RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 40, NUMBER 7 1 SEPTEMBER 1989

Ferromagnetism in the one-band Hubbard model

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(Received 4 April 1989)

We consider the question of ferromagnetism in the one-band Hubbard model on the square lattice with infinite on-site repulsion using exact diagonalization techniques. Our results show a nonmonotonic behavior as a function of the number of holes N_h away from half filling. We find that the spin per electron is generally finite but less than its maximum value and, for a fixed hole number, *increases* with increasing system size. We interpret this as indicating that the infinite-U Hubbard model is ferromagnetic in the thermodynamic limit for a finite fraction of holes, but that there are nonferromagnetic states which are very close in energy.

The considerable activity in trying to understand high-temperature superconductors has aroused interest, once again, in the Hubbard model. While most of the work has investigated the possibility of superconductivity, there remains another long-standing puzzle regarding this model: Namely, is there a ferromagnetic phase? Since the Hubbard model is proposed as a model of itinerant magnetism, among other things, and many itinerant magnets are ferromagnetic, this is obviously a relevant question. A ferromagnetic phase is predicted for large Coulomb repulsion U by the Hartree-Fock approximation[1] and also, though only for even larger values of U, by recent slave-boson mean-field theories.[2]

Since a finite value of U induces an effective *antiferromagnetic* coupling (see below), the most probable region to find ferromagnetism is for $U \to \infty$. Indeed, Nagaoka[3] has proved rigorously that for infinite U, the ground state with one hole away from half filling is a fully aligned ferromagnet for bipartite lattices with periodic boundary conditions. However, one is really interested in knowing whether ferromagnetism persists for a finite *fraction* of holes in the thermodynamic limit and one cannot infer whether or not this is the case from Nagaoka's result. In a recent paper, Shastry, Krishnamurthy, and Anderson[4] prove rigorously that the fully aligned ferromagnetic state (Nagaoka state) cannot be the ground state on the square lattice for hole fraction δ greater than 0.49. In addition, based on their variational calculations, they argue that the Nagaoka state is surprisingly robust. There is, however, no rigorous result that ferromagnetism exists in this model in the thermodynamic limit for any finite hole density.

Here we report on results of the $U=\infty$ one-band Hubbard model on the square lattice obtained by exact diagonalization of clusters of up to $N=16$ sites for various numbers of holes away from half filling. We find a highly nonmonotonic behavior as the number of holes is increased. For one hole with periodic boundary conditions we recover the fully aligned Nagaoka state with spin S given by $S=N_e/2$ where N_e is the number of electrons (so $N_e=N-1$ here, where N is the number of sites). By contrast, the ground state is a singlet for 2 and 6 holes with periodic boundary conditions and has the minimum possible total spin, $S=\frac{1}{2}$, for 1 hole with mixed boundary conditions which are periodic in one direction and antiperiodic in the other. The probable reason for this behavior will be given below. For other numbers of holes we find that S is nonzero, though smaller than $N_e/2$, and increases as N increases. These results indicate that the ground state is presumably ferromagnetic in the thermodynamic limit for $U=\infty$ and a small but finite concentration of holes, but the issue is clearly quite delicate.

The Hubbard Hamiltonian is given by

$$H=-t\sum_{\langle i,j\rangle,\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+c_{j\sigma}^{\dagger}c_{i\sigma})+U\sum_{i}n_{i\uparrow}n_{i\downarrow}\,, \tag{1}$$

where $\langle i,j\rangle$ indicates nearest-neighbor pairs, $c_{i\sigma}^{\dagger}$, $c_{i\sigma}$ are the creation and annihilation operators of an electron in the site i, and $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$. For $U=\infty$, doubly occupied sites never occur and we simply have a problem of constrained hopping, i.e.,

$$H_{\text{eff}}=-t\sum_{\langle i,j\rangle,s}(\tilde{c}_{i\sigma}^{\dagger}\tilde{c}_{j\sigma}+\tilde{c}_{j\sigma}^{\dagger}\tilde{c}_{i\sigma})\,, \tag{2}$$

where $\tilde{c}_{i\sigma}=c_{i\sigma}(1-n_{i,-\sigma})$ and $n_i=n_{i\uparrow}+n_{i\downarrow}$. For U large but finite one can still project out the doubly occupied sites but there is, in addition, an antiferromagnetic term $J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j$, where $\mathbf{S}_i$ is the spin at site i, and $J=4t^2/U$. Hence ferromagnetism is most likely to occur for $U=\infty$, which is the case we consider from now on.

We consider clusters of size $N=L\times L$ where $L=4,\sqrt{10}$ (the sides of this cluster are rotated by $\tan^{-1}\frac{1}{3}$ from the lattice vectors), $\sqrt{8}$ (rotated by $\pi/4$ relative to the lattice), and 2. Our results for the energy as a function of spin for different hole concentrations are summarized in Tables I–IV. Because the calculations are performed in a subspace of fixed total S_z we are unable to compute the energy for spin values less than the spin S_c with minimum energy, because, for $S_z<S_c$, we inevitably obtain the exact ground state with $S=S_c$. However, for $S_z>S_c$, we have $S=S_z$ provided the energy increases monotonically with S, as generally seems to be the case, so the energy can be obtained as a function of S for $S\geq S_c$.

TABLE I. Energy, as a function of hole number and spin, for the $\sqrt{8}\times\sqrt{8}$ lattice with periodic boundary conditions. N_h is the number of holes away from half filling and S_c is the spin of the ground state. For 4 holes, the $S=0$ and 1 states are degenerate.

N_h	S_c	S	Energy
1	$\frac{7}{2}$	$\frac{7}{2}$	−4.000000
2	0	3	−4.000000
		2	−4.690416
		1	−4.690416
		0	−4.898979
3	$\frac{1}{2}$	$\frac{5}{2}$	−4.000000
		$\frac{3}{2}$	−5.179262
		$\frac{1}{2}$	−5.325920
4	0,1	2	−4.000000
		1	−5.830952
5	$\frac{1}{2}$	$\frac{3}{2}$	−4.000000
		$\frac{1}{2}$	−6.332638
6	0	1	−4.000000
		0	−6.928203

In Fig. 1 we plot the spin of the ground state per electron against the hole fraction $\delta=N_h/N$, where N_h is the number of holes away from half filling (i.e., $N_e+N_h=N$) for hole numbers from 1 to 5 with periodic boundary conditions. We see that Nagaoka's result that $S=N_e/2$ for one hole is correctly reproduced, but that $S=0$ for two holes, at least for the sizes studied. For the smaller sizes this result had been anticipated by Takahashi.[5] For greater than two holes, we obtain results which are intermediate between the one and two hole cases, namely S/N_e is finite and increases as $N\rightarrow\infty$. We plot in Fig. 2 the spin of the ground state for the $L=4$ lattice with periodic boundary conditions and with mixed boundary conditions which are periodic in one direction and antiperiodic in the

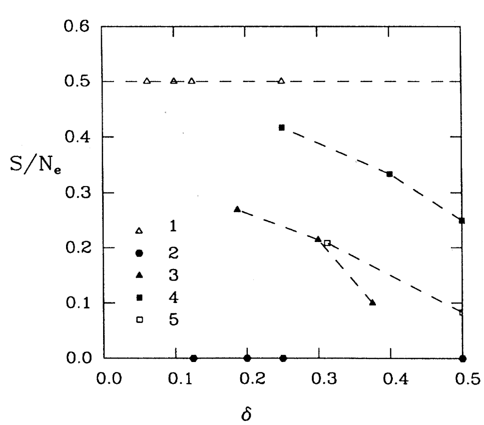

FIG. 1. Spin of the ground state per electron against the hole fraction $\delta=N_h/N$ for periodic boundary conditions. Each symbol represents data for a fixed hole number, as indicated in the legend, for different lattice sizes.

TABLE II. Energy, as a function of hole number and spin, for the $\sqrt{10}\times\sqrt{10}$ lattice with periodic boundary conditions.

N_h	S_c	S	Energy
1	$\frac{9}{2}$	$\frac{9}{2}$	−4.000000
2	0	3	−5.000000
		2	−5.686138
		1	−5.847487
		0	−6.000000
3	$\frac{3}{2}$	$\frac{7}{2}$	−6.000000
		$\frac{5}{2}$	−6.935965
		$\frac{3}{2}$	−7.082377
4	2	3	−7.000000
		2	−8.502177
5	$\frac{1}{2}$	$\frac{5}{2}$	−8.000000
		$\frac{3}{2}$	−8.316343
		$\frac{1}{2}$	−8.343385
6	0	2	−7.000000
		1	−7.993904
		0	−8.004121
7	$\frac{1}{2}$	$\frac{3}{2}$	−6.000000
		$\frac{1}{2}$	−7.617354
8	0	1	−5.000000
		0	−7.211103

other. We see that the behavior is nonmonotonic and depends on the boundary conditions.

How can we understand the curious nonmonotonic behavior in Figs. 1 and 2? It is instructive to consider the Nagaoka state, which is quite simple since the problem is

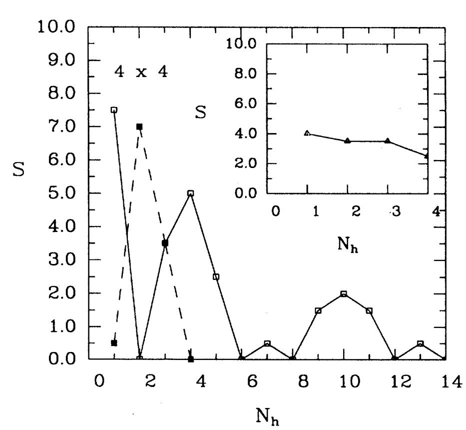

FIG. 2. The open squares show the total spin S, for the 4×4 lattice with periodic boundary conditions for different values of the hole number N_h. The solid squares are the same but with mixed boundary conditions, periodic in one direction and antiperiodic in the other. Inset: The average over these two boundary conditions and is seen to vary much more smoothly with hole concentration than the data for each boundary condition separately.

TABLE III. Energy, as a function of hole number and spin, for the 4×4 lattice with periodic boundary conditions. Except for 5 holes, the energy decreases monotonically as S decreases from $S_{\max}$ to S_c.

N_h	S_c	S	Energy
1	$\frac{15}{2}$	$\frac{15}{2}$	−4.000000
2	0	7	−6.000000
		6	−6.278097
		5	−6.411703
		4	−6.523772
		3	−6.568688
		2	−6.617851
		1	−6.642957
		0	−6.677519
3	$\frac{7}{2}$	$\frac{13}{2}$	−8.000000
		$\frac{11}{2}$	−8.548553
		$\frac{9}{2}$	−8.757522
		$\frac{7}{2}$	−8.820533
4	5	6	−10.00000
		5	−10.81160
5	$\frac{5}{2}$	$\frac{11}{2}$	−12.00000
		$\frac{9}{2}$	−11.90819
		$\frac{7}{2}$	−12.00063
		$\frac{5}{2}$	−12.15913
6	0	5	−12.00000
		4	−12.38707
		3	−12.74177
		2	−13.20195
		1	−13.35133
		0	−13.75547
7	$\frac{1}{2}$	$\frac{9}{2}$	−12.00000
		$\frac{7}{2}$	−12.75661
		$\frac{5}{2}$	−13.31621
		$\frac{3}{2}$	−13.77024
		$\frac{1}{2}$	−14.16114
8	0	4	−12.00000
		3	−13.14163
		3	−13.70990
		1	−14.22336
		0	−14.34751
9	$\frac{3}{2}$	$\frac{7}{2}$	−12.00000
		$\frac{5}{2}$	−13.45856
		$\frac{3}{2}$	−14.06053
10	2	3	−12.00000
		2	−13.80356
11	$\frac{3}{2}$	$\frac{5}{2}$	−12.00000
		$\frac{3}{2}$	−12.34275
12	0	2	−10.00000
		1	−10.79130
		0	−10.81399
13	$\frac{1}{2}$	$\frac{3}{2}$	−8.000000
		$\frac{1}{2}$	−9.194401
14	0	1	−6.000000
		0	−7.569559

then equivalent to that of N_h noninteracting *spin aligned* particles. Because of spin alignment the exclusion principle takes care of the restriction of no double occupancy so the particles are noninteracting. The energy of a hole is, of course, given by $\epsilon = -2t(\cos k_x + \cos k_y)$ where, for the unrotated clusters ($L=2$ or 4 here), $k_x = 2\pi n_x/L$, and $k_y = 2\pi n_y/L$ with periodic boundary conditions, while for the mixed boundary conditions $k_x = 2\pi n_x/L$, and $k_y = 2\pi(n_y + \frac{1}{2})/L$. It is easy to see that with periodic boundary conditions, those cases where S has its minimum value, e.g., $N_h = 2$ and 6, are where the last hole in the Nagaoka state has to go into a single-particle state with a higher energy than that of the other holes. It costs too much energy to promote the last hole in this way and the system gains energy by making a substantial change in the spin arrangement. For the case of 3, 4, and 5 holes with periodic boundary conditions the last hole goes in a state with the same energy as the second hole. Hence these states are not quite so unfavorable as the Nagaoka state with 2 holes, so the spin background does not have to be modified as much and the ground-state spin is intermediate between 0 and $N_e/2$. For a large system and a finite fraction of holes we presume that this nonmonotonic behavior, occurring when the next hole in the Nagaoka state goes in a level of higher energy, will tend to be washed out. For mixed boundary conditions, we also observe an irregular variation with hole number, though the condition for minimum total spin observed for periodic boundary conditions does not seem to be true for this case.

For a finite number of holes our results suggest that the energy of the Nagaoka state and the exact ground state become degenerate as $N \to \infty$, as has been argued by Trugman.[6] This indicates that the holes repel rather than form a bound state, as found earlier[7] for finite U.

While this work was near completion we received copies of unpublished work from Fang *et al.*[8] and Doucot and Wen.[9] Fang *et al.* have shown, by numerical computation, that the Nagaoka state with 2 holes is unstable for periodic boundary conditions and, like us, demonstrated that the ground state is a singlet for $N=8$ and 10. Doucot and Wen have given an analytic argument that the Nagaoka state is unstable with two holes for periodic boundary conditions. Incidentally, it is straightforward to show[10] that with our mixed boundary conditions the trial state of Doucot and Wen for 2 holes gives a *higher* energy than the Nagaoka state. This is consistent with our result that the Nagaoka state is the ground state in this case.

To conclude, we have seen that the spin varies nonmonotonically with hole number but that the main features of this can be understood by looking at the energy

TABLE IV. Energy, as a function of hole number and spin, for the 4×4 lattice with mixed boundary conditions, periodic in one direction and antiperiodic in the other.

N_h	S_c	S	Energy
1	$\frac{1}{2}$	$\frac{15}{2}$	−3.414 214
		$\frac{3}{2}$	−3.557 152
		$\frac{1}{2}$	−3.608 845
		$\frac{9}{2}$	−3.650 197
		$\frac{7}{2}$	−3.682 401
		$\frac{5}{2}$	−3.707 192
		$\frac{3}{2}$	−3.724 825
		$\frac{1}{2}$	−3.736 199
2	7	7	−6.828 428
3	$\frac{7}{2}$	$\frac{13}{2}$	−8.242 641
		$\frac{11}{2}$	−8.688 184
		$\frac{9}{2}$	−8.720 847
		$\frac{7}{2}$	−8.754 569
4	0	6	−9.656 855
		5	−10.232 66
		4	−10.658 63
		3	−10.705 50
		2	−10.788 69
		1	−10.839 35
		0	−10.902 98

of the Nagaoka state. It is reasonable to assume that these rapid variations in S will be washed out for a very large system with a finite *density* of holes. If so, then one may get a better feeling for what happens in the thermodynamic limit by averaging over different boundary conditions. In fact, the total spin *does* vary fairly smoothly when averaged over the two boundary conditions used, as shown in the inset to Fig. 2, for the 4×4 lattice. Furthermore, we find that S/N_e never decreases with increasing size but generally increases, as illustrated in Fig. 1. From these remarks we infer that the one-band Hubbard model with $U=\infty$ probably is ferromagnetic in the thermodynamic limit with a finite density of holes but it appears that there are nonferromagnetic states very close in energy. It is, however, unclear to us whether the ground state is the fully aligned Nagaoka state, or whether the magnetization takes a smaller nonzero value.

One of us (A.P.Y.) would like to thank D. M. Edwards for discussions over several years on the difficulties of understanding itinerant ferromagnetism, which stimulated his interest in this problem. He is also grateful to S. Koonin for a very helpful discussion and to S. Shastry for some stimulating conversations about the work in this paper and Ref. 4. This work was supported in part by National Science Foundation Grant No. DMR 87-21673. J.A.R. is financially supported by the Consejo Nacional de Investigaciones Científicas y Técnicas de la Argentina.

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