PHYSICAL REVIEW B VOLUME 40, NUMBER 4 1 AUGUST 1989

Instability of the Nagaoka state with more than one hole

B. Doucot
Centre de Recherches sur les Très Basses Temperatures, Centre National de la Recherche Scientifique, Boîte Postale No. 166X, 38042 Grenoble CEDEX, France

X. G. Wen
Institute for Theoretical Physics, University of California, Santa Barbara, California 93106
(Received 24 February 1989)

The infinite-U Hubbard model with a finite number of holes is studied. With two holes, the Nagaoka state is shown not to be the ground state of the model in any dimensions. The one-dimensional model with an arbitrary number of holes is also studied in detail.

The discovery of high-temperature superconductors has stimulated a lot of recent interest for the problem of the motion of holes in quantum antiferromagnets. One of the key ideas of the resonating-valence-bond (RVB) theory is that spin and charge degrees of freedom may decouple in a spin liquid state.[1] However, most studies address the problem of one hole moving in an antiferromagnetic spin background.[2,3] Because hopping of the hole interchanges spins on different sites, one expects to find much weaker antiferromagnetic correlations in the vicinity of the hole. The dipolar texture discussed in Ref. 2 describes the asymptotic configuration of the antiferromagnetic order parameter far from the core region, whose size is expected to grow as t/J increases. When the doping is large enough, these core regions surrounding the holes are likely to overlap, and one obtains a new phase which is determined by the properties of the core. It is then difficult to describe the new ground state of the system by starting from the antiferromagnetic vacuum.

In this limit it becomes interesting to understand better the nature of the spin background which minimizes the kinetic energy of the holes. For this reason we would like to present some new results on the infinite-U limit ($J=0$) of the Hubbard model, where only the kinetic energy term remains in the Hamiltonian. The model has been extensively studied already.[4-6] The main result has been obtained by Nagaoka,[4] who showed that for one hole the ground state has the maximal value of the total spin (we will call such a state a Nagaoka state). More recent work has been devoted to understanding the instability of the ferromagnetic state when a small J is switched on or when there is a finite concentration of holes.[4-6] Although many approximate approaches suggest that the Nagaoka state is stable for small concentrations of holes (with $J=0$), there is no rigorous proof of this assertion and the stability of the Nagaoka state is still an unresolved problem.

Exact diagonalizations of small clusters[7] suggest, however, that the Nagaoka state is destroyed in the presence of two holes, even when J is still set to zero. This is because the exchange energy of the system is lowered in the spin-flipped state. A similar result is obtained using a variational approach for finite concentration of holes ($n>0.5$ on square lattice).[8]

In this paper, we shall first give a detailed discussion of the one-dimensional (1D) case with an arbitrary number of holes. Then the problems associated with generalization to higher dimensions are outlined. In higher dimensions we eventually exhibit a wave function for two holes in a nonferromagnetic state which has a lower energy than the Nagaoka state, proving explicitly that this instability is indeed a quite general phenomenon.

Let us first discuss the 1D Hubbard model in the infinite-U limit. The Hamiltonian may be written as

$$H=-t\sum_{\langle i,j\rangle}(1-n_{i,\sigma})c^{\dagger}_{i,\sigma}c_{j,\sigma}(1-n_{j,-\sigma})\,. \tag{1}$$

In this limit the Bethe-ansatz wave function[9] takes a very simple form. Let us denote by $x_1,\ldots,x_M$ ($x_{M+1},\ldots,x_N$) the coordinates of the up (down) spin electrons, respectively. For an open chain and a given ordering Q of the electrons $x_{Q1}<x_{Q2}<\cdots<x_{QN}$ we have

$$\Psi(x_1,\ldots,x_N)=F(Q)\mathrm{Det}(e^{ik_\alpha x_\beta})\,. \tag{2}$$

The Slater determinant above enforces the antisymmetry of the wave function with respect to the sets of up and down spin coordinates, respectively. Furthermore, it satisfies the constraint of no double occupancy. By simple counting arguments the wave functions (2) span a space of dimension $C_L^N C_N^M$ (where L is the total number of sites on the chain), which is the correct one for M up electrons and $N-M$ down electrons on L sites with no double occupancy.

For a closed chain, Ψ has to satisfy periodic boundary conditions. Ψ is invariant under the change $x_{Q1}\to X_{Q1}+L$ and $Q\to QC$, where C denotes the cyclic permutation

$$\begin{bmatrix}1 & 2 & \cdots & N-1 & N\\ 2 & 3 & \cdots & N & 1\end{bmatrix}.$$

The invariance of Ψ under such a substitution yields

$$F(QC)e^{ik_\alpha L}=F(Q),\quad \alpha=1,\ldots,N\,. \tag{3}$$

Since $C^N=1$, we may summarize the result for the following set of equations:

$$e^{ik_\alpha L}=e^{i\Lambda},\quad F(QC)=e^{-i\Lambda}F(Q)\,,$$
$$e^{i\Lambda N}=1\,,\quad E=-2t\sum_{\alpha=1}^{N}\cos k_\alpha\,. \tag{4}$$

These equations provide a complete solution to the infinite-U Hubbard model for arbitrary numbers of electrons. Let us discuss further the case when L is even, corresponding to an unfrustrated ring. If $N=L-1$ (one hole) the lowest-energy state is obtained for $\Lambda=0$ and a k distribution where the $k=\pi$ state is empty. $\Lambda=0$ is compatible with the Nagaoka state, in agreement with Nagaoka theorem. However, in 1D the ground state has larger degeneracy since the energy depends only on the crystal momentum Λ of the associated spin chain, rather than on the total spin.

If now $N=L-2$ (two holes) and $\Lambda=0$, the lowest-energy state is obtained by removing $k=\pi$ and $k=\pi-2\pi/L$ (or $k=\pi+2\pi/L$) from the k distribution. The energy of such a state is

$$E_0=-2\left(1+\cos\frac{2\pi}{L}\right)=-4+\frac{4\pi^2}{L^2}+O(L^{-4})\,. \quad (5)$$

In (5) and henceforth we set $t=1$. However, if $\Lambda=\pi$ from (4), the k distribution is shifted by π/L and the ground state corresponds to removing $k=\pi-\pi/L$ and $k=\pi+\pi/L$, leading to

$$E_\pi=-2\left(2\cos\frac{\pi}{L}\right)=-4+\frac{2\pi^2}{L^2}+O(L^{-4})\,. \quad (6)$$

We have then $E_\pi-E_0=-2\pi^2/L^2+O(L^{-4})$. As a result the ground state has a spin crystal momentum (Λ) of π, and hence the state is orthogonal to the Nagaoka state. We note that E_0 and E_π correspond to the ground-state energies of two spinless fermions and two hard-core bosons, respectively. It turns out that the crystal momentum of the spins can be used to absorb the minus sign arising from the exchange of two fermions, and thus keep their orbital wave function nodeless. This results in a lower kinetic energy.

Now we ask whether the above mechanism can be transposed to higher dimensions. We know the holes in the Nagaoka state behave as free fermions. As we add holes to the system, the holes have to go to states with higher and higher energy due to the Pauli principle. We may view such an increase in energy as a result of frustration caused by the fermionic statistics. Another way to understand the frustration is to notice that the wave function of the holes changes sign upon interchanging two holes. Thus the wave function must contain nodes which increase the kinetic energy of holes. It therefore might be advantageous to eliminate some of the nodes in the hole wave function and to thereby lower the kinetic energy. This may be achieved by transferring some nodes to the spin part of the wave function at a much lower energy cost. Removing nodes from the hole wave function in some sense resembles changing the statistics of the holes from fermionic to bosonic. Of course there is a competition between this exchange mechanism and the direct Nagaoka effect which favors the ferromagnetic Nagaoka state. We thus expect that the ground-state energy of a system with δN holes to be higher than that of a hard-core boson system, but lower than that of spinless fermion system of equal holes concentration.

These ideas have some special consequences in two dimensions, where one can imagine binding the holes to a texture of the ferromagnetic state which would behave as flux tube and thus change the statistics of the holes. In our 1D example with two holes, the path of exchanging the two holes covers the whole ring. Giving the spin configuration a crystal momentum π completely removes the minus sign coming from the fermionic statistics of the holes, since exchanging the two holes shifts the spin configuration by one lattice spacing. In higher dimensions there are many paths for exchanging the two holes. One may try to assign a crystal momentum π to the spin configurations along the exchange path, but it is impossible to do this consistently for every such path, since the crystal momentum operators for different paths may not commute. A partial solution of this problem would be to bind each hole to a skyrmion in the ferromagnetic state. A skyrmion is a texture in which the order parameter is uniform at infinity and wraps the order-parameter sphere exactly once. When the hole hops in a skyrmion background, the skyrmion texture acts like a "magnetic" flux to the hole. The skyrmion-hole band state is similar to a charge-flux bond state. One might expect that the minus sign associated with part of the exchange paths is removed by the skyrmion texture.

The main drawback of the above proposal is that the presence of the texture renormalizes the hopping amplitude by a factor less than unity even in the large skyrmion limit. This reduces the bandwidth and increases the energy of the holes near the bottom of the band. Strong quantum fluctuations are required beyond this semiclassical picture in order to restore the full hopping amplitude of the hole.

In this paper we take an alternative approach. Instead of binding the holes to a spin texture, we are going to study hole hopping in a fixed spin texture, and see whether a proper fixed spin texture can remove some of the frustration arising from the fermionic statistics and lower the kinetic energy of the holes.

The idea about removing frustration by a fixed spin texture is best illustrated in a system of one hole on a torus with a magnetic flux Φ going through the torus (Fig. 1). Let the torus be a $L\times L$ lattice. In the Nagaoka state, the states of the system are labeled by the positions of the hole, i. The magnetic flux (in a given gauge) changes the boundary conditions on the hole wave function

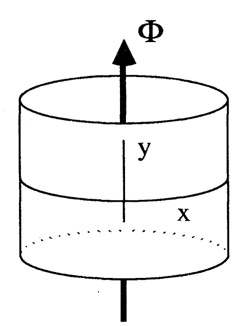

FIG. 1. The torus with a magnetic flux going through it. The two circles on the top and the bottom of the cylinder are identified.

$\psi(i_x,i_y)=e^{i\Phi}\psi(i_x+L,i_y)$. In this gauge, the hopping matrix elements remain real. The energy levels of the holes are given by

$$\varepsilon=-2\left[\cos\left(n_x\kappa_0\frac{\Phi}{L}\right)+\cos(n_y\kappa_0)\right], \tag{7}$$

where n_x and n_y are integers and $\kappa_0=2\pi/L$. We see that the energy of the ground state for nonzero flux is higher than that for zero flux. This increase of the ground-state energy can be interpreted as an effect of frustration introduced by the flux. The frustration is reflected in that the hole wave function acquires a nonzero phase when the hole hops around the cylinder. Notice that such frustration exists only when the hole can hop coherently around the cylinder. When some spins in the Nagaoka state are flipped, the flipped spins may partially destroy the coherence of the hole hopping around the cylinder. Therefore, we expect that with nonzero flux Φ, the Nagaoka state with one hole may not have the lowest energy due to the frustration induced by the flux. The state with flipped spins has less frustration and thus may have lower energy. In fact we have shown that when $\Phi=\pi$ the ground-state energy for one hole and one flipped spin is lower than that of the Nagaoka state (one hole and no flipped spin) by an amount of order $O(N^{-2})$, where $N=L^2$ is the total number of sites.

Now let us consider the hole hopping in a twisted spin configuration. The spin state on site i is given by

$$|S_i\rangle=\begin{pmatrix}\cos(i_x\theta/2)\\ \sin(i_x\theta/2)\end{pmatrix},\quad \theta=\frac{2\pi}{L}, \tag{8}$$

except at the site where the hole is located. This time the states under consideration are again labeled by the position of the hole (Fig. 2). We denote these states by

$$|i,\alpha\rangle=\bigotimes_{j\neq i}|S_j\rangle,\quad i_x,i_y=0,\ldots,L-1, \tag{9}$$

where $|S_j\rangle$ is given in (8). Notice that the spin state $|S_j\rangle$ is independent of j_y.

To obtain the ground state of the (reduced) system we may restrict our attention to states with momentum in y direction $k_y=0$. The problem is thus reduced to a one-dimensional problem. The effective hopping amplitude of the hole in the twisted spin background is given by

$$t_{i_x+1,i_x}=\langle(i_x+1,i_y),\alpha|H|(i_x,i_y),\alpha\rangle=-\cos\frac{\theta}{2},$$
$$t_{0,L-1}=\langle(0,i_y),\alpha|H|(L-1,i_y),\alpha\rangle=+\cos\frac{\theta}{2}. \tag{10}$$

The change in sign of $t_{0,L-1}$ is due to the fact that $|S_0\rangle$ and $|S_L\rangle$, although describing the same spin state, have different signs, i.e., $|S_0\rangle=-|S_L\rangle$. Thus, the hole hopping in the twisted spin background sees a fictitious flux π going through the cylinder. The energy of the hole is given by

$$\varepsilon=-2-2\cos\left(n\kappa_0-\frac{\pi}{L}+\frac{\Phi}{L}\right)\cos\frac{\theta}{2}, \tag{11}$$

where we have included a possible real magnetic flux Φ. We see that when $\Phi=\pi$, the hole in the Nagaoka state and in the twisted spin state have the same energy $\varepsilon=-2-2\cos\pi/L=-2-2\cos\theta/2$. This degeneracy is due to two effects of the twisted spin state which cancel each other: First, the twisted spin state reduces the hopping amplitude and increases the energy of the hole at the bottom of the band; second, the twisted spin state also induces a fictitious flux which cancels the frustration introduced by the external magnetic flux. This second effect reduces the energy of the hole.

In the previous discussion, we only considered the hole hopping in a rigid spin background. We did not include the possibility that the hole may be dressed by spin waves. In this case the local spin configuration near the hole may be distorted and the hopping amplitude can be enhanced by the polarization. To show this, let us consider a modified state of the hole at site i:

$$|i\rangle=\alpha|i,\alpha\rangle+\beta|i\beta\rangle, \tag{12}$$

where α and β are real and $|i,\beta\rangle$ is given by

$$|(i_x,i_y),\beta\rangle=\hat{T}_{(i_x-1,i_y)}|(i_x,i_y),\alpha\rangle-\hat{T}_{(i_x+1,i_y)}|(i_x,i_y),\alpha\rangle. \tag{13}$$

The operator $\hat{T}_i$ flips the spin at site i and is given by $\hat{T}_i=i\sigma^2$. For such a dressed hole the hopping amplitude in x direction is

$$t_{i_x+1,i_x}\equiv-t_x=\langle i_x+1|H|i_x\rangle=-\alpha^2\cos\frac{\theta}{2}-2\alpha\beta\sin\frac{\theta}{2}+\beta^2\cos\frac{\theta}{2}, \tag{14}$$
$$t_{0,L-1}=\langle 0|H|L-1\rangle=+t_x,$$

assuming L is even. The hopping amplitude in y direction is $\langle i_y+1|H|i_y\rangle\equiv-t_y=-\alpha^2$. The energy of the dressed hole becomes

$$\varepsilon=-2t_y-2t_x\cos\left(n\kappa_0-\frac{\pi}{L}+\frac{\Phi}{L}\right). \tag{15}$$

When $\Phi=\pi$, the ground-state energy is $\varepsilon_0=-2t_y-2t_x$. Using the relation $\langle i|i\rangle=\alpha^2+2\beta^2=1$ and minimizing ε_0 by changing β, we obtain

$$\beta=\frac{-\sin\theta/2}{3\cos\theta/2+2}\simeq\tfrac{1}{10}\theta,$$
$$\varepsilon_0=-4+\tfrac{3}{20}\theta^2. \tag{16}$$

The hole in the Nagaoka state with $\Phi=\pi$ has a ground-state energy $-2-2\cos\pi/L=-4+\frac{1}{4}\theta^2$. The dressed hole in the twisted spin background has a lower energy by an amount $\frac{1}{10}\theta^2=(2\pi^2/5)N^{-1}$. We therefore obtain a

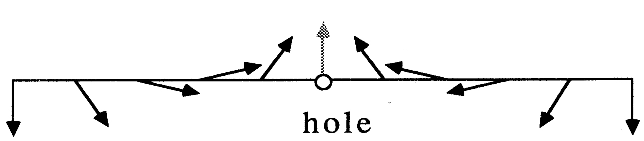

FIG. 2. A hole in a twisted spin configuration.

trial wave function $|\chi\rangle=\sum_i|i\rangle$ such that $\langle\chi|H|\chi\rangle=\varepsilon_0\langle\chi|\chi\rangle$, and hence the Nagaoka state with one hole cannot be the ground state when $\Phi=\pi$ (assuming L is even). We also see that the twisted spin state, lowering the energy by an amount of order $O(N^{-1})$, is much better than the one-spin-flipped state. Certainly the Nagaoka theorem, which only applies to the case with $\Phi=0$, is still correct. The Nagaoka state becomes unstable only after the flux Φ is introduced.

Using the above method we can easily show that the Nagaoka state with two holes is unstable (not the ground state) even in the absence of the magnetic-flux Φ. The Nagaoka state with two holes has the ground-state energy $\varepsilon_N=-6-2\cos\kappa_0=-8+\kappa_0^2$. In the twisted spin background, the two states carrying momentum $\kappa_0/2$ and $-\kappa_0/2$ have the same energy (for the dressed hole):

$$\varepsilon_1=-2t_y-2t_x\cos\frac{\kappa_0}{2}=-4+\tfrac{2}{5}\kappa_0^2\,. \qquad (17)$$

In the ground state, the two states $|\kappa_0/2\rangle$ and $|-\kappa_0/2\rangle$ are occupied by the two holes. The energy of the ground state is given by $-8+\frac{4}{5}\kappa_0^2$. Therefore, the ground-state energy of the two dressed holes in the twisted spin state is lower than that of two holes in the Nagaoka state. The Nagaoka state with two holes cannot be the ground state of the system.

In the above discussion we have treated the two dressed holes as free fermions. This is not quite correct. The two dressed holes interact when they are next to each other. However, such a short-ranged interaction can contribute to the ground-state energy at most a term of order N^{-2}. This is because the wave function of the two holes approaches zero when the two holes are near each other. The energy difference between the Nagaoka state with two holes and the twisted spin state with two holes is $\frac{1}{5}\kappa_0^2=(4\pi^2/5)N^{-1}$. Thus inclusion of the interaction between the holes will not change our previous result when N is large.

We would like to make two remarks. First, although the above discussion is for two-dimensional systems, it can be easily generalized to arbitrary dimensions. Our result still holds in higher dimensions. Second, the spin configuration discussed above does not carry definite crystal momentum. However, the crystal momenta are sharply concentrated near $(k_x,k_y)=(\pi,0)$.[10]

In this paper we have studied the infinite-U Hubbard model. We showed that the Nagaoka state with two holes is not the ground state. Spin configurations may generate a fictitious flux which can reduce the frustration induced by the fermionic statistics and lower the kinetic energy of the holes. This result is supportive of the idea of statistics transmutation in the spin liquid state.[1]

We stress that we have simply found a state with a lower energy than the Nagaoka state. This does not mean our state is close to the true ground state. The most important and unresolved question is what is the ground state of the infinite-U Hubbard model at finite hole concentration. We hope the discussion presented in this paper may shed some light on this problem.

We would like to thank D. Arovas and R. Rammal for helpful discussions. We have learned that Y. Fang, A. Ruckenstein, E. Dagotto, and S. Schmitt-Rink also obtained some of the results in this paper independently using a different approach.[11] This research was supported in part by the National Science Foundation under Grant No. PHY82-17853, supplemented by funds from the National Aeronautics and Space Administration, at the University of California at Santa Barbara.

[1]P. W. Anderson, Science **235**, 1196 (1987); S. Kivelson, D. Rokhsar, and J. Sethna, Phys. Rev. B **35**, 8865 (1987); V. Kalmeyer and R. B. Laughlin, Phys. Rev. Lett. **59**, 2095 (1987); I. Dzyaloshinsky, A. M. Polyakov, and P. B. Wiegmann, Phys. Lett. A **127**, 112 (1988); P. B. Wiegmann, Phys. Rev. Lett. **60**, 821 (1988); Z. Zou, B. Doucot, and B. S. Shastry, Phys. Rev. B **39**, 11 424 (1989); X. G. Wen and A. Zee (unpublished); X. G. Wen, F. Wilczek, and A. Zee, Phys. Rev. B **39**, 11 413 (1989).

[2]B. I. Shraiman and E. D. Siggia, Phys. Rev. Lett. **50**, 740 (1988); **61**, 467 (1988); S. Trugman, Phys. Rev. B **37**, 1597 (1988).

[3]S. Schmitt-Rink, C. M. Varma, and A. E. Ruckenstein, Phys. Rev. Lett. **60**, 2793 (1988); C. Kane, P. Lee, and N. Read (unpublished).

[4]Y. Nagaoka, Phys. Rev. **147**, 392 (1966).

[5]L. B. Ioffe and A. I. Larkin, Phys. Rev. B **37**, 5730 (1988).

[6]L. Roth, J. Phys. Chem. Solids **28**, 1549 (1967); Phys. Rev. **186**, 428 (1969); D. M. Edwards and J. A. Hertz, J. Phys. F **3**, 2191 (1973); J. Kanamori, Prog. Theor. Phys. **30**, 275 (1963); G. Kotliar and A. E. Ruckenstein, Phys. Rev. Lett. **57**, 1362 (1986).

[7]M. Takahashi, J. Phys. Soc. Jpn. **51**, 8475 (1982); Y. Hasegawa and D. Poiblanc (unpublished); J. Bonca, P. Prelovsek, and I. Sega (unpublished).

[8]B. S. Shastry, H. R. Kirshnamurthy, and P. W. Anderson (unpublished).

[9]E. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).

[10]F. D. M. Haldane, Phys. Rev. Lett. **57**, 1488 (1986).

[11]Y. Fang, A. Ruckenstein, E. Dagotto, and S. Schmitt-Rink (unpublished).