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The binding energy and the charged gaps in the negative-*U* Hubbard model: some rigorous results

Guang-Shan Tian

Theoretical Physics, Oxford University, Keble Road, Oxford OX1 3NP, UK
Department of Physics, Peking University, People's Republic of China

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Abstract. By applying Lieb's spin-reflection-positivity method and exploiting a commutation relation satisfied by the negative-U Hubbard Hamiltonian, we prove two rigorous theorems on the binding energy of fermions, the one-particle and the two-particle gaps for the model on an arbitrary finite lattice.

In the study of condensed matter physics, superconductivity has always been a focus of physicists' interest. Its beauty has also fascinated many mathematical physicists. Since Bardeen, Cooper and Schrieffer introduced their extremely successful (BCS) theory on superconductivity [1], great efforts have been made to justify this variational theory on a more rigorous basis [2–8]. For example, in a recent paper [9], Bursill and Thompson showed that, under some very general conditions, the free energy density calculated by the BCS variational scheme is actually exact in the thermodynamic limit.

After the discovery of high-temperature superconductivity in the rare-earth-based cooper oxides [10], superconductivity in the narrow-band systems has also attracted great interest from condensed matter physicists. In this field, the so-called negative-U Hubbard model has been widely used as a phenomenological model [11]. For this model, the main concerns of physicists are the possible existence of the superfluid off-diagonal, long-range order [12, 13] in the model and its low-energy excitations [11]. On the other hand, the binding energy of fermions and the one-particle charged gap have also been discussed by several authors for the one-dimensional case [14–16], in which the Hubbard model is exactly solvable [17].

In this paper, we shall study the binding energy of fermions and the charged gaps for the negative-U Hubbard model defined on an *arbitrary* d-dimensional lattice. By applying some recently developed rigorous techniques [18–23], we prove two theorems on these quantities. They confirm the previous results derived in [14–16] for the one-dimensional negative-U Hubbard model. Moreover, we believe that the general approach given in this paper should also be applicable to other narrow-band superconducting models.

To begin with, we would like to introduce some definitions and useful terminologies.

Take a finite d-dimensional lattice Λ with N_Λ lattice sites. Then, the Hamiltonian of the negative-U Hubbard model can be written as

$$H_\Lambda(\mu, -\{U_i\}) = \sum_\sigma \sum_{\langle ij\rangle} t_{ij}(c^\dagger_{i\sigma}c_{j\sigma} + c^\dagger_{j\sigma}c_{i\sigma}) - \sum_{i\in\Lambda} U_i(n_{i\uparrow} - \mu)(n_{i\downarrow} - \mu) \qquad (1)$$

where $c_{i\sigma}^\dagger(c_{i\sigma})$ is the fermion creation (annihilation) operator which creates (annihilates) a fermion with spin σ at lattice site $\boldsymbol{i}$. $\langle \boldsymbol{ij}\rangle$ denotes a pair of lattice sites. $\{t_{\boldsymbol{ij}}\}$ and $U_{\boldsymbol{i}} > 0$ are parameters representing the kinetic energy and the on-site attraction of fermions, respectively. They are allowed to be site-dependent. $n_{\boldsymbol{i}\sigma} = c_{\boldsymbol{i}\sigma}^\dagger c_{\boldsymbol{i}\sigma}$ and μ is the chemical potential coefficient. In the following, without special notice, we shall *not* assume lattice Λ to be bipartite with respect to $H_\Lambda(\mu, -\{U_{\boldsymbol{i}}\})$.

It is easy to see that $H_\Lambda(\mu, -\{U_{\boldsymbol{i}}\})$ commutes with the total up-spin and down-spin fermion number operators, $\hat{N}_\uparrow$ and $\hat{N}_\downarrow$, respectively. Here, $\hat{N}_\sigma = \sum_{\boldsymbol{i}\in\Lambda} n_{\boldsymbol{i}\sigma}$. Consequently, the Hilbert space of $H_\Lambda(\mu, -\{U_{\boldsymbol{i}}\})$ can be divided into numerous subspaces $\{V(N_\uparrow, N_\downarrow)\}$. Each of them is characterized by a pair of specific fermion numbers, $N_\uparrow$ and $N_\downarrow$. We define subspace $V(N)$ by

$$V(N) = \sum_{N_\uparrow + N_\downarrow = N} \oplus V(N_\uparrow, N_\downarrow). \tag{2}$$

The Hubbard Hamiltonian enjoys the spin symmetry, too. Namely, $H_\Lambda(\mu, -\{U_{\boldsymbol{i}}\})$ commutes with the spin operators $\hat{S}_x$, $\hat{S}_y$ and $\hat{S}_z$ defined by

$$\hat{S}_x = \frac{1}{2}\sum_{\boldsymbol{i}\in\Lambda}(c_{\boldsymbol{i}\uparrow}^\dagger c_{\boldsymbol{i}\downarrow} + c_{\boldsymbol{i}\downarrow}^\dagger c_{\boldsymbol{i}\uparrow}) \qquad \hat{S}_y = \frac{1}{2\mathrm{i}}\sum_{\boldsymbol{i}\in\Lambda}(c_{\boldsymbol{i}\uparrow}^\dagger c_{\boldsymbol{i}\downarrow} - c_{\boldsymbol{i}\downarrow}^\dagger c_{\boldsymbol{i}\uparrow})$$
$$\hat{S}_z = \frac{1}{2}\sum_{\boldsymbol{i}\in\Lambda}(n_{\boldsymbol{i}\uparrow} - n_{\boldsymbol{i}\downarrow}). \tag{3}$$

Consequently, both S^2 and S_z are conserved quantities.

Furthermore, if lattice Λ is *bipartite* and $\mu = \frac{1}{2}$, $H_\Lambda(\frac{1}{2}, -\{U_{\boldsymbol{i}}\})$ also commutes with the so-called pseudospin operators [21, 24], which are defined by

$$\hat{J}_x = \frac{1}{2}\sum_{\boldsymbol{i}\in\Lambda}\epsilon(\boldsymbol{i})(c_{\boldsymbol{i}\uparrow}^\dagger c_{\boldsymbol{i}\downarrow}^\dagger + c_{\boldsymbol{i}\downarrow} c_{\boldsymbol{i}\uparrow}) \qquad \hat{J}_y = \frac{1}{2\mathrm{i}}\sum_{\boldsymbol{i}\in\Lambda}\epsilon(\boldsymbol{i})(c_{\boldsymbol{i}\uparrow}^\dagger c_{\boldsymbol{i}\downarrow}^\dagger - c_{\boldsymbol{i}\downarrow} c_{\boldsymbol{i}\uparrow})$$
$$\hat{J}_z = \frac{1}{2}\sum_{\boldsymbol{i}\in\Lambda}(n_{\boldsymbol{i}\uparrow} + n_{\boldsymbol{i}\downarrow} - 1). \tag{4}$$

Here, by definition, Λ is bipartite in terms of Hamiltonian $H_\Lambda(\mu, -\{U_{\boldsymbol{i}}\})$, if it can be split into two sublattices, A and B, such that fermions can only hop from a site of one sublattice to a site of another sublattice. Function $\epsilon(\boldsymbol{i})$ is defined by $\epsilon(\boldsymbol{i}) = 1$, if $\boldsymbol{i} \in A$; and $\epsilon(\boldsymbol{i}) = -1$, if $\boldsymbol{i} \in B$. It is an easy excise to check that operators $\hat{J}_x$, $\hat{J}_y$ and $\hat{J}_z$ satisfy the conventional commutation relations of the angular momentum operators. Therefore, both J^2 and J_z are also conserved quantities in this case.

In the following, we shall exploit these symmetries of $H_\Lambda(\mu, -\{U_{\boldsymbol{i}}\})$ to prove our theorems.

For the negative-U Hubbard model, one would expect that the fermions are bound by the attractive interaction into the Cooper pairs. In other words, the ground state of the negative-U Hubbard model should be a liquid of the paired fermions with up-spin and down-spin at the same lattice site. Whenever a pair is broken, extra energy will be needed. More precisely, if we let $E_0(N)$ be the ground-state energy of $H_\Lambda(\mu, -\{U_{\boldsymbol{i}}\})$ in subspace $V(N)$, we should expect that the following inequality

$$-E_\mathrm{B} \equiv E_0(2N+2) + E_0(2N) - 2E_0(2N+1) < 0 \tag{5}$$

hold for any integer $0 < N < N_\Lambda$. In many-body theory, E_B is defined to be the binding energy of fermions. Furthermore, at the *absolute* ground-state energy $E_0(2N_0)$, we should also expect that the one-particle charged gap Δ is non-vanishing, i.e. inequality

$$\Delta \equiv E_0(2N_0+1) + E_0(2N_0-1) - 2E_0(2N_0) > 0 \tag{6}$$

should hold for $E_0(2N_0)$. For the negative-U Hubbard model defined on a one-dimensional lattice, these relations have been exactly established [14–16]. However, for $d > 1$ cases, only results derived by either the mean-field theories or the numerical calculations on small size samples are available [11]. In this paper, as the first step of a rigorous investigation, we shall prove that both inequalities (5) and (6) hold for the negative-U Hubbard model on an arbitrary *finite* d-dimensional lattice Λ.

With these preparations, we now proceed to the statement and proof of our first theorem.

Theorem 1. Let Λ be an arbitrary *finite* lattice with N_Λ sites. Then, for any integer $0 < N < N_\Lambda$, the ground-state energies of the negative-U Hubbard Hamiltonian in subspaces $V(2N+2)$, $V(2N+1)$ and $V(2N)$ satisfy inequality (5).

Proof. To prove this theorem, we shall apply a recently generalized version [20] of Lieb's spin-reflection-positivity technique [18–21]. In [20], Lieb and Nachtergaele applied this method to show the stability of the Peierls instability for ring-shaped molecules. Naturally, in the following, we shall further tailor this method into a form which is more suitable for our purpose.

As the first step, we would like to write Hamiltonian $H_\Lambda(\mu, -\{U_i\})$ into a direct product form of operators acting separately on up-spin and down-spin configurations. To achieve this purpose, following [20], we introduce the following new fermion operators:

$$\hat{c}_{i\uparrow} \equiv c_{i\uparrow} \qquad \hat{c}_{i\downarrow} \equiv (-1)^{\hat{N}_\uparrow} c_{i\downarrow}. \tag{7}$$

Note that the operators $\{\hat{c}_{i\downarrow}\}$ now *commute* with $\{\hat{c}_{i\uparrow}\}$. Consequently, $H_\Lambda(\mu, -\{U_i\})$ can be written as

$$H_\Lambda(\mu, -\{U_i\}) = \hat{T}_\uparrow \otimes \hat{I} + \hat{I} \otimes \hat{T}_\downarrow - \sum_{i\in\Lambda} U_i(\hat{n}_{i\uparrow} - \mu) \otimes (\hat{n}_{i\downarrow} - \mu) \tag{8}$$

where $\hat{T}_\sigma = \sum_{\langle ij\rangle} t_{ij}(\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma})$ and $\hat{I}$ is the identity operator. Each operator in (8) acts on a corresponding subspace $\mathcal{H}_\sigma$ of fermions with spin σ.

Next, let us consider the ground-state $\Psi_0(2N+1)$ of $H_\Lambda(\mu, -\{U_i\})$ in subspace $V(2N+1)$. Since the spin operators $\hat{S}_+$ and $\hat{S}_-$ commute with the Hamiltonian, by applying these operators an appropriate number of times, we can always transform $\Psi_0(2N+1)$ into a state satisfying the condition $N_\uparrow - N_\downarrow = 1$. This state is degenerate with $\Psi_0(2N+1)$ and has quantum number $S_z = \frac{1}{2}$. In the following, we shall exclusively use $\Psi_0(2N+1)$ to denote this state.

Wavefunction $\Psi_0(2N+1)$, which has $(N+1)$ up-spin fermions and N down-spin fermions, can be naturally written as

$$\Psi_0(2N+1) = \sum_{m,n} W_{mn}\chi^\uparrow_m \otimes \chi^\downarrow_n. \tag{9}$$

In (9), χ^σ_k is a state vector defined by

$$\chi^\sigma_k \equiv \hat{c}^\dagger_{i_1\sigma}\cdots\hat{c}^\dagger_{i_M\sigma}|0\rangle \tag{10}$$

where $(\boldsymbol{i}_1, \ldots, \boldsymbol{i}_M)$, $M = N+1$, for $\sigma = \uparrow$; $M = N$, for $\sigma = \downarrow$, denote the positions of fermions with spin σ. Apparently, the entire set $\{\chi^\sigma_k\}$ gives a natural basis for $V_\sigma(M)$, the subspace of M fermions with spin σ. However, we should note that, if we naively choose $\mathcal{H}_\uparrow = V_\uparrow(N+1)$ and $\mathcal{H}_\downarrow = V_\downarrow(N)$, then the coefficient matrix $\mathcal{W} = (W_{mn})$ will be an $C^{N+1}_{N_\Lambda} \times C^N_{N_\Lambda}$ matrix, which is not a square matrix. Mathematically, it is rather difficult to deal with such a matrix. To avoid this nuisance, we shall choose both $\mathcal{H}_\uparrow$ and $\mathcal{H}_\downarrow$ by $\mathcal{H}_\sigma = V_\sigma(N) \oplus V_\sigma(N+1)$. Consequently, the natural bases in $\mathcal{H}_\uparrow$ and $\mathcal{H}_\downarrow$ have the same number of state vectors and, hence, matrix $\mathcal{W}$ can now be written as a $D \times D$ *square* matrix with $D = C_{N_\Lambda}^{N} + C_{N_\Lambda}^{N+1}$. Explicitly, we have

$$\mathcal{W} = \begin{pmatrix} O & \mathcal{M} \\ \mathcal{M}^\dagger & O \end{pmatrix} \tag{11}$$

where $\mathcal{M}$ is an $C_{N_\Lambda}^{N+1} \times C_{N_\Lambda}^{N}$ non-zero matrix. For such a square matrix, we have the following polar factorization theorem in matrix theory [25].

Lemma 1. Let A be an $n \times n$ matrix. Then, there are two $n \times n$ *unitary* matrices U, V and an $n \times n$ *diagonal* semi-positive definite matrix H such that

$$A = UHV \qquad h_{mn} = h_m \delta_{mn} \qquad \text{and} \qquad h_m \geqslant 0, m = 1, \ldots, n. \tag{12}$$

The proof of this lemma can be found in a standard textbook of matrix theory. For the reader's convenience, we shall give its proof in the appendix.

By the lemma, there exist two unitary matrices U, V and a diagonal positive semidefinite matrix H, such that $W = UHV$. Consequently, $\Psi_0(2N+1)$ can be rewritten as

$$\Psi_0(2N+1) = \sum_{m,n=1}^{D} W_{mn} \chi_m^\uparrow \otimes \chi_n^\downarrow = \sum_{m,\,n=1}^{D} (UHV)_{mn} \chi_m^\uparrow \otimes \chi_n^\downarrow = \sum_{l=1}^{D} h_l \psi_l^\uparrow \otimes \phi_l^\downarrow \tag{13}$$

with

$$\psi_l^\uparrow = \sum_{m=1}^{D} U_{ml} \chi_m^\uparrow \qquad \phi_l^\downarrow = \sum_{n=1}^{D} V_{ln} \chi_n^\downarrow. \tag{14}$$

Since U and V are unitary, $\{\psi_l^\uparrow\}$ and $\{\phi_l^\downarrow\}$ are also orthonormal bases in subspaces $\mathcal{H}_\uparrow$ and $\mathcal{H}_\downarrow$, respectively. Furthermore, since $\Psi_0(2N+1)$ is an eigenvector of $\hat{N}_\uparrow$ and $\hat{N}_\downarrow$, the following constraint conditions should hold for $\Psi_0(2N+1)$:

$$\langle \Psi_0(2N+1)|\hat{N}_\uparrow|\Psi_0(2N+1)\rangle = \sum_{l_1=1}^{D}\sum_{l_2=1}^{D} h_{l_1} h_{l_2} \langle \psi_{l_2}|\hat{N}|\psi_{l_1}\rangle = N+1 \tag{15}$$

and

$$\langle \Psi_0(2N+1)|\hat{N}_\downarrow|\Psi_0(2N+1)\rangle = \sum_{l_1=1}^{D}\sum_{l_2=1}^{D} h_{l_1} h_{l_2} \langle \phi_{l_2}|\hat{N}|\phi_{l_1}\rangle = N. \tag{16}$$

In both equations (15) and (16), the spin indices are dropped in the sums because, in each equation, only one species of spin is involved. These conditions will be used in the following.

In terms of this new form of $\Psi_0(2N+1)$, the ground-state energy of $H_\Lambda(\mu, -\{U_i\})$ in subspace $V(2N+1)$ is given by

$$\begin{aligned} E_0(2N+1) &= \langle \Psi_0(2N+1)|H_\Lambda(\mu, -\{U_i\})|\Psi_0(2N+1)\rangle \\ &= \sum_{l=1}^{D} h_l^2 [\langle \psi_l^\uparrow|\hat{T}_\uparrow|\psi_l^\uparrow\rangle + \langle \phi_l^\downarrow|\hat{T}_\downarrow|\phi_l^\downarrow\rangle] \\ &\quad - \sum_{i\in\Lambda} U_i \left(\sum_{l_1=1}^{D}\sum_{l_2=1}^{D} h_{l_1} h_{l_2} \langle \psi_{l_2}^\uparrow|n_{i\uparrow} - \mu|\psi_{l_1}^\uparrow\rangle \langle \phi_{l_2}^\downarrow|n_{i\downarrow} - \mu|\phi_{l_1}^\downarrow\rangle \right). \end{aligned} \tag{17}$$

Applying inequality $|ab| \leqslant \frac{1}{2}(|a|^2 + |b|^2)$ to each term in the last sum and dropping the spin indices, we obtain

$$E_0(2N+1) \geqslant \frac{1}{2}\sum_{l=1}^{D} h_l^2[\langle\psi_l|\hat{T}|\psi_l\rangle + \langle\psi_l|\hat{T}|\psi_l\rangle] + \frac{1}{2}\sum_{l=1}^{D} h_l^2[\langle\phi_l|\hat{T}|\phi_l\rangle + \langle\phi_l|\hat{T}|\phi_l\rangle]$$
$$-\frac{1}{2}\sum_{i\in\Lambda} U_i\left(\sum_{l_1=1}^{D}\sum_{l_2=1}^{D} h_{l_1}h_{l_2}\langle\psi_{l_2}|n_i-\mu|\psi_{l_1}\rangle\overline{\langle\psi_{l_2}|n_i-\mu|\psi_{l_1}\rangle}\right)$$
$$-\frac{1}{2}\sum_{i\in\Lambda} U_i\left(\sum_{l_1=1}^{D}\sum_{l_2=1}^{D} h_{l_1}h_{l_2}\langle\phi_{l_2}|n_i-\mu|\phi_{l_1}\rangle\overline{\langle\phi_{l_2}|n_i-\mu|\phi_{l_1}\rangle}\right). \tag{18}$$

Now, we introduce new wavefunctions Ψ_1 and Ψ_2 by

$$\Psi_1 = \sum_{l=1}^{D} h_l\psi_l^{\uparrow}\otimes\bar{\psi}_l^{\downarrow} \qquad \Psi_2 = \sum_{l=1}^{D} h_l\phi_l^{\uparrow}\otimes\bar{\phi}_l^{\downarrow} \tag{19}$$

where $\bar{\psi}_l$ and $\bar{\phi}_l$ are the complex conjugate of ψ_l and ϕ_l, respectively. Apparently, we have

$$\langle\Psi_1|\Psi_1\rangle = \langle\Psi_2|\Psi_2\rangle = \sum_{l=1}^{D} h_l^2 = \langle\Psi_0(2N+1)|\Psi_0(2N+1)\rangle = 1. \tag{20}$$

Since $\hat{T}$ is Hermitian and $\{n_i - \mu\}$ are real, in terms of Ψ_1 and Ψ_2, inequality (18) can be rewritten as

$$E_0(2N+1) \geqslant \tfrac{1}{2}\langle\Psi_1|H_\Lambda(\mu, -\{U_i\})|\Psi_1\rangle + \tfrac{1}{2}\langle\Psi_2|H_\Lambda(\mu, -\{U_i\})|\Psi_2\rangle. \tag{21}$$

On the other hand, we note that Ψ_1 and Ψ_2 are actually wavefunctions in subspaces $V(N+1, N+1)$ and $V(N, N)$, respectively. For example, by using the constraint condition (15), we have

$$\langle\Psi_1|\hat{N}_\uparrow|\Psi_1\rangle = \langle\Psi_1|\hat{N}_\downarrow|\Psi_1\rangle = \sum_{l_1=1}^{D}\sum_{l_2=1}^{D} h_{l_1}h_{l_2}\langle\psi_{l_2}|\hat{N}|\psi_{l_1}\rangle = N+1. \tag{22}$$

Therefore, by the variational principle, we obtain

$$E_0(2N+1) \geqslant \tfrac{1}{2}E_0(2N+2) + \tfrac{1}{2}E_0(2N). \tag{23}$$

Finally, we would like to show that inequality (23) is strict. This will end our proof of theorem 1.

In proving inequality (23), we used inequality $|uv| \leqslant \frac{1}{2}|u|^2 + \frac{1}{2}|v|^2$. It becomes an identity if and only if $u = v$ holds. Therefore, under the condition $U_i > 0$ for any $i \in \Lambda$, inequality (23) should be strict if one can find a set (i, l_1, l_2), such that the following conditions,

$$h_{l_1} \neq 0 \qquad h_{l_2} \neq 0 \qquad \text{and} \qquad \langle\psi_{l_2}|n_i-\mu|\psi_{l_1}\rangle \neq \langle\phi_{l_2}|n_i-\mu|\phi_{l_1}\rangle \tag{24}$$

hold simultaneously. In fact, by constraint conditions (15) and (16), we have

$$\sum_{i\in\Lambda}\sum_{l_1=1}^{D}\sum_{l_2=1}^{D} h_{l_1}h_{l_2}\langle\psi_{l_2}|n_i-\mu|\psi_{l_1}\rangle = N+1-\mu N_\Lambda$$
$$\neq N-\mu N_\Lambda = \sum_{i\in\Lambda}\sum_{l_1=1}^{D}\sum_{l_2=1}^{D} h_{l_1}h_{l_2}\langle\phi_{l_2}|n_i-\mu|\phi_{l_2}\rangle. \tag{25}$$

This implies that there must be at least one set (i, l_1, l_2) for which all the above-mentioned conditions are satisfied. Therefore, inequality (23) is strict. □

Theorem 1 tells us that, for the negative-U Hubbard model on a *finite* lattice, the binding energy E_{B} of fermions is always positive. Consequently, fermions will be bound into pairs and each pair of fermions behaves like a hard-core boson. Therefore, for a specific admissible μ and a finite lattice Λ, there is an integer $0 < N_0 < N_\Lambda$ such that $\Psi_0(2N_0)$ is the *absolute* ground state of $H_\Lambda(\mu, -\{U_i\})$. On the other hand, by theorem 1 we have

$$\begin{aligned} E_0(2N_0+1) + E_0(2N_0-1) - 2E_0(2N_0) &> \tfrac{1}{2}[E_0(2N_0+2) + E_0(2N_0)] \\ &\quad + \tfrac{1}{2}[E_0(2N_0) + E_0(2N_0-2)] - 2E_0(2N_0) \\ &= \tfrac{1}{2}[E_0(2N_0+2) + E_0(2N_0-2) - 2E_0(2N_0)]. \end{aligned} \tag{26}$$

Note that the right-hand side of this inequality is non-negative by the definition of $\Psi_0(2N_0)$. Therefore, the following corollary of theorem 1 holds.

Corollary. For a specific admissible μ and a finite lattice Λ, inequality (6) holds for the *absolute* ground state $\Psi_0(2N_0)$ of $H_\Lambda(\mu, -\{U_i\})$. In other words, there is a non-vanishing one-particle charged gap at $E_0(2N_0)$.

Here, we would like to emphasize that, although we have shown that both the binding energy of fermions and the one-particle charged gap for the negative-U Hubbard model on a *finite* lattice are non-vanishing (both inequalities (5) and (6) are strict), they may tend to zero in the thermodynamic limit. To exclude this possibility, more careful calculations on the differences $|\langle\psi_{l_2}|n_i|\psi_{l_1}\rangle - \langle\phi_{l_2}|n_i|\phi_{l_1}\rangle|^2$ are needed. Further investigations on this problem are being continued.

In the above analysis, we did not assume that the absolute ground state $\Psi_0(2N_0)$ is a Bose–Einstein condensate of the paired fermions. Under this additional assumption, we can further show that the energy difference in the last line of inequality (26) tends to zero in the thermodynamic limit. In other words, if $\Psi_0(2N_0)$ is a superfluid, then its two-particle excitation gap must be absent in the thermodynamic limit. This is our second theorem in this paper. To give a more precise statement of this theorem, we need to introduce the following definition of the off-diagonal long-range order in a superfluid system.

Definition. Let $f(\boldsymbol{i})$ be a complex function defined on lattice Λ such that $|f(\boldsymbol{i})|^2 = 1$. Let

$$\hat{O}(f) \equiv \frac{1}{\sqrt{N_\Lambda}} \sum_{i\in\Lambda} f(\boldsymbol{i}) c_{\boldsymbol{i}\downarrow} c_{\boldsymbol{i}\uparrow}. \tag{27}$$

An eigenstate Ψ of $H_\Lambda(\mu, -\{U_i\})$ in $V(N)$ has a momentum-f, off-diagonal long-range order if and only if there is a constant $\alpha > 0$ independent of N_Λ such that inequality

$$\langle\Psi|\hat{O}^\dagger(f)\hat{O}(f)|\Psi\rangle \geqslant \alpha N_\Lambda \tag{28}$$

holds for the correlation function of $\hat{O}(f)$ as $N_\Lambda \to \infty$ and $N/N_\Lambda \to \rho \neq 0$.

Historically, the concept of off-diagonal, long-range order was proposed by Penrose and Onsager to characterize a superfluid phase in an interacting boson system [25]. Their definition was later generalized to the fermion systems by Yang [12]. Here, we follow Yang's definition. When Λ is a d-dimensional simple cubic lattice, function $f(\boldsymbol{i})$ can be taken as $f(\boldsymbol{i}) = \exp(-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{i})$, where $\boldsymbol{q}$ is a reciprocal vector of the lattice. Obviously, operator $\hat{O}(f)$ is the Fourier transformation of operator $c_{\boldsymbol{i}\downarrow}c_{\boldsymbol{i}\uparrow}$ and inequality

(28) implies that Ψ is a Bose–Einstein condensate of the Cooper pairs at momentum $\boldsymbol{q}$.

With the definition of the off-diagonal long-range order for the negative-U Hubbard model, we now prove theorem 2.

Theorem 2. Let $\Psi_0(2N_0)$ be the absolute ground state of $H_\Lambda(\mu, -\{U_i\})$ on a finite lattice Λ with a specific admissible μ. Assume that $\Psi_0(2N_0)$ has a momentum-f, off-diagonal long-range order as $N_\Lambda \to \infty$ and $2N_0/N_\Lambda \to \rho \neq 0$. Then, the two-particle charged gap at $E_0(2N_0)$ vanishes in the thermodynamic limit. In other words, the limit

$$\lim_{N_\Lambda \to \infty} E_0(2N_0+2) + E_0(2N_0-2) - E_0(2N_0) = 0 \tag{29}$$

holds under these conditions.

Proof. To prove this theorem, we shall take a general approach, which was used in [22] and [23] to show the vanishing spin excitation gaps in some strongly correlated fermion and boson systems. The starting point is the following identity,

$$\begin{aligned}\langle\Psi_0(2N_0)|[\hat{O}^\dagger(f), [H_\Lambda(\mu, -\{U_i\}), \hat{O}(f)]]|\Psi_0(2N_0)\rangle \\ = \sum_n (E_n - E_0(2N_0))[|\langle\Psi_n|\hat{O}(f)|\Psi_0(2N_0)\rangle|^2 + |\langle\Psi_n|\hat{O}^\dagger(f)|\Psi_0(2N_0)\rangle|^2]\end{aligned} \tag{30}$$

where $\{|\Psi_n\rangle\}$ is a complete set of eigenvectors of $H_\Lambda(\mu, -\{U_i\})$. By the definition of $\hat{O}(f)$, the left-hand side of identity (30) is equal to

$$\begin{aligned}&\langle\Psi_0(2N_0)|[\hat{O}^\dagger(f), [H_\Lambda(\mu, -\{U_i\}), \hat{O}(f)]]|\Psi_0(2N_0)\rangle \\ &\quad = \frac{1}{N_\Lambda}\sum_{\langle ij\rangle}(-t_{ij})[f(\boldsymbol{i}) + f(\boldsymbol{j})][\overline{f(\boldsymbol{i})}\langle\Psi_0(2N_0)|c^\dagger_{\boldsymbol{i}\uparrow}c_{\boldsymbol{j}\uparrow} \\ &\qquad + c^\dagger_{\boldsymbol{i}\downarrow}c_{\boldsymbol{j}\downarrow}|\Psi_0(2N_0)\rangle + \overline{f(\boldsymbol{j})}\langle\Psi_0(2N_0)|c^\dagger_{\boldsymbol{j}\uparrow}c_{\boldsymbol{i}\uparrow} + c^\dagger_{\boldsymbol{j}\downarrow}c_{\boldsymbol{i}\downarrow}|\Psi_0(2N_0)\rangle] \\ &\qquad - (1-2\mu)\frac{2N_0 - N_\Lambda}{N_\Lambda}.\end{aligned} \tag{31}$$

Obviously, the last term on the right-hand side of equation (31) is a quantity of O(1) as $N_\Lambda \to \infty$. On the other hand, since $|f(\boldsymbol{i})|^2 = 1$, the sum on the right-hand side of equation (31) is bounded above by $(8/N_\Lambda)\sum_\sigma\sum_{\langle ij\rangle}|t_{ij}||\langle c^\dagger_{i\sigma}c_{j\sigma}\rangle|$. When $\{t_{ij}\}$ are short ranged, it is also a quantity of O(1) in the thermodynamic limit. Consequently, the left-hand side of identity (30) is, at most, a quantity of O(1) as $N_\Lambda \to \infty$.

Next, let us consider the right-hand side of identity (30). It can be rewritten as

$$\begin{aligned}&\sum_n (E_n - E_0(2N_0))[|\langle\Psi_n|\hat{O}(f)|\Psi_0(2N_0)\rangle|^2 + |\langle\Psi_n|\hat{O}^\dagger(f)|\Psi_0(2N_0)\rangle|^2] \\ &\quad = \sum_n{}' (E_n(2N_0-2) - E_0(2N_0))|\langle\Psi_n(2N_0-2)|\hat{O}(f)|\Psi_0(2N_0)\rangle|^2 \\ &\qquad + \sum_m{}' (E_m(2N_0+2) - E_0(2N_0))|\langle\Psi_m(2N_0+2)|\hat{O}^\dagger(f)|\Psi_0(2N_0)\rangle|^2\end{aligned} \tag{32}$$

where $\sum'_n$ and $\sum'_m$ represent the partial sums over the states in subspaces $V(2N-2)$ and $V(2N+2)$, respectively. Other matrix elements are zero because $\hat{O}(f)$ and $\hat{O}^\dagger(f)$) are two-particle annihilation and creation operators. Since $\Psi_0(2N_0)$ is the *absolute* ground state of $H_\Lambda(\mu, -\{U_i\})$, each term in the right-hand side of equation (32) is a non-negative quantity.

By replacing $E_n(2N_0-2)-E_0(2N_0)$ and $E_m(2N_0+2)-E_0(2N_0)$ with $E_0(2N_0-2)-E_0(2N_0)$ and $E_0(2N_0+2)-E_0(2N_0)$ respectively, equation (32) can be further written into an inequality

$$\begin{aligned}
&\sum_n (E_n - E_0(2N_0))[|\langle\Psi_n|\hat{O}(f)|\Psi_0(2N_0)\rangle|^2 + |\langle\Psi_n|\hat{O}^\dagger(f)|\Psi_0(2N_0)\rangle|^2] \\
&\qquad \geqslant (E_0(2N_0-2) - E_0(2N_0)) \sum_n |\langle\Psi_n|\hat{O}(f)|\Psi_0(2N_0)\rangle|^2 \\
&\qquad\quad +(E_0(2N_0+2) - E_0(2N_0)) \sum_m [|\langle\Psi_m|\hat{O}^\dagger(f)|\Psi_0(2N_0)\rangle|^2] \\
&\qquad = (E_0(2N_0-2) - E_0(2N_0))\langle\Psi_0(2N_0)|\hat{O}^\dagger(f)\hat{O}(f)|\Psi_0(2N_0)\rangle \\
&\qquad\quad +(E_0(2N_0+2) - E_0(2N_0))\langle\Psi_0(2N_0)|\hat{O}^\dagger(f)\hat{O}(f)|\Psi_0(2N_0)\rangle \\
&\qquad = (E_0(2N_0-2) + E_0(2N_0+2) - E_0(2N_0))\langle\Psi_0(2N_0)|\hat{O}^\dagger(f)\hat{O}(f)|\Psi_0(2N_0)\rangle \\
&\qquad\quad +(E_0(2N_0+2) - E_0(2N_0))\langle\Psi_0(2N_0)|[\hat{O}^\dagger(f), \hat{O}(f)]|\Psi_0(2N_0)\rangle.
\end{aligned} \tag{33}$$

In equation (33), the sums are over *all* the eigenstates of $H_\Lambda(\mu, -\{U_{\boldsymbol{i}}\})$, although most of the matrix elements are actually zero. A little algebra yields

$$\langle\Psi_0(2N_0)|[\hat{O}^\dagger(f), \hat{O}(f)]|\Psi_0(2N_0)\rangle = \frac{1}{N_\Lambda}\langle\Psi_0(2N_0)|N_\Lambda - \hat{N}|\Psi_0(2N_0)\rangle = \frac{N_\Lambda - 2N_0}{N_\Lambda}. \tag{34}$$

This is a quantity of O(1) as $N_\Lambda \to \infty$. Therefore, the product in the last line of inequality (33) is of O(1) in the thermodynamic limit.

By combining equations (30), (31), (33) and (34), we finally obtain

$$\begin{aligned}
\mathrm{O}(1) &\geqslant (E_0(2N_0-2) + E_0(2N_0+2) - E_0(2N_0))\langle\Psi_0(2N_0)|\hat{O}^\dagger(f)\hat{O}(f)|\Psi_0(2N_0)\rangle \\
&\geqslant 0.
\end{aligned} \tag{35}$$

This holds for any admissible function $f(\boldsymbol{i})$. On the other hand, by the definition of the off-diagonal long-range order and the assumption of the theorem, for some admissible function $f_0(\boldsymbol{i})$, the correlation function $\langle\Psi_0(2N_0)|\hat{O}^\dagger(f_0)\hat{O}(f_0)|\Psi_0(2N_0)\rangle$ is a quantity of $\mathrm{O}(N_\Lambda)$ as $N_\Lambda \to \infty$ and $2N_0/N_\Lambda \to \rho \neq 0$. This requires that the energy difference $E_0(2N_0+2)+E_0(2N_0-2)-E_0(2N_0)$ tends to zero in the thermodynamic limit. Otherwise, inequality (35) will be eventually violated.

Our proof is accomplished. □

As an explicit illustration of theorem 1 and theorem 2 proved above, let us consider a special case of the negative-U Hubbard model. We assume that the model is defined on a *bipartite* lattice Λ. In this case, as we mentioned at the beginning of this paper, when $\mu = \frac{1}{2}$, Hamiltonian $H_\Lambda\left(\frac{1}{2}, -\{U_{\boldsymbol{i}}\}\right)$ commutes with the pseudospin operators $\hat{J}_x$, $\hat{J}_y$ and $\hat{J}_z$. Furthermore, there is also a *unitary* transformation $\hat{U}_1$ defined by

$$\hat{U}_1^\dagger c_{\boldsymbol{i}\uparrow}\hat{U}_1 = c_{\boldsymbol{i}\uparrow} \qquad \hat{U}_1^\dagger c_{\boldsymbol{i}\downarrow}\hat{U}_1 = \epsilon(\boldsymbol{i})c_{\boldsymbol{i}\downarrow}^\dagger \tag{36}$$

such that, under $\hat{U}_1$, we have

$$\hat{U}_1^\dagger H_\Lambda\left(\tfrac{1}{2}, -\{U_{\boldsymbol{i}}\}\right)\hat{U}_1 = H_\Lambda\left(\tfrac{1}{2}, \{U_{\boldsymbol{i}}\}\right) \tag{37}$$

and

$$\hat{U}_1^\dagger \hat{J}_x\hat{U}_1 = \hat{S}_x \qquad \hat{U}_1^\dagger \hat{J}_y\hat{U}_1 = \hat{S}_y \qquad \hat{U}_1^\dagger \hat{J}_z\hat{U}_1 = \hat{S}_z. \tag{38}$$

In the literature, $\hat{U}_1$ is called the partial particle–hole transformation [21, 24].

As a result of the pseudospin symmetry and the partial particle–hole symmetry, one can show that the absolute ground states of both $H_\Lambda\left(\frac{1}{2}, -\{U_i\}\right)$ and $H_\Lambda\left(\frac{1}{2}, \{U_i\}\right)$ coincide with their ground states in the half-filled subspace $V(N = N_\Lambda)$ [20, 24]. Furthermore, if the number of the lattice sites, N_A, in sublattice A is not equal to the number of lattice sites, N_B, in sublattice B, Lieb [19] showed that the ground state $\Psi_0(\{U_i\})$ of the *positive-U* Hubbard Hamiltonian $H_\Lambda\left(\frac{1}{2}, \{U_i\}\right)$ at half-filling has a total spin

$$S = \tfrac{1}{2}|N_A - N_B|. \tag{39}$$

By applying $\hat{U}_1^{-1}$, the inverse of the partial particle–hole transformation, these states will be mapped back onto their counterparts $\Psi_0(-\{U_i\})$ for the negative-U Hubbard Hamiltonian. These new states have a total pseudospin $J = \frac{1}{2}|N_A - N_B|$ due to the dual relation (38) between the spin and the pseudospin operators under the partial particle–hole transformation. Consequently, the absolute ground states of the negative-U Hubbard model at half-filling are degenerate and coincide with the ground states of $H_\Lambda\left(\frac{1}{2}, -\{U_i\}\right)$ in subspaces $V(2N)$, $2N_\Lambda - |N_A - N_B| \leqslant 2N \leqslant 2N_\Lambda + |N_A - N_B|$ [21]. Therefore, for the ground states of $H_\Lambda\left(\frac{1}{2}, -\{U_i\}\right)$ in these subspaces, we have

$$E_0(2N + 2) + E_0(2N - 2) - 2E_0(2N) \equiv 0. \tag{40}$$

On the other hand, when $|N_A - N_B| = \mathrm{O}(N_\Lambda)$, it has been shown that these ground states have actually both superfluid off-diagonal, long-range order and charge-density-wave, diagonal, long-range order [26]. In other words, they are supersolid. Apparently, these previous results are completely consistent with theorem 2. Now, theorem 1 tells us something more about these states. For each of these states, the binding energy of fermions and the one-particle charged gap are non-vanishing.

In summary, in this paper, by applying some recently developed techniques, we have proven two theorems on the binding energy, the one-particle and the two-particle charged gaps of the negative-U Hubbard model on an arbitrary finite lattice Λ.

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Appendix

The polar factorization lemma can be found in a standard textbook in matrix theory. The following proof of this lemma is given in [27].

Polar Factorization Lemma. Let A be an $n \times n$ matrix. Then, there exist two $n \times n$ unitary matrices U and V as well as an $n \times n$ *diagonal* positive semidefinite matrix H, such that

$$A = UHV. \tag{41}$$

The matrices U and V are uniquely determined if and only if A is non-singular.

Proof. Consider the positive semidefinite matrix $A^\dagger A$. Let $h_1^2, \ldots, h_n^2$ be its eigenvalues and let $(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n)$ be the corresponding orthonormal eigenvectors. Assume that $h_j > 0$ for $j = 1, 2, \ldots, k$ and $h_j = 0$ for $j = k+1, \ldots, n$. For $1 \leqslant i, j \leqslant k$, we have

$$\left(\frac{A\boldsymbol{x}_i}{h_i}, \frac{A\boldsymbol{x}_j}{h_j}\right) = \frac{1}{h_i h_j}(A\boldsymbol{x}_i, A\boldsymbol{x}_j) = \frac{1}{h_i h_j}(\boldsymbol{x}_i, A^\dagger A\boldsymbol{x}_j) = \frac{h_j^2 \delta_{ij}}{h_i h_j}. \tag{42}$$

Consequently, the vectors $\boldsymbol{z}_j = A\boldsymbol{x}_j/h_j$, for $j = 1, \ldots, k$, are orthonormal. Take additional $n-k$ orthonormal vectors $\boldsymbol{z}_{k+1}, \ldots, \boldsymbol{z}_n$ from subspace $V^\perp(\boldsymbol{z}_1, \ldots, \boldsymbol{z}_k)$, which is the perpendicular subspace to the subspace spanned by vectors $\boldsymbol{z}_1, \ldots, \boldsymbol{z}_k$. Let X and Z be the unitary matrices defined by $X^{(j)} = \boldsymbol{x}_j$ and $Z^{(j)} = \boldsymbol{z}_j$, where $X^{(j)}$ ($Z^{(j)}$) represents the jth column of matrix X (Z). We have $AX^{(j)} = h_j Z^{(j)}$, or, with $H = \mathrm{diag}(h_1, \ldots, h_n)$,

$$AX = ZH. \tag{43}$$

Now, by letting $U = Z$ and $V = X^\dagger$, we obtain

$$UHV = ZHX^\dagger = AXX^\dagger = A. \tag{44}$$

The lemma is proved. □

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