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The spin reversal symmetry of the ground state of the half-filled Hubbard model

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Abstract. Using a method based on Lieb's theorems and SU(2) symmetry for the half-filled Hubbard model on a bipartite lattice with $|A| = |B| = N$ (where $|A|$ ($|B|$) is the number of sites in the A (B) sublattice), we show that the ground-state wave function has even (odd) symmetry with respect to the spin reversal operator when N is even (odd) for both $U > 0$ and $U < 0$ cases. These rigorous results hold in all dimensions without the necessity for a periodic boundary condition.

The discovery of high-T_c superconductivity renewed interest in the study of the ground-state properties of the Hubbard model. There has been an enormous amount of work in this field, but among them rigorous results and exact solutions are rare. For the one-dimensional case, exact results were obtained by Lieb and Wu [1]. For the higher-dimensional case, Yang and Zhang [2, 3] discovered that the Hubbard model possesses simultaneously a pseudospin SU(2) symmetry and a true SU(2) symmetry. Lieb [4] obtained several theorems about the ground state. In this paper, a new rigorous result about the ground state of the half-filled Hubbard model is stated and proved. It is shown that the ground state has even symmetry under spin reversal when N is even and odd symmetry under spin reversal when N is odd.

The Hubbard model on a finite lattice $2N$ is defined by the Hamiltonian

$$H = -t \sum_{\langle ij \rangle \sigma} (C_{i\sigma}^{+} C_{j\sigma} + \mathrm{HC}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}. \tag{1}$$

We consider the $2N$ lattice as a bipartite lattice with $|A| = |B| = N$, where $|A|$ ($|B|$) is the number of sites in the A (B) sublattice. The spin operators are defined as

$$S^{Z} = \frac{1}{2} \sum_{i} (n_{i\uparrow} - n_{i\downarrow}) \qquad S^{+} = (S^{-})^{+} = \sum_{i} C_{i\uparrow}^{+} C_{i\downarrow} \tag{2}$$

and the Hamiltonian (1) has the SU(2) symmetry

$$[S^{\pm} H] = 0. \tag{3}$$

Then for an arbitrary eigenstate ψ of H with the energy E, we have

$$H S^{\pm} \psi = E S^{\pm} \psi. \tag{4}$$

If $S^{\pm}\psi \neq 0$, $S^{\pm}\psi$ is a degenerate state of state ψ. On the other hand, Lieb's theorems point out that the ground state ψ_g of the Hamiltonian (1) on a bipartite lattice with $|A| = |B|$ is non-degenerate and has $S = 0$ for both $U > 0$ and $U < 0$ cases. Then we obtain

$$S^{\pm} \psi_g = 0. \tag{5}$$

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Of course, we believe that there exist other eigenstates that have the same property as ψ_g, but now we only know ψ_g is non-degenerate, and our interest is in the ground state.

It is well known that the Hubbard model has spin reversal symmetry. The spin reversal operator $\hat{R}^s$, which changes all the signs of the electron spin at each, site is defined as

$$\hat{R}^s \prod_{i=1}^{N} C_{i,\sigma_i}^{+} |0\rangle = \prod_{i=1}^{N} C_{i,-\sigma_i}^{+} |0\rangle \tag{6}$$

and its eigenvalues $R^s = \pm 1$. Because the ground state is unique, it must have even symmetry ($R^s = 1$) or odd symmetry ($R^s = -1$)

$$\hat{R}^s \psi_g = \pm \psi_g. \tag{7}$$

Exact diagonalization results [5] for small clusters have shown that when the number of sites is four, the ground state at half filling has even symmetry ($R^s = 1$), and when the number of sites is two or six, the ground state at half filling has odd symmetry ($R^s = -1$). These results seem to indicate that the ground state for a half-filled Hubbard system on a bipartite lattice $2N$ with $|A| = |B| = N$ has even (odd) symmetry with respect to the spin reversal operator when N is even (odd). The aim here is to confirm that this conjecture is correct.

We know that for the large-U case the half-filled Hubbard Hamiltonian maps into a Heisenberg model with $J = 4t^2/U$. In the following, we first give the proof of the rigorous result on the Heisenberg model, and then apply the method to the Hubbard model.

At the first step, we need a convention to define a appropriate set of basis vectors. For a $2N$ lattice the dimension of the invariant subspace with $S^z = 0$ is $(2N)!/(N!)^2$. We order the sites in an arbitrary way and decompose $2N$ sites into two groups that consist of N sites $\{X_1, \ldots, X_k, \ldots, X_N\}$ and $\{Y_1, \ldots, Y_k, \ldots, Y_N\}$, where X_k, Y_k denote the coordinates of the sites on the $2N$ lattice. When the two groups of sites are fixed, all the basis vectors ψ^l with $S^z = 0$ can be constructed by the following method. The first basis vector is

$$\phi_N^0 = \psi_\uparrow^N(X_1, \ldots, X_k, \ldots, X_N) \otimes \psi_\downarrow^N(Y_1, \ldots, Y_k, \ldots, Y_N)$$

where $\psi_\uparrow^N(X_1, \ldots, X_k, \ldots, X_N)$ represents a state in which the spins of all electrons at the sites $\{X_1, \ldots, X_k, \ldots, X_N\}$ are up, and $\psi_\downarrow^N(Y_1, \ldots, Y_k, \ldots, Y_N)$ represents a state in which the spins of all electrons at the sites $\{Y_1, \ldots, Y_k, \ldots, Y_N\}$ are down. Based on the basis vector ϕ_N^0, we can construct a group of new basis vectors $\phi_N^1(s_1|t_1)$ by changing the signs of the spin of the electrons at sites X_{s_1} and Y_{t_1}, i.e.

$$\begin{aligned}\phi_N^1(s_1|t_1) = {} & \psi_\uparrow^{N-1}(X_1, \ldots, X_{s_1-1}, X_{s_1+1}, \ldots, X_N) \otimes \psi_\downarrow^{N-1}(Y_1, \ldots, Y_{t_1-1}, Y_{t_1+1}, \ldots, Y_N) \\ & \otimes \psi_\downarrow^1(X_{s_1}) \otimes \psi_\uparrow^1(Y_{t_1}) \qquad (s_1, t_1 = 1, 2, \ldots, N).\end{aligned}$$

If we change the signs of j electrons ($j = 1, 2, \ldots, N$) at the sites $\{X_k\}$ and $\{Y_k\}$, we can obtain the jth group of new basis vectors

$$\begin{aligned}&\phi_N^j(s_1, s_2, \ldots, s_j|t_1, t_2, \ldots, t_j) \\ &= \psi_\uparrow^{N-j}(X_1, \ldots, X_{s_1-1}, X_{s_1+1}, \ldots, X_{s_l-1}, X_{s_l+1}, \ldots, X_{s_j-1}, X_{s_j+1}, \ldots, X_N) \\ &\qquad \otimes \psi_\downarrow^{N-j}(Y_1, \ldots, Y_{t_1-1}, Y_{t_1+1}, \ldots, Y_{t_l-1}, Y_{t_l+1}, \ldots, Y_{t_j-1}, Y_{t_j+1}, \ldots, Y_N) \\ &\qquad \otimes \psi_\downarrow^j(X_{s_1}, \ldots, X_{s_l}, \ldots, X_{s_j}) \otimes \psi_\uparrow^j(Y_{t_1}, \ldots, Y_{t_l}, \ldots, Y_{t_j}) \\ &\qquad (s_1 \neq s_2 \neq \ldots \neq s_j, t_1 \neq t_2 \neq \ldots \neq t_j = 1, 2, \ldots, N).\end{aligned}$$

The number of vectors in the jth group is

$$D_j = \binom{N}{j}^2.$$

Then the total number of the vectors constructed by this method is

$$D = \sum_{j=0}^{N} D_j = \frac{(2N)!}{(N!)^2}$$

which is equal to the dimension of the subspace with $S^z = 0$, so the basis vectors constructed by this method are complete. When $j = N$, the basis vector in the jth group is

$$\phi_N^N = \psi_\uparrow^N(Y_1, \ldots, Y_k, \ldots, Y_N) \otimes \psi_\downarrow^N(X_1, \ldots, X_k, \ldots, X_N)$$

so we have

$$\hat{R}^s \phi_N^0 = \phi_N^N. \tag{8}$$

The ground state ψ_g can then be written as $\psi_g = \sum_{l=1}^{D} C_l \psi^l$; the coefficients C_l corresponding to the basis vector $\phi_N^j(s_1, \ldots, s_j|t_1, \ldots, t_j)$ can be denoted as $A^j(s_1, \ldots, s_j|t_1, \ldots, t_j)$. Applying S^- to the ground state ψ_g, from equation (5) we can obtain the following equations for the coefficients:

$$\sum_q A^j(s_1, \ldots, s_{q-1}, s_{q+1}, \ldots, s_{j+1}|t_1, \ldots, t_l, \ldots, t_j) \tag{9}$$

$$+ \sum_u A^{j+1}(s_1, \ldots, s_l, \ldots, s_{j+1}|t_1, \ldots, t_l, \ldots, t_j, u) = 0$$

$$(j = 0, 1, 2, \ldots, N-1).$$

Defining A^j as the sum of all the coefficients corresponding to the vectors in the jth group, we have

$$\sum_{s_1 \neq s_2 \neq \ldots \neq s_j} \sum_{t_1 \neq t_2 \neq \ldots \neq t_j} A^j(s_1, s_2, \ldots, s_j|t_1, t_2, \ldots, t_j) = (j!)^2 A^j \tag{10}$$

and

$$\sum_{s_1 \neq s_2 \neq \ldots \neq s_j \neq s_{j+1}} \sum_{t_1 \neq t_2 \neq \ldots \neq t_j} A^j(s_1, s_2, \ldots, s_j|t_1, t_2, \ldots, t_j) = (j!)^2 (N-j) A^j. \tag{11}$$

Using equations (10) and (11), summing equation (9) we obtain

$$(N-j)A^j + (j+1)A^{j+1} = 0 \qquad (j = 0, 1, \ldots, N-1). \tag{12}$$

Solving these equations (12), we obtain

$$A^j = (-1)^j \frac{N!}{(N-j)!j!} A^0 \qquad (j = 1, 2, \ldots, N). \tag{13}$$

Then

$$A^N = (-1)^N A^0. \tag{14}$$

Because the basis vector ϕ_N^0 is chosen in an arbitrary way, we can obtain the same relation as equation (14) for any basis vectors with $S^z = 0$. From equation (8) and the above result we get

$$\hat{R}^s \psi_g = (-1)^N \psi_g. \tag{15}$$

Then we know that the ground state for the half-filled Hubbard Hamiltonian with large U (AF Heisenberg model) has even (odd) symmetry under the spin reversal if N is even (odd). In fact, this result is not new, this property follows from the 'Marshall sign rule' [6].

Now we analyse the Hubbard model on a bipartite lattice $2N$ ($|A| = |B|$) with $U > 0$ and $U < 0$. For such a Hamiltonian, the dimension of the subspace with $S^z = 0$ is much larger than that of Heisenberg model. The basis vectors can be written in the form

$$\Phi = \psi_{\mathrm{D}}^{m}(X_1, \ldots, X_m) \otimes \psi_{\mathrm{V}}^{m}(Y_1, \ldots, Y_m) \otimes \phi_{N-m}^{j} \qquad (m = 0, 1, \ldots, N; j = 0, 1, \ldots, N - m) \tag{16}$$

where $\psi_{\mathrm{D}}^{m}(X_1, \ldots, X_m)$ representa the fact that at each site of the $\{X_1, \ldots, X_m\}$ there are two electrons with unparallel spin (doubly occupied state), and ψ_{V}^{m} represents the fact that at each site of the $\{Y_1, \ldots, Y_m\}$ there are no electrons (vacancy). For example

$$\psi_{\mathrm{D}}^{2}(X_1, X_2) = C_{X_1\uparrow}^{+} C_{X_1\downarrow}^{+} C_{X_2\uparrow}^{+} C_{X_2\downarrow}^{+} |0\rangle. \tag{17}$$

Notice that the vector $\psi_{\mathrm{D}}^{m}(X_1, \ldots, X_m) \otimes \psi_{\mathrm{V}}^{m}(Y_1, \ldots, Y_m)$ has the property

$$\hat{R}^{s} \psi_{\mathrm{D}}^{m}(X_1, \ldots, X_m) \otimes \psi_{\mathrm{V}}^{m}(Y_1, \ldots, Y_m) = (-1)^m \psi_{\mathrm{D}}^{m}(X_1, \ldots, X_m) \otimes \psi_{\mathrm{V}}^{m}(Y_1, \ldots, Y_m) \tag{18}$$

and

$$(S)^{\pm} \psi_{\mathrm{D}}^{m}(X_1, \ldots, X_m) \otimes \psi_{\mathrm{V}}^{m}(Y_1, \ldots, Y_m) = 0. \tag{19}$$

The spin reversal property for the Hubbard model depends only on the relations of the coefficients of the basis vectors with the same doubly occupied and vacant state, and from equations (5) and (19) one can find that the Hamiltonian matrix elements between states of different m does not affect the relation between the coefficients of these basis vectors. Thus for a group of basis vectors with the same doubly occupied and vacant state, we can still establish the equations for the coefficients by regarding Φ as the basis vectors of the Heisenberg model on a $2N - 2m$ lattice. Using the same method, we obtain the following result for the half-filled Hubbard model:

$$\hat{R}^{S} \psi_g = (-1)^m (-1)^{N-m} \psi_g = (-1)^N \psi_g. \tag{20}$$

Then we know that the ground state for the half-filled Hubbard Hamiltonian with arbitrary U has even (odd) symmetry under the spin reversal if N is even (odd).

In summary, based on Lieb's theorem we have shown that the ground-state wave function of the half-filled Hubbard model on a bipartite lattice with $|A| = |B|$ has even (odd) symmetry with respect to the spin reversal operator when N is even (odd). this conclusion is in agreement with the exact diagonalization results for the two-, four-, and six-site Hubbard model [5] and provides some new information about the Hubbard ground state.

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