Ferrimagnetic Long-Range Order of the Hubbard Model

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In this paper, we show rigorously that there exists the ferrimagnetic long-range order in the ground state of the positive-U Hubbard model at half filling on some bipartite lattices. When $N_A > N_B$ (N_A and N_B are the total site numbers of two sublattices **A** and **B**), except for the ferromagnetism which was found by Lieb [Phys. Rev. Lett. **62**, 1201 (1989)], there also exists the antiferromagnetic long-range order in the ground state. This result only requires $U > 0$ and is independent of the dimension of the lattices.

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The existence of antiferromagnetic long-range order in an itinerant electron system has been an open problem for a long time. Four years ago, Lieb showed that the unique ground state of the Hubbard model on some bipartite lattices at half filling has the total spin $S = |N_A - N_B|/2$ [1]. When $N_A > N_B$, it is nonzero macroscopically. However, in the large-U case, this model is very close to an antiferromagnetic Heisenberg model. It is believed that the ground state should favor the antiferromagnetism, or more accurately, the ferrimagnetism. Except for the nonzero spin, the ferrimagnetism also possesses the antiferromagnetic long-range order. Thus whether there exists such a long-range order is the subject of this paper.

After some preliminary definitions and introduction, we present a theorem on two-point spin correlation function in the Hubbard model. Then incorporating Lieb's theorem [1], we prove that when $N_A > N_B$ [2] and at half-filling, i.e., $N_e = N_A+N_B$, the ground state possesses the ferrimagnetic long-range order. To our knowledge, this is the first example that the ferrimagnetic long-range order exists exactly in an itinerant electron system.

The positive-U Hubbard model on a finite bipartite lattice Λ is defined by

$$H = -t \sum_{(ij),\sigma} C^\dagger_{i\sigma} C_{j\sigma} + |U| \sum_i (n_{i\uparrow} - \tfrac{1}{2})(n_{i\downarrow} - \tfrac{1}{2}), \quad (1)$$

where $C_{i\sigma}$ and $C^\dagger_{i\sigma}$ are the annihilation and creation operators of electron with spin σ ($=\uparrow,\downarrow$) at site i, respectively. (ij) means all pairs of the nearest neighbor sites and i and j belong to two sublattices. This model possesses SO(4) symmetry [3] and the global ground state must belong to the subspace, $N_\uparrow = N_\downarrow$ ($N_\uparrow$ and $N_\downarrow$ are the total numbers of electron with spin-up and spin-down, respectively, and both are the good quantum number of the system). Therefore we limit our discussion in this subspace.

The raising and lowering spin operators are

$$\mathbf{S}_i^+ = C^\dagger_{i\uparrow} C_{i\downarrow}, \quad \mathbf{S}_i^- = C^\dagger_{i\downarrow} C_{i\uparrow}, \quad (2)$$

and the z component is

$$\mathbf{S}_i^z = \tfrac{1}{2}(n_{i\uparrow} - n_{i\downarrow}). \quad (3)$$

Two correlation functions that we are interested in are defined by

$$m(0) = \frac{1}{N_\Lambda} \left\langle \left(\sum_i \mathbf{S}_i^+\right)\left(\sum_i \mathbf{S}_i^-\right)\right\rangle \quad (4)$$

and

$$m(Q) = \frac{1}{N_\Lambda} \left\langle \left(\sum_i \epsilon(i)\mathbf{S}_i^+\right)\left(\sum_i \epsilon(i)\mathbf{S}_i^-\right)\right\rangle, \quad (5)$$

where $\epsilon(i) = 1$ when $i \in \mathbf{A}$, and -1 when $i \in \mathbf{B}$ and the angular brackets denote the ground state expectation. The existence of ferromagnetic (antiferromagnetic) long-range order requires that $m(0)$ $[m(Q)]$ has order of N_Λ ($N_\Lambda = N_A+N_B$), i.e., $m(0) = O(N_\Lambda)$. The ferrimagnetism requires that both $m(0)$ and $m(Q)$ have order of N_Λ. Now we present Theorem I.

Theorem I.—In the positive-U Hubbard model on the bipartite lattice Λ and at half-filling,

$$\langle \mathbf{S}_i^+ \mathbf{S}_j^- \rangle \begin{cases} \geq 0, \text{when } (i,j) \in \mathbf{A} \text{ or } \mathbf{B}, \\ \leq 0, \text{ when } i \in \mathbf{A} \text{ (or } \mathbf{B}) \text{ and } j \in \mathbf{B} \text{ (or } \mathbf{A}). \end{cases} \quad (6)$$

Proof.—The proof of this theorem is based on the particle-hole symmetry of H on the bipartite lattice and the uniqueness of the ground state of a negative-U Hubbard model with even number of electrons.

The partial particle-hole transformation is defined as [4]

$$C_{i\uparrow} \to \epsilon(i) b^\dagger_{i\uparrow}, \quad C_{i\downarrow} \to b_{i\downarrow}. \quad (7)$$

Under this transformation, the Hamiltonian [Eq. (1)] is

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transformed into a negative-U Hubbard model:

$$\bar{H} = -t \sum_{(ij),\sigma} b^\dagger_{i\sigma} b_{i\sigma} - |U| \sum_i (n_{bi\uparrow} - \tfrac{1}{2})(n_{bi\downarrow} - \tfrac{1}{2}), \quad (8)$$

where $n_{bi\sigma} = b^\dagger_{i\sigma} b_{i\sigma}$. This transformation maps one eigenstate of H onto that of $\bar{H}$. When the system is exactly half filled (N_Λ is even), the number of particles do not change and the global-ground states of H are mapped onto the global ground state of $\bar{H}$ [5]. The ground state of $\bar{H}$ is unique [1] and its wave function has the form

$$|\Psi\rangle = \sum_{\alpha\beta} C_{\alpha\beta} |\Psi_{\alpha\uparrow}\rangle \otimes |\Psi_{\beta\downarrow}\rangle, \quad (9)$$

where $\{\Psi_\alpha\}$ is a real orthonormal basis for $N_\uparrow = N_\downarrow = N_e/2$ fermions [6]. $C_{\alpha\beta}$ is the coefficient and the matrix $\hat{C} = \{C^{\alpha\beta}\}$ is Hermitian and positive (or negative) definite (here we choose a positive one which does not affect the final result). Using this wave function [Eq. (9)], one can find that for any pair i and j, the quantity $\langle b_{i\uparrow} b_{i\downarrow} b^\dagger_{j\downarrow} b^\dagger_{j\uparrow}\rangle$ is always non-negative:

$$\langle b_{i\uparrow} b_{i\downarrow} b^\dagger_{j\downarrow} b^\dagger_{j\uparrow}\rangle = \sum_{\alpha,\beta,\gamma,\delta} C^*_{\alpha\beta} C_{\gamma\delta} \langle \Psi_{\alpha\uparrow}| b_{i\uparrow} b^\dagger_{j\uparrow} |\Psi_{\gamma\uparrow}\rangle \langle \Psi_{\beta\downarrow}| b_{i\downarrow} b^\dagger_{j\downarrow} |\Psi_{\delta\downarrow}\rangle = \mathrm{Tr}(\hat{C}^\dagger \hat{B} \hat{C} \hat{B}^\dagger) \geq 0, \quad (10)$$

where $(\hat{B})_{\alpha\beta} = \langle \Psi_\alpha | b_i b^\dagger_j | \Psi_\beta\rangle$ (the spin index is dropped). Since $\{\Psi_\alpha\}$ is a real orthonormal basis, $(\hat{B})_{\alpha\beta}$ is also real and $\hat{B}^T = \hat{B}^\dagger$. At the last step, we have made use of the positive definition of $\hat{C}$. Inequality (10) was also found by one of us in a previous paper [7]. Now we transform $\langle b_{i\uparrow} b_{i\downarrow} b^\dagger_{j\downarrow} b^\dagger_{j\uparrow}\rangle$ back to the original representation, then we have

$$\epsilon(i)\epsilon(j)\langle \mathbf{S}^+_i \mathbf{S}^-_j\rangle \geq 0. \quad (11)$$

From this inequality, one can easily obtain the inequalities in Eq. (6). Q.E.D.

Remark (1). This theorem is valid for any bipartite lattice. It also holds for the antiferromagnetic Heisenberg model. Its physical meaning is very clear: the spins of the electrons on different sublattices tend to favor different directions. In an antiferromagnetic system, it is very well understood, but in an itinerant electron system such as the Hubbard model, it is not trivial and transparent. After the discovery of the relevance between high-T_c superconductors and the Hubbard model, one has been expecting that the ground state at half filling would be an antiferromagnetic one [8]. But there is no rigorous proof to this conjecture until now. We guess Theorem I may be of some relevance to the above conjecture. The fact that this property holds for the copper-oxygen lattice (high-T_c superconductors) could underline the physical relevance of this results.

A direct corollary of Theorem I is the following

Corollary.—Under the condition of Theorem I,

$$m(Q) \geq m(0). \quad (12)$$

Proof of corollary.—Since $\epsilon(i)\epsilon(j)\langle \mathbf{S}^+_i \mathbf{S}^-_j\rangle$ is always non-negative for any pair of i and j, we have

$$\begin{aligned} m(0) &= \frac{1}{N_\Lambda} \sum_{ij} \langle \mathbf{S}^+_i \mathbf{S}^-_j\rangle \\ &\leq \frac{1}{N_\Lambda} \sum_{ij} |\langle \mathbf{S}^+_i \mathbf{S}^-_j\rangle| \\ &= \frac{1}{N_\Lambda} \sum_{i,j} \epsilon(i)\epsilon(j)\langle \mathbf{S}^+_i \mathbf{S}^-_j\rangle = m(Q). \end{aligned} \quad (13)$$

Q.E.D.

From this corollary, $m(Q)$ is always greater than $m(0)$. This is a very natural conclusion for an antiferromagnetic system. If $m(0)$ has order of N_Λ, $m(Q)$ must also be of order of N_Λ, and in this case, there must exist the ferrimagnetic long-range order. In his second theorem for a repulsive case in Ref. [1], Lieb showed the following:

Lieb's Theorem. When $N_e = N_\Lambda$ and on a bipartite lattice, the unique ground state of the Hubbard model has the total spin $S = |N_A - N_B|/2$.

We can express this theorem in the language of $m(0)$

$$\begin{aligned} m(0) &= \frac{1}{N_\Lambda} \left\langle \left(\sum_i \mathbf{S}^+_i\right)\left(\sum_i \mathbf{S}^-_i\right)\right\rangle \\ &= \frac{1}{N_\Lambda} \langle \mathbf{S}^+ \mathbf{S}^-\rangle \\ &= \frac{1}{4}\left(\frac{N_A}{N_\Lambda} - \frac{N_B}{N_\Lambda}\right)^2 N_\Lambda + O(1). \end{aligned} \quad (14)$$

When $N_A > N_B$, $m(0)$ is order of N_Λ, i.e.,

$$\lim_{N_\Lambda \to \infty} \frac{1}{N_\Lambda} m(0) > 0. \quad (15)$$

Combining this theorem and the corollary of Theorem I, we have Theorem II.

Theorem II.—In the positive-U Hubbard model on the bipartite lattice Λ with $N_A > N_B$ and $N_e = N_\Lambda$,

$$m(Q) \geq m(0) = O(N_\Lambda). \quad (16)$$

Both the antiferromagnetic and ferromagnetic long-range order coexist in the ground state. In another word, the ground state possesses ferrimagnetic long-range order.

Now we make two remarks:

Remark (i): Theorem II also holds in the antiferromagnetic Heisenberg model on a bipartite lattice with $N_A > N_B$. In this model, the existence of the ferromagnetism in the ground state was shown by Lieb and Mattis [9] three decades ago.

Remark (ii): When $N_A = N_B$, $m(0) = 0$. In this case, no ferromagnetic order appears and whether the antiferromagnetic long-range order exists or not is still unclear. As the ground state of the antiferromagnetic Heisenberg model on a cubic lattice has long-range order [10], we believe that at least in the large-U case, $m(Q)$ also has order of N_Λ.

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[1] E. H. Lieb, Phys. Rev. Lett. **62**, 1201 (1989); **62**, 1927 (1989).

[2] In this paper, $N_A > N_B$ means that in every unit cell, the number of sites belonging to the sublattice **A** is greater than that to **B**.

[3] C. N. Yang and S. C. Zhang, Mod. Phys. Lett. B **4**, 759 (1990); Int. J. Mod. Phys. B **5**, 977 (1991).

[4] H. Shiba, Prog. Theor. Phys. **48**, 2171 (1972); Y. Nagaoka, *ibid.* **52**, 1716 (1974); V. J. Emery, Phys. Rev. B **14**, 2989 (1972); S. Robaszkiewicz, R. Micnas, and K. A. Chao, Phys. Rev. B **23**, 1447 (1981); R. Micnas, J. Ranninger, and S. Robaszkiewicz, Rev. Mod. Phys. **62**, 113 (1990).

[5] Shun-Qing Shen and Zhao-Ming Qiu, Phys. Rev. Lett. **71**, 4238 (1993).

[6] The real orthonormal basis means that each Ψ_α is a real, homogeneous polynomial of n in the $b_i^\dagger$'s acting on the vacuum. See Ref. [1].

[7] G. S. Tian, Phys. Rev. B **45**, 3145 (1992).

[8] P. W. Anderson, Science **235**, 1196 (1987).

[9] E. Lieb and D. Mattis, J. Math. Phys. **3**, 749 (1962).

[10] F. Dyson, E. H. Lieb, and B. Simon, J. Stat. Phys. **18**, 335 (1978); T. Kennedy, E. H. Lieb, and B. S. Shastry, *ibid.* **58**, 1019 (1988).