−0.279 237	−0.120 178
0.2	−0.371 506	−0.240 356
0.3	−0.466 585	−0.360 534
0.4	−0.563 352	−0.480 712
0.6	−0.760 078	−0.721 068
0.8	−0.959 552	−0.961 424
1.0	−1.160 85	−1.201 78
2.0	−2.183 10	−2.403 56

To get an intuitive feeling as to why the ground state has a finite $\mathbf{k}$ we solved analytically the 2×2 lattice. Since the total spin is conserved it suffices to consider only the total $S_z=\frac{1}{2}$ manifold, which contains three spin states, $S=\frac{3}{2}$, $\frac{1}{2}$, and $\frac{1}{2}$. The $\frac{3}{2}$ state corresponds to a hole freely hopping in a passive ferromagnetic background, while the doublets are dynamically mixed as the hole hops. The nonzero $\mathbf{k}$ of the ground state is a direct consequence of the nonzero phase of the overlap of the initial and final spin states of a hole move. It is instructive to map this problem onto an effective one-body Hamiltonian in one dimension,

$$H=J\left[\frac{\sigma_z}{2}-1\right]+t\sum_{n=1}^{4}\left(e^{i\sigma_y 2\pi/3}a_{n+1}^{\dagger}a_n+\text{H.c.}\right). \qquad (2)$$

This describes a hole with pseudospin $\frac{1}{2}$ (representing the two spin-$\frac{1}{2}$ states in the physical problem) hopping around a 4-site ring (a_n is a hole operator). The energy eigenvalues are

$$E_{k\pm}=-J+\cos k\pm(J^2/4+3\sin^2 k)^{1/2},$$

with allowed values of k of 0, $\pm\pi/2$, and π. The lowest energy is for $k=\pm\pi/2$ and with the lowest-energy doublet $(-)$ (for $J_c\le J\simeq1$). We believe that the renormalization of the bandwidth, the nonzero $\mathbf{k}$ of the ground state, and related effects on large square lattices all follow from the effect encountered here; as the hole moves the overlap of the spin states is reduced from unit magnitude and has a nontrivial phase ϕ. This phase induces a counter phase from the momentum in order to obtain a low-energy state leading to $k\neq0$.

It is instructive to study a special case of Eq. (2). Consider the limit of $J=0$ in the 2×2 lattice and let us work

TABLE II. Ground-state energy for the six independent momentum sectors on a 4×4 lattice at different values of the coupling J. The error is in the last digit.

k	$J=0.0$	0.2	0.4	1.0	2.0
(0,0)	−0.250 00	−0.355 23	−0.521 66	−1.086 21	−2.081 24
$\left(\frac{\pi}{2},0\right)$	−0.245 25	−0.362 15	−0.546 99	−1.136 63	−2.156 24
$\left(\frac{\pi}{2},\frac{\pi}{2}\right)$	−0.240 09	−0.371 51	−0.563 35	−1.160 85	−2.183 10
$(\pi,0)$	−0.240 09	−0.371 51	−0.563 35	−1.160 85	−2.183 10
$\left(\frac{\pi}{2},\pi\right)$	−0.236 04	−0.365 17	−0.554 58	−1.154 00	−2.182 67
(π,π)	−0.232 46	−0.356 08	−0.526 60	−1.107 49	−2.153 56

in the sector of spin $S=\frac{1}{2}$. We know that for $J=0$ the ground state in fact is in the $S=\frac{3}{2}$ (ferromagnetic phase). However, it is instructive to analyze the subspace that contains the state that will become the ground state for $J\geq J_c$. We solved this problem in a basis where the hole is fixed in a given site while the spins are combined in two linearly independent spin-$\frac{1}{2}$ states represented schematically by

$$\psi^{\pm}=(|\uparrow\downarrow\uparrow\rangle+\gamma_{\pm}|\uparrow\uparrow\downarrow\rangle+\gamma_{\pm}^{2}|\downarrow\uparrow\uparrow\rangle)/\sqrt{3}\ ,$$

where $\gamma=e^{\pm i2\pi/3}$. In this basis the Hamiltonian in the subspace of each of the two doublets can be written as a 4×4 matrix

$$H=\begin{bmatrix} 0 & -t\bar{\gamma} & 0 & -t\gamma \\ -t\gamma & 0 & -t\bar{\gamma} & 0 \\ 0 & -t\gamma & 0 & -t\bar{\gamma} \\ -t\bar{\gamma} & 0 & -t\gamma & 0 \end{bmatrix}. \tag{3}$$

This result is a special case of Eq. (2) after a rotation to the z axis in "isospin" space. By inspection we realize that this matrix is isomorphic to that of a single particle moving on a 2×2 lattice in a nontrivial background gauge field or a particle moving around a 4-site ring coupled to a gauge field. This gauge field ($A_{\mathrm{i,i}+\hat{\mathrm{e}}}=\pm 2\pi/3$) corresponds to a nonzero magnetic field in each plaquette (it cannot be contracted to zero). The ground state of Eq. (2) has a total momentum $\mathbf{k}=(0,\pi)$ or $(\pi,0)$ (or $k=\pm\pi/2$ for a ring) but not (0,0). If we take $\gamma=1$ we obtain the Hamiltonian matrix of a free particle hopping without external fields. That corresponds to a total spin maximum, $S=\frac{3}{2}$ and the ground state has $\mathbf{k}=(0,0)$. We hope to generalize this equivalent Hamiltonian mapping to lattices of arbitrary size. It seems likely that one can always find a basis where the Hamiltonian in the sector with lowest spin (singlet or doublet) can be written as a $N\times N$ matrix (N=number of sites) equivalent to the Hamiltonian of a single particle moving in an external magnetic field. This result may be a first step towards an understanding of some recent speculative ideas about "flux" phases in the Hubbard model.[12]

Note that the momenta of the ground state for $J\geq J_c$ are equal to those of a hole in a Hubbard model with $U=0$ (free theory) with a half-filled band. In fact, we have also solved exactly the Hubbard model on a 2×2 lattice (without any strong-coupling approximation). The results are in excellent agreement with the picture previously presented. After some (very large) critical coupling $U_c\approx 18$ the ground state has momentum $(0,\pi)$ or $(\pi,0)$ and that state continuously maps into the ground state of a hole in a free theory. However, as previously shown, we believe that the physical explanation for the finite **k** of the ground state in strong coupling lies in the phase factors coming from the overlap of rotated wave functions. So the intuitive physics of both limits appears to be different. Nonetheless, it is remarkable that in many respects there is a smooth interpolation between the strong- and weak-coupling regions. Both regions are continuously connected at least in the one-hole sector.

One of the consequences of the ground state having a finite **k** is that spatially extended observables measured with respect to a reference frame moving with the hole may appear nonsymmetric around the hole. In fact the shape observed in some variables resembles the cigarlike distributions found in Hartree-Fock calculations in the context of the spin-bag approach for small U.[4,13] They are a simple consequence of the nontrivial fact that the ground state has a finite momentum. As an example, in Fig. 2 we present our results for $\langle S^z(\mathbf{m})S^z(\mathbf{m}+\hat{\mathbf{e}})\rangle$ (where $\mathbf{m},\mathbf{m}+\hat{\mathbf{e}}$ are two-dimensional vectors corresponding to nearest-neighbor sites measured with respect to a reference frame located at the hole). The diagonal distortion can clearly be seen.

At small J we observed a change in the ground state. At $J_c\approx 0.075$, there is a crossing of levels leading to a new ground state for $J<J_c$ with zero total momentum (other states with total spin between the maximum and minimum are the ground state in a narrow region around J_c so the transition is not completely abrupt). This is reasonable since for $J=0$ we would expect a behavior

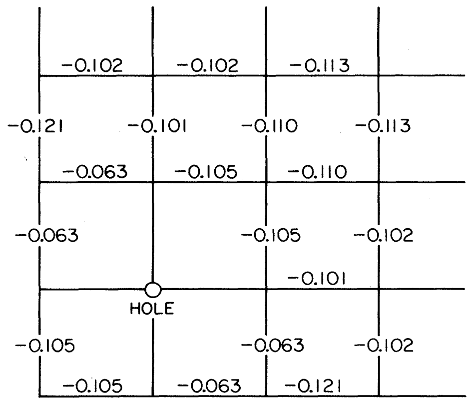

FIG. 2. Correlation functions for a dynamical hole showing asymmetry along a diagonal. [$J=0.4$, $t=1$, $\mathbf{k}=(\pi/2,\pi/2)$].

corresponding to that of a single particle in its lowest energy state at zero momentum and all spins parallel, consistent with Nagaoka's theorem.[14] To test the ferromagnetism expected in this new ground state we measured the total spin $S_{\rm tot}=\langle \mathbf{S}^2\rangle$. For $J<J_c$ we obtain a result $\langle \mathbf{S}^2\rangle=63.7500(1)$ which is in excellent agreement with the maximum spin state of 15 particles, i.e., $\frac{15}{2}(\frac{15}{2}+1)$. In contrast, for $J\geq J_c$ we found $S_{\rm tot}=0.750\,000(1)$ which corresponds to the minimum spin state of our 15 fermions, i.e., $\frac{1}{2}(\frac{1}{2}+1)$. Note that these results are difficult to obtain numerically unless the ground-state wave function is known with high accuracy.[15] Another important detail we learn from measurements of the total spin is that the energies quoted in Table II correspond to states with different values of $\langle \mathbf{S}^2\rangle$. Then, in principle, they should not be interpreted as belonging to the same band.

What is surprising in our results is that while the Nagaoka picture is lost very quickly increasing J, the ground state simultaneously acquires a finite $\mathbf{k}$. The smallness of the critical coupling J_c corresponds to the loss of exchange energy in the ferromagnetic state which scales as the number of spins while the delocalization energy of the hole is approximately independent of the size of the system. For a 2×2 lattice $J_c=0.2629$ (exact result), while it is approximately 0.075 for a 4×4 lattice. Presumably $J_c\to0$ in the thermodynamic limit.[16–18] However, if we interpret our results on a 4×4 lattice with one hole as a good approximation to the bulk limit results at a finite doping fraction ($\frac{1}{16}$), then J_c and the ferromagnetic phase acquire a physical meaning. This is currently under investigation.

We have also obtained information about the bag surrounding the hole. For $0.1\leq J\leq0.4$, correlation function $\langle S^z(\mathbf{m})S^z(\mathbf{m}+\hat{\mathbf{e}})\rangle$ measurements show that the weakest correlation is along a diagonal, due to the elongated shape of the bag, and is between 40% and 50% of the result far from the hole (see, also, Fig. 2). These strong-coupling results are in good agreement with the expected behavior of the spin distortion around the hole as predicted by the spin-bag theory.[4] We have also carried out a numerical calculation of the spin correlation in the Ising limit of Eq. (1) using a random-walk Monte Carlo technique.[19] The Ising model is studied because in this case there are no problems associated with negative signs. Our Monte Carlo study on lattices up to 8×8 sites similarly finds that the antiferromagnetic spin correlation near the hole is reduced about 50% relative to the correlation at large distances from the hole.

In a separate publication we will also discuss results on a 8-, 10-, and 16-site lattice showing that for large J two holes in the Heisenberg model form a bound state. Dynamical properties of the t-J model will also be discussed in that publication.[20]

After completion of this work we received unpublished work[21] with results about one and two holes in the t-J model and where the nonzero $\mathbf{k}$ of the ground state in the one-hole sector is also briefly mentioned.

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[7]Convergence to the ground state is faster for large J in Eq. (1).

[8]The present calculation is close to the limit that can be achieved given the presently known algorithms to attack many-fermion problems. A study of larger lattices using Lanczos algorithms would be very difficult since the dimension of the Hilbert space grows exponentially with the number of lattice sites. On the other hand, Monte Carlo simulations with fermions have the notorious problem of negative determinants at low temperatures even in the one-hole sector of the Heisenberg model.

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[15]To get an accuracy of 10^{-6} in the total spin, we need to get the ground-state energy (used as a criterion for convergence) to an accuracy of 10^{-12}.

[16]Exact calculations on a 3×3 lattice (see Ref. 11) show that there are only two phases as a function of J.

[17]Naively another criterion to check Nagaoka's theorem may have been the calculation of $M(\mathbf{m})=\langle S^z(\mathbf{m})\rangle$, where the distance $\mathbf{m}$ is measured with respect to a reference frame moving with the dynamical hole. We find that for the static case $M(\mathbf{m})$ is staggered, but reducing J we arrive to a situation in which $M(\mathbf{m})$ is positive everywhere, and that may be confused with the ferromagnetic phase. However, $M(\mathbf{m})$ becomes everywhere positive at $J\approx0.5\pm0.1$ on the 4×4 lattice, which is much larger than the actual value $J_c\approx0.075$. $M(\mathbf{m})$ just tell us the way in which the spin-$\frac{1}{2}$ is distributed near the hole.

[18]From the exact solution of the 2×2 lattice we also noticed that for large J there is another crossing of levels this time from $\mathbf{k}=(0,\pi)$ to (π,π). But at large J Eq. (1) is no longer a good approximation to the Hubbard model. The Hubbard model exactly solved on a 2×2 lattice shows only one transition at small J.

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[20]We have also studied the special case $t=0$ (that we define as the static limit). The ground-state energy per site is approximately -1.055 at $J=1$. In this limit there is no dependence on momentum of the energy (infinitely massive hole). We have evaluated the correlation function $C(\mathbf{m},\mathbf{n})=\frac{1}{3}\langle\mathbf{S}(\mathbf{m})\cdot\mathbf{S}(n)\rangle$ in the ground state, where $\mathbf{m}$ and $\mathbf{n}$ are measured with respect to the position of the hole. For the special case where $\mathbf{m}$ is at a distance of one lattice spacing from the hole and $\mathbf{n}$ is at distance two along this axis we found $C(1,2)=-0.1220$, while its value for the Heisenberg model without holes is -0.1170 for a 4×4 lattice [J. Oitmaa and D. D. Betts, Can. J. Phys. **56**, 897 (1978); J. Reger and A. Young, Phys. Rev. B **37**, 5978 (1988)]. (As a check we note that the latter result is approximately recovered at the $\mathbf{m},\mathbf{n}$ pair furthest from the hole.) The increase is approximately of 4%. This result suggests that antiferromagnetism is enhanced in the vicinity of a static hole. This is in agreement with a recent spin-wave calculation in the static limit [N. Bulut, D. Hone, E. Loh, and D. Scalapino, Phys. Rev. Lett. **62**, 2192 (1989); K. Schonhammer (private communication); see, also, R. Joynt, Phys. Rev. B **37**, 7979 (1988)]. Of course dynamical holes quickly reverse this effect as t is increased from zero, thus reducing antiferromagnetism below the value found for a half-filled band. Like in the case of Nagaoka's theorem, it would have been misleading to try to verify the spin-wave prediction by measuring $M(\mathbf{m})=\langle S^z(\mathbf{m})\rangle$. Doing this, the result is that $M(1)$ takes a value -0.207 while $M(2)$ is already 0.152, slowly decreasing to smaller values at a large distance instead of approaching its asymptotic value around 0.3. This is reasonable for a finite lattice, since tunneling between the two possible staggered ground states gives a net staggered magnetization equal to zero. So the fact that $M(1)>M(2)$ cannot be considered as a check of the spin-wave prediction since real effects and tunneling cannot be clearly distinguished.

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