Ferromagnetism in the Infinite-$U$ Hubbard Model

Shoudan Liang and Hanbin Pang

Department of Physics,
Pennsylvania State University,
University Park, PA 16802

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Abstract

We have studied the stability of the ferromagnetic state in the infinite-$U$ Hubbard model on a square lattice by approximate diagonalization of finite lattices using the density matrix renormalization group technique. By studying lattices with up to 100 sites, we have found the ferromagnetic state to be stable below the hole density of $\delta_c = 0.22$. Beyond $\delta_c$, the total spin of the ground state decreased gradually to zero with increasing hole density.

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The origin of many unusual electronic properties of high $T_c$ superconductors can be traced to strong electron-electron repulsion in the $CuO$ planes. The Hubbard model is the simplest description of such repulsive interactions. Because of its simplicity the Hubbard model plays a role in many-body problems similar to that of the Ising model in phase transition problems. However, the Hubbard model is still very difficult to analyze. After forty years of research, we are still unsure of even its most basic features \[1,2\]. In this letter, we focus on the infinite-$U$ limit to begin looking for unusual behaviors suggested recently \[3,4\]. There are several reasons for studying this limit. First of all, the antiferromagnetic state at half filling in the large $U$ limit is incompatible with the motion of holes in the metallic phase \[5\]. It is interesting to learn about the spin background preferred by the motion of the holes without the complication of the antiferromagnetic interaction. A well understood infinite-$U$ limit also provides a starting point for systematic expansion in $t/U$. Furthermore, the ground state of the infinite-$U$ Hubbard model at small doping is believed to be ferromagnetic. This provides a mechanism for itinerant ferromagnetism \[6\]. But it is controversial whether there is a finite range of hole density where the ground state is ferromagnetic. This letter provides strong evidence that such a finite region indeed exists for the square lattice. We used the recently developed density matrix renormalization group(DMRG) method to compute the critical hole doping \[7\].

The investigation of the infinite-$U$ Hubbard model has a long history. The earliest rigorous result is due to Nagaoka \[8\], and independently Thouless \[9\], showing that in the case of one hole, the ground state on a bipartite lattice is the ferromagnetic state (also known as
Nagaoka state), where all the spins are aligned in the same direction. Since then, progress on this difficult problem has been slow \[10–16\]. Recently, it has been shown \[17,18\] that for two holes the Nagaoka state is not the ground state. However, the proposed two-hole trial state \[17\] has essentially local ferromagnetic correlation. Shastry et al. considered \[19\] the instability of one spin flip of the Nagaoka state at finite hole density. They shown that the Nagaoka state is unstable when the hole density exceeds \(\delta_c = 0.49\). This result has been improved \[20\] to yield \(\delta_c = 0.41\). The single spin flip state has also been studied by von der Linden and Edwards \[21\] using a more general trial wave function. They shown that the Nagaoka state is unstable against a single spin flip for \(\delta > 0.29\).

By comparing the high temperature expansion coefficients of the infinite-\(U\) Hubbard model with that of a free spinless fermion Hamiltonian, Yedidia \[22\] conjectured that the transition to the non-ferromagnetic state occurs at \(\delta \simeq 3/11\). The high temperature expansion has been extended to higher order by Putikka et al. \[23\]. When the free energy is extrapolated to zero temperature, their calculation suggests \(\delta_c = 0\).

An extensive exact diagonalization investigation \[24,25\] has been carried out using Lanczos method, which is limited to small clusters. A very large finite-size effect has been observed. On a square lattice with periodic boundary conditions, the Nagaoka state is stabilized for the close-shell configurations when the number of holes is 1, 5, 9, .... At other hole fillings the Nagaoka state tends to be destabilized on small lattices because the energy change from one shell to the next is too large. Because of this, the ground-state magnetization oscillates with the number of holes \[24\].
We have studied the stability of the Nagaoka state as well as the nature of the transition to the paramagnetic state by approximate diagonalization on finite lattices. The recently developed density matrix renormalization group method by White [7] and our own extension [26] to two dimensions allow us to perform calculations on much larger lattices than previously possible and with high accuracy.

For $L_x \times L_y$ lattices, when $L_y > 2L_x$ the difficulty of the calculation depends only weakly on $L_y$ [26]. By making $L_y$ suitably long, spacing between the nearest $k_y$ can be made as small as we want and thus the close-shell effect can be eliminated.

Based on diagonalizations of $L_x \times L_y$ lattices with $L_y = 20$, we find the critical hole concentrations for the onset of instability in the Nagaoka state to be almost the same for $L_x = 2, 3$ and 4. This suggests that the critical hole doping we calculated, $\delta_c = 0.22$, is close to the bulk limit. This value is close to but lower than $\delta_c = 0.29$ obtained from Edwards trial wave function [21] for the case of single spin flip. We show in contrary to previous finding [23] that a finite region of hole doping exists below 0.22 where the fully ferromagnetic state is stable.

We calculate the ground-state energy of small clusters using the DMRG method, in which one reduces degrees of freedom by keeping the eigenstates of the density matrix [7]. This is in contrast to the conventional real space renormalization group method where the low energy eigenstates of the block Hamiltonian are kept. An iterative procedure [7] is used to systematically improve the approximation to the density matrix. The DMRG method proves to be highly accurate for one dimensional systems. For quantum spin chains, the
ground-state energy can be calculated to a high accuracy of \(10^{-6}\) \[1\]. When the method is applied to the quasi-one dimensional system of several coupled chains \[20\], the number of states needed to compute the energy to a fixed accuracy grows exponentially with the number of chains, but is independent of the length of the chains. It can also be shown \[26\] that the energy calculated in the finite cluster DMRG method always provides a variational upper bound to the ground-state energy.

We study the one-band Hubbard model with \(U = \infty\) on \(L_x \times L_y\) square lattices with free boundary conditions in both directions. We are restricted to small \(L_x\) because the accuracy of the DMRG method deteriorates at large \(L_x\). In this work, the calculations are done on strips with \(L_x = 2, 3, 4, 5\) and \(L_y = 20\). The large value of \(L_y\) used reduces finite size effects due to the \(k\)-space shell closing discussed previously.

Let \(E_N(Q, S_z)\) be the energy calculated for the system with \(Q\) holes (the number of electrons is \(N - Q\)) and total \(z\)-direction spin \(S_z\) on an \(L_x \times L_y\) lattice with \(N\) sites. The critical hole doping \(\delta_c\) is determined by comparing \(E_N(Q, S_z = 0)\) with the energy of the Nagaoka state, \(E_{\text{nag}}(Q)\), which is the energy of \(N - Q\) spin up electrons on the same lattice. (We assume the number of electrons \(N - Q\) is even. When \(N - Q\) is odd, set \(S_z = 1/2\).) Because of the global SU(2) symmetry of the Hubbard model, the Nagaoka state with total spin \(S = (N - Q)/2\) is \((2S + 1)\)-fold degenerate. One of these states has \(S_z = 0\). Since the DMRG method calculates a variational upper bound to the ground-state energy, we have \(E_N(Q, S_z = 0) \geq E_{\text{nag}}(Q)\), if the ground state is the Nagaoka state. On the other hand, if \(E_N(Q, S_z = 0) < E_{\text{nag}}(Q)\) the ground state is not the Nagaoka state. The smallest hole
doping for which this occurs determines the critical doping \( \delta = Q/N \). Since energy computed in the DMRG method is a variational upper bound, the critical doping \( \delta_c \) we estimated from the condition \( E_N(Q, S_z = 0) < E_{nag}(Q) \) is an upper bound to the true \( \delta_c \).

Since below \( \delta_c \) the exact \( E_N(Q, S_z = 0) \) is equal to \( E_{nag}(Q) \), the difference between the actual \( E_N(Q, S_z = 0) \) calculated and the corresponding Nagaoka energy provides an estimate for the accuracy of our calculations. The accuracy of our calculations in the relevant doping region varies from 0.03% for \( 2 \times 20 \) (with \( M = 52 \)) to 0.5% for \( 4 \times 20 \) lattices (with \( M = 102 \)) (Fig. 1), where \( M \) is the number of states kept.

In Fig. 1, the energy difference \( E_N(Q, S_z = 0) - E_{nag}(Q) \) between the calculated energy and the Nagaoka energy is shown as a function of hole doping \((S_z = 1/2 \text{ if the number of electrons is odd})\). The energies are normalized to \( E_{nag}(Q) \). At critical doping \( \delta_c \), the energy difference changes from positive to negative. The calculated energy \( E_N(Q, S_z = 0) \) reported here are for the largest number of internal states kept. We have not attempted the extrapolation to the infinite-\( M \) limit because we are uncertain about the validity of such an extrapolation and because at the largest \( M \), \( E_N(Q, S_z) \) gives a nice variational upper bound. For \( \delta < \delta_c \), the energy difference is positive and flat. For \( \delta > \delta_c \) the energy difference turns negative abruptly and decreases linearly with \( \delta - \delta_c \) (at least for \( L_x = 2, 4 \)). In Fig. 1(a), the data for \( 2 \times 20 \) and \( 2 \times 30 \) are almost indistinguishable from each other indicating that \( L_y = 20 \) is large enough. Since the number of states needed for calculations with fixed accuracy grows exponentially with the \( L_x \), the errors for \( 5 \times 20 \) (Fig. 1(d)) are considerably larger. Because of this, the energy difference becomes negative at a higher doping.
The condition $E_N(Q, S_z = 0) \geq E_{nag}(Q)$ is a necessary condition for the stability of the Nagaoka state. It only suggests but does not prove the ground state is ferromagnetic. However, for the $2 \times 20$ and $2 \times 30$ lattices when hole doping is smaller than 0.22, $E_N(Q, S_z = 0) - E_{nag}(Q)$ is as small as $10^{-5}E_{nag}(Q)$ which strongly suggest that the true $E_N(Q, S_z = 0)$ is in fact equal to $E_{nag}(Q)$. The ferromagnetic state is at least a degenerated ground state. The similarity between the data for $L_x = 3, 4$ and $L_x = 2$ suggests that the Nagaoka state is stable below about 20 percent doping. Also, the critical hole dopings change very little for $L_x = 2, 3, 4$. This insensitivity indicates that $\delta_c = 0.22$ is close to the bulk limit.

Near $\delta_c$ we also calculated the energy of the lowest state with one spin flipped ($S_z = \frac{N-Q}{2} - 1$). We expect to achieve higher energy accuracy because the dimensions of the Hilbert space is reduced from the $S_z = 0$ case. We have verified that for $L_x = 2, 3, 4$, the $\delta_c$ inferred from the energy with one spin flipped is the same as the $S_z = 0$ case.

To investigate the effects of lattice shape anisotropy on the critical doping $\delta_c$, we introduced hopping anisotropy: $t_x = 0.5$ and $t_y = 1$ on $L_x \times L_y$ lattice with $L_x = 4, L_y = 20$. Remarkably, the critical doping for this system (Fig. 2) is very close to $\delta_c = 0.22$ of the isotropic case (when $t_x = t_y = 1$ in Fig. 1(c)). This insensitivity to hopping anisotropy gives us some confidence that $\delta_c = 0.22$ is close to the bulk limit.

We now discuss the nature of the ferromagnetic to paramagnetic transition after the doping exceeds $\delta_c$. There are two possibilities: (i) the total spin $S$ of the ground state changes discontinuously from the maximum $\frac{N-Q}{2}$ to zero, or (ii) as the hole concentration $\delta$ exceeds the critical doping, the ground-state total spin reduces gradually to zero as $\delta$ is
increased. We can in principle distinguish between these two possibilities by computing the ground state energy $E_N(Q, S_z)$ as a function of $S_z$. In case (i), the energy $E_N(Q, S_z)$ decreases until $S_z$ reaches zero. For case (ii), $S_z$ stops decreasing at $S_c(Q)$ and $S_c(Q)$ goes to zero when $Q$ is increased.

Our data is consistent with case (ii) above namely that there exists a doping region $\delta_c < \delta < \delta_{c1}$ where the ground-state total spin is between $S_{\text{max}} = \frac{N-Q}{2}$ and zero. For $\delta > \delta_{c1}$ the ground-state total spin becomes zero. Fig.3 shows some representative data. In Fig.3(a) for $\delta = 0.3$ on $2 \times 30$ lattice, the ground-state energy $E(Q, S_z)$ drops quickly with decreasing $S_z$ until $S_z = 0.5S_{\text{max}}$. After that the energy is flat. The total spin of the ground state is then $S = 0.5S_{\text{max}}$. The slight increase in the energy from $S_z = 0.5S_{\text{max}}$ to $S_z = 0$ is due to the increased Hilbert space at small $S_z$ which makes the calculation less accurate. At $\delta = 0.5$ (Fig.3(b)), the energy decreases continuously to $S_z = 0$. This implies that the ground state has zero total spin. Similar behaviors are observed for $L_x = 4$. We are unable to determine $\delta_{c1}$ accurately. But it is close to 0.40.

We now discuss technical details of the DMRG calculation specific to the infinite-$U$ limit. A general discussion of DMRG procedures for quasi-one-dimensional systems can be found in Ref. [26]. The chief computational advantage of the infinite-$U$ limit over the full Hubbard model is the reduced Hilbert dimensions. When expanding a block, we add three states per site (empty, spin up and spin down).

The one dimensional system is used to initialize the environment blocks [7,26]. One particular difficulty in the infinite-$U$ limit is that in one dimension all the spin configurations
have exactly the same energy. The total angular momentum is therefore undefined. In the quasi-one-dimensional system, however, this degeneracy is lifted and the ground state has well defined total angular momentum. One can get around this problem by starting from the one dimensional Hubbard model with large $U$ which lifts the degeneracy.

Typically six iterations are performed for each of several values of $M$ (number of internal states kept) starting from small $M$. To preserve the $SU(2)$ symmetry, we always keep the states with the same weight so that the actual number of states kept may be larger than the assigned $M$.

The programming for the DMRG method is much more complex than Lanczos exact diagonalization. Our code for the two dimensional Hubbard model contains over 4000 lines. A crucial issue is how to make sure that the computer program is correct. Our computer code has passed two non-trivial tests. *(i)* Hubbard model satisfies a global spin $SU(2)$ symmetry. For states with zero total spin, the internal states retained should exhibit the $SU(2)$ symmetry. In particular, the states come in $2S + 1$ multiplets, *i.e.* whenever we have a state with $z$-component of spin $S_z = S$ we should also find states having identical weight (the diagonals of density matrix) with $z$-direction of spin being $S - 1, S - 2, ..., -S + 1, -S$.

*(ii)* For spin polarized state with $S_z = \frac{N-Q}{2}$, the computed energy approaches the exact answer.

In conclusion, we have studied the stability of the Nagaoka state in the infinite-$U$ Hubbard model in two dimensions using the density matrix renormalization group method. We found the ferromagnetic state to be stable for a finite doping range near half filling. By computing
energy upper bounds on $L_x \times 20$ lattices with $L_x$ up to 5, we have shown that the Nagaoka state becomes unstable for hole doping larger than 22 percent. The ground-state total spin decreases gradually as the hole doping is increased and becomes zero for more than about 40 percent doping.

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FIGURES

FIG. 1. The critical doping $\delta_c$ is obtained by comparing a variational upper bound of energy, $E$, calculated at doping $\delta$ and $S_z = 0$ (and $S_z = 1/2$ if the number of electrons is odd) with the energy of Nagaoka state, $E_{nag}$. The energy difference, normalized to the Nagaoka energy, is plotted as a function of hole doping. The Nagaoka state becomes unstable when the energy difference is negative. (a) $2 \times 20$ and $2 \times 30$ lattices. The number of states kept in the calculation $M = 52$. The energy accuracy of the variational bounds are 0.03 percent. (b) $3 \times 20$ lattice with $M=62$. (c) $4 \times 20$ lattice with $M=102$. (d) $5 \times 20$ lattice with $M=120$.

FIG. 2. Same as Fig.1(c) but with anisotropic hoping $t_x = 0.5$ (in the short direction of the lattice) and $t_y = 1$. $M$ is 120.

FIG. 3. The ground-state energy $E(S_z)$ as a function of $S_z$ calculated at $M=62$. (a) At doping $\delta = 0.3$, the energy decreases as the spins are flipped from the Nagaoka state until $S_z \simeq 0.5S_{max}$, where the $S_{max}$ is the spin of the Nagaoka state. The total spin of the ground state is then close to $0.5S_{max}$. (b) At larger doping $\delta = 0.5$, the energy decreases continuously. The ground-state total spin is zero.
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E(S_z) vs. S_z/S_{max}

2X30, δ=0.3
$E(S_z) \propto 2X30, \delta=0.5$