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Holes in the infinite-U Hubbard model: Instability of the Nagaoka state

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The solution of a three-body Schrödinger equation (for two holes and a spin flip) shows that in the $U=\infty$ Hubbard model the saturated ferromagnetic state with two holes is unstable (in a finite volume and for periodic boundary conditions). The ground state carries a finite momentum, and becomes degenerate with the Nagaoka state in the thermodynamic limit. This is in agreement with exact diagonalization results for small lattices where, in addition, we find that the true two-hole ground state is a singlet. As a result, our notions of ferromagnetism in the Hubbard model might need revision.

The Hubbard model was proposed twenty years ago as the simplest model expected to incorporate the essential features of strong correlations. In spite of the great amount of effort in solving this model, very few precise results are available, except in one dimension (1D) where many properties are accessible through the exact Bethe-ansatz solution. Most recently, the Hubbard model has received renewed attention especially motivated by Anderson's[1] suggestion that superconductivity in the high-T_c oxides can be understood already within this simplest model. In this Rapid Communication we do not address the possibility of superconductivity (which is still a highly debated question). Rather, we would like to present new results concerning ferromagnetism, one of the original motivations for the introduction of the model.

Much of the early work on the subject was based on weak-coupling mean-field theory and predicted Stoner-like ferromagnetism[2] for U greater than or equal to the bandwidth, W. More recent slave-boson mean-field theories[3] and variational Monte Carlo–Gutzwiller calculations[4] suggest that if ferromagnetism exists in the Hubbard model it must be restricted to very large values of $U(\gg W)$. We note that the latter results are consistent with the absence of ferromagnetism in intermediate-coupling Monte Carlo simulations.[5] Unfortunately, the only exactly known limits are restricted to $U=\infty$. In particular, for one single hole and $U=\infty$, Nagaoka[6] proved that the ground state of a finite (but arbitrary size) bipartite lattice is a saturated ferromagnet. Also, by working from the paramagnetic, high-hole-density limit, Kanamori[7] showed that a ferromagnetic phase could exist with decreasing hole concentration δ, starting around quarter filling. It is amusing that the slave-boson mean-field theory[3] leads to conclusions consistent with these results.

The above discussion suggests that if ferromagnetism exists at all in the Hubbard model it originates as a continuation of the Nagaoka state to a finite hole concentration and finite values of U. In this paper we will consider the stability of the fully polarized $U=\infty$ state with respect to a single spin flip. We first consider the already nontrivial case of two holes in two dimensions (2D), and then comment on the results of simple variational calculations for the ground state of a single spin flip in the presence of a finite hole concentration. Exact diagonalization results for more than one spin flip, and more than two holes will also be discussed.

We begin with the $U=\infty$ Hubbard Hamiltonian, written in terms of composite creation and annihilation operators, $\tilde{c}_{i\sigma}^{\dagger}=c_{i\sigma}^{\dagger}(1-n_{i-\sigma})$ and $\tilde{c}_{i\sigma}$, respectively, which already contain the constraint of no double occupancy,

$$H=-t\sum_{i,\mathbf{h},\sigma}\tilde{c}_{i+\mathbf{h}\sigma}^{\dagger}\tilde{c}_{i\sigma}\,, \tag{1}$$

where $\mathbf{h}$ is a vector pointing in the direction of the nearest neighbors with a magnitude a equal to the lattice spacing, t is the nearest-neighbor hopping matrix element, and $\sigma=\pm1$ denotes up and down spin components. Two holes in the fully polarized state act as spinless fermions: The bottom of the two-particle band, $E_B=-2t[3+\cos(2\pi a/L)]$, corresponds to occupying the lowest two single-particle states on a size L^2 lattice. One may expect that by modifying the spin background one can reduce the effect of Fermi statistics and regain part of the kinetic energy lost through the antisymmetrization. This is indeed true, as we will now demonstrate by considering the case of a single spin flip.

Starting from the saturated ferromagnetic state (polarized along the $+z$ direction), $|F\rangle$, the most general two-hole single-spin-flip wave function can be written as

$$|\Psi\rangle=\sum_{n,l_1,l_2}\Phi(n,l_1,l_2)S_n^-\tilde{c}_{l_1\uparrow}\tilde{c}_{l_2\uparrow}|F\rangle\,. \tag{2}$$

n,l_1,l_2 represent the positions of the spin flip and two holes, respectively; and $S_n^-=\tilde{c}_{n\downarrow}^{\dagger}\tilde{c}_{n\uparrow}$. The wave function $\Phi(n,l_1,l_2)$ is antisymmetric with respect to the interchange of l_1 and l_2; in addition, it satisfies the "hard-core" constraint $\Phi(n,n,l_2)=\Phi(n,l_1,n)=0$, which prohibits a hole and the spin flip from occupying the same site. The relevant Schrödinger equation is easily derived from Eqs. (1) and (2) and reads,

$$E\Phi(n,l_1,l_2)=t\sum_{\mathbf{h}}[\Phi(n,l_1+\mathbf{h},l_2)(1-\delta_{l_1,n})+\Phi(n,l_1,l_2+\mathbf{h})(1-\delta_{l_2,n})]+t\sum_{\mathbf{h}}[\Phi(l_1,n,l_2)\delta_{l_1,n+\mathbf{h}}+\Phi(l_2,l_1,n)\delta_{l_2,n+\mathbf{h}}]\,. \quad (3)$$

The first two terms on the right-hand side describe the hopping of two independent holes, while the last two describe the interchange of a hole and the spin flip on nearest-neighbor sites.

It is easiest to proceed in momentum space, where Eq. (3) becomes

$$[E-t(k_1)-t(k_2)]\tilde{\Phi}(k_1,k_2;Q)=\frac{1}{N}\sum_{k'}t(Q-k_1-k_2-k')[\tilde{\Phi}(k',k_2;Q)-\tilde{\Phi}(k',k_1;Q)] \quad (4)$$
$$+\frac{g}{N}\sum_{k'}[\tilde{\Phi}(k',k_2;Q)-\tilde{\Phi}(k',k_1;Q)]\,.$$

Here

$$\tilde{\Phi}(k_1,k_2;Q)\equiv\textstyle\sum_{n,l_1,l_2}\exp\{-i[k_1l_1+k_2l_2+(Q-k_1-k_2)n]\}\Phi(n,l_1,l_2)\,,$$

and $t(q)=2t[\cos(q_xa)+\cos(q_ya)]$. In (4) we have already used the antisymmetry with respect to interchanging the two holes; also, we have introduced a fictitious repulsion g which is to be taken to infinity to enforce the hard-core constraint, $\sum_{k'}\tilde{\Phi}(k',k;Q)=0$. The solution is further simplified by rewriting (4) as a $5L^2\times5L^2$ matrix equation for the five quantities,

$$\Psi(k;Q)=\textstyle\sum_{k'}\tilde{\Phi}(k',k;Q)\,,$$

$$\Psi_a^c(k;Q)=\textstyle\sum_{k'}\cos(k_a'a)\tilde{\Phi}(k',k;Q)\,,$$

and

$$\Psi_a^s(k;Q)=\textstyle\sum_{k'}\sin(k_a'a)\tilde{\Phi}(k',k;Q)\ (a=x,y)\,.$$

In addition to solving (4) numerically, we have also studied the low-lying states by a Lanczos exact diagonalization method.[8] In both cases we used periodic boundary conditions.

Our results are summarized in Tables I and II. For the 4×4 lattice (Table I) we compare the eigenvalues for all Q calculated from (4) with those obtained by exact diagonalization. Note that all eigenvalues lie below the bottom of the two-hole band in the Nagaoka state (−6 in units in which $t=1$), and form a very narrow band. The agreement between the two methods required a value of g of at most 10^4. The lowest eigenvalue is threefold degenerate [the degeneracy between (0,0) and (0,π) is a special feature of the 4×4 lattice, while the remaining degeneracy follows trivially from π/2 rotations]. For larger sizes ($N=36$, 64, and 100) the ground state is twofold degenerate and carries momentum (0,π) or (π,0).[9] The ground-state energy for the 6×6 lattice is −7.08876 and for the 10×10 lattice, −7.62400. Our two-dimensional results do not appear to follow a simple (i.e., linear in $1/L^2$) scaling law.

As a simple check of our calculation, we note that, when applied to an even-site one-dimensional Hubbard chain (again in the case of two holes and one spin flip), Eq. (3) leads to a ground state with $Q=\pi$ and $E=-4t(1-\pi^2/2L^2)$, $-2t\pi^2/L^2$ lower than the fully spin-polarized state, in exact agreement with the Bethe-ansatz results.[10] As explained in Ref. 10, in 1D the exact decoupling of spin and charge allows one to remove the node in the two-hole wave function, by absorbing the antisymmetry of the hole wave function into a crystal momentum π for the spin flip. This is equivalent to turning the holes into hard-core bosons, resulting in a lowering of the kinetic energy. There is no similar argument in 2D since there is no simple decoupling of spin and charge degrees of freedom. As already hinted above, it is appealing to interpret the instability of the Nagaoka state (in the finite system) as a result of decreasing the effect of the Fermi statistics through the presence of the spin flip. We believe that, in 2D, the frustration of the spin background arises as a result of the increased degeneracy of the low-lying states available to holes in the presence of the spin flip. At the moment it is not clear to us whether the apparent (discrete) symmetry breaking suggested by a ground state with momentum (0,π) or (π,0) is a special feature of the two-hole problem or whether it is a more

TABLE I. Ground-state energy and momentum for a 4×4 lattice using the exact diagonalization method (Lanczos) and the three-body Schrödinger equation with $g=10^6$. The error is in the last digit.

Lanczos	Schrödinger equation	Q
−6.27808	−6.27808	(0,0),(0,π),(π,0)
−6.14016	−6.14016	(±π/2,±π/2), (π,π)
−6.21184	−6.21184	(0,±π/2), (±π/2,0), (±π/2,π), (π,±π/2)

TABLE II. Ground-state energy and momentum for an 8×8 lattice ($g=10^4$). We show all points along directions [0,1] and [1,1] with energy below the bottom of the two-hole band, $E_B=-7.41440$. The error is in the last digit.

Q	Energy
(0,0)	−7.41696
(π/4,π/4)	−7.41824
(π/2,π/2)	−7.42528
(3π/4,3π/4)	−7.41952
(π,π)	−7.41568
(0,π/2)	−7.43168
(0,3π/4)	−7.43872
(0,π)	−7.44000

general phenomenon.[9] We also mention that our results are consistent with the work of Hashimoto,[11] who showed that *in the thermodynamic limit* there exists a spin-density-wave state [with momentum $(0,\pi)$ or $(\pi,0)$] degenerate with the Nagaoka state.

Although our calculation proves the instability of the Nagaoka state in the case of two holes, we do not yet know the exact ground state in this case. Our Lanczos diagonalization for the 4×4 lattice shows that for two holes further spin flips (we have considered so far at most three spin flips) lower the ground-state energy. This suggests that for two holes the true ground state is a singlet, as we in fact find for eight- and ten-site lattices, in agreement with early numerical indications on very small lattices due to Takahashi.[12,13] Also, this is consistent with the notion that the minimum cost of antisymmetrization is achieved in the spin background with highest degeneracy. (As expected, we have found numerically that the ground state remains a singlet for finite U.) It is, in fact, easy to see how to construct a singlet state with energy lower than those given in Table I, if one starts from the minimum $(S=\frac{1}{2})$ spin sector of a single hole in the Heisenberg antiferromagnet (at $J=0$).[14,15] This state is fourfold degenerate and a singlet state of two holes can thus be constructed by occupying two of the four possible states (at $\pm\pi/2$, $\pm\pi/2$),[16] with little energy cost in antisymmetrization due to the orthogonality of these states. This implies that the ground state carries either momentum close to $(0,0)$ or $(0,\pi),(\pi,0)$ and only degenerate perturbation theory starting from the fourfold degenerate single-hole ground states can select the correct two-hole ground state.

Our quantitative results for more than two holes are very limited. For a 4×4 lattice we find that the fully polarized state is also unstable with respect to a single spin flip for three and four holes. In addition, for an eight-site lattice we also found that the ground state for two or more holes carries the minimum total spin ($S=0$ or $S=\pm\frac{1}{2}$, for an even or odd number of holes, respectively). Qualitatively, since the fourfold degeneracy of the single-hole ground state in the minimum spin sector can accommodate up to four holes, we find it plausible that the ground state for three and four holes carries minimum spin. We cannot, however, rule out the possibility that for more holes the ground-state magnetization increases or even oscillates.

Of course, ultimately one hopes to build a mean-field theory of magnetism in the large-U Hubbard model for finite filling on the basis of the physics learned from simple but nontrivial few-body problems. To this end, we have attempted to study the problem of one spin flip and a finite concentration of holes in the otherwise fully polarized state by using the systematic formulation of the many-body theory for composite operators (such as the $\tilde{c}_{i\sigma}$) proposed by two of these authors. Within the simplest conserving approximation[17] (analogous to the Hartree-Fock approximation of conventional perturbative approaches) the quasiparticle energy of a down-spin electron can be written as

$$E_{k\downarrow}=-(1-n_\uparrow)t(k)+\frac{1}{1-n_\uparrow}\frac{1}{N}\sum_{k'}n_{k'\uparrow}\left[t(k')+\frac{1}{N}\sum_{k''}t(k+k'-k'')n_{k''\uparrow}\right], \tag{5}$$

where $n_{k\uparrow}$ is the free-electron distribution function describing the up spins, and $n_\uparrow$ is the up-spin concentration.[18] It is remarkable that at zero temperature the same result follows from the Gutzwiller wave function[19] (with the *exact* calculation of the kinetic energy) and thus the $(k=0)$ ground-state energy obtained from (5), after adding the contribution from the free up-spin Fermi sea, is a variational bound.[17,18,20] An expression *identical* to (5) can also be derived from a more conventional, perturbative approach which treats three-particle correlations (between the down-spin electron and one-particle hole pair of the up-spin Fermi sea) by solving analytically the three-body Fadeev equations in the infinite U limit.[17,18]

Gutzwiller wave functions [leading to the same expression for $E_{k\downarrow}$ as obtained from (5) at $T=0$] have been also discussed recently by Shastry, Krishnamurthy, and Anderson,[20] who independently studied the single spin flip in the $U=\infty$ Hubbard model. They evaluated (5) for various lattices and found that within this approximation the destabilization of the fully polarized state occurs only for relatively large values of the hole concentration (around quarter filling). In our opinion, the implications of this result are somewhat disappointing since, on the basis of Kanamori's Bethe-Goldstone theory[7] and from the slave-boson calculations,[3] one expects the *complete* destruction of ferromagnetism at similar values of the filling. In fact, the possibility of an instability for very small hole concentrations may be outside the scope of a Gutzwiller-type ansatz. This is best understood by noting that, e.g., in 1D and very close to half filling such an ansatz leads to a ground-state energy *higher* than that obtained for a *fixed* (i.e., infinite mass) spin flip.[17,21] In other words, the local constraint implied by the Gutzwiller wave function simply leads to too rapid a spatial variation of the many-body wave function, and thus to a very high kinetic energy for the spin flip. It then requires a significant hole concentration before flipping the spin balances the Fermi energy.

The physics ignored in the Gutzwiller treatment is the dynamical reaction of the Fermi sea to the motion of the spin flip. In analogy with the two-hole problem, the frustration of the spin background (i.e., the stabilization of the spin flip) should be enhanced by increasing the density of low-lying excitations associated with the x-ray edge like effects of spin flips in the presence of the Fermi sea. In our context, this problem is difficult to treat with (well) known techniques: We are presently attempting to discuss it within our many-body approach for composite operators.[17]

In this Rapid Communication we have shown that the Nagaoka state with two holes is unstable in a finite system. Although in our calculation this appears entirely as a finite-size effect, we expect that the presence of zero-energy bound states (in the thermodynamic limit) may lead to a destabilization of the saturated ferromagnet (i.e., a decrease in the magnetization) for arbitrarily small values of (i) the exchange interaction J and (ii) the hole concentration.

Recently, Trugman[22] has constructed a rigorous proof that for $U=\infty$ and *finite* number of holes (i) there are no two-hole bound states in any spin sector, and (ii) the ferromagnetic state is either the ground state *or* becomes asymptotically degenerate with the ground state in the infinite-volume limit, consistent with our findings.

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