Two Theorems on Pseudo-spin in the Hubbard Model *

Sze-Shiang Feng,
1. CCAST(World Lab.), P.O. Box 8730, Beijing 100080
2. Department of Astronomy and Applied Physics
University of Science and Technology of China, 230026, Hefei, China
e-mail: sshfeng@yahoo.com

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Abstract

An inequality of the eigenvalues of the reduced density matrix $\rho_2$ at finite temperature in the Hubbard model is obtained by means of the Bogolyubov inequality. The quasi-average of $\bar{S}^+$ in a simple symmetry-breaking perturbation of the Hamiltonian for a bipartite lattice is shown to be zero.

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Hubbard models and its extensions such as the SO(5) model[1] are currently believed to be able to account for the high-$T_c$ superconductivity of cuprates. The possibility of existence at finite temperature of $s$-wave pairing, generalized $\eta$-pairing and $d_{x^2-y^2}$ in one and two dimensional Hubbard model and Anderson model seems to have been be ruled out[2](of course, the conclusions are only valid with respect to the special kind of symmetry-breaking perturbations, there may exist some other kinds of perturbations for which the quasi-average of the order parametres do not suffer from those limitations, and thus are possibly non-vanishing). On the other hand, there do exist some states in some Hubbard models exhibit

*On leave of absence from the Physics Department, Shanghai University, 201800, Shanghai, China
superconductivity[3]. Therefore, the relevance to superconductivity of Hubbard models still calls for further investigations. A convenient concept is off-diagonal long-range order (ODLRO) discussed in detail in[5] which can be studied by \( \eta \)-pairing[5] and its variants. The existence of ODLRO can be recognized if the largest eigenvalue of the two-body reduced density matrix \( \rho_2 \) is of the order of the total number of the fermions[5]. A novel property of \( \eta \)-pairing is that it constitutes a pseudo-spin algebra. Lieb used this algebra and partial particle-hole transform and exactly proved for the first time that ferromagnetism may exist in itinerant electrons [6]. Based on Lieb’s results, it is shown that for some specific lattice structure and electron-filling, the ground-state of negative-\( U \) Hubbard may support ODLRO[4]. In this letter, we first prove an inequality of the eigenvalues of \( \rho_2 \) by means of Bogolyubov inequality. Then we show by means of fluctuation-dissipation theorem that the grand canonical quasi-average of \( \tilde{S}^+ \) vanishes for both positive and negative-\( U \) Hubbard models.

The grand-canonical Hamiltonian for the Hubbard model is

\[
K = \sum_{\langle ij \rangle} \sum_\sigma t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu N
\]  

(1)

where \( c_{i\sigma}^\dagger \) and \( c_{i\sigma} \) are the creation and annihilation operators of the electrons with spin \( \sigma = \uparrow, \downarrow \) at site \( i \). The hopping matrix \( \{ t_{ij} \} \) are required to be real and symmetric. The number operators are \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \), while the \( U \) denotes the on-site Coulomb interaction. It is further assumed that the lattice \( \Lambda \) is bipartite in the sense that it can be divided into sublattices \( A \) and \( B \), i.e. \( \Lambda = A \cup B \), such that \( t_{ij} = 0 \) whenever \( \{ ij \} \in A \) or \( \{ ij \} \in B \). As usual, the spin \( S \) and pseudo-spin \( \tilde{S} \) are defined as follows

\[
S^+ = \sum_{i \in \Lambda} c_{i\uparrow}^\dagger c_{i\downarrow}, \quad S^- = \sum_{i \in \Lambda} c_{i\downarrow}^\dagger c_{i\uparrow}, \quad S^z = \frac{1}{2} \sum_{i \in \Lambda} (c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}) = \frac{1}{2} (N_{\uparrow} - N_{\downarrow})
\]

(2)

\[
\tilde{S}^+ = \sum_{i \in \Lambda} \epsilon(i) c_{i\uparrow}^\dagger c_{i\downarrow}, \quad \tilde{S}^- = \sum_{i \in \Lambda} \epsilon(i) c_{i\downarrow}^\dagger c_{i\uparrow}, \quad \tilde{S}^z = \frac{1}{2} \sum_{i \in \Lambda} (1 - n_{i\uparrow} - n_{i\downarrow})
\]

(3)

where \( \epsilon(i) = 1 \) when \( i \in A \) and \(-1 \) when \( i \in B \). Both the spin and the pseudo-spin operators constitute \( SU(2) \) algebra and they commute with each other, i.e. \( [\tilde{S}, S] = 0 \), so they form an \( SU(2) \otimes SU(2) \) algebra. It is not difficult to show that \( [H, \tilde{S}^2] = [H, S] = [H, \tilde{S}_z] = 0 \).

Therefore, Hubbard model enjoys \( SU(2) \otimes U(1) \otimes U(1) \) symmetry. Yang and Zhang[7] showed that ODLRO exists whenever the expectation value of \( \tilde{S}^2 - \tilde{S}_z^2 \) is of order \( N^2_\Lambda \), where
\( N_A \) is the number of the sites of the lattice considered.

The well-known Bogolyubov inequality\(^8\) says that for any two operators \( C \) and \( Q \), the following inequality always holds
\[
\langle CC^\dagger + C^\dagger C \rangle \geq \frac{2}{\beta} \left| \frac{\langle [Q(t), C(t)] \rangle^2}{\langle [Q^\dagger(t), K] \rangle^2} \right|
\]
where \( \langle O \rangle \) denote the statistical average of the mechanical quantity \( O \). This inequality has been utilized in\(^2\). We employ it here to prove a relation the eigenvalues of the reduced density \( \rho_2 \) should satisfy. Let us recognize some fundamental properties of the eigenvalues before presenting the relation. Firstly, it is not difficult to show that the onset of ODLRO can be guaranteed if the largest eigenvalue of either \( \langle \epsilon(j)\eta_j^\dagger \epsilon(i)\eta_i \rangle \) or \( \langle \eta_j^\dagger \eta_i \rangle \), where the \( \eta \) pairing is defined as \( \eta_i = c_{it}c_{i\downarrow} \), is of the order of \( N_A \). In fact, we have the following lemma.

**Lemma 1** The matrices \( \langle \epsilon(j)\eta_j^\dagger \epsilon(i)\eta_i \rangle \) and \( \langle \eta_j^\dagger \eta_i \rangle \) have the same eigenvalues.

**Proof** Suppose \( \sum_i \langle \eta_j^\dagger \eta_i \rangle u_i = \lambda u_j \), then we have
\[
\sum_i \langle \epsilon(j)\eta_j^\dagger \epsilon(i)\eta_i \rangle u_i = \epsilon(j) \sum_i \langle \eta_j^\dagger \eta_i \rangle u_i = \lambda \epsilon(j) u_j
\]
and this proves the lemma. Q.E.D.

Secondly, the eigenvalues are non-negative.

**Lemma 2** The matrix \( \langle \epsilon(j)\eta_j^\dagger \epsilon(i)\eta_i \rangle \) is positive semi-definite.

**Proof** For an arbitrary vector \( u_i \), define \( O = \sum_i \epsilon_i\eta_i u_i \), then
\[
\sum_{i,j} u_j^* \langle \eta_j^\dagger \epsilon(j)\eta_i \rangle u_i = \langle O^\dagger O \rangle \geq 0
\]
Therefore, all the eigenvalues are non-negative. Q.E.D.

Beside the above two lemmas, we will use the next lemma in the following.

**Lemma 3** Let \( A \) be an \( N \times N \) matrix whose entries satisfy \( a_{mn} = a_{m-n} \). Then all the eigenvalues of \( A \) are given by \( \lambda_q = \frac{1}{N} \sum_{m=1}^N \sum_{n=1}^N a_{mn} e^{iq(m-n)} \), where \( q = \frac{2\pi}{N} k \) with \( k = 0, 1, \cdots, N - 1 \).

This lemma has been used in\(^9\) and\(^10\) and a proof is presented in\(^10\). Now we are ready to present our first result.

**Theorem 1** The eigenvalues of \( \langle \eta_j^\dagger \eta_i \rangle \) can be denoted by wave vectors \( k \) as \( \lambda_k \), \( k \) belong to the first Brillouin zone. If the system is translationally invariant and the lattice is bipartite, the following inequality holds
\[
\lambda_k \geq |x| \frac{1}{\beta} \frac{1}{|2\mu - U|} \delta_{k,0} - \frac{x}{2}
\]
where \( x = 1 - \rho_e \).

**Proof** For our purpose, we choose

\[ Q = \tilde{S}^- \]  

(8)

and

\[ C_k = \sum_j e^{ik \cdot R_j} \epsilon(j) \eta_j = \sum_j e^{ik \cdot R_j} \epsilon(j) c_j \hat{c}_j \]  

(9)

Making use of the relation \([\eta_i^\dagger, \eta_j] = \delta_{ij} (n_{i\uparrow} + n_{i\downarrow} - 1)\), we have

\[ [Q, C_k] = \sum_j e^{ik \cdot R_j} (n_j - 1) \]  

(10)

Since

\[ [\tilde{S}^-, K] = (2\mu - U)\tilde{S}^- \]  

(11)

we have

\[ [Q^\dagger, K] = (U - 2\mu)\tilde{S}^+ \]  

(12)

\[ [Q, [Q^\dagger, K]] = 2(2\mu - U)\tilde{S}_z \]  

(13)

By direct calculation, we have

\[ C_k^\dagger C_k + C_k C_k^\dagger = 2 \sum_{ij} e^{ik \cdot (R_i - R_j)} \epsilon(i) \epsilon(j) \eta_j^\dagger \eta_i - \sum_i (n_i - 1) \]  

(14)

Therefore, using Bogolyubov inequality, we have

\[ 2 \sum_{ij} e^{ik \cdot (R_i - R_j)} \epsilon(i) \epsilon(j) < \eta_j^\dagger \eta_i > - \sum_i < n_i - 1 > \geq \frac{2}{\beta} \frac{|< \sum_j e^{ik \cdot R_j} (n_j - 1) > |^2}{|2(2\mu - U)|| < \tilde{S}_z > |} = \frac{2}{\beta} \frac{2 \sum_{ij} e^{ik \cdot (R_i - R_j)} < n_i - 1 > < n_j - 1 >}{2|2\mu - U| \cdot \frac{1}{2} \sum_j < 1 - n_j >} \]  

(15)

Since we consider the translationally invariant system, \( < n_i > = N_e/N_A = \rho_e \), accordingly

\[ 2 \sum_{ij} e^{ik \cdot (R_i - R_j)} \epsilon(i) \epsilon(j) < \eta_j^\dagger \eta_i > + N_A x \geq \frac{2}{\beta} \frac{\sum_{ij} e^{ik \cdot (R_i - R_j)} x^2}{|2\mu - U| \cdot N_A |x|} = \frac{2}{\beta} |x| \frac{\delta_{k,0} N_A}{|2\mu - U|} \]  

(16)

where we have used that \( \sum_{ij} e^{ik \cdot (R_i - R_j)} = N_A^2 \delta_{k,0} \). Or

\[ 2 \sum_{ij} e^{ik \cdot (R_i - R_j)} < \epsilon(j) \eta_j^\dagger \epsilon(i) \eta_i > \geq \frac{2}{\beta} |x| \frac{\delta_{k,0} N_A}{|2\mu - U|} - N_A x \]  

(17)

On the other hand, lemma 3 tells us that the eigenvalues of the \( N_A \times N_A \) matrix \( < \epsilon(j) \eta_j^\dagger \epsilon(i) \eta_i > \) are

\[ \lambda_k = \frac{1}{N_A} \sum_{ij} e^{ik \cdot (R_i - R_j)} < \epsilon(j) \eta_j^\dagger \epsilon(i) \eta_i > \]  

(18)
and this proves the theorem. Q.E.D.

We make some remarks here. In the case of at half-filling, \( x = 0 \). in this case, the theorem provides no new information because lemma 2 has told us that all the eigenvalues are non-negative. It should be mentioned that Tian showed in [10] that at half-filling, for the negative—\( U \) case, the lowest eigenvalue is zero in the ground-state. Our result is in accordance with Tian’s, though the zero-temperature limit of a grand-canonical average does not necessarily coincide with the ground state expectation value in general such as [11] and [1]. But, if the system is at over half-filling, \( x \) will be negative and the r.h.s. of (7) is positive. in this case, the theorem tells us that there exists lower positive bound to each eigenvalue. Unfortunately, the lower bound to the largest eigenvalue the theorem provides is only a constant other than a number proportional to \( N_e \).

Our second result is

**Theorem 2** Assuming the lattice is bipartite, for the \( U(1) \) symmetry-breaking Hamiltonian

\[
H = \sum_{(ij)} \sum_{\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \Delta \tilde{S}^+ + \Delta^* \tilde{S}^-
\]  

(19)

we have for the grand canonical average of \( \tilde{S}^+ \)

\[
\lim_{\Delta \to 0} \lim_{N_A \to \infty} \frac{1}{N_A} < \tilde{S}^+ > = 0
\]

(20)

**Proof** The grand canonical Hamiltonian is \( K = H - \mu \hat{N} \). We use the fluctuation-dissipation theorem as in [11]. to calculate \( < \tilde{S}^+ \tilde{S}^- > \). The evolution equation of the double-time Green function \( < \tilde{S}^- | \tilde{S}^+ >_\omega \) is [12]

\[
\omega < \tilde{S}^- | \tilde{S}^+ >_\omega = < [\tilde{S}^-, \tilde{S}^+] > + < [\tilde{S}^-, K] | \tilde{S}^+ >_\omega
\]

(21)

It can be calculated directly that

\[
[\tilde{S}^-, K] = (2\mu - U)\tilde{S}^- - 2\Delta \tilde{S}_z
\]

(22)

Accordingly, we have

\[
\omega < \tilde{S}^- | \tilde{S}^+ >_\omega = -2 < \tilde{S}_z > + (2\mu - U) < \tilde{S}^- | \tilde{S}^+ > - 2\Delta < \tilde{S}_z | \tilde{S}^+ >_\omega
\]

(23)

Using again the equation of motion, we can obtain

\[
\omega < \tilde{S}^- | \tilde{S}^+ >_\omega = - < \tilde{S}^+ > - \Delta < \tilde{S}^- | \tilde{S}^+ >_\omega + \Delta^* < \tilde{S}^- | \tilde{S}^+ >_\omega
\]

(24)
where these three equations eq.(23)-eq.(25) are enough to determine the three unknowns $\ll \tilde{S}^-|\tilde{S}^+\gg_{\omega}$, $\ll \tilde{S}^+|\tilde{S}^+\gg_{\omega}$, and $\ll \tilde{S}^z|\tilde{S}^+\gg_{\omega}$. Especially, we have

$$\ll \tilde{S}^-|\tilde{S}^+\gg_{\omega} = \frac{c_1}{\omega} + \frac{c_2}{\omega - \omega_2} + \frac{c_3}{\omega - \omega_3}$$

where

$$c_1 = \frac{[2\Delta(2\mu - U) < \tilde{S}^+ > - 4|\Delta|^2 < \tilde{S}_z >]}{4|\Delta|^2 - (2\mu - U)^2}$$

$$c_2 = \frac{1}{\omega_2(\omega_2 - \omega_3)} \{2\Delta < \tilde{S}^+ > (\omega_2 + 2\mu - U) - 2[\omega_2(\omega_2 + 2\mu - U) + 2|\Delta|^2] < \tilde{S}_z > \}$$

$$c_3 = \frac{1}{\omega_3(\omega_3 - \omega_2)} \{2\Delta < \tilde{S}^+ > (\omega_3 + 2\mu - U) - 2[\omega_3(\omega_3 + 2\mu - U) + 2|\Delta|^2] < \tilde{S}_z > \}$$

$$\omega_{2,3} = \pm \sqrt{(2\mu - U)^2 - 4|\Delta|^2}$$

Thus from the fluctuation-dissipation theorem

$$< \tilde{S}^+ \tilde{S}^- > = \frac{i}{2\pi} \int_{-\infty}^{+\infty} d\omega \frac{< \tilde{S}^-|\tilde{S}^+\gg_{\omega+i\eta} - < \tilde{S}^-|\tilde{S}^+\gg_{\omega-i\eta}}{e^{\beta\omega} - 1}$$

we know that $c_1$ must vanish, otherwise, there will be $< \tilde{S}^+ \tilde{S}^- > = \infty$ for finite $N_A$. Thus

$$\frac{1}{N_A} < \tilde{S}^+ > = \frac{2\Delta^*}{2\mu - U} \frac{1}{N_A} < \tilde{S}_z >$$

Taking the limit in (20), one can immediately arrive at the conclusion Q.E.D.

According to Bogolyubov[13], symmetry-breaking properties should be discussed by quasi-averages, i.e. giving some symmetry-breaking perturbation and letting it vanish finally. Theorem 2 states that the quasi-average of $\tilde{S}^+$ is zero. This does not mean the pairing

$$\lim_{\Delta \to 0} \lim_{N_A \to \infty} < c_i^+ c_i^- > = 0.$$ If the two sub-lattices are homogeneous, denote $\tilde{s}^+_A$ for $i \in A/B$. Theorem 2 implies that $\rho_A \tilde{s}^+_A - \rho_B \tilde{s}^+_B = 0$, where $\rho_A/B = N_A/B/N_A$.

We make some conclusional discussions. It can be understood that we can not obtain a lower limit of the order of $N_A$ for the largest eigenvalue of the reduce density $\rho_2$ by means of the Bogolyubov identity (4) because the times of sum $\sum_i$ in both the numerator and the denominator in the right hand side of (4) are equal. Thus the value will not be of order $N_A$. As the conclusions in [2] hold only for the specific quasi-averages therein, our theorem 2 refers to only a special way of symmetry breaking, or a special quasi-average too.
It can not surely rule out the possibility for non-vanishing $\langle \tilde{S}^+ \rangle$ for other quasi-averages. Similar discussions seem to apply to other models such as Kondo lattice model and periodic Anderson model. Finally, we would like to stress that both theorems do not rule out the possible existence of ODLRO in Hubbard models.

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