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A new method to show the absence of some long-range orderings

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Abstract. In this article, we shall show that the correlation function of a local operator B_i decays if there is another local operator A_i satisfying $[H, A_i] = \alpha B_i$, where H is the Hamiltonian of the many-body system under consideration and α is a constant. Finally, as an application of this theorem, we shall rigorously show that the RVB states, which were proposed by P W Anderson and his collaborators to explain high-temperature superconductivity, are absent in the Hubbard model at half-filling. We also give an argument, which indicates that the existence of the RVB ground states in the doped cases is highly improbable.

It is well known that the existence of a specific long-range ordering in a many-body system is very difficult to prove or disprove rigorously. For example, the famous Heisenberg model [1] was proposed in 1928 to explain the magnetic properties of insulators. However, it took about 40 years to show that the magnetic long-range order of this model at a finite temperature in one or two dimensions did not exist [2]. The existence of the antiferromagnetic long-range order in three dimensions was established much later and the existence of the ferromagnetic long-range order still remains an open problem [3–6]. Here, a great challenge to theorists is to find the proper methods for a concrete model.

In this article, we shall introduce a new method to prove the absence of some long-range orderings. We shall show that, if the relevant local operator is generated by the commutator of the Hamiltonian of a many-body system with another local operator, then the two-point correlation function of this operator will rapidly decay. As an application of this theorem, we shall prove rigorously that the ground state of the Hubbard model at half-filling cannot be a resonanting valence bond (RVB) state, which was proposed by Anderson to explain newly discovered high-temperature superconductivity [7, 8]. We also show strong evidence which indicates the non-existence of the RVB states even in a doped Hubbard model.

Before stating our theorem in a more precise form, we would like to recall several definitions and introduce some useful notation.

As far as solid state physics is concerned, most models are defined on a lattice. In other words, their Hamiltonians have discrete forms. Naturally, we shall concentrate on such models in the following. For definiteness, we take a finite d-dimensional simple cubic lattice Λ and impose the periodic boundary condition on it. For a concrete model, we let V_i be the relevant Hilbert space at site $i \in \Lambda$ (for instance, V_i is spanned by $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, and $|\uparrow\downarrow\rangle$ in the Hubbard model). Then, the total Hilbert space V_Λ is given by $\bigotimes_{i\in\Lambda} V_i$. Now, H_Λ, which is the restriction of the Hamiltonian in lattice Λ, can be written as a matrix. We denote its normalized global ground-state wavefunction by $\Psi_0(\Lambda)$. Let B_i be a local operator centred at site i. Following Yang [9], we define a matrix M by

$$M_{ij} \equiv \langle\Psi_0(\Lambda)|B_i^\dagger B_j|\Psi_0(\Lambda)\rangle. \qquad (1)$$

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Then, $\Psi_0(\Lambda)$ supports a long-range ordering characterized by B_i if and only if the largest eigenvalue $\lambda_{\max}$ of the matrix M satisfies the following inequality

$$\lambda_{\max} \geqslant \beta N_\Lambda \tag{2}$$

where N_Λ is the number of sites in lattice Λ and β is a positive constant independent of Λ. It is not difficult to show [9] that inequality (2) implies

$$\lim_{|i-j|\to\infty} \lim_{\Lambda\to\infty} \langle\Psi_0(\Lambda)|B_i^\dagger B_j|\Psi_0(\Lambda)\rangle \neq 0 \tag{3}$$

and *vice versa*. In particular, if the Hamiltonian is translational invariant, one can show that all the eigenvalues of M are of the following form

$$\lambda_q = \frac{1}{N_\Lambda}\sum_{i\in\Lambda}\sum_{j\in\Lambda}\langle\Psi_0(\Lambda)|B_i^\dagger B_j|\Psi_0(\Lambda)\rangle \exp[\mathrm{i}q\cdot(i-j)] \equiv \langle\Psi_0(\Lambda)|B_q^\dagger B_q|\Psi_0(\Lambda)\rangle \tag{4}$$

with

$$B_q \equiv \frac{1}{\sqrt{N_\Lambda}}\sum_{j\in\Lambda} B_j \exp[-\mathrm{i}q\cdot j] \tag{5}$$

and $q = (q_1, q_2, \ldots, q_d)$ is a reciprocal vector subject to the conditon $0 \leqslant q_i \leqslant 2\pi$. A detailed discussion on this point can be found in [10]. Therefore, the largest eigenvalue $\lambda_{\max}$ corresponds to some reciprocal vector q_0 and inequality (2) can be rewritten as $\lambda_{q_0} \geqslant \beta N_\Lambda$. A direct corollary is that, if

$$\lambda_q \equiv \langle\Psi_0(\Lambda)|B_q^\dagger B_q|\Psi_0(\Lambda)\rangle = \mathrm{O}(1) \tag{6}$$

for any reciprocal vector q as lattice Λ tends to infinity, then the long-range order of B_i does not exist.

With these definitions and notation, we now summarize our main result in the following theorem.

Theorem. Let $H_\Lambda = H_0 + \sum_{i\neq j} V(i-j)$ be the Hamiltonian of a lattice–fermion (boson) model, where H_0 represents the kinetic energy of independent particles and $V(i-j)$ is the interaction of two particles located at sites i and j. We assume that the interaction $V(i-j)$ is short-ranged and $|V|$ is bounded. Let A_i and B_i be two local operators centred at site i. If they satisfy

$$\alpha B_i = [H, A_i] \tag{7}$$

where $\alpha \neq 0$ is a constant, and

$$\langle\Psi_0(\Lambda)|B_q|\Psi_0(\Lambda)\rangle = \langle\Psi_0(\Lambda)|B_q^\dagger|\Psi_0(\Lambda)\rangle = 0 \tag{8}$$

then, for any reciprocal vector q,

$$\langle\Psi_0(\Lambda)|B_q^\dagger B_q|\Psi_0(\Lambda)\rangle = \mathrm{O}(1) \tag{9}$$

as lattice Λ tends to infinity. In other words, the global ground state $\Psi_0(\Lambda)$ of H_Λ does not support a long-range ordering of B_i.

Remark. Before we proceed to the proof of this theorem, we would like to emphasize that equations (7) and (8) are sufficient conditions for the non-existence of a long-range ordering of B_i in $\Psi_0(\Lambda)$. Ignoring mathematical rigour, this theorem can be understood by the following intuitive argument. Let Ψ_0 be the ground state of the Hamiltonian H defined on the infinite lattice Z^d and let E_0 be the energy of the ground state . Notice that the absolute value of E_0 is ill defined and, in fact, an infinity. For definiteness, we assume that a long-range ordering of B_i in Ψ_0 exists at $q = 0$. Then, this long-range ordering can be characterized by a non-vanishing expectation value of B_i in Ψ_0, i.e. $\langle\Psi_0|B_i|\Psi_0\rangle \neq 0$. (For a finite lattice, this expectation value is generally zero. Instead, one has to study the correlation functions of B_i.) However, if equation (7) holds, then this expectation value must vanish since

$$\langle\Psi_0|B_i|\Psi_0\rangle = \frac{1}{\alpha}\langle\Psi_0|[H, A_i]|\Psi_0\rangle = \frac{1}{\alpha}(E_0 - E_0)\langle\Psi_0|A_i|\Psi_0\rangle = 0. \tag{10}$$

Therefore, a long-range ordering of B_i in Ψ_0 cannot exist.

Proof of the theorem. Let $\{\Psi_n(\Lambda)\}$ be a complete set of orthonormal eigenvectors of H_Λ. We introduce

$$S_\Lambda(q, B_i) \equiv \langle\Psi_0(\Lambda)|B_q^\dagger B_q|\Psi_0(\Lambda)\rangle + \langle\Psi_0(\Lambda)|B_q B_q^\dagger|\Psi_0(\Lambda)\rangle. \tag{11}$$

Obviously,

$$S_\Lambda(q, B_i) \geqslant \langle\Psi_0(\Lambda)|B_q^\dagger B_q|\Psi_0(\Lambda)\rangle \geqslant 0 \tag{12}$$

for any q. Inserting $\{\Psi_n(\Lambda)\}$ between $B_q^\dagger$ and B_q, we obtain

$$S_\Lambda(q, B_i) = \sum_n [|\langle\Psi_n(\Lambda)|B_q|\Psi_0(\Lambda)\rangle|^2 + |\langle\Psi_n(\Lambda)|B_q^\dagger|\Psi_0(\Lambda)\rangle|^2]. \tag{13}$$

Using the condition $\langle\Psi_0(\Lambda)|B_q|\Psi_0(\Lambda)\rangle = \langle\Psi_0(\Lambda)|B_q^\dagger|\Psi_0(\Lambda)\rangle = 0$, we can write this sum as

$$\begin{aligned} S_\Lambda(q, B_i) = &\sum_n \frac{|\langle\Psi_n(\Lambda)|B_q|\Psi_0(\Lambda)\rangle|}{\sqrt{E_n(\Lambda) - E_0(\Lambda)}} \left(|\langle\Psi_n(\Lambda)|B_q|\Psi_0(\Lambda)\rangle|\sqrt{E_n(\Lambda) - E_0(\Lambda)}\right) \\ &+ \sum_n \frac{|\langle\Psi_n(\Lambda)|B_q^\dagger|\Psi_0(\Lambda)\rangle|}{\sqrt{E_n(\Lambda) - E_0(\Lambda)}} \left(|\langle\Psi_n(\Lambda)|B_q^\dagger|\Psi_0(\Lambda)\rangle|\sqrt{E_n(\Lambda) - E_0(\Lambda)}\right) \end{aligned} \tag{14}$$

where $E_n(\Lambda)$ is the eigenvalue of H_Λ corresponding to $\Psi_n(\Lambda)$. Since $E_0(\Lambda)$ is the lowest eigenvalue of H_Λ, the square root of $E_n(\Lambda) - E_0(\Lambda)$ is well defined. By Cauchy's inequality $(\sum |a_n b_n|)^2 \leqslant (\sum |a_n|^2)(\sum |b_n|^2)$, we obtain

$$\begin{aligned} 0 \leqslant S_\Lambda^2(q, B) \leqslant &\left[\sum_n \frac{|\langle\Psi_n(\Lambda)|B_q|\Psi_0(\Lambda)\rangle|^2 + |\langle\Psi_n(\Lambda)|B_q^\dagger|\Psi_0(\Lambda)\rangle|^2}{E_n(\Lambda) - E_0(\Lambda)}\right] \\ &\times \left[\sum_n (|\langle\Psi_n|B_q|\Psi_0\rangle|^2 + |\langle\Psi_n|B_q^\dagger|\Psi_0\rangle|^2)(E_n - E_0)\right]. \end{aligned} \tag{15}$$

It is easy to check that the second factor on the right-hand side of inequality (15) is equal to

$$m_\Lambda(q, B_i) \equiv \langle \Psi_0(\Lambda)|[B_q^\dagger, [H, B_q]]|\Psi_0(\Lambda)\rangle. \tag{16}$$

We now simplify the first factor by applying commutation relation (7), which is equivalent to the following identity

$$\begin{aligned}\alpha\langle \Psi_n(\Lambda)|B_q|\Psi_0(\Lambda)\rangle &= \langle \Psi_n(\Lambda)|[H_\Lambda, A_q]|\Psi_0(\Lambda)\rangle \\ &= (E_n(\Lambda) - E_0(\Lambda))\langle \Psi_n(\Lambda)|A_q|\Psi_0(\Lambda)\rangle. \end{aligned}\tag{17}$$

Substituting this identity into the first factor on the right-hand side of inequality (15), we are able to rewrite it as

$$\begin{aligned}\alpha^{-2}m_\Lambda(q, A_i) &\equiv \alpha^{-2}\sum_n [|\langle \Psi_n(\Lambda)|A_q|\Psi_0(\Lambda)\rangle|^2 + |\langle \Psi_n(\Lambda)|A_q^\dagger|\Psi_0(\Lambda)\rangle|^2](E_n(\Lambda) - E_0(\Lambda)) \\ &= \alpha^{-2}\langle \Psi_0(\Lambda)|[A_q^\dagger, [H_\Lambda, A_q]]|\Psi_0(\Lambda)\rangle. \end{aligned}\tag{18}$$

Therefore,

$$0 \leqslant \langle \Psi_0(\Lambda)|B_q^\dagger B_q|\Psi_0(\Lambda)\rangle \leqslant S_\Lambda(q, B) \leqslant \alpha^{-1}\sqrt{m_\Lambda(q, A_i)m_\Lambda(q, B_i)}. \tag{19}$$

If we can show that both $m_\Lambda(q, A_i)$ and $m_\Lambda(q, B_i)$ are of O(1) as Λ tends to infinity for any q, then our theorem is established.

For definiteness, let us consider $m_\Lambda(q, A_i)$. By the definition of $m_\Lambda(q, A_i)$, it is the expectation value of $[A_q^\dagger, [H_\Lambda, A_q]]$ in the ground state $\Psi_0(\Lambda)$ and hence, it is a positive quantity. On the other hand, due to the fact that A_i is a local operator and V is short-ranged, the commutator must be of the following form

$$\begin{aligned}[A_q^\dagger, [H_\Lambda, A_q]] &= \frac{1}{N_\Lambda}\sum_{i\in\Lambda}\sum_{j\in\Lambda}[A_i^\dagger, [H, A_j]]\exp\{\mathrm{i}q\cdot(i-j)\} \\ &= \frac{1}{N_\Lambda}\sum_{i\in\Lambda} O_i(q)\end{aligned}\tag{20}$$

where $\{O_i(q)\}$ are some local operators dependent of q. In general, they are polynomials of the creation and annihilation operators of fermions or bosons. These statements can be easily checked by calculating the commutator for a concrete model. For instance, one can check equation (20) with the Hubbard Hamiltonian (definition (24)) and the operator $A_q \equiv (1/N_\Lambda)^{1/2}\sum_{i\in\Lambda}\exp[-\mathrm{i}q\cdot j]c_{i\uparrow}c_{i\downarrow}$. Therefore,

$$0 \leqslant \langle \Psi_0(\Lambda)|[A_q^\dagger, [H_\Lambda, A_q]]|\Psi_0(\Lambda)\rangle \leqslant \frac{1}{N_\Lambda}N_\Lambda \max_{i,q}|\langle \Psi_0(\Lambda)|O_i(q)|\Psi_0(\Lambda)\rangle|. \tag{21}$$

Since $|V|$ is bounded, we can find a positive constant C, which is independent of i, q and Λ, such that

$$|\langle \Psi_0(\Lambda)|O_i(q)|\Psi_0(\Lambda)\rangle| \leqslant C. \tag{22}$$

Combining (20), (21) and (22) yields

$$m_\Lambda(q, A_i) = \mathrm{O}(1)$$

as Λ tends to infinity. Similarly, one can show that $m_\Lambda(q, B_i)$ is also of O(1). Therefore, $S_\Lambda(q, B_i)$ and $\langle \Psi_0(\Lambda)|B_q^\dagger B_q|\Psi_0(\Lambda)\rangle$ are at most O(1) for any reciprocal vector q. Namely, a long-range ordering of B_i is absent.

Our proof is accomplished. □

Some remarks are in order.

Remark 1. A similar inequality was used in [5] to show the existence of the antiferromagnetic long-range order in the ground state of a three-dimensional spin-$\frac{1}{2}$ Heisenberg model.

Remark 2. Inequality (22) can be formally proven by using the well known Gershgorin's theorem in matrix theory [11]. One can find a short proof of this theorem and its application to Nagaoka theorem for the infinite-U Hubbard model in [12] and [13].

Remark 3. In the following, we shall study the Hubbard model. With the concrete forms of H_Λ and the relevant local operators A_i (B_i) being given, one can easily check the validity of all the statements contained in (20), (21) and (22) about $m_\Lambda(q, A_i)$ ($m_\Lambda(q, B_i)$).

As an application of our theorem, we now show the absence of the resonanting valence bond (RVB) states in the Hubbard model.

The Hubbard Hamiltonian is of the following form

$$H_\Lambda = -t \sum_\sigma \sum_{\langle ij \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_{i\in\Lambda} (n_{i\uparrow} - \mu)(n_{i\downarrow} - \mu) \tag{24}$$

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 i. $n_{i\uparrow}$ ($n_{i\downarrow}$) is the fermion number operators which measures the number of fermions with upspin (downspin) at site i. $\langle ij \rangle$ denotes a pair of nearest-neighbour sites of Λ. $t > 0$ and $U > 0$ are two parameters representing the kinetic energy and the on-site Coulomb repulsion of fermions, respectively. μ is the chemical potential. It is easy to see that this Hamiltonian commutes with $N_\uparrow$ ($N_\downarrow$), the number operator of upspin (downspin) fermions. Consequently, the total number of fermions is also a conserved quantity. When $N_\uparrow + N_\downarrow = N_\Lambda$, the lattice is half-filled. For obvious reasons, the system is called doped with holes if $N_\uparrow + N_\downarrow < N_\Lambda$.

Originally, this model was introduced [14] to explain the itinerant electron ferromagnetism [15] and Mott metal–insulator transition [16]. After the discovery of high-temperature superconductivity in the rare-earth-based copper oxides, Anderson and his collaborators proposed [7, 8] that the physical properties of these materials can be described by a two-dimensional Hubbard model and the ground state of this model should be an RVB state. By definition, an RVB state $\widetilde{\Psi}$ is characterized by a non-vanishing expectation value of the following operator

$$b_{\langle ij \rangle} \equiv c_{i\uparrow} c_{j\downarrow} - c_{i\downarrow} c_{j\uparrow} \tag{25}$$

in it. In definition (25), i and j are two nearest-neighbour sites. By definition, it is easy to see that $b_{\langle ij \rangle} = b_{\langle ji \rangle}$. We shall use this relation in the following. We would also like to emphasize that $\widetilde{\Psi}$ is an eigenstate of H, not H_Λ. While the former is defined on the whole infinite lattice, the latter is only its restriction on the finite lattice Λ. For an eigenstate Ψ_Λ of H_Λ, the expectation value of $b_{\langle ij \rangle}$, which contains only particle annihilation operators, will be identically zero because Ψ_Λ must be an eigenvector of the total particle number operator $\hat{N}$. On the other hand, $\widetilde{\Psi}$ may not be an eigenvector of $\hat{N}$ if spontaneous symmetry breaking occurs. Based on his proposal, Anderson developed a new theory for high-temperature superconductivity.

However, as research goes into more depth, more and more results show evidence which disfavour the existence of the RVB states in the Hubbard model. For example, by using the second-order perturbation theory and mapping the Hubbard Hamiltonian to an antiferromagnetic Heisenberg model in the large-U limit, Baskaran and Anderson [17] argued that the ground state at half-filling cannot be an RVB state. More precisely, they showed that, under the gauge transformation $c_{i\sigma} \to \exp(i\theta_i)c_{i\sigma}$, the Heisenberg Hamiltonian is invariant. Therefore, $\langle\widetilde{\Psi}|b_{\langle ij\rangle}|\widetilde{\Psi}\rangle$ must be zero by a theorem due to Elitzur [18]. Their conclusion has been conformed by Zhang [19]. By exploiting the following commutation relation satisfied by the Hubbard Hamiltonian,

$$[H, c_{i\uparrow}c_{i\downarrow}] = t\sum_k b_{\langle ik\rangle} - (1-2\mu)Uc_{i\uparrow}c_{i\downarrow} \tag{26}$$

where the sum is over all the nearest-neighbour sites of i, Zhang showed that

$$\langle\widetilde{\Psi}|\sum_k b_{\langle ik\rangle}|\widetilde{\Psi}\rangle = \left[\frac{(1-2\mu)U}{t}\right]\langle\widetilde{\Psi}|c_{i\uparrow}c_{i\downarrow}|\widetilde{\Psi}\rangle. \tag{27}$$

Therefore, the order parameter of the RVB states is related to the on-site s-wave pairing amplitude. In particular, the right-hand side of (27) will vanish at half-filling since $\mu = 1/2$ in this case. In the following, we shall take a different approach. By using the theorem proven above, we show that the off-diagonal-long-range-order (ODLRO) correlation function of $b_{\langle ij\rangle}$ decays. Therefore, the RVB ground states do not exist in the Hubbard model. In this way, we are able to make Zhang's argument mathematically rigorous.

Let us first consider the half-filled case. For technical convenience, we define

$$A_i \equiv c_{i\uparrow}c_{i\downarrow} \qquad B_i \equiv \sum_k b_{\langle ik\rangle}. \tag{28}$$

Then, the totality of the matrix elements M_{hl} defined by equation (1) is, in fact, the ODLRO correlation function of $\sum_k b_{\langle ik\rangle}$, which is proportional to the ODLRO correlation function of $b_{\langle ij\rangle}$ since $b_{\langle ij\rangle} = b_{\langle ji\rangle}$. Therefore, if M_{hl} tends to zero as $|h-l|$ tends to infinity, the ground state of the Hubbard model cannot be an RVB state.

To apply the theorem, there are two problems which have to be solved.

(i) Commutator (26) is not exactly in form (7).

(ii) The ground state $\Psi_0(\Lambda)$ may not be the global ground state of H_Λ.

Fortunately, these difficulties can be simultaneously overcome by letting $\mu = 1/2$ in definition (24). Now, commutation relation (26) is reduced to the standard form (7) and it is well known [20] that $\Psi_0(\Lambda)$ at half-filling is the global ground state of H_Λ with $\mu = 1/2$. Therefore, without further ado, we immediately find that $\lambda_q = O(1)$ for any q as Λ tends to infinity. As we have said above, it implies the absence of an RVB ordering in the Hubbard model at half-filling.

Next, we study the doped cases. Although we cannot prove it rigorously, we shall argue that the existence of the RVB long-range order in the ground states with doping is highly impossible. Our strategy is, by using inequality (15), to show that the existence of a RVB long-range ordering implies the existence of an on-site pairing long-range ordering (OSPLRO). Then, we argue that the existence of OSPLRO in the Hubbard model is impossible when the on-site Coulomb repulsion U is large.

Since the spectra of H_Λ in these cases are not clearly known, we have to make some plausible assumptions. Let $\Psi_0(\Lambda, N_h)$ be the ground state of H_Λ in the sector of

$N_h \equiv N_\Lambda - (N_\uparrow + N_\downarrow) \neq 0$. We first assume that, by fine tuning the value of μ, one can make $\Psi_0(\Lambda, N_h)$ the global ground state of H_Λ and this specific $\tilde{\mu}$ is determined by

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\mu} E_0(\Lambda, N_h, \mu)|_{\mu=\tilde{\mu}} &= \langle \Psi_0(\Lambda, N_h)| \frac{\partial}{\partial \mu} H_\Lambda(\tilde{\mu}) |\Psi_0(\Lambda, N_h)\rangle \\ &= [-(N_\uparrow + N_\downarrow) + 2\tilde{\mu} N_\Lambda] U \\ &= 0 \end{aligned} \tag{29}$$

where $E_0(\Lambda, N_h, \tilde{\mu}) \equiv \langle \Psi_0(\Lambda, N_h)|H_\Lambda(\tilde{\mu})|\Psi_0(\Lambda, N_h)\rangle$. Solving equation (29), we obtain

$$\tilde{\mu} = \frac{(N_\uparrow + N_\downarrow)}{2N_\Lambda} \leqslant \frac{1}{2} \tag{30}$$

and hence, $1 - 2\tilde{\mu} \geqslant 0$ in the doped cases. If we further assume that the ground-state wavefunction $\Psi_0(\Lambda, N_h)$ satisfies

$$\langle \Psi_0(\Lambda, N_h)|N_\uparrow|\Psi_0(\Lambda, N_h)\rangle = \langle \Psi_0(\Lambda, N_h)|N_\downarrow|\Psi_0(\Lambda, N_h)\rangle \tag{31}$$

then $\tilde{\mu}$ can be rewritten as

$$\tilde{\mu} = \langle n_\uparrow \rangle = \langle n_\downarrow \rangle \tag{32}$$

where $\langle n_\uparrow \rangle$ and $\langle n_\downarrow \rangle$ are the averaged density of the particles with upspin and downspin, respectively. Now, the Hubbard Hamiltonian reads

$$H_\Lambda = -t \sum_\sigma \sum_{\langle ij \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_{i \in \Lambda} (n_{i\uparrow} - \langle n_\uparrow \rangle)(n_{i\downarrow} - \langle n_\downarrow \rangle). \tag{33}$$

From this form of the Hamiltonian, we see immediately that deviation of $n_{i\uparrow}$ and $n_{i\downarrow}$ from $\langle n_\uparrow \rangle$ and $\langle n_\downarrow \rangle$ will make the Coulomb repulsion energy larger and hence, the energy of the system higher. This is consistent with our assumptions.

Now, equation (26) gives

$$\begin{aligned}&\langle \Psi_n(\Lambda, N_h)| \sum_k b_{\langle ik \rangle} |\Psi_0(\Lambda, N_h)\rangle \\ &\quad = \left[\frac{E_n - E_0 + (1 - 2\tilde{\mu})U}{t} \right] \langle \Psi_n(\Lambda, N_h)| c_{i\uparrow} c_{i\downarrow} |\Psi_0(\Lambda, N_h)\rangle. \end{aligned} \tag{34}$$

A similar identity holds for $\sum_k b_{\langle ik \rangle}^\dagger$, in which the factor $[E_n - E_0 + (1-2\tilde{\mu})U]/t$ is replaced with $[E_n - E_0 - (1-2\tilde{\mu})U]/t$. Therefore, the theorem cannot be directly applied. To proceed further, a slight change in inequality (15) has to be made. Noticing $1 - 2\tilde{\mu} \geqslant 0$, we can safely replace $\sqrt{E_n - E_0}$ in equation (14) with $\sqrt{E_n - E_0 + (1 - 2\tilde{\mu})U}$ and inequality (19) now reads

$$\begin{aligned}S_q^2\left(\Lambda, \sum_k b_{\langle ik \rangle}\right) &\leqslant t^{-2} [m_\Lambda(q, c_{i\uparrow} c_{i\downarrow}) + (1 - 2\mu) U S_q(\Lambda, c_{i\uparrow} c_{i\downarrow})] \\ &\quad \times \left[m_\Lambda\left(q, \sum_k b_{\langle ik \rangle}\right) + (1 - 2\mu) U S_q\left(\Lambda, \sum_k b_{\langle ik \rangle}\right) \right]. \end{aligned} \tag{35}$$

Now, if we assume that $S_{q_0}(\Lambda, \sum_k b_{\langle ik \rangle}) = O(N_\Lambda)$ for some reciprocal verctor q_0, i.e. there is an RVB long-range ordering. Then, the left-hand side of inequality (35) will be of order $O(N_\Lambda^2)$. Since both $m_\Lambda(q_0, c_{i\uparrow}c_{i\downarrow})$ and $m_\Lambda(q_0, \sum_k b_{\langle ik \rangle})$ are of O(1), that requires

$$S_{q_0}(\Lambda, c_{i\uparrow}c_{i\downarrow}) = O(N_\Lambda). \tag{36}$$

Otherwise, inequality (35) fails. Therefore, the existence of an RVB long-range ordering implies the existence of an on-site pairing long-range ordering. However, when the on-site Coulomb repulsion U is large, the probability amplitude of the configurations with doubly occupied sites in the ground state will be greatly suppressed. Therefore, an on-site pairing long-range ordering can hardly exist. Consequently, we would expect that the RVB states to be absent even in the doped Hubbard models.

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