The Nagaoka state in the one-hand Hubbard model with two and more holes

The Nagaoka state in the one-band Hubbard model with two and more holes

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Abstract. The infinite-U Hubbard model with two holes on a two-dimensional square lattice is explicitly studied. We show that the energy of the Nagaoka state and the exact ground state become degenerate in the thermodynamic limit, i.e. there exists no energy gap between the ground state and the first excited state. Finally, we discuss briefly how to generalize this result to cases in which there is a finite number of holes and the structure of the lattice is more complicated.

Since the discovery of superconductivity in the rare-earth-based copper oxides, there has been growing interest in the Hubbard model. The physics of this model is complex and far from being fully understood. Nagaoka's theorem [1-5] is one of few rigorous results known to physicists. The Hamiltonian of the Hubbard model has the following simple form:

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

where $c_{i\sigma}^{+}(c_{i\sigma})$ and $n_{i\sigma}$ are, respectively, creation (annihilation) operators and number operators of electrons with spin σ. Nagaoka's theorem tells us that the ground state of the Hubbard model has the maximum total spin when U is infinite and the following conditions are satisfied:

(i) there is exactly one hole;

(ii) the lattice can be divided into two sublattices such that t_{ij} is always zero if both i and j belong to the same sublattice;

(iii) $t_{ij} \geqslant 0$.

As far as the multi-hole cases are concerned, there are still no rigorous results known. Recently, these cases have been vigorously discussed in the literature [6-9]. There is some numerical evidence which indicates that the energy of the Nagaoka state and the exact ground state become degenerate in the thermodynamic limit [7]. In this paper, we shall give this conjecture a rigorous proof.

Let us first introduce some preliminary definitions.

Definition 1. We denote simple cubic lattice by SC, body-centred cubic lattice by BCC, face-centred cubic lattice by FCC and hexagonal close-packed lattice by HCP.

Definition 2. We call a lattice Λ divisible with respect to the Hubbard Hamiltonian (1) if it can be divided into two sublattices A and B such that

(i) each site of Λ belongs to either A or B;

(ii) if sites i and j belong to the same sublattice, say A, then $t_{ij} = 0$.

Definition 3. Let Λ be a sublattice. We define N_Λ to be the number of sites in Λ, $N_\uparrow$ the number of the up-spin electrons, $N_\downarrow$ the number of the down-spin electrons and $N_e = N_\uparrow + N_\downarrow$ the total number of electrons. $n = N_\Lambda - N_e$ is naturally defined to be the number of holes when it is positive.

Since the Hubbard Hamiltonian preserves $N_\uparrow$ and $N_\downarrow$, we can divide all the possible electron configurations into several disconnected sectors. In each sector, $N_\uparrow$ and $N_\downarrow$ are specified integers. In particular, we call the sector, in which all the electrons have up-spin, the all-spin-up sector (ASUS).

Definition 4. The Nagaoka state is defined to be the eigenstate corresponding to the lowest eigenvalue of the Hamiltonian restricted in the all-spin-up sector.

Remark. By definition, the Nagaoka state may not be the exact ground state of the Hubbard model. Only for the one-hole case have they been proved identical [2].

Our main result is the following theorem.

Theorem. Let Λ be a finite sublattice. Assume that

$$t_{ij} = \begin{cases} t & \text{if sites } i \text{ and } j \text{ are the nearest neighbours} \\ 0 & \text{otherwise.} \end{cases} \tag{2}$$

Suppose that

(i) $U = \infty$

(ii) $n = N_\Lambda - N_e \geqslant 2$ but finite;

(iii) the parameter t is positive for an FCC or HCP lattice, and either positive or negative for an SC or BCC lattice.

Then the energy of the Nagaoka state and the energy of the exact ground-state approach to the same limit as the sublattice tends to infinity in Van Hove's sense. Furthermore, the thermodynamic limit of the energy is $-nzt$ where z is the number of nearest neighbours of each site of Λ.

Some remarks are in order.

Remark 1. For an SC or BCC lattice, the sign of t does not really matter since they are divisible with respect to the Hubbard Hamiltonian with t_{ij} defined in (2). A proper canonical transformation can reverse this sign but leaves the spectrum of the Hamiltonian unaffected. For an indivisible FCC or HCP lattice, the positive condition on t cannot be relaxed. Readers can find a detailed discussion in [2].

Remark 2. To avoid unnecessary nuisance, we do not give the phrase 'lattice Λ tends to infinity in Van Hove's sense' a mathematically rigorous definition. Roughly speaking, lattice Λ would grow like a balloon rather than a sausage.

The strategy of our proof can be outlined as follows. Let $E_g(\Lambda)$ be the energy of the exact ground state. We first seek some lower and upper bounds to $E_g(\Lambda)$. Then we take the thermodynamic limit. To find a lower bound, $E_L(\Lambda)$, to $E_g(\Lambda)$, we write the Hubbard Hamiltonian in a suitable matrix form and then use the technique which we developed in [5]. For the upper bound to $E_g(\Lambda)$, we use the variational principle. Notice that $E_g(\Lambda)$ bounded above by the energy of the Nagaoka state $E_{Na}(\Lambda)$ for the lowest eigenvalue of the restricted Hamiltonian in a sector is never less than the lowest eigenvalue of the total Hamiltonian. Then, by the variational principle, $E_{Na}(\Lambda)$ is less than the energy of some proper trial state vector, $E_{Tr}(\Lambda)$.

For simplicity, we shall only consider the Hamiltonian on a two-dimensional square lattice with two holes in the following. The proof can be easily extended to more general cases.

Before proving this theorem, we would like to introduce several notations and collect some simple facts which will be useful.

(*a*) Let Λ be an $M_1 \times M_2$ two-dimensional square sublattice, where M_1 and M_2 are integers. For convenience, we impose the open boundary condition on Λ. Choose a site of Λ as the original point. Then a pair of integer coordinates (x, y) can be assigned to each lattice site. We can now define an order among the lattice sites. In the following, we shall assume the alphabetical order, i.e. site $i = (x_1, y_1)$ is ahead of site $j = (x_2, y_2)$ if

(i) $x_1 < x_2$, or

(ii) $x_1 = x_2$ but $y_1 < y_2$.

(*b*) As $U = \infty$, there can be at most one electron at each site.

(*c*) Each sector of the electron configurations can be marked by a pair of integers $(N_\uparrow, N_\downarrow)$ such that

$$N_e = N_\uparrow + N_\downarrow. \tag{3}$$

In sector $(N_\uparrow, N_\downarrow) = (n_1, n_2)$, a complete set of orthogonal and normalized state vectors can be defined in the following way

$$\Psi_{\{hk,\alpha\}} = (-1)^{h-1}(-1)^{k-2} C_{1,\sigma(1)}^+ \cdots C_{h-1,\sigma(h-1)}^+ C_{h+1,\sigma(h+1)}^+ \cdots C_{k-1,\sigma(k-1)}^+$$
$$\times C_{k+1,\sigma(k+1)}^+ \cdots C_{N_\Lambda,\sigma(N_\Lambda)}^+ |0\rangle \tag{4}$$

where h and k are the positions of holes and α denotes the spin configuration

$$\{\sigma(1), \ldots, \sigma(h-1), \sigma(h+1), \ldots, \sigma(k-1), \sigma(k+1), \ldots, \sigma(N_\Lambda)\}. \tag{5}$$

The phase factor is introduced for a purpose.

In terms of this basis, the Hubbard Hamiltonian can be written in the following matrix form:

$$H = \begin{pmatrix} H(N_\Lambda - 2, 0) & & & & \\ & H(N_\Lambda - 3, 1) & & & 0 \\ & & \ddots & & \\ 0 & & & H(0, N_\Lambda - 2) \end{pmatrix}. \tag{6}$$

Each submatrix is a square matrix.

(*d*) For a specified submatrix $H(n_1, n_2)$, we now calculate its elements. Since the Hamiltonian contains only hopping terms, a non-zero element must be either $-t$ or t. If two state vectors Ψ and Φ contribute a non-zero matrix element $\langle \Psi | H(n_1, n_2) | \Phi \rangle$, then we call them super-neighbours (SN). It is obvious that a hole at site k in Ψ should appear at a nearest neighbour site of k in Φ if Ψ and Φ are SN. In a two-dimensional square sublattice, each site has $z = 4$ nearest neighbours. Therefore, any state vector Ψ can have at most $2z = 8$ SN (there are two holes). In other words, there are at most $2z$ non-zero elements in each row of the submatrix $H(n_1, n_2)$.

Furthermore, if the non-zero matrix element is $-t$, we call Ψ and Φ good super-neighbours (GSN). Otherwise, they are called bad super-neighbours (BSN). Rewriting the Hamiltonian in the form

$$H = \sum_\sigma \sum_{\langle ij \rangle} t c_{i\sigma}^+ c_{j\sigma} = \sum_\sigma \sum_{\langle ij \rangle} (-t) c_{j\sigma} c_{i\sigma}^+ \tag{7}$$

one can easily see that a state vector Φ is a BSN of Ψ if, and only if, the order of holes in Φ and Ψ is reversed.

Let the positions of two holes be $h = (x_1, y_1)$ and $k = (x_2, y_2)$ in Ψ. To calculate the non-zero elements contributing from SN of Ψ, several cases have to be considered separately.

(i) $|x_1 - x_2| \geqslant 2$ (see figures $1(a)$ and $1(b)$). In figure $1(a)$, both holes are in the interior of Λ, i.e. $x_1, x_2 \neq 0$ or M_1. In this case, each state vector has $2z = 8$ GSN. Therefore, the corresponding row in $H(n_1, n_2)$ contains exactly $2z$ non-zero elements $(-t)$. We shall use N_{Ia} to denote the total number of such state vectors in the all-spin-up sector (ASUS).

In figure $1(b)$, one of the holes is on the boundary. In this case, Ψ has fewer than $2z$ GSN. For instance, the state vector corresponding to figure $1(b)$ has $2z - 1 = 7$ GSN. Let N_{Ib} be the number of such state vectors in ASUS. Then

$$N_{Ib} \leqslant 2(M_1 + M_2)N_{\Lambda}. \tag{8}$$

(Fix a hole on the boundary. Another hole can occupy any position two blocks away. The number of these positions is certainly less than N_{Λ}. For the fixed hole, there are $2(M_1 + M_2)$ positions available.)

Next, we consider the state vectors Ψs represented by the configurations in which $|x_1 - x_2| = 0$ or 1.

(ii) $|x_1 - x_2| = 0$ (see figure 2). A state vector Ψ satisfying this condition has several BSN and hence fewer than $2z$ GSN. For example, the state vector corresponding to the
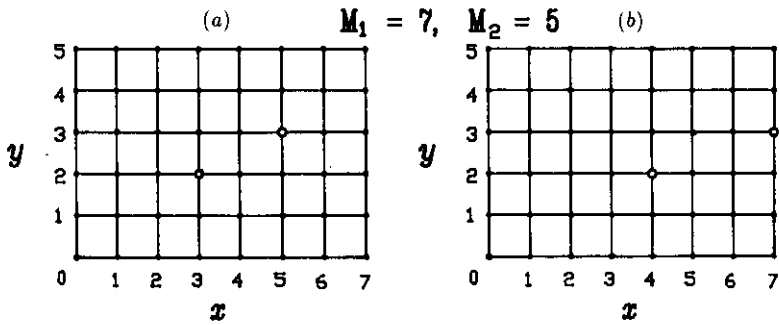

Figure 1 (a) $|x_1 - x_2| \geqslant 2$ and both holes are inside of Λ. (b) $|x_1 - x_2| \geqslant 2$ and one hole is on the boundary of Λ. $\bullet$ = electron; $\circ$ = hole.
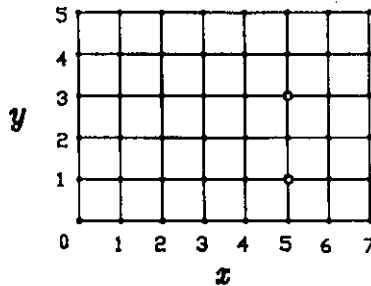

Figure 2. $|x_1 - x_2| = 0$. $\bullet$ = electron; $\circ$ = hole.

configuration shown in figure 2 has two BSN and $2z - 2 = 6$ GSN. Let N_{II} be the number of such state vectors in ASUS. Then

$$N_{II} \leqslant M_2^2 M_1 = M_2 N_A. \tag{9}$$

(iii) $|x_1 - x_2| = 1$ (see figures $3(a)$ and $3(b)$). Most of the state vectors satisfying this condition have some BSN and hence fewer than $2z$ GSN (figure $3(a)$). But some of them have fewer than $2z$ GSN because of topological restriction (figure $3(b)$). Let the number of the state vectors satisfying condition (iii) in ASUS be N_{III}. Then

$$N_{III} \leqslant M_2^2 M_1 = M_2 N_A. \tag{10}$$

The above analysis is lengthy but otherwise straightforward. For the higher-dimensional and more general lattices, similar conclusions can be easily obtained. We shall use these results to derive an upper bound to the energy of the exact ground state.
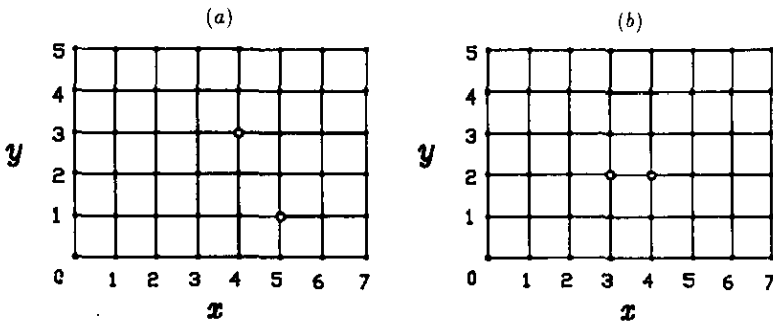

Figure 3. (a) $|x_1 - x_2| = 1$ but $|y_1 - y_2| \neq 0$. (b) $|x_1 - x_2| = 1$ and $|y_1 - y_2| = 0$. $\bullet$ = electron; $\circ$ = hole.

(e) By means of the creation and annihilation operators, we can write the total spin operator and its z-component operator in the following form [5]:

$$S_{\text{total}}^2 = \tfrac{1}{2} \left(\sum_i c_{i\uparrow}^+ c_{i\downarrow} \right) \left(\sum_j c_{j\uparrow}^+ c_{j\downarrow} \right) + \tfrac{1}{2} \left(\sum_i c_{i\downarrow}^+ c_{i\uparrow} \right) \left(\sum_j c_{j\downarrow}^+ c_{j\uparrow} \right)$$

$$+ \tfrac{1}{4} \left\{ \sum_i (n_{i\uparrow} - n_{i\downarrow}) \right\} \left\{ \sum_j (n_{j\uparrow} - n_{j\downarrow}) \right\} \tag{11}$$

$$S_z = \tfrac{1}{2} \sum_i (n_{i\uparrow} - n_{i\downarrow}). \tag{12}$$

A little algebra shows that any state vector in ASUS

$$\Psi_{hk} = (-1)^{h-1} (-1)^{k-2} C_1^+ \dots C_{h-1}^+ C_{h+1}^+ \dots C_{k-1}^+ C_{k+1}^+ \dots C_{N_A}^+ |0\rangle \tag{13}$$

(we have dropped index α for all the spins are up in this state) has

$$S_z = S_{\text{total}} = S_{\max} = \tfrac{1}{2} N_e = \tfrac{1}{2} (N_A - 2). \tag{14}$$

Therefore, as a linear combination of these state vectors, the Nagaoka state has the maximum total spin.

Now, we are ready to prove our theorem.

Proof. We first show that

$$E_g(\Lambda) \geq -2zt = -8t. \tag{15}$$

Since the Hamiltonian matrix has the block structure shown in (6), the energy of the exact ground state must be the lowest eigenvalue of some submatrix $H(n_1, n_2)$. Let D be the number of rows (columns) of $H(n_1, n_2)$. Take an arbitrary eigenvalue λ of $H(n_1, n_2)$. There is a non-zero vector u_λ such that

$$H(n_1, n_2)u_\lambda = \lambda u_\lambda. \tag{16}$$

Suppose that $|u_m|$ is the maximum of the absolute values of the components of u_λ, i.e.

$$|u_m| = \max_{1 \leq j \leq D} |u_j|. \tag{17}$$

Consider the mth row of equation (16),

$$\sum_{n=1}^{D} H_{mn}u_n = \lambda u_m. \tag{18}$$

Using the definition of $|u_m|$, we obtain the following inequality:

$$
\begin{aligned}
|\lambda u_m| &= \left| \sum_{n=1}^{D} H_{mn}u_n \right| \\
&\leq \sum_{n=1}^{D} |H_{mn}||u_n| \\
&\leq \left(\sum_{n=1}^{D} |H_{mn}| \right) |u_m|.
\end{aligned}
\tag{19}
$$

Therefore,

$$|\lambda| \leq \sum_{n=1}^{D} |H_{mn}| \leq 2zt. \tag{20}$$

In (20), we used the fact that, in each row of $H(n_1, n_2)$, there are at most $2z$ non-zero elements $-t$ or t (see the discussion in (d) above).

Since $H(n_1, n_2)$ is Hermitian, any eigenvalue of it must be real. Inequality (20) gives

$$\lambda \geq -2zt. \tag{21}$$

In particular, it holds for the lowest eigenvalue of $H(n_1, n_2)$, $E_g(\Lambda)$, i.e.

$$E_g(\Lambda) \geq -2zt. \tag{22}$$

Next, we seek an upper bound to $E_g(\Lambda)$.

$E_g(\Lambda)$ is trivially bounded above by $E_{Na}(\Lambda)$. On the other hand, the variational principle tells us that

$$E_{Na}(\Lambda) = \min_{\Psi \in ASUS} \frac{(\Psi, H(N_\Lambda - 2, 0)\Psi)}{(\Psi, \Psi)} \tag{23}$$

over the all-spin-up sector. Choosing the following trial vector

$$\Psi_{tr} = \sum_{\{hk\}} \Psi_{hk} \tag{24}$$

and inserting it into (23), we get

$$E_g(\Lambda) \leq E_{Na}(\Lambda) \leq \frac{(\Psi_{tr}, H(N_\Lambda - 2, 0)\Psi_{tr})}{(\Psi_{tr}, \Psi_{tr})}. \tag{25}$$

The denominator in (25) is simply the dimension of ASUS. It is the number of ways in which one can choose two sites from N_Λ sites:

$$(\Psi_{tr}, \Psi_{tr}) = C_{N_\Lambda}^2 \equiv \frac{N_\Lambda!}{2!(N_\Lambda - 2)!}. \tag{26}$$

The estimate of the numerator is a little cumbersome but straightforward.

Let N_g and N_b be the numbers of pairs of GSN and BSN in ASUS, respectively. Then

$$(\Psi_{tr}, H(N_\Lambda - 2, 0)\Psi_{tr}) = \sum_{\{hk\}} \sum_{\{h'k\}} (\Psi_{hk}, H(N_\Lambda - 2, 0)\Psi_{h'k'})$$

$$= -2tN_g + 2tN_b. \tag{27}$$

The factor 2 is from double counting in the sum.

From the discussion in (d), we see that each state vector in ASUS represented by figure $1(a)$ has $2z$ GSN and no BSN. Therefore

$$N_g \geq \frac{(2zN_{Ia})}{2}. \tag{28}$$

On the other hand, each state vector in ASUS represented by figures $1(b)$, 2, $3(a)$ and $3(b)$ contributed fewer than $2z$ or zero BSN and hence

$$N_b \leq \frac{2z(N_{Ib} + N_{II} + N_{IIIa} + N_{IIIb})}{2}. \tag{29}$$

Inserting (28) and (29) into (27), we obtain

$$(\Psi_{tr}, H(N_\Lambda - 2, 0)\Psi_{tr})$$

$$\leq -2ztN_{Ia} + 2zt(N_{Ib} + N_{II} + N_{IIIa} + N_{IIIb})$$

$$= -2zt(N_{Ia} + N_{Ib} + N_{II} + N_{IIIa} + N_{IIIb})$$

$$+ 4zt(N_{Ib} + N_{II} + N_{IIIa} + N_{IIIb}). \tag{30}$$

The sum in the first term is the number of all the possible state vectors in ASUS and thus the dimension of ASUS, $C_{N_\Lambda}^2$. The sum in the second term is less than $4M_2 N_\Lambda + 2M_1 N_\Lambda$, using the conclusions of discussions in $(d(i)-(iii))$. Therefore,

$$(\Psi_{tr}, H(N_\Lambda - 2, 0)\Psi_{tr}) \leq (-2zt)C_{N_\Lambda}^2 + 16ztM_2 N_\Lambda + 8ztM_1 N_\Lambda. \tag{31}$$

Substituting (26) and (31) into (25), we obtain

$$E_g(\Lambda) \leq E_{Na}(\Lambda)$$

$$\leq \frac{-2ztC_{N_\Lambda}^2 + 16ztM_2 N_\Lambda + 8ztM_1 N_\Lambda}{C_{N_\Lambda}^2}$$

$$= -2zt + \frac{32ztM_2 N_\Lambda + 16ztM_1 N_\Lambda}{N_\Lambda(N_\Lambda - 1)}$$

$$= -2zt + 32zt\left(\frac{M_2}{N_\Lambda - 1}\right) + 16zt\left(\frac{M_1}{N_\Lambda - 1}\right). \tag{32}$$

Combining (22) and (32) yields

$$-2zt \leq E_g(\Lambda) \leq (-2zt) + 32zt\left(\frac{M_2}{N_\Lambda - 1}\right) + 16zt\left(\frac{M_1}{N_\Lambda - 1}\right). \tag{33}$$

Letting Λ tend to infinity in Van Hove's sense, i.e.

$$N_\Lambda = M_1 M_2 \to \infty \quad \text{and} \quad \frac{M_1}{M_2} \to K \tag{34}$$

where K is a constant, the thermodynamic limit of the energy of the exact ground state is obtained

$$\lim_{\Lambda \to \infty} E_g(\Lambda) = -2zt = -8t. \quad \square \tag{35}$$

We would like to make some remarks.

Remark 1. Noticing that the energy of the ground state in the one-hole case is $-zt$ [5], it would be safe to say that, for $U = \infty$, holes tend to avoid each other. In this way, each hole can be regarded almost independent, and each of them contributes the same amount to the energy of the ground state.

Remark 2. This theorem can be easily generalized to more complicated cases by mimicking the above proof.

Suppose that there are n holes (n is a finite constant integer) and the Hubbard Hamiltonian is defined on a d-dimensional SC, BCC, FCC or HCP lattice. We impose the open boundary condition on the system and order the lattice sites by alphabetical order. We now define a set of orthogonal and normalized state vectors by

$$\Psi_{\{i_1,\dots,i_n;\alpha\}} = (-1)^{i_1-1}\dots(-1)^{i_n-n}c^+_{1,\sigma_1}\dots c^+_{i_1-1,\sigma_{i_1-1}}c^+_{i_1+1,\sigma_{i_1+1}}$$
$$\dots c^+_{i_n-1,\sigma_{i_n-1}}c^+_{i_n+1,\sigma_{i_n+1}}\dots c^+_{N_\Lambda,\sigma_{N_\Lambda}}|0\rangle \tag{36}$$

where $\{i_1,\dots,i_n\}$ are the positions of holes. Under condition (2) imposed on t_{ij}, any state vector $\Psi_{\{i_1,\dots,i_n;\alpha\}}$ can have at most nz SN. When N_Λ is sufficiently large, there is at least one state vector which has nz SN. Therefore, without ado, we get

$$E_g(N_\Lambda) \geq -nzt. \tag{37}$$

On the other hand, by the variational principle, $E_g(N_\Lambda)$ is bounded above by

$$\frac{\langle \Psi_{tr}|H|\Psi_{tr}\rangle}{\langle \Psi_{tr}|\Psi_{tr}\rangle} \tag{38}$$

where $\Psi_{tr} = \Sigma_{\{i_1,\dots,i_n\}} \Psi_{\{i_1,\dots,i_n\}}$ belongs to ASUS. The denominator $\langle \Psi_{tr}|\Psi_{tr}\rangle$ simply equals $C^n_{N_\Lambda}$. We shall concentrate on calculating the numerator in the following.

From the above proof, we see that, when N_Λ is sufficiently large, the majority of the state vectors should have exactly nz GSN. Only a few state vectors have BSN or less than nz GSN because some holes are 'too close' to each other or on the boundary of lattice Λ. We shall call them the state vectors with defects. A little algebra shows that the numerator is bounded above by

$$-nztC^n_{N_\Lambda} + K_1 \{\text{number of state vectors having defects}\} \tag{39}$$

where K_1 is a constant independent of N_Λ. Unlike the two-hole case, a hole-interchanging does not necessarily contribute a positive matrix element t. As a matter of

fact, when a hole changes positions with an even number of holes, the corresponding matrix element $\langle \Psi | H | \Phi \rangle$ is still $-t$. Such subtleties make calculation of the quantity in the braces of (39) very difficult. Fortunately, we may ignore them. A crude estimate on the number of the state vectors having defects is good enough for our purpose. Let us assume that any pair of state vectors Ψ and Φ contributes a positive non-zero matrix t if some holes change their positions in Ψ and Φ. It is obvious that, under this assumption, the number of state vectors having defects is greatly inflated. We now argue that this inflated quantity is bounded above by $K_2 C_{N_\Lambda-2}^{n-2}(N_\Lambda)^{2-1/d}$, where K_2 is a constant independent of N_Λ. We first take two holes and put them 'close' enough such that their changing positions produces BSN. Then, we fix their positions and let the rest of holes occupy the remaining lattice sites arbitrarily. The total number of such configurations is $C_{N_\Lambda-2}^{n-2}$. Finally, we move that pair of holes around but still keep them 'close'. Using the conclusions of (d) in the proof, we see that this operation produces another factor which is less than $K_2(N_\Lambda)^{2-1/d}$. Therefore, expectation (38) is bounded above by

$$-nzt + \frac{K_1 K_2 C_{N_\Lambda-2}^{n-2}(N_\Lambda)^{2-1/d}}{C_{N_\Lambda}^{n}}. \tag{40}$$

The second term of (40) is of order $(N_\Lambda)^{-1/d}$ when N_Λ is sufficiently large. Taking the thermodynamic limit, we obtain

$$\lim_{\Lambda \to \infty} E_g(N_\Lambda) = -nzt. \tag{41}$$

Obviously, the above argument can be made rigorous.

Although we do not obtain the exact ground state of the infinite-U Hubbard model with more than two holes in this article (numerical results show that the Nagaoka's state cannot be the ground state for a finite size sample), our result does indicate that there is no energy gap between the ground state and the first excited state in the thermodynamic limit.

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