Spin and charged gaps in strongly correlated electron systems with negative or positive couplings

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Abstract

In this paper, by introducing a simplified version of Lieb's spin-reflection-positivity method, we show that the spin-excitation gap in a strongly correlated fermion model with *attracting interactions* is always larger than or equal to its charged gap, *at any admissible filling* . As another application of this method and a comparison to the above statement, we also give a detailed proof to an *opposite* inequality, which is satisfied by the spin gap and the charged gap in the half-filled Kondo lattice model, a strongly correlated electron model with *positive couplings.*

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I. INTRODUCTION

In the study of strongly correlated electron systems, the possible existence of charged gaps and spin gaps in their excitation spectrum attracts many physicists' interest. The quantum transport and the magnetic properties of these systems are mainly affected by these gaps. In particular, if a strongly correlated electron system has a nonzero charged gap at certain filling, it becomes an insulator. For instance, in a seminal paper [1], Lieb and Wu solved exactly the one-dimensional Hubbard model and showed that, for any on-site Coulomb repulsion $U > 0$, the system has a nonvanishing charged gap at half-filling. Consequently, it is always a Mott insulator and the metal-insulator transition happens at $U_c = 0$ in this model. In higher dimensions, it is still not very clear whether the half-filled Hubbard model has a metal-insulator transition at a nonzero U_c [2,3].

For the Kondo lattice model, another strongly correlated electron model which is currently under intensive study [4], the interplay between its charged excitation and spin excitation has been one of the focusing points of research in the past several decades. The super-exchange interaction in this system leads to a RKKY effective interaction between the localized spins. It competes with the Kondo screening effect on the localized spins. Consequently, when J, the super-exchange coupling, is much smaller than the bandwidth of itinerant electrons, the RKKY interaction becomes dominant and the localized spins are antiferromagnetically ordered at half-filling. Therefore, the spin-excitation gap of the system is vanishing. On the other hand, when J is sufficiently large, the Kondo interaction will eventually win over and the system becomes paramagnetic. This phase is characterized by a nonzero spin gap and the system is a spin liquid. As a result, for the half-filled Kondo lattice model, a quantum phase transition from an antiferromagnetic insulator to a paramagnetic insulator would be expected to occur at some critical value $J_c > 0$.

In a paper published in 1992, Tsunetsugu *et al* studied this transition in a one-dimensional Kondo lattice by numerical diagonalization [5]. After introduction of the density matrix renormalization group technique [6], Yu and White could investigate the same model on

a larger sample [7]. These authors found that the expected transition actually occurs at $J_c = 0$. In other words, a finite spin gap exists for any $J > 0$ in the one-dimensional Kondo lattice model. Moreover, they also observed that *the charged gap of this model is always larger than its spin excitation gap.* These conclusions were confirmed by further numerical investigations on both one-dimensional periodic Anderson model and Kondo lattice model [8–10]. One can find a detailed review on these results in Ref. [11].

Recently, by applying a generalized version of Lieb's spin-reflection-positivity technique [12–14], we were able to re-establish rigorously some observations made in these previous works. More precisely, we proved that, *in any dimensions*, both the quasiparticle gaps and the charged gaps of the positive-U Hubbard model, the periodic Anderson model and the Kondo lattice model at half-filling are larger than their spin excitation gaps [15,16]. Our analysis showed clearly that this conclusion strongly depends on the particle-hole symmetry possessed by these models at half-filling and the repulsive interactions between electrons. Therefore, a natural question arose is whether this statement still holds true for either the same models with doping or some phenomenological models with an *attracting interaction* between fermions, such as the negative-U Hubbard model [17].

In fact, for the doped Kondo lattice model, some recent numerical results have already indicated that a nonvanishing spin gap may sustain, while the charged gap becomes zero [18]. Further investigations are needed to confirm this observation. On the other hand, for the negative-U Hubbard model, one believes that the attracting potential between fermions makes Cooper pairs formed. Consequently, the spin fluctuations in this system should be strongly suppressed. As a result, a spin pseudo-gap may appear even before temperature is lowered below the superconducting temperature T_c [19]. When temperature is below T_c, these preformed Cooper pairs are coherently correlated and the system becomes superconducting. As a result, the charged gap (Not the quasi-particle gap) of the model vanishes. Therefore, one would expect that, at temperature $T = 0$, the spin gap of the negative-U Hubbard model should be larger than or equal to its charged gap at *any finite filling.* In other words, for both the doped Kondo lattice chain and the negative-U Hubbard model,

their spin-excitation gaps may be larger than their charged gaps.

The purpose of the present paper is twofolds. First, we would like to establish rigorously a relation between the charged gap and the spin-excitation gap in a strongly correlated fermion model with *attracting* potentials. More precisely, by taking the negative-U Hubbard model as an example, we shall show that its spin-excitation gap is indeed larger than its charged gap *at any admissible filling.*

In the meantime, we shall introduce a simplified version of the spin-reflection-positivity method for the strongly correlated fermion systems containing *an odd number* of particles. This new approach is based on the singular polar decomposition theorem in matrix theory. Then, as another application of this more straightforward technique, we shall show that *an opposite inequality* is satisfied by the charged gap and the spin gap in *the half-filled strongly correlated electron models with positive couplings* (We take the Kondo lattice model as a concrete example).

From a technical point of view, by studying these concrete models in details, we shall demonstrate how to apply Lieb's spin-reflection-positivity method to the strongly correlated electron systems which have *unequal* numbers of up-spin and down-spin fermions. We believe that this technique should be very useful in studying other interesting properties of these models. On the other hand, since the conclusions derived in this paper are actually based on some very general properties shared by many strongly correlated electron models, such as the periodic Anderson model and the double-exchange model [20], they can be easily extended to these models without further ado.

This paper is organized in the following way: In section II, we introduce the Hamiltonians of both the Hubbard model and the Kondo lattice model. We shall also explain some symmetries of these models; In section III, we define charged gaps and spin-excitation gaps for the strongly correlated electron systems. Then, we state our main results in two theorems; In section IV, we prove theorem 1 for the negative-U Hubbard model, a typical phenomenological strongly correlated fermion model with *negative couplings.* In the meantime, we shall also introduce a simplified version of the spin-reflection-positivity method for the strongly

correlated electron systems with *unequal numbers* of up-spin and down-spin fermions; In section V, we apply this method again to the half-filled strongly correlated electron systems with *positive couplings*. We show that their charged gaps and spin-excitation gaps satisfy *an opposite inequality*; Section VI is for some conclusions. And, finally, in the appendix of this paper, for the reader's convenience, we give a shortened proof of the singular polar decomposition which we used to prove our main results in this paper.

II. THE HAMILTONIANS OF THE HUBBARD MODEL AND THE KONDO LATTICE MODEL

To begin with, we now introduce some definitions and useful notation.

Take a finite d-dimensional simple cubic lattice Λ with N_Λ lattice sites. We impose the open boundary condition on it. Then, the Hamiltonian of the negative-U Hubbard model can be written as

$$H_H(-U) = -t \sum_{\sigma} \sum_{<\mathbf{ij}>} \left(c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + c^\dagger_{\mathbf{j}\sigma} c_{\mathbf{i}\sigma} \right) - U \sum_{\mathbf{i}\in\Lambda} \left(n_{\mathbf{i}\uparrow} - \frac{1}{2} \right) \left(n_{\mathbf{i}\downarrow} - \frac{1}{2} \right) - \mu \hat{N} \tag{1}$$

In Eq. (1), $c^\dagger_{\mathbf{i}\sigma}$ ($c_{\mathbf{i}\sigma}$) is the fermion creation (annihilation) operator which creates (annihilates) an *itinerant* electron of spin σ at lattice site $\mathbf{i}$. $<\mathbf{ij}>$ denotes a pair of nearest-neighbor lattice sites. The parameters $t > 0$ and $U > 0$ represent the kinetic energy and the on-site attracting potential between itinerant electrons, respectively. μ is the chemical potential. We would like to emphasize that, in terms of $H_H(-U)$, the simple cubic lattice is bipartite. In other words, the lattice can be divided into two separated sublattices A and B such that, fermions can only hop from a site of one sublattice to a site in another sublattice.

In literature, the negative-U Hubbard model is frequently used as a phenomenological model to study either the strong coupling superconductors [17] or the strong static binding of electrons at localized centers in amorphous semiconductors [21].

Similarly, the Hamiltonian of the Kondo lattice model has the following form

$$H_K = -t\sum_{\sigma}\sum_{<\mathbf{ij}>}\left(c^{\dagger}_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma} + c^{\dagger}_{\mathbf{j}\sigma}c_{\mathbf{i}\sigma}\right) + J\sum_{\mathbf{i}\in\Lambda}\sigma_{\mathbf{i}}\cdot\mathbf{s}_{\mathbf{i}} - \mu\hat{N} \tag{2}$$

In Eq. (2), $c_{\mathbf{i}\sigma}$ is the fermion operator for itinerant electrons at lattice site $\mathbf{i}$. $\sigma_{\mathbf{i}}$ and $\mathbf{s}_{\mathbf{i}}$ represent the spin operators of itinerant electrons and localized electrons, respectively. In terms of the spin-1/2 fermion operators, they can be written as

$$\sigma_{\mathbf{i}x} \equiv \frac{1}{2}\left(c^{\dagger}_{\mathbf{i}\uparrow}c_{\mathbf{i}\downarrow} + c^{\dagger}_{\mathbf{i}\downarrow}c_{\mathbf{i}\uparrow}\right), \quad \sigma_{\mathbf{i}y} \equiv \frac{1}{2i}\left(c^{\dagger}_{\mathbf{i}\uparrow}c_{\mathbf{i}\downarrow} - c^{\dagger}_{\mathbf{i}\downarrow}c_{\mathbf{i}\uparrow}\right),$$
$$\sigma_{\mathbf{i}z} \equiv \frac{1}{2}\left(n^{c}_{\mathbf{i}\uparrow} - n^{c}_{\mathbf{i}\downarrow}\right) \tag{3}$$

and

$$s_{\mathbf{i}x} \equiv \frac{1}{2}\left(f^{\dagger}_{\mathbf{i}\uparrow}f_{\mathbf{i}\downarrow} + f^{\dagger}_{\mathbf{i}\downarrow}f_{\mathbf{i}\uparrow}\right), \quad s_{\mathbf{i}y} \equiv \frac{1}{2i}\left(f^{\dagger}_{\mathbf{i}\uparrow}f_{\mathbf{i}\downarrow} - f^{\dagger}_{\mathbf{i}\downarrow}f_{\mathbf{i}\uparrow}\right),$$
$$s_{\mathbf{i}z} \equiv \frac{1}{2}\left(n^{f}_{\mathbf{i}\uparrow} - n^{f}_{\mathbf{i}\downarrow}\right) \tag{4}$$

$J > 0$ is the antiferromagnetic super-exchange interaction between them. In Eq. (4), $f^{\dagger}_{\mathbf{i}\sigma}$ and $f_{\mathbf{i}\sigma}$ represent the localized fermion operators. Unlike the fermion operators of itinerant electrons, they are subject to the following constraint conditions

$$n^{f}_{\mathbf{i}} = f^{\dagger}_{\mathbf{i}\uparrow}f_{\mathbf{i}\uparrow} + f^{\dagger}_{\mathbf{i}\downarrow}f_{\mathbf{i}\downarrow} = 1. \tag{5}$$

In other words, at each lattice site, there must be a localized fermion with either up-spin or down-spin. It is a very strict constraint condition on the possible form of the ground state wave functions of the Kondo lattice Hamiltonian H_K and has to be dealt with carefully.

In terms of Hamiltonian (2), the simple cubic lattice is also bipartite. This fact can be easily visualized by introducing a "double layer lattice structure" [22]. For definiteness, let us consider a two dimensional square lattice with lattice constant $a = 1$ for example. We take two identical copies of this lattice, Λ_1 and Λ_2, and make a doubly-layered lattice $\tilde{\Lambda}$ by connecting their corresponding sites with bonds of unit length. Now, each point of $\tilde{\Lambda}$ has coordinates $\mathbf{r} = (\mathbf{i}, m)$ with $m = 1, 2$ and, obviously, $\tilde{\Lambda}$ has $2N_{\Lambda}$ lattice points. If we define new fermion operators $e_{\mathbf{r}\sigma}$ by

$$e_{\mathbf{r}\sigma} = \begin{cases} c_{\mathbf{i}\sigma}, & \text{if } m = 1; \\ f_{\mathbf{i}\sigma}, & \text{if } m = 2. \end{cases} \tag{6}$$

then lattice $\tilde{\Lambda}$ can be divided into two separated sublattices A and B such that, the electron hopping and the spin exchanging only happen between sites in the different sublattices. Therefore, $\tilde{\Lambda}$ as well as Λ are bipartite.

As usual, by exploring the symmetries of a specific model, one can often simplify his analysis on the system. We notice that both the negative-U Hubbard Hamiltonian and the Kondo lattice Hamiltonian enjoy some common symmetries.

First, Hamiltonians (1) and (2) commute with the total particle number operators $\hat{N}$. Consequently, their Hilbert spaces can be divided into numerous subspaces $\{V(N)\}$. Each of these subspaces is characterized by an integer N, the total number of fermions in the system. In particular, the subspaces $V(N = N_\Lambda)$ and $V(N = 2N_\Lambda)$ are called the half-filled subspaces for the negative-U Hubbard Hamiltonian and the Kondo lattice Hamiltonian, respectively.

Furthermore, it is easy to check that both Hamiltonians $H_H(-U)$ and H_K commute with the total spin operators $\hat{S}_+ = \hat{S}_x + i\hat{S}_y$, $\hat{S}_- = \hat{S}_x - i\hat{S}_y$ and $\hat{S}_z$, which are defined to be summations of the spin operators in Eqs. (3) and (4) over all the lattice sites, respectively. Therefore, S^2 and S_z are good quantum numbers of these systems: Any eigenstate Ψ_n of either $H_H(-U)$ or H_K with quantum number $\hat{S}^2 = S(S+1)$ must have $2S+1$ isotopes $\{\Psi_n(M)\}$ with $-S \leq M \leq S$.

In addition, when $\mu = 0$, both $H_H(-U)$ and H_K have another symmetry: They also commute with the so-called pseudo-spin operators, which are defined by

$$\begin{aligned} \hat{J}_+ &\equiv \sum_{\mathbf{i}\in\Lambda} \epsilon(\mathbf{i}) \left(c^\dagger_{\mathbf{i}\uparrow} c^\dagger_{\mathbf{i}\downarrow} \right), \quad \hat{J}_- \equiv \hat{J}^\dagger_+, \\ \hat{J}_z &\equiv \frac{1}{2} \sum_{\mathbf{i}\in\Lambda} \left(n^c_{\mathbf{i}\uparrow} + n^c_{\mathbf{i}\downarrow} - 1 \right), \end{aligned} \tag{7}$$

for the negative-U Hubbard Hamiltonian and

$$\hat{J}_+ \equiv \sum_{\mathbf{i}\in\Lambda} \epsilon(\mathbf{i}) \left(c^\dagger_{\mathbf{i}\uparrow} c^\dagger_{\mathbf{i}\downarrow} - f^\dagger_{\mathbf{i}\uparrow} f^\dagger_{\mathbf{i}\downarrow} \right), \quad \hat{J}_- \equiv \hat{J}^\dagger_+,$$

$$\hat{J}_z \equiv \frac{1}{2}\sum_{\mathbf{i}\in\Lambda}\left(n^c_{\mathbf{i}\uparrow}+n^c_{\mathbf{i}\downarrow}+n^f_{\mathbf{i}\uparrow}+n^f_{\mathbf{i}\downarrow}-2\right), \tag{8}$$

for the Kondo lattice Hamiltonian. In the above equations, $\epsilon(\mathbf{i}) = 1$, for $\mathbf{i} \in A$; $\epsilon(\mathbf{i}) = -1$, for $\mathbf{i} \in B$. These operators satisfy the commutation relations of the conventional spin operators. Consequently, both J^2 and J_z are also good quantum numbers. In other words, each eigenstate of $H_H(-U)$ or H_K can be also characterized by a quantum number J and a quantum number J_z with $-J \leq J_z \leq J$.

Remark 1: It has been shown that, when $\mu = 0$, *the global ground states* of both $H_H(-U)$ and H_K on a simple cubic lattice coincide with their corresponding ground states in the half-filled subspaces. Furthermore, they have quantum numbers $S = 0$ and $J = 0$ [12,23].

III. CHARGED GAPS AND SPIN GAPS OF STRONGLY CORRELATED ELECTRON MODELS

With these preparations, we now introduce the definitions of the spin-excitation gap and the charged gaps for both the negative-U Hubbard model and the Kondo lattice model.

When the systems are half-filled, the chemical potential $\mu = 0$. In this case, both S^2 and J^2 are good quantum numbers. Therefore, following Refs. [5] and [7], we can simply define the spin-excitation gap of these models by

$$\Delta_s \equiv E_0(J = 0,\ S = 1) - E_0(J = 0,\ S = 0) \tag{9}$$

where $E_0(J = j,\ S = s)$ is the lowest eigenvalue of the corresponding Hamiltonian in the subspace with quantum numbers $J = j$ and $S = s$. Similarly, the charged gap of these models at half-filling are defined by [5,7]

$$\Delta_c \equiv E_0(J = 1,\ S = 0) - E_0(J = 0,\ S = 0) \tag{10}$$

For both the Hubbard Hamiltonian and the Kondo lattice Hamiltonian at half-filling, these quantities are well defined, since $E_0(J = 0,\ S = 0)$ coincide with their global ground

state energies, as we recalled in Remark 1. However, when these models are at *an arbitrary admissible filling*, the chemical potential μ is, in general, nonzero. In this case, the pseudospin symmetry is violated, although S^2 is still a conserved quantity. Consequently, we have to revise both definitions (9) and (10). For the spin-excitation gap in a *doped* strongly correlated electron system, its extension is actually quite straightforward. Following Ref. [18], we define

$$\Delta_s \equiv E_0(N,\ S=1) - E_0(N,\ S=0) \tag{11}$$

In Eq. (11), N is required to be *an even integer*. Apparently, when the systems are half-filled, Eq. (11) coincides with definition (9).

On the other hand, the revision of the definition for the charged gap in the doped case demands a little thinking. We notice that, by the definition of the pseudospin operators, $E_0(J=1,\ S=0)$ in Eq. (10) actually coincides with the ground state energies of the Hamiltonians in both subspaces $V(N=\widetilde{N}+2)$ and $V(N=\widetilde{N}-2)$. Here, $\widetilde{N}=N_\Lambda$ for the Hubbard model and, $\widetilde{N}=2N_\Lambda$ for the Kondo lattice model. Therefore, following Ref. [18] again, it is natural to extend definition (10) as

$$\Delta_c \equiv \frac{1}{2}\left(E_0(N+2)+E_0(N-2)-2E_0(N)\right) \tag{12}$$

with N being an even integer. In Eq. (12), $E_0(N)$ should be taken as *the global ground state energies* of the Hamiltonians at filling $\rho = N/\widetilde{N}$. It is easy to check that, when $N=\widetilde{N}$, Eq. (12) is reduced to Eq. (10), too.

Now, we are ready to state and prove our main results, which can be summarized in the following theorems.

Theorem 1: For the negative-U Hubbard model on an d-dimensional simple cubic lattice, the following inequality

$$\Delta_s \geq \Delta_c \tag{13}$$

holds at *any filling ratio* $0 < N/N_\Lambda < 2$ with N being an even integer.

Theorem 2: For the positive-U Hubbard model, the periodic Anderson model and the Kondo lattice model on an d-dimensional simple cubic lattice, *when the system is half-filled*,

their charged gap Δ_c is larger than their spin-excitation gap Δ_s. Namely, the following inequality

$$\Delta_c \geq \Delta_s \tag{14}$$

is satisfied.

In the introduction of this paper, we have argued why theorem 1 should be expected on a physical basis. Actually, it can be proven by applying the same techniques which we employed in our previous papers [15,16]. In the following, however, we would like to prove it in a more straightforward way. The new approach is based on the singular polar decomposition theorem in matrix theory and is considerably simpler, when one has to deal with *localized spin freedoms* in a strongly correlated electron system. We shall make this point more clear by giving a new proof to theorem 2, which we have established in Refs. [15] and [16] by a rather complicated approach.

IV. PROOF OF THEOREM 1

First, we prove theorem 1.

Proof of theorem 1: For the negative-U Hubbard model, Lieb showed that its ground state has spin $S = 0$, when there are an *even number* of particles in the system [12]. Therefore, the ground state of $H_H(-U)$ has quantum numbers $N_\uparrow = M$ and $N_\downarrow = M$, when the total number of particles in the system is $N = 2M$. In this case, we denote the ground state of $H_H(-U)$ by $\Psi_0(M,\, M)$ and its energy by $E_0(M,\, M)$. By fine-tuning the chemical potential μ, we can assume that $\Psi_0(M,\, M)$ is the *global ground state* of Hamiltonian $H_H(-U,\, \mu)$.

Next, let us consider $\Psi_0(M+1,\, M-1)$ and $\Psi_0(M-1,\, M+1)$, the ground states of $H_H(-U,\, \mu)$ in the spin triplet sector. We denote their energies by $E_0(M+1,\, M-1)$ and $E_0(M-1,\, M+1)$, respectively. Since $H_H(-U,\, \mu)$ commutes with spin operators $\hat{S}_+$, $\hat{S}_-$ and $\hat{S}_z$, both the ground states $\Psi_0(M+1,\, M-1)$ and $\Psi_0(M-1,\, M+1)$ are, in fact, degenerate. Therefore, we have identity

$$E_0(M+1,\ M-1) = E_0(M-1,\ M+1)$$
$$= E_0(2M,\ S=1) \tag{15}$$

To apply the spin-reflection-positivity technique, we re-write Hamiltonian (1) into a sum of direct products of up-spin fermion operators with down-spin fermion operators. For this purpose, we shall follow Ref. [13] and introduce the following quasi-fermion operators by letting

$$\hat{C}_{\mathbf{i}\uparrow} \equiv c_{\mathbf{i}\uparrow},\quad \hat{C}_{\mathbf{i}\downarrow} \equiv (-1)^{\hat{N}_\uparrow} c_{\mathbf{i}\downarrow} \tag{16}$$

In Eq. (16), $\hat{N}_\uparrow$ represents the total number operator of up-spin fermions in the system. It is easy to check that the conventional anticommutation relations

$$\{\hat{C}_{\mathbf{i}\sigma},\ \hat{C}_{\mathbf{j}\sigma}\} = \{\hat{C}^\dagger_{\mathbf{i}\sigma},\ \hat{C}^\dagger_{\mathbf{j}\sigma}\} = 0,\quad \{\hat{C}^\dagger_{\mathbf{i}\sigma},\ \hat{C}_{\mathbf{j}\sigma}\} = \delta_{\mathbf{ij}} \tag{17}$$

still hold for operators with *the same spin indices*. However, operators $\{\hat{C}_{\mathbf{i}\uparrow}\}$, now, *commute with* $\{\hat{C}_{\mathbf{i}\downarrow}\}$. Therefore, Hamiltonian (1) can be re-written as

$$H_H(-U,\ \mu) = \hat{T}_\uparrow \otimes \hat{I}_\downarrow + \hat{I}_\uparrow \otimes \hat{T}_\downarrow$$
$$- U \sum_{\mathbf{i}\in\Lambda} \left(n_{\mathbf{i}\uparrow} - \frac{1}{2}\right) \otimes \left(n_{\mathbf{i}\downarrow} - \frac{1}{2}\right) - \mu \hat{N} \tag{18}$$

In Eq. (18), $\hat{T}_\sigma$ stands for the hopping term of spin-σ fermions and $\hat{I}_\sigma$ is the identity operator, acting in the Hilbert space of spin-σ fermions.

With the quasi-fermion operators and the direct-product form (18) of the negative-U Hubbard Hamiltonian, the wave function of $\Psi_0(M+1,\ M-1)$ can be simply written as

$$\Psi_0(M+1,\ M-1) = \sum_{m,\,n} W_{mn} \psi^\uparrow_m \otimes \psi^\downarrow_n. \tag{19}$$

In Eq. (19), ψ^σ_k is a configuration of spin-σ fermions defined by

$$\psi^\sigma_k \equiv \hat{C}^\dagger_{\mathbf{i}_1\sigma} \cdots \hat{C}^\dagger_{\mathbf{i}_L\sigma} \mid 0\rangle \tag{20}$$

where $(\mathbf{i}_1, \ldots, \mathbf{i}_L)$, with $L = M+1$, for $\sigma = \uparrow$; $L = M-1$, for $\sigma = \downarrow$, indicate the positions of fermions with spin σ in the lattice. Apparently, the entire set $\{\psi^\sigma_k\}$ gives a natural basis of $V_\sigma(L)$, the subspace of L fermions with spin σ.

By letting m be the row index and n be the column index, we can further write the coefficients $\{W_{mn}\}$ of $\Psi_0(M+1,\ M-1)$ into a matrix $\mathcal{W}$. However, in general, this matrix *is not a square matrix.* That is due to the fact that, for $\sigma =\uparrow$, $V_\uparrow(M+1)$ has dimension $C_{N_\Lambda}^{M+1}$, while the dimension of $V_\downarrow(M-1)$ is $C_{N_\Lambda}^{M-1}$. *Generally, they are not equal.* Mathematically, it is rather difficult to deal with a nonsquare matrix. In our previous work [15,16], we amended this problem by enlarging the Hilbert subspaces and constructing a new coefficient matrix $\widetilde{W}$, *which is square.* To this matrix, we can apply the standard polar decomposition theorem in matrix theory [24]. However, in this process, many unphysical states, *which are not eigenvectors of the particle number operators* $\hat{N}_\uparrow$ *and* $\hat{N}_\downarrow$, are created. To eliminate these states, we had to set their coefficients in the expansion of the wave function to be zero. That made our previous approach rather complicated.

In the following, we shall introduce a more straightforward approach, which is based on the following *singular polar decomposition theorem for the nonsquare matrices* in matrix theory.

Lemma (Singular Polar Decomposition Theorem): Let A be an $m \times n$ matrix with $m \neq n$.

(i) If $m < n$, then there exist an $m \times m$ unitary matrix U_1, an $m \times m$ diagonal semipositive definite matrix Λ_1 and one $m \times n$ matrix V_1 such that

$$A = U_1 \Lambda_1 V_1 \tag{21}$$

Moreover, the m rows of matrix V_1 are orthonormal vectors.

(ii) Similarly, if $m > n$, then there exist an $m \times n$ matrix V_2, an $n \times n$ diagonal semipositive definite matrix Λ_2 and one $n \times n$ unitary matrix U_2 such that

$$A = V_2 \Lambda_2 U_2 \tag{22}$$

with the n columns of V_2 being orthonormal.

The proof of this theorem can be found in a standard textbook on matrix theory [24]. However, for reader's convenience, we shall give a short proof of it in the appendix of this paper.

For definiteness, let us assume that the coefficient matrix $\mathcal{W}$ has more rows than columns. In this case, the singular polar decomposition theorem tells us that we can find three matrices U, V and Λ such that

$$\mathcal{W} = V\Lambda U \tag{23}$$

with U being an $C_{N_\Lambda}^{M-1} \times C_{N_\Lambda}^{M-1}$ square unitary matrix and V being an $C_{N_\Lambda}^{M+1} \times C_{N_\Lambda}^{M-1}$ matrix with orthonormal columns. Moreover, Λ is an $C_{N_\Lambda}^{M-1} \times C_{N_\Lambda}^{M-1}$ diagonal matrix with $\lambda_l \geq 0$. Consequently, the wave function $\Psi_0(M+1,\ M-1)$ can be re-written as

$$\begin{aligned}\Psi_0(M+1,\ M-1) &= \sum_{m,\,n} W_{mn}\psi_m^{\uparrow} \otimes \psi_n^{\downarrow} \\ &= \sum_{m,\,n} (V\Lambda U)_{mn}\, \psi_m^{\uparrow} \otimes \psi_n^{\downarrow} \\ &= \sum_{l=1}^{D} \lambda_l \xi_l^{\uparrow} \otimes \phi_l^{\downarrow}\end{aligned} \tag{24}$$

with $D = C_{N_\Lambda}^{M-1}$. In Eq. (24), $\xi_l^{\uparrow}$ and $\phi_l^{\downarrow}$ are defined by

$$\xi_l^{\uparrow} = \sum_m V_{ml}\psi_m^{\uparrow}, \quad \phi_l^{\downarrow} = \sum_n U_{ln}\psi_n^{\downarrow}. \tag{25}$$

Since U is unitary and V has columns which are orthonormal, the new sets of vectors $\{\xi_l^{\uparrow}\}$ and $\{\phi_l^{\downarrow}\}$ are orthonormal, too. More importantly, *these new vectors* $\{\xi_l^{\uparrow}\}$ *and* $\{\phi_l^{\downarrow}\}$ *are also the eigenvectors of the particle number operators* $\hat{N}_{\uparrow}$ *and* $\hat{N}_{\downarrow}$, *respectively.* Furthermore, because the ground state wave function $\Psi_0(M+1,\ M-1)$ is normalized, we have

$$\mathrm{Tr}\mathcal{W}^{\dagger}\mathcal{W} = \sum_{l=1}^{D} \lambda_l^2 = 1 \tag{26}$$

With the simple form (24) for $\Psi_0(M+1,\ M-1)$, we calculate the ground state energy $E_0(M+1,\ M-1)$.

$$\begin{aligned}&E_0(M+1,\ M-1) \\ &= \sum_{l=1}^{D} \lambda_l^2 \left[\langle \xi_l^{\uparrow} \mid \hat{T}_{\uparrow} \mid \xi_l^{\uparrow}\rangle + \langle \phi_l^{\downarrow} \mid \hat{T}_{\downarrow} \mid \phi_l^{\downarrow}\rangle\right] \\ &- U\sum_{\mathrm{i}\in\Lambda}\left(\sum_{l_1,\,l_2=1}^{D} \lambda_{l_1}\lambda_{l_2}\langle \xi_{l_2}^{\uparrow} \mid n_{\mathrm{i}\uparrow} - \frac{1}{2} \mid \xi_{l_1}^{\uparrow}\rangle\right. \\ &\left.\times\ \langle \phi_{l_2}^{\downarrow} \mid n_{\mathrm{i}\downarrow} - \frac{1}{2} \mid \phi_{l_1}^{\downarrow}\rangle\right) - 2\mu M\end{aligned} \tag{27}$$

Next, we apply inequality $\mid ab \mid \leq \frac{1}{2}(\mid a \mid^2 + \mid b \mid^2)$ to each term in the last summation of Eq. (27). Dropping the spin indices, we obtain

$$
\begin{aligned}
& E_0(M+1,\ M-1) \\
\geq\ & \frac{1}{2}\sum_{l=1}^{D}\lambda_l^2\left[\langle\xi_l \mid \hat{T} \mid \xi_l\rangle + \langle\xi_l \mid \hat{T} \mid \xi_l\rangle\right] \\
+\ & \frac{1}{2}\sum_{l=1}^{D}\lambda_l^2\left[\langle\phi_l \mid \hat{T} \mid \phi_l\rangle + \langle\phi_l \mid \hat{T} \mid \phi_l\rangle\right] \\
-\ & \frac{U}{2}\sum_{\mathrm{i}\in\Lambda}\left(\sum_{l_1,\,l_2}\lambda_{l_1}\lambda_{l_2}\langle\xi_{l_2} \mid n_{\mathrm{i}} - \frac{1}{2} \mid \xi_{l_1}\rangle\right. \\
\times\ & \left.\overline{\langle\xi_{l_2} \mid n_{\mathrm{i}} - \frac{1}{2} \mid \xi_{l_1}\rangle}\right) \\
-\ & \frac{U}{2}\sum_{\mathrm{i}\in\Lambda}\left(\sum_{l_1,\,l_2}\lambda_{l_1}\lambda_{l_2}\langle\phi_{l_2} \mid n_{\mathrm{i}} - \frac{1}{2} \mid \phi_{l_1}\rangle\right. \\
\times\ & \left.\overline{\langle\phi_{l_2} \mid n_{\mathrm{i}} - \frac{1}{2} \mid \phi_{l_1}\rangle}\right) - 2\mu M
\end{aligned}
\tag{28}
$$

The right hand side of Eq. (28) can be put into a more compact form by introducing new wave functions

$$
\Psi_1 = \sum_{l=1}^{D}\lambda_l\xi_l^{\uparrow}\otimes\bar{\xi}_l^{\downarrow},\quad \Psi_2 = \sum_{l=1}^{D}\lambda_l\phi_l^{\uparrow}\otimes\bar{\phi}_l^{\downarrow},
\tag{29}
$$

where $\bar{\xi}_l^{\sigma}$ and $\bar{\phi}_l^{\sigma}$ are the complex conjugate of ξ_l^{σ} and ϕ_l^{σ}, respectively. In terms of Ψ_1 and Ψ_2, inequality (28) now reads

$$
\begin{aligned}
& E_0(M+1,\ M-1) \\
\geq\ & \frac{1}{2}\langle\Psi_1 \mid H_H \mid \Psi_1\rangle + \frac{1}{2}\langle\Psi_2 \mid H_H \mid \Psi_2\rangle.
\end{aligned}
\tag{30}
$$

By their constructions, Ψ_1 and Ψ_2 are actually wave functions in the subspaces $V(M+1,\ M+1)$ and $V(M-1,\ M-1)$, respectively. That is due to the fact that $\{\xi_l^{\sigma}\}$ ($\{\phi_l^{\sigma}\}$) are the eigenvectors of the particle number operators $\hat{N}_{\sigma}$ with the same eigenvalue $N_{\sigma} = M+1$ $(M-1)$. Furthermore, they are also normalized. Therefore, by the variational principle, inequality (30) implies that

$$
\begin{aligned}
& E_0(M+1,\ M-1) \\
\geq\ & \frac{1}{2}E_0(M+1,\ M+1) + \frac{1}{2}E_0(M-1,\ M-1)
\end{aligned}
\tag{31}
$$

Following the similar procedure, we can also show that

$$\begin{aligned} & E_0(M-1,\ M+1) \\ \geq & \frac{1}{2}E_0(M-1,\ M-1)+\frac{1}{2}E_0(M+1,\ M+1) \end{aligned} \tag{32}$$

Combining Eq. (31) with Eq. (32) and using identity (15), we obtain

$$\begin{aligned} & 2E_0(M+1,\ M-1) \\ \geq & E_0(M-1,\ M-1)+E_0(M+1,\ M+1) \end{aligned} \tag{33}$$

Finally, by subtracting $2E_0(M,\ M) = 2E_0(2M)$ from both sides of inequality (33) and dividing the resultant equation by factor 2, we establish inequality (13).

Theorem 1 is proven. **QED**.

Before proceeding to the proof of theorem 2, we would like to make a remark.

Remark 2: As shown in the proof of inequality (13), we mainly exploited the spin interchange symmetry and the negative interactions between up-spin and down-spin fermions in the negative-U Hubbard Hamiltonian. As a matter of fact, it is the on-site attracting potential between fermions which greatly suppresses the spin fluctuation in the system. Consequently, a spin gap opens. Therefore, we shall expect that theorem 1 can be easily extend to other strongly correlated fermion models with attracting potentials and the spin symmetry. Consequently, inequality (13) should also hold true for these models.

V. PROOF OF THEOREM 2

Now, we turn to the proof of theorem 2.

Proof of theorem 2: In the following, we shall take the Kondo lattice model as a concrete example.

For the half-filled Kondo lattice model at half-filling, the standard definitions (9) and (10) of the spin-excitation gap and the charged gap are applicable, since both the quantum numbers S^2 and J^2 are conserved quantities. By these definitions, we see that inequality (14) is actually equivalent to

$$E_0(J=1,\ S=0) \geq E_0(J=0,\ S=1) \tag{34}$$

In the following, we shall show that, indeed, inequality (34) holds true for the ground state energies of the Kondo lattice model in the subspaces $V(J=1,\ S=0)$ and $V(J=0,\ S=1)$.

First, let us investigate the ground state wave function $\Psi_0(J=1,\ S=0)$. By the definition of the pseudospin operators, $\Psi_0(J=1,\ S=0)$ has a representative with $J_z=1$, which belongs to the subspace $V(N_\Lambda+1,\ N_\Lambda+1)$. In the following, we shall exclusively use $\Psi_0(J=1,\ S=0)$ and $E_0(J=1,\ S=0)$ to denote this state and its energy.

Unlike the negative-U Hubbard model, a direct application of the spin-reflection-positivity method to the Kondo lattice Hamiltonian is impossible. The main difficulty is caused by the positive super-exchange interaction in the model. However, this technical problem can be easily overcome by applying the so-called partial particle-hole transformation $\hat{U}_K$ to the Kondo lattice Hamiltonian. Under this transformation, H_K will be mapped onto a unitarily equivalent Hamiltonian with *negative couplings*.

Following Ref. [23], we define $\hat{U}_K$ by

$$\begin{aligned}
&\hat{U}_K^\dagger c_{\mathbf{i}\uparrow}\hat{U}_K = c_{\mathbf{i}\uparrow}, \quad \hat{U}_K^\dagger c_{\mathbf{i}\downarrow}\hat{U}_K = \epsilon(\mathbf{i})c_{\mathbf{i}\downarrow}^\dagger, \\
&\hat{U}_K^\dagger f_{\mathbf{i}\uparrow}\hat{U}_K = f_{\mathbf{i}\uparrow}, \quad \hat{U}_K^\dagger f_{\mathbf{i}\downarrow}\hat{U}_K = -\epsilon(\mathbf{i})f_{\mathbf{i}\downarrow}^\dagger.
\end{aligned} \tag{35}$$

It is well known that $\hat{U}_K$ is a unitary transformation. Under this transformation, the Hamiltonian H_K is transformed into [23]

$$\begin{aligned}
\widetilde{H}_K &= \hat{U}_K^\dagger H_K \hat{U}_K \\
&= -t\sum_\sigma \sum_{<\mathbf{ij}>} \left(c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{j}\sigma} + c_{\mathbf{j}\sigma}^\dagger c_{\mathbf{i}\sigma}\right) \\
&- \frac{J}{4}\sum_\sigma \sum_{\mathbf{i}\in\Lambda} \left(c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{i}\sigma} + f_{\mathbf{i}\sigma}^\dagger f_{\mathbf{i}\sigma}\right) \\
&+ \frac{J}{2}\sum_{\mathbf{i}\in\Lambda} \left(c_{\mathbf{i}\uparrow}^\dagger c_{\mathbf{i}\uparrow} f_{\mathbf{i}\uparrow}^\dagger f_{\mathbf{i}\uparrow} + c_{\mathbf{i}\downarrow}^\dagger c_{\mathbf{i}\downarrow} f_{\mathbf{i}\downarrow}^\dagger f_{\mathbf{i}\downarrow}\right) \\
&- \frac{J}{2}\sum_{\mathbf{i}\in\Lambda} \left(c_{\mathbf{i}\uparrow}^\dagger f_{\mathbf{i}\uparrow} c_{\mathbf{i}\downarrow}^\dagger f_{\mathbf{i}\downarrow} + f_{\mathbf{i}\uparrow}^\dagger c_{\mathbf{i}\uparrow} f_{\mathbf{i}\downarrow}^\dagger c_{\mathbf{i}\downarrow}\right).
\end{aligned} \tag{36}$$

We notice that $\widetilde{H}_K$ is symmetric with respect to the fermion spin indices and the sign of its last sum, which represents the couplings between the up-spin fermions and the down-spin

fermions, *is negative*. These characteristics of the new Hamiltonian allow us to apply the spin-reflection-positivity method.

Under the transformation $\hat{U}_K$, the constraint condition (5) now reads

$$f^\dagger_{\mathrm{i}\uparrow} f_{\mathrm{i}\uparrow} = f^\dagger_{\mathrm{i}\downarrow} f_{\mathrm{i}\downarrow}. \tag{37}$$

It requires that, in the eigenstates of the transformed Hamiltonian $\widetilde{H}_K$, each localized orbital is either completely empty or occupied by a pair of f-fermions. This condition causes some mathematical problem which we shall carefully deal with in the following.

Remark 3: Another important fact which we would like to emphasize is that, under the partial particle-hole transformation, the spin operators $\hat{S}_+$, $\hat{S}_-$ and $\hat{S}_z$ are mapped onto the pseudo-spin operators $\hat{J}_+$, $\hat{J}_-$ and $\hat{J}_z$ defined in Eq. (8), and *vice versa*. Consequently, after the transformation, an eigenstate $\Psi(J = j,\ S = s)$ of the original Hamiltonian H_K is mapped onto an eigenstate $\widetilde{\Psi}(J = s,\ S = j)$ of $\widetilde{H}_K$.

As before, we introduce the quasi-fermion operators and re-write Hamiltonian $\widetilde{H}_K$ into a sum of direct products of up-spin fermion operators with down-spin fermion operators. Namely, we let

$$\begin{aligned} &\hat{c}_{\mathrm{i}\uparrow} \equiv c_{\mathrm{i}\uparrow}, \quad \hat{f}_{\mathrm{i}\uparrow} \equiv f_{\mathrm{i}\uparrow}, \quad \hat{c}_{\mathrm{i}\downarrow} \equiv (-1)^{\hat{N}_\uparrow} c_{\mathrm{i}\downarrow}, \\ &\hat{f}_{\mathrm{i}\downarrow} \equiv (-1)^{\hat{N}_\uparrow} f_{\mathrm{i}\downarrow} \end{aligned} \tag{38}$$

where $\hat{N}_\uparrow$ is the total number operator of fermions with up-spin in the system. Then, Hamiltonian (36) can be re-written as

$$\begin{aligned} \widetilde{H}_K = &\hat{G}_\uparrow \otimes \hat{I}_\downarrow + \hat{I}_\uparrow \otimes \hat{G}_\downarrow \\ &- \frac{J}{2} \sum_{\mathrm{i}\in\Lambda} \left(\hat{c}^\dagger_{\mathrm{i}\uparrow} \hat{f}_{\mathrm{i}\uparrow} \otimes \hat{c}^\dagger_{\mathrm{i}\downarrow} \hat{f}_{\mathrm{i}\downarrow} + \hat{f}^\dagger_{\mathrm{i}\uparrow} \hat{c}_{\mathrm{i}\uparrow} \otimes \hat{f}^\dagger_{\mathrm{i}\downarrow} \hat{c}_{\mathrm{i}\downarrow} \right). \end{aligned} \tag{39}$$

In Eq. (39), $\hat{G}_\sigma$ represents all the terms in $\widetilde{H}_K$ which contain solely the fermion operators of spin σ.

Now, let us consider how the eigenstate $\Psi_0(J = 1,\ J_z = 1,\ S = 0)$ of H_K is transformed under $\hat{U}_K$. As we noticed in Remark 3, this state is mapped onto the eigenstate $\widetilde{\Psi}_0(J = 0,\ S = 1,\ S_z = 1)$ of $\widetilde{H}_K$ in subspace $V(N_\Lambda + 1,\ N_\Lambda - 1)$. Therefore, we have identity

$$E_0(J=1,\ S=0;\ H_K) = E_0(J=0,\ S=1;\ \widetilde{H}_K). \tag{40}$$

since the transformation $\hat{U}_K$ is unitary. Consequently, instead of studying the ground state $\Psi_0(J=1,\ S=0)$ of H_K, we are now concentrating on $\tilde{\Psi}_0(J=0,\ S=1)$, the ground state of the transformed Hamiltonian $\widetilde{H}_K$.

In terms of the basis vectors

$$\psi_k^\sigma \equiv \hat{c}^\dagger_{\mathrm{i}_1\sigma} \cdots \hat{f}^\dagger_{\mathrm{i}_h\sigma} \cdots \hat{c}^\dagger_{\mathrm{i}_L\sigma} \mid 0\rangle \tag{41}$$

with $L = N_\Lambda + 1$, for $\sigma = \uparrow$ and $L = N_\Lambda - 1$, for $\sigma = \downarrow$, we write the wave function of $\tilde{\Psi}_0(J=0,\ S=1)$ as

$$\begin{aligned}\tilde{\Psi}_0(J=0,\ S=1) &= \tilde{\Psi}_0(N_\Lambda+1,\ N_\Lambda-1) \\ &= \sum_{m,\,n} W_{mn}\psi_m^\uparrow \otimes \psi_n^\downarrow.\end{aligned} \tag{42}$$

However, in constructing the wave function $\tilde{\Psi}_0(N_\Lambda+1,\ N_\Lambda-1)$, *constraint condition (37) must be strictly observed.* Therefore, if $\psi_m^\uparrow$ and $\psi_n^\downarrow$ have different f-fermion distributions, the coefficient of $\psi_m^\uparrow \otimes \psi_n^\downarrow$ in the expansion of $\tilde{\Psi}_0(N_\Lambda+1,\ N_\Lambda-1)$ should be put to zero. Consequently, $\tilde{\Psi}_0(N_\Lambda+1,\ N_\Lambda-1)$ has a form of "partial summations", i.e.,

$$\begin{aligned}&\tilde{\Psi}_0(N_\Lambda+1,\ N_\Lambda-1) \\ &= \sum_{m,\,n}{}^{(1)} W^{(1)}_{mn}\psi^{(1)\uparrow}_m \otimes \psi^{(1)\downarrow}_n + \cdots \\ &+ \sum_{m,\,n}{}^{(s)} W^{(s)}_{mn}\psi^{(s)\uparrow}_m \otimes \psi^{(s)\downarrow}_n + \cdots\end{aligned} \tag{43}$$

In each partial sum, the distribution of f-fermions is specified, subject to the constraint condition (37).

For example, let us consider a partial sum $\sum^{(r)} W^{(r)}_{mn}\psi^{(r)\uparrow}_m \otimes \psi^{(r)\downarrow}_n$. Assume that the total number of f-fermion pairs in this sector is n_f. Then, in an admissible configuration $\psi^{(r)\uparrow}_m \otimes \psi^{(r)\downarrow}_n$, which satisfies the constraint condition (37), there are $n^c_\uparrow = N_\Lambda + 1 - n_f$ up-spin and $n^c_\downarrow = N_\Lambda - 1 - n_f$ down-spin itinerant fermions. In general, $n^c_\uparrow \neq n^c_\downarrow$. Since $\{\psi^{(r)\uparrow}_m\}$, the set of up-spin fermion configurations in this partial sum, contains $C^{n^c_\uparrow}_{N_\Lambda}$ vectors

and $\{\psi_n^{(r)\downarrow}\}$ has $C_{N_\Lambda}^{n_\downarrow^c}$ vectors, the coefficient matrix $\mathcal{W}^{(r)}$ of this partial sum is an $C_{N_\Lambda}^{n_\uparrow^c} \times C_{N_\Lambda}^{n_\downarrow^c}$ matrix, which is, in general, *not a square matrix*. As done above, we apply the singular polar decomposition theorem to this matrix and rewrite the partial sum as

$$\sum_{m,\,n}^{(r)} W_{mn}^{(r)} \psi_m^{(r)\uparrow} \otimes \psi_n^{(r)\downarrow} = \sum_{l=1}^{D_r} \lambda_l^{(r)} \xi_l^{(r)\uparrow} \otimes \phi_l^{(r)\downarrow} \tag{44}$$

with $\lambda_l \geq 0$ and $\{\xi_l^{(r)\uparrow}\}$ and $\{\phi_l^{(r)\downarrow}\}$ being orthonormal. Naturally, these new sets of vectors are eigenvectors of the particle number operators $\hat{N}_\uparrow$ and $\hat{N}_\downarrow$ with $N_\uparrow = N_\Lambda + 1$ and $N_\downarrow = N_\Lambda - 1$, respectively. More importantly, both of them have the same distribution of f-fermion and hence, the right hand side of Eq. (44) satisfies automatically the constraint condition (37).

By repeating this process to each partial sum in Eq. (43), we are able to write the wave function $\tilde{\Psi}_0(N_\Lambda + 1,\, N_\Lambda - 1)$ as

$$\begin{aligned} \tilde{\Psi}_0(N_\Lambda + 1,\, N_\Lambda - 1) &= \sum_{s=1} \sum_{l=1}^{D_s} \lambda_l^{(s)} \xi_l^{(s)\uparrow} \otimes \phi_l^{(s)\downarrow} \\ &\equiv \sum_T \lambda_T \xi_T^\uparrow \otimes \phi_T^\downarrow \end{aligned} \tag{45}$$

with $\lambda_T \geq 0$ and

$$\sum_s \mathrm{Tr} \mathcal{W}^{(s)\dagger} \mathcal{W}^{(s)} = \sum_T \lambda_T^2 = 1 \tag{46}$$

Consequently, we have

$$\begin{aligned} & E_0(J = 0,\, S = 1,\, \widetilde{H}_K) \\ &= E_0(N_\Lambda + 1,\, N_\Lambda - 1,\, \widetilde{H}_K) \\ &= \sum_T \lambda_T^2 \left[\langle \xi_T^\uparrow \mid \hat{G}_\uparrow \mid \xi_T^\uparrow \rangle + \langle \phi_T^\downarrow \mid \hat{G}_\downarrow \mid \phi_T^\downarrow \rangle \right] \\ &- \frac{J}{2} \sum_{\mathrm{i} \in \Lambda} \left(\sum_{T_1,\, T_2} \lambda_{T_1} \lambda_{T_2} \langle \xi_{T_2}^\uparrow \mid \hat{c}_{\mathrm{i}\uparrow}^\dagger \hat{f}_{\mathrm{i}\uparrow} \mid \xi_{T_1}^\uparrow \rangle \right. \\ &\left. \times \langle \phi_{T_2}^\downarrow \mid \hat{c}_{\mathrm{i}\downarrow}^\dagger \hat{f}_{\mathrm{i}\downarrow} \mid \phi_{T_1}^\downarrow \rangle \right) \\ &- \frac{J}{2} \sum_{\mathrm{i} \in \Lambda} \left(\sum_{T_1,\, T_2} \lambda_{T_1} \lambda_{T_2} \langle \xi_{T_2}^\uparrow \mid \hat{f}_{\mathrm{i}\uparrow}^\dagger \hat{c}_{\mathrm{i}\uparrow} \mid \xi_{T_1}^\uparrow \rangle \right. \\ &\left. \times \langle \phi_{T_2}^\downarrow \mid \hat{f}_{\mathrm{i}\downarrow}^\dagger \hat{c}_{\mathrm{i}\downarrow} \mid \phi_{T_1}^\downarrow \rangle \right) \end{aligned} \tag{47}$$

By applying inequality $|\, ab \,| \leq \frac{1}{2}(|\, a \,|^2 + |\, b \,|^2)$ to each term in the last two sums in Eq. (47) and introducing new trial wave functions $\tilde{\Psi}_1$ and $\tilde{\Psi}_2$ by

$$\tilde{\Psi}_1 = \sum_T \lambda_T \xi_T^{\uparrow} \otimes \bar{\xi}_T^{\downarrow}, \quad \tilde{\Psi}_2 = \sum_T \lambda_T \phi_T^{\uparrow} \otimes \bar{\phi}_T^{\downarrow}, \tag{48}$$

we are able to reduce inequality (47) into

$$\begin{aligned} & E_0(N_\Lambda + 1,\, N_\Lambda - 1,\, \widetilde{H}_K) \\ & \geq \frac{1}{2}\langle \tilde{\Psi}_1 \mid \widetilde{H}_K \mid \tilde{\Psi}_1 \rangle + \frac{1}{2}\langle \tilde{\Psi}_2 \mid \widetilde{H}_K \mid \tilde{\Psi}_2 \rangle. \end{aligned} \tag{49}$$

Notice that $\tilde{\Psi}_1$ and $\tilde{\Psi}_2$ are actually wave functions in the subspaces $V(N_\Lambda + 1,\, N_\Lambda + 1)$ and $V(N_\Lambda - 1,\, N_\Lambda - 1)$, respectively. Therefore, inequality (47) implies

$$\begin{aligned} & E_0(J = 0,\, S = 1,\, \widetilde{H}_K) \\ & \geq \frac{1}{2} E_0(N_\Lambda + 1,\, N_\Lambda + 1,\, \widetilde{H}_K) \\ & + \frac{1}{2} E_0(N_\Lambda - 1,\, N_\Lambda - 1,\, \widetilde{H}_K) \end{aligned} \tag{50}$$

On the other hand, it has been shown [23] that, for the Hamiltonian $\widetilde{H}_K$, identities

$$\begin{aligned} & E_0(N_\Lambda + 1,\, N_\Lambda + 1,\, \widetilde{H}_K) \\ & = E_0(N_\Lambda - 1,\, N_\Lambda - 1,\, \widetilde{H}_K) \\ & = E_0(J = 1,\, S = 0,\, \widetilde{H}_K) \end{aligned} \tag{51}$$

hold. Consequently, by substituting Eq. (51) into Eq. (50), we finally obtain

$$E_0(J = 0,\, S = 1,\, \widetilde{H}_K) \geq E_0(J = 1,\, S = 0,\, \widetilde{H}_K) \tag{52}$$

To finish the proof of theorem 2, we apply the inverse of the partial particle-hole transformation $\hat{U}_K^{-1}$ and map $\widetilde{H}_K$ back into the Hamiltonian H_K. As we discussed in Remark 3, under this transformation, $\tilde{\Psi}_0(J = 0,\, S = 1,\, \widetilde{H}_K)$ is unitarily mapped onto $\Psi_0(J = 1,\, S = 0,\, H_K)$ and $\tilde{\Psi}_0(J = 1,\, S = 0,\, \widetilde{H}_K)$ is mapped onto $\Psi_0(J = 0,\, S = 1,\, H_K)$. Therefore, by $\hat{U}_K^{-1}$, Eq. (52) is transformed into Eq. (34), which is equivalent to inequality (14). That ends our proof of theorem 2. **QED**.

As we have shown in the above proof, it is the localized spin constraint in the Kondo lattice model which makes the analysis of the model rather difficult. Comparing with our previous approach in Refs. [15] and [16], one can see that the newly-developed version of the spin-reflection-positivity technique, which is based on the singular polar decomposition theorem, is more straightforward and hence, more effective in dealing with the problems caused by this constraint. Since the same problems may also arise for other strongly correlated electron models with two or more degenerate bands, such as the double-exchange model [20], we expect that this technique provides a very useful tool in analyzing these models.

VI. CONCLUSIONS

In summary, in the present paper, we prove that the spin-excitation gap in a strongly correlated fermion model with *attracting interactions*, such as the negative-U Hubbard model, is always larger than or equal to its charged gap, *at any admissible filling*. In proving this theorem, we introduce a simplified version of Lieb's spin-reflection-positivity method. As another application of this method and a comparison to the above statement, we also show in details that the spin gap and charged gap in the half-filled Kondo lattice model, a strongly correlated electron model with *positive couplings*, satisfy an opposite inequality.

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Appendix

In this appendix, for reader's convenience, we shall give a shortened proof of the singular polar decomposition theorem, which we applied to prove theorem 1 and theorem 2 in this paper. One can find a more detailed discussion of this theorem on page 411 of Ref. [24].

Proof of the singular polar decomposition theorem: First, let us assume that $m < n$. In this case, we consider matrix product $AA^\dagger$. It is an $m \times m$ semipositive definite matrix. Therefore, it has m orthonormal eigenvectors $(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_m)$, which satisfy equations

$$AA^\dagger \mathbf{x}_i = \lambda_i^2 \mathbf{x}_i, \quad 1 \leq i \leq m. \tag{53}$$

Re-organizing $\{\lambda_i\}$ in a decreasing order

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_k > \lambda_{k+1} = \cdots = \lambda_m = 0 \tag{54}$$

we define a diagonal semipositive definite matrix Λ_1 and an $m \times m$ unitary matrix U_1 by

$$\Lambda_1 = \begin{pmatrix} \lambda_1 \cdots 0 \\ \cdots\cdots \\ 0 \cdots \lambda_m \end{pmatrix} \tag{55}$$

and

$$U_1 = (\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_m) \tag{56}$$

where $\mathbf{x}_i$ represents the i^{th} column of matrix U_1.

Next, we construct matrix V_1. The first k rows of V_1 are given by

$$V_1^i = \frac{1}{\lambda_i} \left(A^\dagger \mathbf{x}_i\right)^\dagger \tag{57}$$

Since $\lambda_i \neq 0$ for $1 \leq i \leq k$, these rows are well defined. To define the rest $m - k$ rows of V_1, we notice that *the first k rows defined in Eq. (57) are orthonormal to each other.* Actually, we have

$$\begin{aligned} \overline{\langle V_1^i | V_1^j \rangle} &= \frac{1}{\lambda_i \lambda_j} \langle A^\dagger \mathbf{x}_i | A^\dagger \mathbf{x}_j \rangle \\ &= \frac{1}{\lambda_i \lambda_j} \mathbf{x}_i^\dagger A A^\dagger \mathbf{x}_j = \frac{1}{\lambda_i \lambda_j} \lambda_j^2 \mathbf{x}_i^\dagger \mathbf{x}_j = \delta_{ij} \end{aligned} \tag{58}$$

In the last step of the above derivation, we used the definition of vectors $\{\mathbf{x}_i\}$. On the other hand, since each row V_1^i is an n-dimensional vector, one can find other $m-k$ orthonormal vectors $\mathbf{z}_1^\dagger$, $\mathbf{z}_2^\dagger$, $\cdots$, $\mathbf{z}_{m-k}^\dagger$, which are orthogonal to each V_1^i with $1 \leq i \leq k$. We let them be the rest $m-k$ rows of V_1. Consequently, matrix V_1 has m orthonormal rows.

Finally, we need to show that

$$U_1^\dagger A = \Lambda_1 V_1 \tag{59}$$

holds for the above defined matrices. Obviously, by their definitions, the first k rows of $U_1^\dagger A$ and $\Lambda_1 V_1$ are correspondingly identical. Consequently, we need only to consider the rest $m-k$ rows of both $U_1^\dagger A$ and $\Lambda_1 V_1$. For $\Lambda_1 V_1$, these rows are zero vectors since $\lambda_{k+1} = \cdots = \lambda_m = 0$. We now show that the corresponding rows in $U_1^\dagger A$ are also zero vectors.

Let us take one row $\mathbf{x}_l^\dagger A$ of $U_1^\dagger A$ with $k+1 \leq l \leq m$ and calculate its norm.

$$\begin{aligned}
\langle \mathbf{x}_l^\dagger A | \mathbf{x}_l^\dagger A \rangle &= \sum_{\alpha=1}^{n} \overline{\left(\sum_{\beta=1}^{m} \overline{(\mathbf{x}_l)}_\beta A_{\beta\alpha} \right)} \left(\sum_{\gamma=1}^{m} \overline{(\mathbf{x}_l)}_\gamma A_{\gamma\alpha} \right) \\
&= \sum_{\alpha=1}^{n} \left[\sum_{\beta=1}^{m} \sum_{\gamma=1}^{m} \overline{A_{\beta\alpha}} (\mathbf{x}_l)_\beta A_{\gamma\alpha} \overline{(\mathbf{x}_l)}_\gamma \right] \\
&= \sum_{\alpha=1}^{n} \left[\sum_{\beta=1}^{m} \sum_{\gamma=1}^{m} \overline{(\mathbf{x}_l)}_\gamma A_{\gamma\alpha} A^\dagger_{\alpha\beta} (\mathbf{x}_l)_\beta \right] \\
&= \mathbf{x}_l^\dagger A A^\dagger \mathbf{x}_l = \lambda_l^2 \mathbf{x}_l^\dagger \mathbf{x}_l = 0
\end{aligned} \tag{60}$$

Therefore, $\mathbf{x}_l^\dagger A = 0$ and Eq. (59) is an identity.

Similarly, when $m > n$, one can prove that $A = V_2 \Lambda_2 U_2$ holds by considering matrix product $A^\dagger A$ instead of $A A^\dagger$.

The theorem is proven. **QED**.

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