Stability of the Nagaoka state in the one-band Hubbard model

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We discuss the stability of the saturated ferromagnetic state of the one-band Hubbard model in the thermodynamic limit. We prove rigorously that the Nagaoka state is stable on a d-dimensional ($d=2,3$) simple-cubic lattice if the number of holes N_h is less than N_Λ^α, $0\le\alpha<1/2d$. Finally, we explain briefly why the Nagaoka state is probably unstable when $N_h \gg N_\Lambda^{1/2d}$.

An understanding of strongly-correlated electron systems becomes increasingly important in present-day condensed-matter physics. Apart from its possible relevance to high-temperature superconductivity, the Hubbard model, which is the simplest strongly correlated electron model, could also be the right model for itinerant ferromagnetism. In fact, the only known rigorous result about itinerant ferromagnetism, the Nagaoka theorem,[1-3] was derived from the infinite-U Hubbard model. Unfortunately, despite extensive work over many years, this model and itinerant ferromagnetism are still poorly understood. Recently, many physicists have actively pursued these problems.[4-8] In particular, in Ref. 8, we proved that the Nagaoka saturated ferromagnetic state is stable in the thermodynamic limit when the number of holes, N_h, is finite. However, the problem of whether the Nagaoka state is stable when the density of holes is finite in the thermodynamic limit is still unsettled. The authors of Ref. 7 showed that the Nagaoka state is unstable if the hole concentration is larger than 0.49. Very little is known about smaller-hole-concentration cases.

In a recent paper, Barbieri *et al.*[9] showed that, when $N_h \ll \ln N_\Lambda$ (N_Λ is the number of lattice sites) in two-dimensional or $N_h \ll N_\Lambda^{1/3}$ in three-dimensional lattices, the Nagaoka state is locally stable in the thermodynamic limit. Although the density of holes is zero in their case, their results give us a deeper understanding about the stability of the Nagaoka state. In this article, we show that results of Ref. 9 can be greatly improved in the two-dimensional case, using a technique we developed in Refs. 3 and 8. And our proof is mathematically rigorous.

Our main results can be summarized in the following theorem.

Theorem: Let Λ be a d-dimensional simple-cubic lattice. Let $N_\Lambda=L^d$ be the number of lattice sites and N_h be the number of holes. Then, the Nagaoka state is stable in two dimensions (three dimensions) as $N_\Lambda\to\infty$, if $N_n \sim N_\Lambda^\alpha$ with $0\le\alpha<\frac{1}{4}$ ($0\le\alpha<\frac{1}{6}$).

The strategy of our proof is simple. We first use the variational principle to find an upper bound to E_g, the energy of the exact ground state. In fact, we choose the Nagaoka state as the trial function. Then we obtain a lower bound to E_g by a well-known lemma in matrix theory. Finally, we show that these bounds approach the same quantity in the thermodynamic limit under the conditions stated in the theorem.

This article is organized in the following way. We shall first introduce some necessary notation and terminology. Then we write the Hamiltonian in matrix form and make some important observations. After these preparations, we prove the theorem. Finally, we make several remarks.

Take a finite lattice Λ. With an infinite on-site repulsion, the Hubbard Hamiltonian reduces to

$$H=P\sum_\sigma\sum_{\langle ij\rangle} t(c_{i\sigma}^\dagger c_{j\sigma}+c_{j\sigma}^\dagger c_{i\sigma})P\ , \tag{1}$$

where $c_{i\sigma}^\dagger$, $c_{i\sigma}$ are the creation and annihilation operators of an electron with spin σ at site i and $\langle ij\rangle$ indicates nearest-neighbor pairs. In formula (1),

$$P=\prod_{i\in\Lambda}(1-n_{i\uparrow}n_{i\downarrow}) \tag{2}$$

is the projection operator that projects wave functions to the subspace without double occupation at each site. Although our results can be proven for either sc, bcc, fcc, or hcp lattices, we shall stick with a square lattice with $N_\Lambda=L^2$ sites for definiteness. There is one point that is worth mentioning. With respect to the Hamiltonian (1), sc and bcc lattices are bipartite; i.e., their sites can be divided into two separate groups such that an electron does not hop among sites belonging to the same group. In this case, the sign of t does not make any difference. But, for fcc or hcp lattices, our theorem only holds under the condition $t>0$. One can find a detailed discussion about this subject in Nagaoka's original paper (Ref. 1). Furthermore, we shall impose the open boundary condition on lattice Λ for technical convenience.

Following Nagaoka, we shall introduce a set of orthogonal and normalized many-body wave functions which completely span the Hilbert space. In doing that, we have to be cautious about the order of the electron operators. First of all, we define an order among the lattice sites by alphabetical order. Setting up a coordinate system, we assign a pair of integer coordinates (x,y) to each site of Λ. Take two sites $i=(x_1,y_1)$ and $j=(x,y_2)$. If $x_1<x_2$, then we define $i<j$. When $x_1=x_2$, the order of i and j is determined by their y coordinates. By alphabetical order, $y_1<y_2$ implies that $i<j$. With this order, we now introduce

$$\Psi(j_1,\ldots,j_{N_\Lambda};\alpha)=\prod_{k=1}^{N_h}(-1)^{j_K-k}c^\dagger_{1,\sigma_1}\cdots c^\dagger_{j_1-1,\sigma_{j_1-1}}c^\dagger_{j_1+1,\sigma_{j_1+1}}\cdots c^\dagger_{j_{N_h}-1,\sigma_{j_{N_h}-1}}c^\dagger_{j_{N_h}+1,\sigma_{j_{N_h}+1}}\cdots c^\dagger_{N_\Lambda,\sigma_{N_\Lambda}}|0\rangle \ . \quad (3)$$

In (3), $|0\rangle$ denotes the vacuum state and α stands for the spin configuration

$$(\sigma_1,\ldots,\sigma_{j_1-1},\sigma_{j_1+1},\ldots,\sigma_{j_{N_h}-1},\sigma_{j_{N_h}+1},\ldots,\sigma_{N_\Lambda}) \ . \quad (4)$$

Since there are N_h creation operators missing in $\Psi(j_1,\ldots,j_{N_h};\alpha)$, the wave function contains N_h holes located at sites $j_1<j_2<\cdots<j_{N_h}$. The phase factor in (3) deserves more explanation. With this factor, the signs of the nonzero Hamiltonian matrix elements are negative when one hole changes order with no hole or an even number of holes (for an odd number of holes, the matrix elements are positive). To see that, we rewrite the Hubbard Hamiltonian

$$H=P\sum_\sigma\sum_{\langle ij\rangle}(-t)(c_{j\sigma}c^\dagger_{i\sigma}+c_{i\sigma}c^\dagger_{j\sigma})P \ , \quad (5)$$

and use the anticommutation relations. A direct calculation yields the above conclusions. Letting $(j_1,j_2,\ldots,j_{N_h})$ and α run separately over all the possible configurations, we obtain a set of wave functions. Obviously, they are orthogonal and normalized. It is easy to show that they are a basis of the Hilbert space with N_h holes and without double occupation. In terms of them, we can write the Hamiltonian in a matrix that has the following characteristics.

(i) Since the Hamiltonian preserves $N_\uparrow$ and $N_\downarrow$, which are, respectively, the number of up-spin and down-spin electrons, the matrix H is formed by some square submatrices along its principal diagonal line. Other elements of H are 0's. Each of these submatrices corresponds to a specified pair $N_\uparrow=n_1$ and $N_\downarrow=n_2$. Obviously, the lowest eigenvalue of H coincides with the lowest eigenvalue of some submatrix $H(n_1,n_2)$. Therefore, we can concentrate on these submatrices.

(ii) Since the Hamiltonian contains only hopping terms, all the elements along the principal diagonal line in $H(n_1,n_2)$ are 0's. Furthermore, the nonzero elements are either t or $-t$. For convenience, we call a pair of wave functions $\Psi_1=\Psi(j_1,\ldots,j_{N_h};\alpha)$ and $\Psi_2=\Psi(j'_1,\ldots,j_{N'_h};\beta)$ superneighbors if they contribute a nonzero matrix element $\langle\Psi_1|H|\Psi_2\rangle$. It is not difficult to see that, for Ψ_1 and Ψ_2 being superneighbors, some j_k and j'_k must be nearest-neighbors in the lattice Λ and the rest of the sites should be identical, since the Hamiltonian can only change the position of one electron each time. Therefore, any wave function has, at most, zN_h superneighbors where z is the number of the nearest-neighbors of each site in Λ. On the other hand, if $N_h\le\frac{1}{2}N_\Lambda$, then there is at least one wave function Ψ which has exactly zN_h superneighbors. For instance, Fig. 1 represents such a wave function. In other words, each row of $H(n_1,n_2)$ can have, at most, zN_h nonzero elements, while, for $N_h\le\frac{1}{2}N_\Lambda$, there must be one row which has exactly zN_h nonzero elements.

These observations are indispensable to our proof.

Proof of the theorem. We first find a good lower bound to the lowest eigenvalue E_g of $H(n_1,n_2)$. This is achieved by applying the following lemma.

Lemma: Let $A=(a_{ij})$ be an $n\times n$ matrix. Any eigenvalue λ of it must satisfy at least one of the following inequalities.

$$|\lambda-a_{ii}|\le\sum_{k\ne i}|a_{ik}|, \quad i=1,2,\ldots,n \ . \quad (6)$$

One can find a proof of this lemma in Ref. 3.

In our case, all the matrix elements a_{ii} vanish and $|a_{ik}|$ are either 0 or t.

Therefore, any eigenvalue of $H(n_1,n_2)$ satisfies

$$|\lambda|\le t \text{ times the largest number of the nonzero elements in a row} = t(zN_h) \ , \quad (7)$$

i.e.,

$$-zN_ht\le\lambda\le zN_ht \ . \quad (8)$$

In particular, inequality (8) holds for the lowest eigenvalue E_g. Therefore,

$$-4N_ht\le E_g \quad (9)$$

for $z=4$ in the two-dimensional square lattice.

To get an upper bound to E_g, we take the Nagaoka state as our trial function. Let

$$\Psi_{\text{trial}}=\sum_{\{j_1,\ldots,j_{N_h}\}}\Psi(j_1,\ldots,j_{N_h}) \ . \quad (10)$$

In (10), the spin configuration index α is dropped because all of the spins are up in the Nagaoka state. The variational principle tells us that

$$E_g\le\langle\Psi_{\text{trial}}|H|\Psi_{\text{trial}}\rangle/\langle\Psi_{\text{trial}}|\Psi_{\text{trial}}\rangle \ . \quad (11)$$

Notice that Ψ_{trial} is a linear combination of $\Psi(j_1,\ldots,j_{N_h})$ with equal weight. Therefore, evaluation

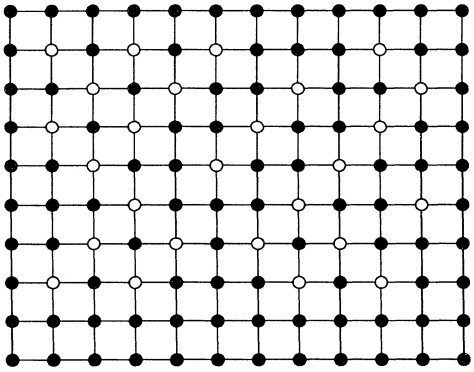

FIG. 1. The configuration of a wave function having exactly zN_h super-neighbors. ● Electron. ○ hole.

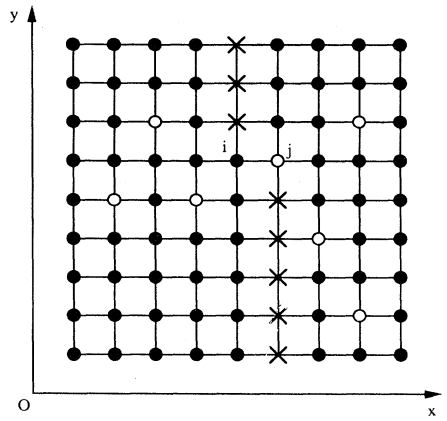

FIG. 2. The positions between sites i and j are marked by a cross.

of (11) can be reduced to a problem of combinatorics. In particular, the denominator in (11) is

$$C_{N_\Lambda}^{N_h}=\frac{N_\Lambda!}{N_h!(N_\Lambda-N_h)!}\ , \tag{12}$$

which is the number of ways to distribute N_h particles among N_Λ lattice sites, subject to the condition that no double occupation is allowed. Calculation of the numerator is also straightforward but a little cumbersome. For the reader's convenience, we shall show it in detail.

Consider a term of H

$$h_{ij}=(-t)P(c_j c_i^\dagger+c_i c_j^\dagger)p \tag{13}$$

(the spin index σ is dropped). The pair of sites i and j are in either a vertical line or a horizontal line. Therefore, the Hamiltonian can be split up into two sums, H_v and H_h. H_v (H_h) contains only vertical hopping terms (horizontal hopping terms). With respect to alphabetical order, a vertical hopping term cannot change the order of holes since i and j have the same x coordinate. Therefore, all the nonzero matrix elements to which a vertical hopping term contributes are $(-t)$'s as we said before. Furthermore, if $\langle\Psi_1|h_{ij}|\Psi_2\rangle=-t$, then either i or j must be a hole and another is occupied. In Ψ_1 and Ψ_2, the hole and the electron change positions. Therefore, the expectation of h_{ij} in the Nagaoka state is $-2tC_{N_\Lambda-2}^{N_h-1}$, which is the number of ways to distribute N_h-1 holes (one hole sticks with bond $\langle ij\rangle$) among $N_\Lambda-2$ available positions (sites i and j are excluded). The factor 2 comes from two possible choices i and j for the hole sticking with them. Since there are more than $N_\Lambda-4L$ vertical bonds in Λ, the expectation of H_v satisfies

$$\langle\Psi_{\text{trial}}|H_v|\Psi_{\text{trial}}\rangle\le-2tC_{N_\Lambda-2}^{N_h-1}(N_\Lambda-4L)\ . \tag{14}$$

Next, we calculate the expectation of H_h, the horizontal part of the Hamiltonian.

Take a horizontal bond $\langle ij\rangle$. Assume that $i<j$. Then, there are $L-1$ lattice sites between them with respect to alphabetical order. In Fig. 2, these sites are marked by crosses. There are two cases which we have to consider separately. (a) There are no holes or an even number of holes between i and j. (b) There are an odd number of holes between i and j.

In case (a), the nonzero matrix elements are $-t$. Assume that there are $2k\le L-1$ holes between i and j. Distributing these holes among $L-1$ available positions gives a factor C_{L-1}^{2k}. Therefore,

$$\langle\Psi_{\text{trial}}|h_{ij}|\Psi_{\text{trial}}\rangle_{2k}=-2tC_{N_\Lambda-(L+1)}^{N_h-(2k+1)}C_{L-1}^{2k} \tag{15}$$

where $\langle\ \rangle_{2k}$ indicates a 2k-holes-between-i-and-j sector.

In case (b), the matrix elements are t's. Therefore,

$$\langle\Psi_{\text{trial}}|h_{ij}|\Psi_{\text{trial}}\rangle_{2k+1}=2tC_{N_\Lambda-(L+1)}^{N_h-(2k+2)}C_{L-1}^{2k+1}\ . \tag{16}$$

Summing up these contributions, we obtain

$$\begin{aligned}\langle\Psi_{\text{trial}}|h_{ij}|\Psi_{\text{trial}}\rangle&=\sum_{k=0}^{L-1}\langle\Psi_{\text{trial}}|h_{ij}|\Psi_{\text{trial}}\rangle_k\\&=2t\sum_{k=0}^{L-1}(-1)^{k+1}C_{N_\Lambda-(L+1)}^{N_h-(k+1)}C_{L-1}^{k}\ .\end{aligned} \tag{17}$$

Under the conditions stated in the theorem, i.e., $N_h\sim N_\Lambda^\alpha$ with $0\le\alpha<1/2d$, the sum in (17) is negative when N_Λ is sufficiently large. (In fact, by following the analysis from (19) to (25), one can show that the sum is approximately $[-2tN_h+o(1)]C_{N_\Lambda}^{N_h}/N_\Lambda$ where $o(1)$ is an infinitesimal quantity) Multiplying this quantity by the number of horizontal bonds in Λ, which is more than $N_\Lambda-4L$, we obtain

$$\langle\Psi_{\text{trial}}|H_h|\Psi_{\text{trial}}\rangle\le2t(N_\Lambda-4L)\left[\sum_{k=0}^{L-1}(-1)^{k+1}C_{N_\Lambda-(L+1)}^{N_h-(k+1)}C_{L-1}^{k}\right]\ . \tag{18}$$

The sum in the curved bracket can be estimated as follows.

$$\sum_{k=0}^{L-1}(-1)^{k+1}C_{N_\Lambda-(L+1)}^{N_h-(k+1)}C_{L-1}^{k}=-\sum_{k=0}^{L-1}C_{N_\Lambda-(L+1)}^{N_h-(k+1)}C_{L-1}^{k}+2\sum_{\substack{k \text{ is odd}\\ k\geq 1}}C_{N_\Lambda-(L+1)}^{N_h-(k+1)}C_{L-1}^{k}$$

$$=-C_{N_\Lambda-2}^{N_h-1}+2\sum_{\substack{k \text{ is odd}\\ k\geq 1}}C_{N_\Lambda-(L+1)}^{N_h-(k+1)}C_{L-1}^{k}\ . \tag{19}$$

Here, we used the fact that the first sum after the first equals sign is the coefficient of t^{N_h-1} in the expansion of

$$(1+t)^{N_\Lambda-(L+1)}(1+t)^{L-1}=(1+t)^{N_\Lambda-2}\ . \tag{20}$$

Combining formulas (11), (12), (14), (18), and (19) yields

$$\begin{aligned}E_g &\leq \langle\Psi_{\text{trial}}|H|\Psi_{\text{trial}}\rangle/\langle\Psi_{\text{trial}}|\Psi_{\text{trial}}\rangle\\ &=(\langle\Psi_{\text{trial}}|H_v|\Psi_{\text{trial}}\rangle+\langle\Psi_{\text{trial}}|H_h|\Psi_{\text{trial}}\rangle)/C_{N_\Lambda}^{N_h}\\ &\leq -4t(N_\Lambda-4L)C_{N_\Lambda-2}^{N_h-1}/C_{N_\Lambda}^{N_h}+4t(N_\Lambda-4L)\sum_{\substack{k \text{ is odd}\\ k\geq 1}}C_{N_\Lambda-(L+1)}^{N_h-(k+1)}C_{L-1}^{k}/C_{N_\Lambda}^{N_h}\ .\end{aligned} \tag{21}$$

A little algebra shows that the first term of (21) is

$$-4N_ht+O(N_hL/N_\Lambda)\ . \tag{22}$$

The second term demands more thinking and the term of $k=1$ in the sum has to be evaluated separately. First, each term of the sum satisfies

$$\begin{aligned}C_{N_\Lambda-(L+1)}^{N_h-(k+1)}C_{L-1}^{k}/C_{N_\Lambda}^{N_h} &\leq (1/k!)[N_h^{k+1}L^k/(N_\Lambda-L)^{k+1}][1-(N_h/N_\Lambda)]^{L-k}\\ &<(1/k!)[N_h^{k+1}L^k/(N_\Lambda-L)^{k+1}]\ .\end{aligned} \tag{23}$$

If

$$N_hL/(N_\Lambda-L)\leq 1\ , \tag{24}$$

then the right-hand side of (23) is a decreasing function of k. In particular, for $N_h\sim N_\Lambda^\alpha, 0\leq\alpha<\frac{1}{4}$, the condition (24) holds when N_Λ is sufficiently large. Replacing the terms in the sum with their upper bounds, we see that the second term of (21) is bounded by

$$\begin{aligned}&4t(N_\Lambda-4L)\sum_{\substack{k \text{ is odd}\\ k\geq 1}}(1/k!)[N_h^{k+1}L^k/(N_\Lambda-L)^{k+1}]\\ &=4t(N_\Lambda-4L)[N_h^2L/(N_\Lambda-L)^2]+4t(N_\Lambda-4L)\sum_{\substack{k \text{ is odd}\\ k\geq 3}}(1/k!)[N_h^{k+1}L^k/(N_\Lambda-L)^{k+1}]\\ &\leq 4t[N_h^2L/(N_\Lambda-L)]+4t(N_\Lambda-4L)(1/3!)[N_h^4L^3/(N_\Lambda-L)^4](L/2)\\ &\approx O(N_h^2L/N_\Lambda)+O(N_h^4L^4/N_\Lambda^3)\ .\end{aligned} \tag{25}$$

Therefore,

$$-4N_ht\leq E_g\leq -4N_ht+O(N_hL/N_\Lambda)+O(N_h^2L/N_\Lambda)+O(N_h^4L^4/N_\Lambda^3)\ . \tag{26}$$

Since $L=N_\Lambda^{1/2}$, the last three terms of the right-hand side of the above inequality approach zero if $N_h\sim N_\Lambda^\alpha$, $0\leq\alpha<\frac{1}{4}$. It implies that the energy of the exact ground state E_g and the energy of the Nagaoka state E_{Na} become degenerate in the thermodynamic limit. And the degenerate energy is $-4N_ht$.

Our proof is accomplished. **QED.**

Some remarks are in order.

Remark 1. Using the same technique described above, we can easily show that the Nagaoka state is stable in three-dimensional simple cubic lattice, if $N_h\sim N_\Lambda^\alpha$ with $0\leq\alpha<\frac{1}{6}$. In this calculation, one should notice that the largest number of holes between i and j is $L^2-1\sim O(N_\Lambda^{2/3})$. Therefore, one has to evaluate the sum in inequality (21) to $k=5$ term.

Remark 2. Our result shows that the energy of the ex-

act ground state approaches $-N_h zt$ in the thermodynamic limit when the number of holes is less than N_Λ^α, $0 \leq \alpha < \frac{1}{2}d$. On the other hand, Nagaoka's theorem tells us that the energy of the ground state is $-zt$ if there is only one hole in the system.[1] Therefore, it seems that each hole behaves like an independent particle and contributes a "Nagaoka energy" $-zt$ to the system. That can be achieved by getting away from other holes as far as possible. In other words, holes tend to flee away from each other to be independent. Certainly, when there are too many holes and space is too crowded, independence is destroyed. In this case, the Nagaoka state becomes unstable. Although we cannot prove it, we doubt that, when $N_h \geq N_\Lambda^\alpha$, $\alpha > 1/2d$, the lattice is already too crowded for holes to be comfortable.

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