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Antiferromagnetism and spin waves in the Hubbard model at half-filling

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Abstract. For a localized quantum spin system, such as the Heisenberg model, one believes that the collective excitations will be gapless if the ground state is antiferromagnetic, by the spin-wave theory. In this paper, we use some rigorous results of Lieb and show that the above conclusion still holds for the Hubbard model at half-filling, which is an itinerant electron system.

The Hubbard model [1] was introduced a long time ago as a model to study the strongly correlated fermion systems. It has been used to interpret the metal–insulator transition [2, 3] and itinerant electron ferromagnetism [4]. It may also provide some new mechanism for the newly discovered high-temperature superconductivity [5]. Naturally, such an important model attracts many physicists' interest. Attempts have been made to solve this model analytically or numerically but, so far, only a few rigorous results have been proved. Among them, the most important ones are probably the exact solution in one dimension [6] and Nagaoka's theorem [4].

In a recent paper [7], Lieb proved rigorously that, for any $U > 0$, the ground state of the Hubbard model at half-filling is non-degenerate and the total spin of the ground state is 0 in a finite simple-cubic lattice. Although the antiferromagnetic long-range order was not established in this paper, these results make further investigations possible. In this paper, based on Lieb's results, we shall show that a well established fact for the localized quantum spin models, such as the Heisenberg model, still holds for the Hubbard model, an itinerant electron system. More precisely, we shall rigorously prove that a closed collective excitation gap is a necessary condition for the antiferromagnetic long-range order in the ground state of the Hubbard Hamiltonian at half-filling.

The Hubbard Hamiltonian is

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

where t and U are parameters representing the hopping energy and the on-site interaction of electrons, respectively. $\langle ij \rangle$ denotes a pair of nearest-neighbour sites. For definiteness, we define the Hamiltonian on a finite simple-cubic lattice Λ. With respect to the Hamiltonian, Λ is bipartite. In this case, the sign of t can be either positive or negative because a suitable canonical transformation always changes it [4]. In the following, U is assumed positive, representing a Coulomb repulsion. Let N_Λ be the number of the lattice sites and N_e be the total number of electrons. When $N_e = N_\Lambda$, the lattice is half-filled. Although Lieb's results tell us that the collective excitation gap is open for any finite Λ at half-filling, one argues that it will be eventually closed in the thermodynamic limit. The argument is based on a common belief that the ground state of the Hubbard model at half-filling is antiferromagnetic. Therefore, by the spin-wave theory, there will be spin wave excitations whose energies are arbitrarily close to the energy of the ground state. Noticing the spin-wave theory is established for the localized quantum spin models, such as the Heisenberg model, we feel that it will be proper to confirm the above argument by a direct and rigorous exploration on the properties of the ground state of the Hubbard model, which is an itinerant electron model. In this paper, we prove the following theorem, by using uniqueness of the ground state of the Hubbard model at half-filling.

Theorem. If the ground state of the Hubbard model at half-filling has the antiferromagnetic long-range order, then the collective excitation gap will be closed in the thermodynamic limit.

Our main tool for the proof of the theorem is the following lemma.

Lemma 1. Let $|\Psi_0\rangle$ be the non-degenerate ground state of a given Hamiltonian H. Let B be an operator such that $\langle\Psi_0|B|\Psi_0\rangle = 0$, then

$$\frac{\langle\Psi_0|[B^+, [H, B]]|\Psi_0\rangle}{\langle\Psi_0|B^+B + BB^+|\Psi_0\rangle} \geq E_1 - E_0 \tag{2}$$

where E_0 is the energy of the ground state and E_1 is the energy of the first excited state.

Proof. Expanding the commutator and using the definition of E_0, we find

$$\frac{\langle\Psi_0|[B^+, [H, B]]|\Psi_0\rangle}{\langle\Psi_0|B^+B + BB^+|\Psi_0\rangle} = \frac{\langle\Psi_0|B^+HB + BHB^+|\Psi_0\rangle}{\langle\Psi_0|B^+B + BB^+|\Psi_0\rangle} - E_0. \tag{3}$$

Since $\langle\Psi_0|B|\Psi_0\rangle = \langle\Psi_0|B^+|\Psi_0\rangle = 0$, the new states $|\Psi_1\rangle = B|\Psi_0\rangle$ and $|\Psi_2\rangle = B^+|\Psi_0\rangle$ are orthogonal to $|\Psi_0\rangle$. By the variational principle, the expectation values of H in these states are larger than E_1. Therefore,

$$\langle\Psi_0|B^+HB|\Psi_0\rangle \geq E_1\langle\Psi_0|B^+B|\Psi_0\rangle \qquad \langle\Psi_0|BHB^+|\Psi_0\rangle \geq E_1\langle\Psi_0|BB^+|\Psi_0\rangle. \tag{4}$$

Substituting them into the right-hand side of (3), we prove the lemma. □

To detect the antiferromagnetic long-range order in the ground state of a localized quantum spin model, one of the standard methods is as follows.

We first introduce the spin-wave operators

$$S_{\boldsymbol{q}} = \frac{1}{\sqrt{N_\Lambda}} \sum_{\boldsymbol{k}\in\Lambda} S_{\boldsymbol{k}z} \exp(-i\boldsymbol{q}\cdot\boldsymbol{k}) \tag{5}$$

where $\boldsymbol{q} = (q_1, q_2, \ldots, q_d)$ is a quasi-momentum vector satisfying $0 \leq q_i < 2\pi$ and $S_{\boldsymbol{k}z}$ is the spin z-component at site $\boldsymbol{k}$. If the ground state has the antiferromagnetic long-range order, we expect that the following condition should be satisfied:

$$g_Q = \langle\Psi_0|S_{-Q}S_Q|\Psi_0\rangle \geq cN_\Lambda \tag{6}$$

where $Q = (\pi, \pi, \ldots, \pi)$ and c is a positive constant independent of N_Λ. In other words, there should be the spin-wave condensation at Q. For details, see [8]. On the other hand, it is well known [7] that, for spin-$\frac{1}{2}$ fermions, the following operators

$$S_x = \tfrac{1}{2}(c_\uparrow^+ c_\downarrow + c_\downarrow^+ c_\uparrow) \qquad S_y = \frac{1}{2i}(c_\uparrow^+ c_\downarrow - c_\downarrow^+ c_\uparrow) \qquad S_z = \tfrac{1}{2}(n_\uparrow - n_\downarrow) \tag{7}$$

satisfy the spin commutation relations

$$[S_\alpha, S_\beta] = i\varepsilon_{\alpha\beta\gamma} S_\gamma. \tag{8}$$

Therefore, we can easily transplant the above method to the Hubbard model by substituting (7) into the definition of S_q.

Some properties of S_q are useful in proving our theorem.

First, it is easy to show that

$$S_q^+ = S_{-q} \qquad \text{and} \qquad [S_q, S_{-q}] = 0. \tag{9}$$

Next, we can prove the following.

Lemma 2. Let Ψ_0 be the non-degenerate ground state of the Hubbard Hamiltonian at half-filling. Then

$$\langle \Psi_0 | S_q | \Psi_0 \rangle = 0 \tag{10}$$

for any q.

Proof. We first notice that the total spin x-component

$$S_x = \sum_{k \in \Lambda} S_{kx} = \frac{1}{2} \sum_{k \in \Lambda} (C_{k\uparrow}^+ C_{k\downarrow} + C_{k\downarrow}^+ C_{k\uparrow}) \tag{11}$$

commutes with the Hamiltonian, i.e.,

$$[S_x, H] = 0. \tag{12}$$

Therefore, for any real number θ, we have

$$\exp(i\theta S_x) H \exp(-i\theta S_x) = H. \tag{13}$$

This implies that any subspace corresponding to an eigenvalue λ of H is invariant under the unitary transformation $U = \exp(i\theta S_x)$. In particular, the subspace spanned by the ground state of H, which is one-dimensional by Lieb [7], is so. Therefore, we must have

$$U(\theta)|\Psi_0\rangle = \exp(i\theta S_x)|\Psi_0\rangle = \exp(i\alpha(\theta))|\Psi_0\rangle \tag{14}$$

where $\alpha(\theta)$ is a real number dependent of θ. We now choose $\theta = \pi$. A little algebra shows that

$$U(\pi) S_{kz} U^+(\pi) = -S_{kz} \tag{15}$$

for any k in Λ. Therefore, $U(\pi) S_q U^+(\pi) = -S_q$ and

$$\langle \Psi_0 | U(\pi) S_q U^+(\pi) | \Psi_0 \rangle = -\langle \Psi_0 | S_q | \Psi_0 \rangle. \tag{16}$$

On the other hand, by (14), we have

$$\begin{aligned} \langle \Psi_0 | U(\pi) S_q U^+(\pi) | \Psi_0 \rangle &= \langle \Psi_0 | \exp(i\alpha(\pi)) S_q \exp(-i\alpha(\pi)) | \Psi_0 \rangle \\ &= \langle \Psi_0 | S_q | \Psi_0 \rangle. \end{aligned} \tag{17}$$

Combining (16) and (17), we obtain

$$\langle\Psi_0|S_{\boldsymbol{q}}|\Psi_0\rangle = 0 \tag{18}$$

for any $\boldsymbol{q}$. □

We are now ready to prove the theorem.

Proof of the theorem. We assume that the collective excitation gap keeps open in the thermodynamic limit.

Let $S_{\boldsymbol{q}}$ be the operator B in lemma 1. Noticing $S_{\boldsymbol{q}}^{+} = S_{-\boldsymbol{q}}$ and $S_{-\boldsymbol{q}}S_{\boldsymbol{q}} = S_{\boldsymbol{q}}S_{-\boldsymbol{q}}$, inequality (2) now reads

$$\langle\Psi_0|[S_{-\boldsymbol{q}}, [H, S_{\boldsymbol{q}}]]|\Psi_0\rangle \geqslant 2(E_1 - E_0)\langle\Psi_0|S_{-\boldsymbol{q}}S_{\boldsymbol{q}}|\Psi_0\rangle. \tag{19}$$

A direct calculation of the commutator gives

$$\langle\Psi_0|[S_{-\boldsymbol{q}}, [H, S_{\boldsymbol{q}}]]|\Psi_0\rangle = -\frac{1}{2dN_\Lambda}\sum_{s=1}^{d}(1-\cos q_s)\langle\Psi_0|T|\Psi_0\rangle \tag{20}$$

where T is the hopping term of the Hubbard Hamiltonian. Its expectation value in the ground state satisfies

$$-aN_\Lambda \leqslant \langle\Psi_0|T|\Psi_0\rangle \leqslant 0 \tag{21}$$

where a is a positive constant independent of N_Λ. While the upper bound in (21) is trivial, one can get the lower bound by using Gershgorin's theorem (see [9] and [10] for its proof and applications to Nagaoka's theorem).

Substituting (20) and (21) into (19) and letting $\boldsymbol{q} = \boldsymbol{Q}$, we finally obtain

$$2^{d-2}(a/d) \geqslant (E_1 - E_0)\langle\Psi_0|S_{-\boldsymbol{Q}}S_{\boldsymbol{Q}}|\Psi_0\rangle. \tag{22}$$

Since the collective excitation gap keeps open in the thermodynamic limit, there must be a positive constant e such that $E_1 - E_0 \geqslant e$ and hence

$$2^{d-2}(a/d) \geqslant e\langle\Psi_0|S_{-\boldsymbol{Q}}S_{\boldsymbol{Q}}|\Psi_0\rangle. \tag{23}$$

Therefore, $g_{\boldsymbol{Q}}$ can be, at most, O(1) as N_Λ approaches infinity. And inequality (6) is not satisfied. It implies that the antiferromagnetic order cannot exist in Ψ_0.

Our proof is accomplished. □

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