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The inseparability of resonating valence bond and on-site pairing long-range orders in doped Hubbard models

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Abstract. The concept of the resonating valence bond (RVB) state was originally proposed by Anderson for the ground state of the positive-U Hubbard model. However, the on-site pairing long-range order is expected to exist in the ground state of the negative-U Hubbard and to be incompatible with the RVB order. In this article, we shall rigorously prove that, in fact, these two long-range orderings either coexist or are suppressed simultaneously in the global ground states of the doped Hubbard models.

Since the discovery of high-T_c superconductivity in the rare-earth-based copper oxides, various new mechanisms have been introduced to explain this remarkable phenomenon [1–3]. In particular, Anderson and his collaborators have proposed [1,4] that the physical properties of these materials be described by a two-dimensional Hubbard model and, hence, have developed a theory of high-T_c superconductivity. According to their theory, when the on-site Coulomb repulsion is sufficiently strong, the configurations with doubly-occupied sites are suppressed in the ground state of the Hubbard model and the spins of electrons are paired into short-range singlets. Such a state is called a resonating valence-bond (RVB) state. After doping, two types of quasiparticles emerge. One type can be intuitively identified with empty lattice sites, which have unit positive charge but no spin freedom. They are bosons and are called holons. The other is an occupied lattice site with unpaired electron spin. These are fermions of spin-$\frac{1}{2}$ and are called spinons. Anderson [1] proposed that the Bose–Einstein condensation of holons makes the system superfluid.

However, with more in-depth research, an increasing number of results provide evidence which disagrees with the existence of the RVB states in the two-dimensional 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 found [5] that the ground state of the Hubbard model at half-filling is not an RVB state. Their conclusion has been confirmed by Zhang [6]. By exploiting a commutation relation satisfied by the Hubbard Hamiltonian, Zhang also showed that a non-vanishing RVB order parameter requires a non-zero on-site pairing order parameter in the doped cases. However, the strong on-site repulsion greatly suppresses the existence of the doubly-occupied sites in the ground state of the Hubbard model, let alone a non-zero on-site pairing order parameter. In a recent article [7], by studying the correlation functions of the RVB operator and the on-site pairing operator, we re-established Zhang's results on a mathematically rigorous basis. We proved that, if the ground state of the doped Hubbard model has RVB long-range order, then it must also have a corresponding on-site pairing long-range order.

A natural question arising from our study of these correlation functions is whether the existence of on-site pairing long-range order in the ground state of the doped *negative-U* Hubbard model also implies the existence of a corresponding RVB long-range order. In other words, we conjecture that the RVB long-range order always coexists with the on-site pairing long-range order in the ground state of the *negative-U* Hubbard model. In this article, we shall give this conjecture a rigorous proof.

Before we proceed to the statement of our theorem and its proof, we would like to introduce some definitions and terminology.

Take a finite d-dimensional simple cubic lattice Λ with $N_\Lambda = L^d$ lattice points (we set the lattice constant $a = 1$). The Hubbard Hamiltonian is of the following form:

$$H_\Lambda(\mu) = -t \sum_{\sigma} \sum_{\langle ij \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_{i \in \Lambda} (n_{i\uparrow} - \mu)(n_{i\downarrow} - \mu) \tag{1}$$

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 i, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, $\langle ij \rangle$ denotes a pair of nearest-neighbour sites of Λ, $t > 0$ and U are two parameters representing the kinetic energy and the on-site interaction of fermions, respectively, and μU is the chemical potential. In the conventional Hubbard Hamiltonian, the parameter U is chosen to be positive for on-site Coulomb repulsion. In this article, we shall consider both positive- and negative-U Hubbard models.

It is easy to see that the Hubbard Hamiltonian commutes with the total electron-number operator $\hat{N} = \sum c_{i\sigma}^\dagger c_{i\sigma}$. Consequently, the total number of electrons is a conserved quantity and the Hilbert space of $H_\Lambda(\mu)$ can be divided into numerous subspaces $\{V(N)\}$. Each of these is characterized by a specific particle number N. In each subspace $V(N)$, $H_\Lambda(\mu)$ has a ground state. By fine tuning the value of μ, we can transform the ground state of a specific subspace $V(N)$ into the global ground state of $H_\Lambda(\mu)$.

Next, let us recall the definitions of the RVB and on-site pairing long-range orders.

Let A_j be a local operator defined on lattice Λ. Define its Fourier transformation by

$$A(q) \equiv \frac{1}{\sqrt{N_\Lambda}} \sum_{j \in \Lambda} A_j \exp(-\mathrm{i} q \cdot j) \tag{2}$$

where q is a reciprocal vector. For a specific μ, let $\Psi_0(\mu, \Lambda)$ be the global ground state of $H_\Lambda(\mu)$. According to Yang [8], $\Psi_0(\mu, \Lambda)$ has a momentum-q_0 long-range order of operator A_j if there is a positive constant α, which is independent of N_Λ, such that

$$\langle \Psi_0(\mu, \Lambda) | A^\dagger(q) A(q) | \Psi_0(\mu, \Lambda) \rangle \geqslant \alpha N_\Lambda$$

or (3)

$$\langle \Psi_0(\mu, \Lambda) | A(q) A^\dagger(q) | \Psi_0(\mu, \Lambda) \rangle \geqslant \alpha N_\Lambda$$

holds for some reciprocal vector q_0. With respect to this definition, a momentum-q RVB correlation and a momentum-q on-site correlation in $\Psi_0(\mu, \Lambda)$ are characterized by the following operators:

$$B_j \equiv \sum_k b_{jk} \equiv \sum_k (c_{j\uparrow} c_{k\downarrow} - c_{j\downarrow} c_{k\uparrow}) \qquad D_j \equiv c_{j\uparrow} c_{j\downarrow} \tag{4}$$

respectively. In the definition of B_j, the sum is over all the nearest-neighbour sites of $\boldsymbol{j}$. Anderson's definition of the RVB state [1, 4] is equivalent to saying that $\Psi_0(\mu, \Lambda)$ has a momentum-0 RVB long-range order.

In [7], by exploiting the commutation relations

$$[H_\Lambda(\mu), D(\boldsymbol{q})] = tB(\boldsymbol{q}) - (1-2\mu)UD(\boldsymbol{q}) \tag{5}$$

$$[H_\Lambda(\mu), D^\dagger(\boldsymbol{q})] = -tB^\dagger(\boldsymbol{q}) + (1-2\mu)UD^\dagger(\boldsymbol{q}) \tag{6}$$

we have proved that the RVB and on-site pairing correlation functions satisfy the following inequality:

$$S^2(B(\boldsymbol{q})) \leqslant t^{-2}\{m_\Lambda(D(\boldsymbol{q})) + |(1-2\mu)U|S(D(\boldsymbol{q}))\}\{m_\Lambda(B(\boldsymbol{q})) + |(1-2\mu)U|S(B(\boldsymbol{q}))\} \tag{7}$$

where

$$S(A(\boldsymbol{q})) \equiv \langle\Psi_0|A^\dagger(\boldsymbol{q})A(\boldsymbol{q})|\Psi_0\rangle + \langle\Psi_0|A(\boldsymbol{q})A^\dagger(\boldsymbol{q})|\Psi_0\rangle$$

and

$$m_\Lambda(A(\boldsymbol{q})) \equiv \langle\Psi_0(\mu,\Lambda)|[A^\dagger(\boldsymbol{q}), [H_\Lambda(\mu), A(\boldsymbol{q})]]|\Psi_0(\mu,\Lambda)\rangle \geqslant 0. \tag{8}$$

Noticing that both $m_\Lambda(B(\boldsymbol{q}))$ and $m_\Lambda(D(\boldsymbol{q}))$ are quantities of order O(1) as $N_\Lambda \to \infty$, inequality (7) tells us that, if the global ground state $\Psi_0(\mu, \Lambda)$ of $H_\Lambda(\mu)$ has a momentum-$\boldsymbol{q}$ RVB long-range order, it must also have a momentum-$\boldsymbol{q}$ on-site pairing long-range order. In particular, if $\Psi_0(\mu, \Lambda)$ is a RVB state, as Anderson defined it, then it must have a momentum-0 on-site pairing long-range order. This is impossible when $U > 0$ is sufficiently large.

Naturally, after reading the above analysis, one would like to ask whether the existence of a momentum-$\boldsymbol{q}$ on-site pairing long-range order in the global ground state $\Psi_0(\mu, \Lambda)$ of the *negative-U* Hubbard model [9] also implies the existence of a corresponding momentum-$\boldsymbol{q}$ RVB long-range order in $\Psi_0(\mu, \Lambda)$. Unfortunately, inequality (7) is not useful on this problem.

In the following, we shall prove a new inequality which is complementary to inequality (7). As a corollary of this inequality, we show that the existence of a momentum-$\boldsymbol{q}$ on-site pairing long-range order indeed implies the existence of a momentum-$\boldsymbol{q}$ RVB long-range order in the doped Hubbard model.

Our main results can be summarized in the following theorem.

Theorem. When the Hubbard model is doped with holes (electrons), at least one of the following inequalities must be satisfied by $\Psi_0(\mu, \Lambda)$, the global ground state of the doped Hamiltonian $H_\Lambda(\mu)$:

$$\langle\Psi_0(\mu,\Lambda)|D^\dagger(\boldsymbol{q})D(\boldsymbol{q})|\Psi_0(\mu,\Lambda)\rangle \leqslant \frac{t^2}{|(1-2\mu)U|^2}\langle\Psi_0|B^\dagger(\boldsymbol{q})B(\boldsymbol{q})|\Psi_0\rangle \tag{9}$$

$$\langle\Psi_0(\mu,\Lambda)|D(\boldsymbol{q})D^\dagger(\boldsymbol{q})|\Psi_0(\mu,\Lambda)\rangle \leqslant \frac{t^2}{|(1-2\mu)U|^2}\langle\Psi_0|B(\boldsymbol{q})B^\dagger(\boldsymbol{q})|\Psi_0\rangle. \tag{10}$$

Proof. When the system is doped, the chemical potential coefficient $\mu \neq \frac{1}{2}$ [10]. Therefore, one of the values $-(1-2\mu)U$ and $(1-2\mu)U$ must be negative. For definiteness, let us assume that $-(1-2\mu)U < 0$ (for the positive-U Hubbard model, this condition holds when the system is doped with holes). We now show that inequality (9) holds.

We assume that

$$\langle\Psi_0(\mu,\Lambda)|D^\dagger(q)D(q)|\Psi_0(\mu,\Lambda)\rangle \neq 0. \tag{11}$$

In fact, if this expectation value is zero, then inequality (9) is certainly true.

Consider the identity

$$\begin{aligned}\langle\Psi_0(\mu,\Lambda)|D^\dagger(q)H_\Lambda(\mu)D(q)|\Psi_0(\mu,\Lambda)\rangle - E_0\langle\Psi_0|D^\dagger(q)D(q)|\Psi_0\rangle \\ = \langle\Psi_0(\mu,\Lambda)|D^\dagger(q)\,[H_\Lambda(\mu),D(q)]\,|\Psi_0(\mu,\Lambda)\rangle.\end{aligned} \tag{12}$$

Let $\{\Psi_m\}$ be the complete set of the eigenstates of $H_\Lambda(\mu)$. Inserting the identity operator $I=\sum_m|\Psi_m\rangle\langle\Psi_m|$ between the operators on the left-hand side of (12), one can easily see that the quantity on the right-hand side of (12) is positive since $E_0(\mu,\Lambda)$ is the lowest eigenvalue of $H_\Lambda(\mu)$. By using commutation relation (5), we obtain

$$\begin{aligned}0 &\leqslant \langle\Psi_0(\mu,\Lambda)|D^\dagger(q)[H_\Lambda(\mu),D(q)]|\Psi_0(\mu,\Lambda)\rangle \\ &= t\langle\Psi_0|D^\dagger(q)B(q)|\Psi_0\rangle - (1-2\mu)U\langle\Psi_0|D^\dagger(q)D(q)|\Psi_0\rangle.\end{aligned} \tag{13}$$

A little algebra yields

$$\langle\Psi_0(\mu,\Lambda)|D^\dagger(q)D(q)|\Psi_0(\mu,\Lambda)\rangle \leqslant \frac{t}{|(1-2\mu)U|}\langle\Psi_0(\mu,\Lambda)|D^\dagger(q)B(q)|\Psi_0(\mu,\Lambda)\rangle. \tag{14}$$

Next, we apply the Cauchy inequality $\sum_n a_n b_n \leqslant (\sum_n|a_n|^2)^{1/2}(\sum_n|b_n|^2)^{1/2}$ to the expectation value on the right-hand side of inequality (14).

$$\begin{aligned}\langle\Psi_0(\mu,\Lambda)|D^\dagger(q)B(q)|\Psi_0(\mu,\Lambda)\rangle &= \sum_m\langle\Psi_0|D^\dagger(q)|\Psi_m\rangle\langle\Psi_m|B(q)|\Psi_0\rangle \\ &\leqslant \langle\Psi_0(\mu,\Lambda)|D^\dagger(q)D(q)|\Psi_0(\mu,\Lambda)\rangle^{1/2}\langle\Psi_0(\mu,\Lambda)|B^\dagger(q)B(q)|\Psi_0(\mu,\Lambda)\rangle^{1/2}.\end{aligned} \tag{15}$$

By substituting inequality (15) into (14), we obtain inequality (9).

Similarly, if $(1-2\mu)U < 0$, one can show that inequality (10) holds by using commutation relation (6) and, then, by following the above proof.

Our proof is accomplished. □

By jointly applying inequalities (7) and (9) (or (10)), we immediately obtain the following corollary.

Corollary of the theorem. For a doped Hubbard model with $\mu \neq \frac{1}{2}$, its global ground state $\Psi_0(\mu,\Lambda)$ has a RVB long-range order if and only if $\Psi_0(\mu,\Lambda)$ also has an on-site pairing long-range order.

Proof. We first assume that $\Psi_0(\mu,\Lambda)$ has a momentum-q RVB long-range order. Then, by definition (3), $S(B(q)) = O(N_\Lambda)$ as $N_\Lambda \to \infty$. Consequently, the quantity on the left-hand side of inequality (7) is of order $O(N_\Lambda^2)$. It forces $S(D(q)) = O(N_\Lambda)$. In other words, $\Psi_0(\mu,\Lambda)$ must also have a momentum-q on-site pairing long-range order.

Similarly, if $\Psi_0(\mu,\Lambda)$ has a momentum-q on-site pairing long-range order, then inequalities (9) and (10) guarantee that $\Psi_0(\mu,\Lambda)$ must also have a momentum-q RVB long-range order. □

At first glance, this corollary may seem contrary to one's intuition. But, in fact, it is consistent with some previous results obtained by approximate methods.

When $U > 0$, as is well known, the ground state of the Hubbard model at half-filling is an insulator with antiferromagnetic long-range order. However, when the system is highly doped, the ground state becomes a paramagnetic state, which has a gap for the spin excitations and, hence, is magnetically disordered. The interesting question is what happens when the system is slightly doped. In this region, the phase diagram of the positive-U Hubbard model is not yet clear. From numerical analysis, we have conjectured the existence of some intermediate phases, such as the RVB phase, which are characterized by various coherent short-ranged antiferromagnetic correlations and called spin liquids in the literature [11]. Our corollary shows that these intermediate phases may actually be absent in the positive-U Hubbard model. In other words, the phase transition from the antiferromagnetically-ordered phase to the completely disordered paramagnetic phase is probably direct as the density of holes increases.

In contrast, for a many-body fermion system with an attracting interaction between particles, we believe that electrons will be paired and that the system will become superfluid, no matter how weak the attraction is. The only difference between a weakly-interacting system and a strongly-interacting system is that the electrons are paired in the reciprocal vector (momentum) space (the BCS theory) in the former case and in the real space in the latter case [12]. However, we have not found a sudden transition occurring between these two limiting patterns as the attraction intensity changes. In some sense, our corollary conforms to this picture. In the negative-U Hubbard model, the attraction is extremely short ranged and strong. Our corollary shows that electrons are not only paired on the same site but also paired on sites with a non-zero distance. Obviously, this is a residual from the BCS pairing in the reciprocal vector space.

Finally, we would like to make some remarks.

Remark 1. We would like to emphasize that the above corollary is not true for the half-filled Hubbard models with $\mu = \frac{1}{2}$. In fact, it has been shown [7] that the RVB long-range order is always absent in this case. However, on-site pairing long-range order may exist in the ground state of the negative-U Hubbard model at half-filling when $|U|$ is sufficiently large [9].

Remark 2. Although we have only proved our theorem and its corollary for the d-dimensional simple cubic lattice, it is not difficult to see that, in fact, these results can be easily extended to Hubbard models on an arbitrary bipartite lattice. Naturally, in that case, we would have to introduce a generalized definition for the Fourier transformation of the local operator A_i since the reciprocal vectors $\{q\}$ may not be well defined. One can find a detailed discussion on this point in [13].

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