Long-Range Correlation of Electron Pairs in the Hubbard Model at Finite Temperatures in Three Dimensions

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Abstract

We show that in the translation invariant case and in the antiferromagnetic phase, the reduced density matrix $\rho_2$ has no off-diagonal long-range order of on-site electron pairs for the single-band Hubbard model on a cubic lattice away from half filling at finite temperatures both for the positive coupling and for the negative coupling. In these cases the model can not give a mechanism for the superconductivity caused by the condensation of on-site electron pairs and the nearest-neighbor electron pairs.

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It was proposed the possibility that the Hubbard model can give a mechanism to characterize high temperature superconductivity\cite{1}. It has been shown that the $\eta$ pairing states for the single band Hubbard model with constant hopping matrix element for nearest neighbor sites have ODLRO\cite{2}. It has also been shown that in the ground state the model with negative coupling has off-diagonal long-range order (ODLRO) on some bipartite lattice\cite{3}. However, as the temperature $T > 0$ whether the reduced density matrix $\rho_2$ has ODLRO is inconclusive. The purpose of this work is to study the ODLRO of $\rho_2$ in the single-band Hubbard model with constant hopping matrix element for nearest neighbor pairs on a cubic lattice at finite temperatures. In the translation invariant case we obtain an equation (10) in the following) which is satisfied by the long-range correlation functions of on-site electron pairs. From which we find that there is no ODLRO of on-site electron pairs. Then we consider the case with an antiferromagnetic background. In this case we will show that there is still no ODLRO of on-site electron pairs.

The Hamiltonian of the model is

$$H = -t \sum_{\langle \mathbf{r}, \mathbf{r'} \rangle} (a^\dagger_{\mathbf{r}} a^{}_{\mathbf{r'}} + b^\dagger_{\mathbf{r}} b^{}_{\mathbf{r'}}) + U \sum_{\mathbf{r}} a^\dagger_{\mathbf{r}} a^{}_{\mathbf{r}} b^\dagger_{\mathbf{r}} b^{}_{\mathbf{r}} - \mu \sum_{\mathbf{r}} (a^\dagger_{\mathbf{r}} a^{}_{\mathbf{r}} + b^\dagger_{\mathbf{r}} b^{}_{\mathbf{r}}), \quad (1)$$

where $a^{}_{\mathbf{r}}$ ($b^{}_{\mathbf{r}}$) is the annihilation operator of the electron with spin up (down) at site $\mathbf{r}$. $U$ and $t$ are constant, and $\mu$ is the chemical potential. $\langle \mathbf{r}, \mathbf{r'} \rangle$ is a pair of nearest-neighbor sites. The lattice is cubic in the three dimensional space. We take the lattice spacing to be unity.

Define the $\eta$–operators as those in \cite{2, 4, 5},

$$\eta_- = \sum_{\mathbf{r}} e^{-i \pi \cdot \mathbf{r}} a^{}_{\mathbf{r}} b^{}_{\mathbf{r}}, \quad \eta_+ = \eta_-^\dagger, \quad \eta_z = \frac{1}{2} \sum_{\mathbf{r}} (a^\dagger_{\mathbf{r}} a^{}_{\mathbf{r}} + b^\dagger_{\mathbf{r}} b^{}_{\mathbf{r}} - 1), \quad (2)$$

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where $\pi = (\pi, \pi, \pi)$. They satisfy

$$[\eta_+, \eta_] = 2\eta_z, \quad [\eta_\pm, \eta_z] = \mp \eta_\pm,$$

and

$$\eta_- H = (H + U - 2\mu)\eta_-.$$  \hspace{1cm} (4)

Consider the average over a grand canonical ensemble

$$\langle \eta_+ \eta_- \rangle = \frac{1}{Z} Tr(\eta_+ \eta_- e^{-\beta H}),$$  \hspace{1cm} (5)

where $Z$ is the grand partition function; $\beta$ the inverse temperature. Using (4) and cyclically permuting the factors under the trace, we obtain $\langle \eta_- \eta_+ \rangle = \langle \eta_+ \eta_- \rangle e^{\beta(U-2\mu)}$. Then the first one of (3) gives, when $U \neq 2\mu$,

$$\langle \eta_+ \eta_- \rangle = 2 \langle \eta_z \rangle e^{\beta(U-2\mu)}/(1 - e^{\beta(U-2\mu)}).$$  \hspace{1cm} (6)

From (2) we have $\langle \eta_z \rangle = (N-M)/2$, where $N = \sum_r \langle a_r^\dagger a_r + b_r^\dagger b_r \rangle$ is the average total number of electrons, $M$ the total number of lattice sites. Denoting the density of the number of electrons as $D = N/M$, (6) leads to

$$\frac{1}{M} \langle \eta_+ \eta_- \rangle = \frac{D - 1}{1 - e^{\beta(U-2\mu)}},$$  \hspace{1cm} (7)

$U \neq 2\mu$ corresponds to the case away from half filling. We will only consider this case below. As $T = \beta^{-1} = finite$ and away from half filling, the right hand side of (7) shows that $1/M \langle \eta_+ \eta_- \rangle$ is a finite intensive quantity, which is still finite in the thermodynamic limit ($M \to \infty, N \to \infty$ with $D = N/M$ and $\beta$ fixed).

On the other hand, by the definition of $\eta_\pm$, we can write

$$\frac{1}{M} \langle \eta_+ \eta_- \rangle = \frac{1}{M} \sum_{r,s} \langle b_r^\dagger a_s a_s^\dagger b_s \rangle e^{i\pi \cdot (r-s)}.$$  \hspace{1cm} (8)
First we consider the case without the spontaneous breaking of the translation symmetry on the lattice, and take the periodic boundary condition. We have
\[
\frac{1}{M} \langle \eta_+ \eta_- \rangle = \sum_r \langle b_r^\dagger a_r a_o b_o \rangle e^{i\pi \cdot r}.
\] (9)

In the thermodynamic limit, the right hand side of (9) becomes an infinite series. As we show above that \( \frac{1}{M} \langle \eta_+ \eta_- \rangle \) is finite, thus the infinite series \( \sum_r \langle b_r^\dagger a_r a_o b_o \rangle e^{i\pi \cdot r} \) is convergent.

Let us take the thermodynamic limit first, then, for the aim to investigate the behavior of \( \langle b_r^\dagger a_r a_o b_o \rangle \) at large \(|r|\), consider a cube of volume \((2S)^3\) in the infinitely large system. The center of the cube is at the origin of the coordinates. Let \( f(L) = \sum_{faces} \langle b_r^\dagger a_r a_o b_o \rangle e^{i\pi \cdot r} \), where \( r = (l, m, n), -L \leq l, m, n \leq L, l, m, n, L \) are integers, and \( L \leq S \). \( \sum_{faces} \) is the sum over the six faces of the cube with volume \((2L)^3\), i.e.,
\[
\sum_{faces} = \sum_{l,m=-L}^{L} \sum_{n=-L(n=\pm L)}^{L} + \sum_{n=-L(m=\pm L)}^{L} + \sum_{m,-L(l=\pm L)}^{L} + \sum_{m,-L(l=\pm L)}^{L} + \sum_{n,-L(l=\pm L)}^{L} + \sum_{m,-L(l=\pm L)}^{L}.
\]

It is clear that the sum of \( \langle b_r^\dagger a_r a_o b_o \rangle e^{i\pi \cdot r} \) over the cube of volume \((2S)^3\) can be written as \( \sum_r \langle b_r^\dagger a_r a_o b_o \rangle e^{i\pi \cdot r} = \sum_{L=0}^{S} f(L) \). Since as \( S \to \infty \) this series is convergent, we have \( \lim_{L \to \infty} f(L) = 0 \), namely,
\[
\lim_{L \to \infty} \sum_{faces} \langle b_r^\dagger a_r a_o b_o \rangle e^{i\pi \cdot r} = 0.
\] (10)

Eq.(10) is a strong restriction on the long-range correlation functions. We will show that it determines \( \langle b_r^\dagger a_r a_o b_o \rangle \) completely in the limit \(|r| \to \infty\).

From the algebraic approach to the quantum statistical mechanics we know that the correlation functions in the equilibrium states of a pure thermodynamic phase have the spatial cluster properties, which is a rigorous
result. It enables us to write
\[ \langle b_\mathbf{r}^\dagger a_\mathbf{r}^\dagger a_\mathbf{0} b_\mathbf{0} \rangle \to \langle b_\mathbf{r}^\dagger a_\mathbf{r}^\dagger \rangle \langle a_\mathbf{0} b_\mathbf{0} \rangle, \text{ as } |\mathbf{r}| \to \infty. \] (11)

In the translation invariant case \( \langle a_\mathbf{r} b_\mathbf{r} \rangle = \langle a_\mathbf{0} b_\mathbf{0} \rangle \), thus \( \langle b_\mathbf{r}^\dagger a_\mathbf{r}^\dagger a_\mathbf{0} b_\mathbf{0} \rangle \to |\langle a_\mathbf{0} b_\mathbf{0} \rangle|^2 \), as \( |\mathbf{r}| \to \infty \). In (11) \( \langle a_\mathbf{r} b_\mathbf{r} \rangle \) should be understood as Bogolubov’s quasi-average, i.e., a \( U(1) \) symmetry breaking term was added to the Hamiltonian, and after taking the thermodynamic limit it has been sent to zero. \( \langle a_\mathbf{r} b_\mathbf{r} \rangle \) does not vanish, if there is on-site electron pair condensation, otherwise it vanishes. In the calculation of \( \langle b_\mathbf{r}^\dagger a_\mathbf{r}^\dagger a_\mathbf{0} b_\mathbf{0} \rangle \) the symmetry breaking term is not necessary. Since \( b_\mathbf{r}^\dagger a_\mathbf{r}^\dagger a_\mathbf{0} b_\mathbf{0} \) is an invariant under the global \( U(1) \) gauge transformation, its usual average ( in the Hamiltonian without the symmetry breaking term) and the quasi-average are the same.

It is a well established empirical fact that in the second-order phase transition the correlation length is divergent at the critical point, and it is finite away from the critical point. The modern theories of critical phenomena (the scaling hypothesis, the renormalization group approach, etc.) are based on it. We assume that this empirical fact works in the present problem, which is consistent with the superconducting transition being a second-order phase transition. Define \( G(\mathbf{r}) = \langle b_\mathbf{r}^\dagger a_\mathbf{r}^\dagger a_\mathbf{0} b_\mathbf{0} \rangle - |\langle a_\mathbf{0} b_\mathbf{0} \rangle|^2 \) for arbitrary \( \mathbf{r} \). Suppose that the system is in a noncritical thermodynamic state, then \( G(\mathbf{r}) \) can not decay slower than \( O(|\mathbf{r}|^{-3}) \) as \( |\mathbf{r}| \to \infty \), otherwise the correlation length for \( G(\mathbf{r}) \) will diverge to infinity at a noncritical point. So \( \lim_{L \to \infty} \sum_{\text{faces}} G(\mathbf{r}) e^{i\pi \cdot \mathbf{r}} = 0 \). Hence (11) shows that we can write
\[ \lim_{L \to \infty} \sum_{\text{faces}} \langle b_\mathbf{r}^\dagger a_\mathbf{r}^\dagger a_\mathbf{0} b_\mathbf{0} \rangle e^{i\pi \cdot \mathbf{r}} = |\langle a_\mathbf{0} b_\mathbf{0} \rangle|^2 \lim_{L \to \infty} \sum_{\text{faces}} e^{i\pi \cdot \mathbf{r}}. \] (12)
It can be shown that
\[ \sum_{fans} e^{i\pi \mathbf{r}} = (-1)^L 2, \quad \text{for } L \geq 1. \] (13)

Then (10) leads to \((-1)^L 2 |\langle a_o b_o \rangle|^2 \to 0\). Therefore we obtain \(\langle a_o b_o \rangle = 0\), and by translation invariance,
\[ \langle a_r b_r \rangle = 0, \quad \text{at any site } r. \] (14)

Furthermore (11) and (14) show that
\[ \langle b_r^\dagger a_r^\dagger a_s b_s \rangle \to 0, \quad \text{as } |\mathbf{r}| \to \infty. \] (15)

Eq. (14) shows that there is no condensation of on-site electron pairs, and (15) shows that the reduced density matrix \(\rho_2\) has no ODLRO for on-site electron pairs. These two statements are equivalent.

Using (14) and taking the quasi-average of \([H, a_r b_r]\), it can be shown [9]
\[ \langle a_r b_{r'} \rangle = 0, \] (16)
where \(r, r'\) are nearest neighbor sites. From the cluster property of correlation functions, we can write \(\langle b_r^\dagger a_r^\dagger a_s b_{s'} \rangle \to 0\), where \(|\mathbf{r} - \mathbf{r}'| = 0 \text{ or } 1, \quad |s - s'| = \text{finite}, \) and \(|\mathbf{r} - \mathbf{s}| \to \infty\).

The above results are obtained for the translation invariant case. The antiferromagnetic order breaks the translation symmetry. But we can show that the existence of antiferromagnetic order, if any, is not in contradiction with (14)-(16). In the antiferromagnetic phase there are two kinds of translations, i.e., the displacement \(\Delta \mathbf{r} = (\Delta x, \Delta y, \Delta z), \Delta x + \Delta y + \Delta z = \text{even integer}, \)
and $\Delta x + \Delta y + \Delta z = \text{odd integer}$. The first one does not break the translation symmetry, but the second one does. The second kind of translations is equivalent to exchange the up spins and the down spins, so it is easily seen that

$$
\langle a_r b_r \rangle = e^{i\pi \cdot r} \langle a_o b_o \rangle \quad \text{and} \quad \langle b_r^\dagger a_r^\dagger a_s b_s \rangle = \langle b_{r-s}^\dagger a_{r-s}^\dagger a_o b_o \rangle. \tag{17}
$$

Thus (9) and (10) are still valid, but (12) should be replaced by

$$
\lim_{L \to \infty} \sum_{\text{faces}} \langle b_r^\dagger a_r^\dagger a_o b_o \rangle e^{i\pi \cdot r} = |\langle a_o b_o \rangle|^2 \lim_{L \to \infty} \sum_{\text{faces}} 1
\quad = |\langle a_o b_o \rangle|^2 \lim_{L \to \infty} 2(12L^2 + 1). \tag{18}
$$

So we can show that (14)-(16) still hold, i.e., there is no ODLRO for on-site electron pairs.

In the derivation of (14)-(16), the sign of $U$ plays no role whatsoever, so the above results apply to the cases both for $U > 0$ and for $U < 0$.

In summary, we have shown that for the translation invariant case or in the antiferromagnetic phase the reduced density matrix $\rho_2$ has no ODLRO of on-site electron pairs for the single band Hubbard model on a cubic lattice away from half filling at finite temperatures both for $U > 0$ and for $U < 0$. In these cases the model can not give a mechanism for the superconductivity caused by the condensation of on-site electron pairs and nearest neighbor electron pairs. To derive the above results we have assumed that in the case away from the critical point the correlation length is finite, and no other ad hoc assumption is needed. The above discussion can be easily generalized to any dimensions. Our results are not incompatible with [2] and [3], since their results are not the ensemble average at $T > 0$.

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