Journal of Statistical Physics, Vol. 116, Nos. 1/4, August 2004 (© 2004)

Lieb's Spin-Reflection-Positivity Method and Its Applications to Strongly Correlated Electron Systems

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Received June 18, 2003; accepted October 2, 2003

In this paper, we discuss the spin-reflection-positivity method introduced by Lieb [E. H. Lieb, *Phys. Rev. Lett.* **62**:1201 (1989)] and its applications to strongly correlated electron systems in a pedagogical manner. We emphasize the important role played by the sign rule of the ground-state wave function in studying a many-body system. To make our explanation more readable, we shall first review some well-known one-dimensional examples and recall the Lieb–Mattis theorem on the Heisenberg localized spin models. Then, after introducing the general theory of spin-reflection positivity, we show in detail how to use it to overcome the sign problem caused by the fermion characteristics of itinerant electrons in strongly correlated models. Finally, we establish several rigorous results on the Hubbard model, the periodic Anderson model and the Kondo lattice model.

KEY WORDS: Strongly correlated electron systems; spin-reflection-positivity method; magnetic and superconducting correlation functions.

1. INTRODUCTION

In condensed matter physics, the electronic band theory, which is based on the independent electron approximation, is impressively successful in accounting for nonmagnetic properties, such as transport and thermodynamics, of solids. In this approximation, the repulsive Coulomb interaction between electrons is renormalized into their effective mass and these quasi-electrons move near freely in a background periodic potential provided by the positive ions.[1]

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0022-4715/04/0800-0629/0

However, this theory fails to explain some very important phenomena, such as the magnetic ordering[2] and the Mott metal-insulator transition,[3,4] observed in experiments. For instance, in the transition and rare-earth metals, the ferromagnetic order appears when the samples are cooled below their Curie temperatures. This ordering is attributed to the existence of the partly filled d- or f-electron bands in addition to the conduction band. In these bands, the electron density is concentrated near the ions but sparse between them. In other words, it seems that an electron is "on" a particular ion. This circumstance requires an atomic description of the electrons in d- or f-band. On the other hand, the same electrons in these bands contribute significantly to the low temperature specific heat of the solids. Also, the magnetic moments per ion in the ferromagnetic phase of these materials is far from integral numbers of Bohr magneton. These observations seem to be consistent with the prediction of the band theory based on the itinerant electron picture.

In a seminal paper published in 1963,[5] Hubbard argued that it is the correlation effect caused by the electronic short-ranged intra-atomic interaction in the narrow d- or f-band that makes the electrons exhibiting both atomic and itinerant behavior simultaneously. Roughly speaking, the intra-atomic interaction energy of two electrons on the same ion will be lowered, according to the Hund's rule, if their spins point to same direction, say upwards. Therefore, when the intra-atomic interaction is sufficiently strong to produce appreciable correlation, the state of total spin up on an ion may persist for a period long compared with the d- or f-electron hopping time. In this circumstance, one can think of the spin as being associated with the atom rather than with electrons and the possibility of an atomic model emerges.

To analytically study the correlation effect in a narrow band solid, Hubbard,[5] Gutzwiller,[6] and Kanamori[7] introduced independently a simplified model , which is now known as the Hubbard model. On a finite lattice Λ with N_Λ sites, the Hamiltonian of this model is of the following form

$$H_H = -t \sum_{\sigma} \sum_{\langle \mathbf{ij} \rangle} (\hat{c}^{\dagger}_{\mathbf{i}\sigma} \hat{c}_{\mathbf{j}\sigma} + \hat{c}^{\dagger}_{\mathbf{j}\sigma} \hat{c}_{\mathbf{i}\sigma}) + U \sum_{\mathbf{i} \in \Lambda} (\hat{n}_{\mathbf{i}\uparrow} - \tfrac{1}{2})(\hat{n}_{\mathbf{i}\downarrow} - \tfrac{1}{2}) - \mu \hat{N}, \qquad (1)$$

where $\hat{c}^{\dagger}_{\mathbf{i}\sigma}$ ($\hat{c}_{\mathbf{i}\sigma}$) denotes the fermion creation (annihilation) operator which creates (annihilates) an electron of spin σ at lattice site $\mathbf{i}$. $\langle \mathbf{ij} \rangle$ stands for a pair of lattice sites. $t > 0$ and $U > 0$ are parameters representing the itinerant energy and the short-ranged intra-atomic Coulomb repulsion of electrons, respectively. μ is the chemical potential of the system.

In Hamiltonian (1), the first term is the well-known tight-binding Hamiltonian, which represents electron hopping in the periodic ionic

background potential. The second term gives an on-site (intra-atomic) repulsion interaction between electrons. When two electrons of opposite spins are on the same ion, they repel each other with a short-ranged interaction U. It is this interaction term that induces the correlation between electrons: If an atomic orbital is already occupied by one electron with spin σ, the possibility for another electron with different spin $\bar{\sigma}$ hopping into the same orbital is greatly suppressed by an energy penalty U. Consequently, electrons tend to be localized on the ions.

Obviously, the Hubbard model is an oversimplified model, in which the set of the multiple atomic levels is reduced to a single orbital. Consequently, only one electronic band, the conduction s band, is represented. However, it turns out that this seemingly simple model is actually very difficult to analyze quantitatively. In the past four decades, many physicists have made great efforts to uncover the physics of this model. For example, by a Green function decoupling scheme, Hubbard showed that, at temperature $T = 0$, the single s band is continuously split into a lower and an upper band as U increases.[8] This picture gives a natural explanation of the Mott metal-insulator transition in some solids.[3, 4] However, Hubbard's approach does not provide information on the features of quasi-particles in the system. On the other hand, Brinkman and Rice[9] concentrated on the low-energy behavior of the model and observed the disappearance of the quasiparticle peak at the Mott transition point by applying the Gutzwiller variational method.[6] But, their analysis does not produce the lower and upper Hubbard bands. To create a unified description which treats both the low and high energy features of the Hubbard model on equal footing, various analytical techniques, such as the effective Hamiltonian approach,[10] the quantum Monte Carlo[11] and the Lanczos exact diagonalization[12] numerical methods, and the quantum field machineries,[13] were introduced. In particular, the recently-developed density matrix renormalization group numerical techniques[14] give a very accurate description of the Hubbard model in one dimension, while the dynamical mean-field theory[15, 16] provides exact information of the same model in the limit of infinite dimensionality (or coordination number).

Because of the subtle fermion correlation effects built in the Hubbard model, exact solutions and rigorous results are clearly useful bench marks. However, they are rare. The well-known examples are the exact solution of the Hubbard model in one dimension[17] and the Nagaoka theorem.[18] While the exact solution of Lieb and Wu shows the absence of the Mott transition in the one-dimensional Hubbard model and hence, put the simple picture of the lower and upper Hubbard bands in serious doubt, Nagaoka's theorem reveals the existence of ferromagnetism in the ground state of the model with $U = \infty$ and the electron number $N_e = N_\Lambda - 1$. It is

certainly consistent with Hubbard's original conjecture.[5] Recently, the ferromagnetic order in the finite-U Hubbard model on some special lattices was also proven by Mielke[19] and Tasaki.[20]

One of the the main difficulties in establishing rigorous results for the Hubbard model is caused by the so-called fermion sign problem. As the Pauli principle requires, when two itinerant electrons interchange their positions, an extra negative sign is created. Consequently, the sign of expansion coefficients in the ground-state wave function of the Hubbard model is completely intractable. As we shall explain in the following, it is this problem that makes many mathematical tools developed for analyzing the localized fermion models inapplicable. Fortunately, in the case considered by Nagaoka, this sign problem can be avoided. Since the system has only one hole, electrons are only allowed to interchange their positions in a very restricted way dictated by the infinite Coulomb repulsion.[18] In one dimension, this problem can be also ignored if the electron hopping is restricted to a pair of nearest-neighbor sites. In this case, one can properly arrange the positions of electrons with the different spins on the chain such that the fermion problem is completely eliminated.[21, 22] However, we have to face it in dealing with the finite-U Hubbard model on an arbitrary higher dimensional lattice.

In a paper published in 1989,[23] Lieb made a breakthrough by introducing a completely new approach, which is now called Lieb's spin-reflection-positivity method. By using it, the difficulties caused by the fermion sign problem inherited in the Hubbard model can be overcome in some cases. Therefore, Lieb was able to show that the ground state of the Hubbard model is nondegenerate in these cases. More importantly, some previously-developed techniques for the localized fermion models[24] become also applicable. In particular, with these techniques, Lieb proved that the ground state of the Hubbard model has an unsaturated magnetization under certain conditions, which we shall explain in Section 5.

Inspired by these new developments, many authors, including us, applied subsequently the spin-reflection-positivity method to study the ground states of other strongly correlated electron models,[25–29] such as the periodic Anderson model[30] and the Kondo lattice model,[31, 32] to investigate their correlation functions,[33–35] to prove the existence of the ferrimagnetic long-range order in the ground state of the Hubbard model,[36] and to establish some general relations satisfied by the charged gap, the quasiparticle gap and the spin excitation gap of these models.[37]

The purpose of this paper is to introduce the spin-reflection-positivity method and its consequences to a wide audience. Therefore, without making much efforts on mathematical abstraction and generalization, we shall explain how to explore the properties of the strongly correlated

electron models by applying this method to some concrete systems in a pedagogical manner. This paper is not a complete review in the sense that every contribution is covered, but an attempt has been made to mention, at least, most of topics in this field. Besides, we shall also skip some rigorous results, such as the stability of the Nagaoka ferromagnetic state[38] and the uniform density theorems,[39] whose proofs were achieved by different techniques rather than the spin-reflection-positivity method. Readers can find an excellent review on these topics in ref. 40.

In the following discussion, we shall often take the Hubbard model for example, due to its simplicity. However, we would like to emphasize that the same theorems can be also proven for other strongly correlated electron models. In particular, we have the periodic Anderson model[30] and the Kondo lattice model[31] in mind. These models are widely used in the study of condensed matter physics.[32] In the Fock representation, their Hamiltonians are respectively given by

$$H_A = -t \sum_{\sigma} \sum_{\langle \mathbf{ij} \rangle} (\hat{c}^{\dagger}_{\mathbf{i}\sigma} \hat{c}_{\mathbf{j}\sigma} + \hat{c}^{\dagger}_{\mathbf{j}\sigma} \hat{c}_{\mathbf{i}\sigma}) + V \sum_{\sigma} \sum_{\mathbf{i} \in \Lambda} (\hat{c}^{\dagger}_{\mathbf{i}\sigma} \hat{d}_{\mathbf{i}\sigma} + \hat{d}^{\dagger}_{\mathbf{i}\sigma} \hat{c}_{\mathbf{i}\sigma})$$
$$+ U \sum_{\mathbf{i} \in \Lambda} (\hat{d}^{\dagger}_{\mathbf{i}\uparrow} \hat{d}_{\mathbf{i}\uparrow} - \tfrac{1}{2})(\hat{d}^{\dagger}_{\mathbf{i}\downarrow} \hat{d}_{\mathbf{i}\downarrow} - \tfrac{1}{2}) - \mu \hat{N}, \tag{2}$$

and

$$H_K = -t \sum_{\sigma} \sum_{\langle \mathbf{ij} \rangle} (\hat{c}^{\dagger}_{\mathbf{i}\sigma} \hat{c}_{\mathbf{j}\sigma} + \hat{c}^{\dagger}_{\mathbf{j}\sigma} \hat{c}_{\mathbf{i}\sigma}) + J \sum_{\mathbf{i} \in \Lambda} \hat{\boldsymbol{\sigma}}_{\mathbf{i}} \cdot \hat{\mathbf{s}}_{\mathbf{i}} - \mu \hat{N}. \tag{3}$$

In Eq. (2), $\hat{c}_{\mathbf{i}\sigma}$ and $\hat{d}_{\mathbf{i}\sigma}$ represent the atomic s- and d-orbital fermion operators at lattice site $\mathbf{i}$, respectively. V stands for their hybridization energy. Similarly, in Eq. (3), $\{\hat{\boldsymbol{\sigma}}_{\mathbf{i}}\}$ stands for the spin operators of the itinerant electrons in the s-band and $\{\hat{\mathbf{s}}_{\mathbf{i}}\}$ is the set of the localized spins in the f-band. $J > 0$ is the antiferromagnetic exchange interaction between them. Technically, the existence of the additional d- or f-orbital in these models may cause some minor problems, which we shall address in the proper places.

This paper is organized as follows: In Section 2, we introduce several definitions and notation, which will be used in our discussions. Some common symmetries of these strongly correlated electron models are explained. In Section 3, we recall briefly a few basic definitions and results of the general reflection positivity theory, on which the spin-reflection positivity method is based. In Section 4, we establish sign rules for the ground states of some simple quantum mechanical systems, such as the localized spin models. The technique described in this section will be used to deal with more complicated itinerant electron models. In Section 5, we

discuss on the spin-reflection-positivity method and its applications to strongly correlated electron systems. We show that the ground-state wave function of a spin-reflection positive itinerant electron model satisfies a weaker sign rule, which allows us to overcome the difficulties caused by the fermion sign problem. In Section 6, we consider some strongly correlated electron models with an odd number of electrons. In this case, their Hamiltonian is not spin-reflection positive. However, one can still show that their quasiparticle gaps and charged gaps are larger than their excitation gaps. In Section 7, we explain shortly how to generalize the spin-reflection-positivity method to the case of nonzero temperature. Finally, in Section 8, we summarize this paper. We shall also mention some related issue and open problems.

2. SYMMETRIES OF THE STRONGLY CORRELATED ELECTRON MODELS

To begin with, we would like to introduce several definitions and notation. In particular, we recall some common symmetries shared by these strongly correlated electron models.

In literature, a lattice Λ is called bipartite with respect to the Hubbard Hamiltonian if it can be separated into two sublattices A and B such that, electron hopping takes place only between a site $\mathbf{i}$ in one sublattice to a site $\mathbf{j}$ in another sublattice. One example is the simple cubic lattice. It is bipartite if electron hopping in Hamiltonian (1) is restricted to a pair of nearest-neighbor sites.

When a lattice is bipartite with respect to the Hubbard Hamiltonian, it is also bipartite to the Hamiltonians of the periodic Anderson model and the Kondo lattice model. This fact can be easily understood by introducing a "double layer lattice structure." To illustrate the idea, let us consider the periodic Anderson model on a two-dimensional square lattice. Take two identical copies of this lattice, Λ_1 and Λ_2, and make a doubly-layered lattice $\tilde{\Lambda}$ by connecting the corresponding lattice points of Λ_1 and Λ_2 with bonds of length $a = 1$. Then, each point of $\tilde{\Lambda}$ has coordinates $\mathbf{r} = (\mathbf{i}, m)$ with $m = 1, 2$, and $\tilde{\Lambda}$ has $2N_\Lambda$ lattice points. Next, we define new fermion operators $\hat{e}_{\mathbf{r}\sigma}$ by

$$\hat{e}_{\mathbf{r}\sigma} = \begin{cases} \hat{c}_{\mathbf{i}\sigma}, & \text{if} \quad m = 1; \\ \hat{d}_{\mathbf{i}\sigma}, & \text{if} \quad m = 2. \end{cases} \tag{4}$$

Obviously, with the definitions of $\tilde{\Lambda}$ and $\hat{e}_{\mathbf{r}\sigma}$, Hamiltonian (2) can be thought of as the Hamiltonian of a generalized Hubbard model on the

bipartite lattice $\tilde{\Lambda}$, if V is taken to be the "hopping" constant of $\hat{e}$-fermions between layer 1 and layer 2.

In the following, we shall mainly concentrate on the strongly correlated models on a bipartite lattice.

The Hamiltonians of these strongly correlated electron models enjoy some common symmetries, which we shall exploit in the following. In this section, we recall briefly these symmetries and their consequences. A more detailed discussion on this subject can be found in ref. 41.

(1) Hamiltonians H_H, H_A, and H_K commute with the total particle number operators $\hat{N}$. Consequently, their Hilbert spaces can be divided into numerous subspaces $\{V(N)\}$. Each subspace is characterized by a specific integer N, the total number of electrons in the system. In particular, the subspace $V(N)$ is called half-filled if $N = N_\Lambda$ for the Hubbard model; $N = 2N_\Lambda$ for both the periodic Anderson model and the Kondo lattice model.

As a matter of fact, $N_\uparrow$ and $N_\downarrow$, the particle numbers of electrons with up-spin and down-spin, are also conserved for the Hubbard model and the periodic Anderson model. Consequently, $V(N)$ can be further written as a direct sum of subspaces $\{V(N_\uparrow = N_1, N_\downarrow = N - N_1)\}$ in these cases.

(2) Define the total spin operators, for the Hubbard model by

$$\begin{aligned} &\hat{S}_x \equiv \frac{1}{2}\sum_{\mathbf{i}\in\Lambda}(\hat{c}^\dagger_{\mathbf{i}\uparrow}\hat{c}_{\mathbf{i}\downarrow} + \hat{c}^\dagger_{\mathbf{i}\downarrow}\hat{c}_{\mathbf{i}\uparrow}), \qquad \hat{S}_y \equiv \frac{1}{2i}\sum_{\mathbf{i}\in\Lambda}(\hat{c}^\dagger_{\mathbf{i}\uparrow}\hat{c}_{\mathbf{i}\downarrow} - \hat{c}^\dagger_{\mathbf{i}\downarrow}\hat{c}_{\mathbf{i}\uparrow}), \\ &\hat{S}_z \equiv \frac{1}{2}\sum_{\mathbf{i}\in\Lambda}(\hat{n}_{\mathbf{i}\uparrow} - \hat{n}_{\mathbf{i}\downarrow}), \end{aligned} \tag{5}$$

and for the periodic Anderson model by

$$\begin{aligned} \hat{S}_x &\equiv \frac{1}{2}\sum_{\mathbf{i}\in\Lambda}(\hat{c}^\dagger_{\mathbf{i}\uparrow}\hat{c}_{\mathbf{i}\downarrow} + \hat{d}^\dagger_{\mathbf{i}\uparrow}\hat{d}_{\mathbf{i}\downarrow} + \hat{c}^\dagger_{\mathbf{i}\downarrow}\hat{c}_{\mathbf{i}\uparrow} + \hat{d}^\dagger_{\mathbf{i}\downarrow}\hat{d}_{\mathbf{i}\uparrow}), \\ \hat{S}_y &\equiv \frac{1}{2i}\sum_{\mathbf{i}\in\Lambda}(\hat{c}^\dagger_{\mathbf{i}\uparrow}\hat{c}_{\mathbf{i}\downarrow} + \hat{d}^\dagger_{\mathbf{i}\uparrow}\hat{d}_{\mathbf{i}\downarrow} - \hat{c}^\dagger_{\mathbf{i}\downarrow}\hat{c}_{\mathbf{i}\uparrow} - \hat{d}^\dagger_{\mathbf{i}\downarrow}\hat{d}_{\mathbf{i}\uparrow}), \\ \hat{S}_z &\equiv \frac{1}{2}\sum_{\mathbf{i}\in\Lambda}(\hat{n}^c_{\mathbf{i}\uparrow} + \hat{n}^d_{\mathbf{i}\uparrow} - \hat{n}^c_{\mathbf{i}\downarrow} - \hat{n}^d_{\mathbf{i}\downarrow}). \end{aligned} \tag{6}$$

Then, it is easy to check that these operators satisfy the commutation relations of the angular momentum operators and also commute with the Hamiltonians H_H and H_A, respectively. Therefore, both $\hat{S}^2$ and $\hat{S}_z$ are good

quantum numbers and each eigenvalue $E_n(S)$ of these Hamiltonians corresponds to $2S+1$ eigenstates $\{\Psi_n(M)\}$ with $-S \leqslant M \leqslant S$.

The definition of the spin operators for the Kondo lattice model is slightly different. Certainly, one can define these operators by replacing $\hat{d}$-fermion operators in Eq. (6) with $\hat{f}$-fermion operators, which represent electrons in the localized f-orbitals of the Kondo lattice model. However, unlike the itinerant $\hat{d}$-fermion operators of the periodic Anderson model, the localized $\hat{f}$-fermion operators are required to satisfy the following constraint condition

$$\hat{f}^{\dagger}_{\mathbf{i}\uparrow}\hat{f}_{\mathbf{i}\uparrow} + \hat{f}^{\dagger}_{\mathbf{i}\downarrow}\hat{f}_{\mathbf{i}\downarrow} = 1 \tag{7}$$

imposed at each lattice site $\mathbf{i}$. Although this constraint condition does not violate the spin $SU(2)$ symmetry of the Kondo lattice Hamiltonian, it does cause some problems in applying the spin-positivity-reflection method.

We emphasize that the spin $SU(2)$ symmetry is possessed by the Hamiltonians H_H, H_A, and H_K on any lattice, which may not be bipartite.

(3) When the chemical potential $\mu = 0$, these models on a bipartite lattice have an additional symmetry: Their Hamiltonians also commute with the so-called pseudo-spin operators, which are defined, for the Hubbard model by

$$\hat{J}_x \equiv \frac{1}{2}\sum_{\mathbf{i}\in\Lambda} \epsilon(\mathbf{i})(\hat{c}^{\dagger}_{\mathbf{i}\uparrow}\hat{c}^{\dagger}_{\mathbf{i}\downarrow} + \hat{c}_{\mathbf{i}\downarrow}\hat{c}_{\mathbf{i}\uparrow}), \qquad \hat{J}_y \equiv \frac{1}{2i}\sum_{\mathbf{i}\in\Lambda} \epsilon(\mathbf{i})(\hat{c}^{\dagger}_{\mathbf{i}\uparrow}\hat{c}^{\dagger}_{\mathbf{i}\downarrow} - \hat{c}_{\mathbf{i}\downarrow}\hat{c}_{\mathbf{i}\uparrow}),$$

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

and for the symmetric periodic Anderson model by

$$\begin{aligned}
\hat{J}_x &\equiv \frac{1}{2}\sum_{\mathbf{i}\in\Lambda} \epsilon(\mathbf{i})(\hat{c}^{\dagger}_{\mathbf{i}\uparrow}\hat{c}^{\dagger}_{\mathbf{i}\downarrow} + \hat{c}_{\mathbf{i}\downarrow}\hat{c}_{\mathbf{i}\uparrow} - \hat{d}^{\dagger}_{\mathbf{i}\uparrow}\hat{d}^{\dagger}_{\mathbf{i}\downarrow} - \hat{d}_{\mathbf{i}\downarrow}\hat{d}_{\mathbf{i}\uparrow}),\\
\hat{J}_y &\equiv \frac{1}{2i}\sum_{\mathbf{i}\in\Lambda} \epsilon(\mathbf{i})(\hat{c}^{\dagger}_{\mathbf{i}\uparrow}\hat{c}^{\dagger}_{\mathbf{i}\downarrow} - \hat{c}_{\mathbf{i}\downarrow}\hat{c}_{\mathbf{i}\uparrow} - \hat{d}^{\dagger}_{\mathbf{i}\uparrow}\hat{d}^{\dagger}_{\mathbf{i}\downarrow} + \hat{d}_{\mathbf{i}\downarrow}\hat{d}_{\mathbf{i}\uparrow}),\\
\hat{J}_z &\equiv \frac{1}{2}\sum_{\mathbf{i}\in\Lambda} (\hat{n}^{c}_{\mathbf{i}\uparrow} + \hat{n}^{c}_{\mathbf{i}\downarrow} + \hat{n}^{d}_{\mathbf{i}\uparrow} + \hat{n}^{d}_{\mathbf{i}\downarrow} - 2),
\end{aligned} \tag{9}$$

where $\epsilon(\mathbf{i}) = 1$, for $\mathbf{i} \in A$; $\epsilon(\mathbf{i}) = -1$, for $\mathbf{i} \in B$, is the so-called alternating function. The pseudo-spin operators of the Kondo lattice model are given by replacing the $\hat{d}$-fermion operators in Eq. (9) with the $\hat{f}$-fermion operators, subject to condition (7).

It is easy to check that these operators also satisfy the commutation relations of the angular momentum operators and commute with the corresponding spin operators defined in Eqs. (5) and (6). Therefore, both J^2 and J_z are conserved quantities. In physics, they represent actually the pairing and the charge-density-wave (CDW) freedom of electron pairs.

(4) Except the above-mentioned "trivial" symmetries, these models have also a "hidden" particle-hole symmetry, when they are defined on a bipartite lattice. Take the Hubbard Hamiltonian for example. We define a unitary transformation by ref. 42

$$\hat{U}_H = \left[\prod_{\mathbf{i} \in \Lambda} (\hat{c}^\dagger_{\mathbf{i}\uparrow} + \hat{c}_{\mathbf{i}\uparrow}) \prod_{\mathbf{i} \in \Lambda} (2\hat{n}_{\mathbf{i}\uparrow} - 1) \right] \left[\prod_{\mathbf{i} \in \Lambda} (\hat{c}^\dagger_{\mathbf{i}\downarrow} + \hat{c}_{\mathbf{i}\downarrow}) \prod_{\mathbf{i} \in \Lambda} (2\hat{n}_{\mathbf{i}\downarrow} - 1) \right]. \tag{10}$$

When the number of lattice sites, N_Λ, is an even integer, it is easy to check that, under the transformation, the electron operators are changed by

$$\begin{aligned} \hat{U}^\dagger_H \hat{c}_{\mathbf{i}\uparrow} \hat{U}_H &= \epsilon(\mathbf{i})\, \hat{c}^\dagger_{\mathbf{i}\uparrow}, \qquad & \hat{U}^\dagger_H \hat{c}^\dagger_{\mathbf{i}\uparrow} \hat{U}_H &= \epsilon(\mathbf{i})\, \hat{c}_{\mathbf{i}\uparrow}, \\ \hat{U}^\dagger_H \hat{c}_{\mathbf{i}\downarrow} \hat{U}_H &= \epsilon(\mathbf{i})\, \hat{c}^\dagger_{\mathbf{i}\downarrow}, \qquad & \hat{U}^\dagger_H \hat{c}^\dagger_{\mathbf{i}\downarrow} \hat{U}_H &= \epsilon(\mathbf{i})\, \hat{c}_{\mathbf{i}\downarrow}. \end{aligned} \tag{11}$$

Consequently, the first two terms of the Hubbard Hamiltonian are unchanged by this transformation. But the chemical potential term $-\mu\hat{N}$ becomes $-\mu(2N_\Lambda - \hat{N})$ and the subspace $V(N_1, N_2)$ is mapped into $V(N_\Lambda - N_1, N_\Lambda - N_2)$. Therefore, when $\mu = 0$, $\hat{U}_H$ is a symmetric transformation of the Hubbard Hamiltonian and hence, the global ground state of H_H coincides with its ground state in the corresponding half-filled subspace $V(N_\Lambda/2, N_\Lambda/2)$.[41, 43]

The similar transformation can also be defined for both the periodic Anderson model and the Kondo lattice model. For instance, for the Kondo lattice model, the unitary particle-hole transformation $\hat{U}_K$ is defined by

$$\begin{aligned} \hat{U}^\dagger_K \hat{c}_{\mathbf{i}\uparrow} \hat{U}_K &= \epsilon(\mathbf{i})\, \hat{c}^\dagger_{\mathbf{i}\uparrow}, \qquad & \hat{U}^\dagger_K \hat{c}_{\mathbf{i}\downarrow} \hat{U}_K &= \epsilon(\mathbf{i})\, \hat{c}^\dagger_{\mathbf{i}\downarrow}, \\ \hat{U}^\dagger_K \hat{f}_{\mathbf{i}\uparrow} \hat{U}_K &= -\epsilon(\mathbf{i})\, \hat{f}^\dagger_{\mathbf{i}\uparrow}, \qquad & \hat{U}^\dagger_K \hat{f}_{\mathbf{i}\downarrow} \hat{U}_K &= -\epsilon(\mathbf{i})\, \hat{f}^\dagger_{\mathbf{i}\downarrow}. \end{aligned} \tag{12}$$

It preserves not only the Hamiltonian when $\mu = 0$, but also the constraint condition (7).

3. BASIC REFLECTION POSITIVITY

With the above preparations, we recall the basic definitions and results of reflection positivity theory in this section. The method was first introduced in the quantum field theory by Osterwalder and Schrader.[44] Its

applications to localized spin systems was initialized in refs. 45–47. A detailed review on this subject is given in ref. 48.

The reflection positivity method is based on the following observations: For a given many-body Hamiltonian on a lattice Λ, the set $\mathscr{U}$ of all the relevant operators (observables) of the system is an algebra with the operations of addition, complex scalar multiplication and operator product. In many cases, this algebra can be further written as a direct product of two subalgebras $\mathscr{U}_+$ and $\mathscr{U}_-$, i.e., $\mathscr{U} = \mathscr{U}_+ \otimes \mathscr{U}_-$. Moreover, a one-to-one linear mapping (isomorphism) θ between $\mathscr{U}_+$ and $\mathscr{U}_-$ can be also established.

We take the Hubbard model for example. For this model, the relevant observable algebra $\mathscr{U}$ is the family of polynomials in all the fermion operators $\{\hat{c}^\dagger_{i\sigma}\}$ and $\{\hat{c}_{i\sigma}\}$. We would like to emphasize that, by this definition, the Hubbard Hamiltonian itself is a member of $\mathscr{U}$. We choose $\mathscr{U}_+ = \mathscr{U}_\uparrow$ (resp. $\mathscr{U}_- = \mathscr{U}_\downarrow$) to be the subset of polynomials in $\{\hat{c}^\dagger_{i\uparrow}\}$ and $\{\hat{c}_{i\uparrow}\}$ (resp. $\{\hat{c}^\dagger_{i\downarrow}\}$ and $\{\hat{c}_{i\downarrow}\}$). An natural isomorphism θ between $\mathscr{U}_\uparrow$ and $\mathscr{U}_\downarrow$ is given by $\theta(\hat{c}^\dagger_{i\uparrow}) = \hat{c}^\dagger_{i\downarrow}$ and $\theta(\hat{c}_{i\uparrow}) = \hat{c}_{i\downarrow}$. In this case, θ is called *the spin reflection mapping*. However, we still need to solve a technical problem to write $\mathscr{U}$ into a direct product of $\mathscr{U}_\uparrow$ and $\mathscr{U}_\downarrow$.

The difficulty is caused by the anticommutation relation imposed on the fermion operators with different spins. (In physics, this requirement is unnecessary, although the fermion operators of the same spin must satisfy these relations required by the Pauli principle). To eliminate this problem, we apply a method proposed in ref. 27. Introduce the so-called quasi-fermion operators by

$$\hat{C}_{i\uparrow} \equiv \hat{c}_{i\uparrow}, \qquad \hat{C}_{i\downarrow} \equiv (-1)^{\hat{N}_\uparrow}\, \hat{c}_{i\downarrow}, \tag{13}$$

where $\hat{N}_\uparrow$ is the total number operator of electrons with up-spin in the system and assume that $\hat{c}_{i\uparrow}$ and $\hat{c}_{i\downarrow}$ satisfy the canonical anticommutation relations. Then, one can easily check that $\{\hat{C}_{i\downarrow}\}$, now, *commute with* $\{\hat{C}_{i\uparrow}\}$. By replacing the electron operators with the quasi-fermion operators, we have $\mathscr{U} = \mathscr{U}_\uparrow \otimes \mathscr{U}_\downarrow$. This allows us to rewrite the Hubbard Hamiltonian as

$$H_H = \hat{T}_\uparrow \otimes \hat{I}_\downarrow + \hat{I}_\uparrow \otimes \hat{T}_\downarrow + U \sum_{i \in \Lambda} (\hat{n}_{i\uparrow} - \tfrac{1}{2}) \otimes (\hat{n}_{i\downarrow} - \tfrac{1}{2}) - \mu \hat{N}, \tag{14}$$

where $\hat{T}_\sigma = (-t) \sum_{\langle ij \rangle} (\hat{C}^\dagger_{i\sigma} \hat{C}_{j\sigma} + \hat{C}^\dagger_{j\sigma} \hat{C}_{i\sigma})$ and $\hat{I}_\sigma$ is the identity operator acting in the subalgebra $\mathscr{U}_\sigma$.

Keeping this example in mind, we continue our discussion on the reflection positivity. Take an arbitrary Hermitian polynomial (Hamiltonian)

$\hat{H}$ (Not necessarily the previously given Hamiltonian, say H_H). We define a linear functional by

$$\langle \hat{A} \rangle_{\hat{H}} \equiv Z_{\hat{H}}^{-1} \operatorname{Tr}(\hat{A} \exp^{-\beta \hat{H}}), \tag{15}$$

where $\beta = 1/T$ and $\hat{A}$ is an arbitrary operator in the algebra $\mathscr{U}$. In Eq. (15), $Z_{\hat{H}} = \operatorname{Tr} \exp(-\beta \hat{H})$. In terms of this functional, the Hamiltonian $\hat{H}$ is called *reflection positive* if and only if

$$\langle \hat{A} \overline{\theta(\hat{A})} \rangle_{\hat{H}} \geqslant 0 \tag{16}$$

holds for all $\hat{A} \in \mathscr{U}_+$. In Eq. (16), $\bar{\hat{B}}$ is the complex conjugate (not the Hermitian conjugate) of operator $\hat{B}$.

A sufficient condition for a specific Hamiltonian to be reflection positive is given in the following theorem.

Theorem 3.1. If $\hat{H} \in \mathscr{U}$ can be written as

$$\hat{H} = \hat{B} \otimes \hat{I}_- + \hat{I}_+ \otimes \overline{\theta(\hat{B})} - \sum_{j=1}^{k} \hat{D}_j \otimes \overline{\theta(\hat{D}_j)}, \tag{17}$$

with $\hat{B}, \hat{D}_j \in \mathscr{U}_+$, then $\hat{H}$ is reflection positive.

We emphasize that it is the negative sign in the crossing terms which makes $\hat{H}$ reflection positive.

Another important result is the Dyson–Lieb–Simon theorem.[46]

Theorem 3.2. Assume that Hamiltonian $\hat{H}$ has the form

$$\hat{H} = \hat{H}(\hat{A}, \hat{B}) \equiv \hat{A} \otimes \hat{I}_- + \hat{I}_+ \otimes \hat{B} - \sum_{j=1}^{K} \hat{D}_j \otimes \overline{\theta(\hat{D}_j)} \tag{18}$$

with $\hat{A} = \hat{A}^\dagger \in \mathscr{U}_+$ and $\hat{B} = \hat{B}^\dagger \in \mathscr{U}_-$, then its ground-state energy $E_0(\hat{A}, \hat{B})$ satisfies inequality

$$E_0(\hat{A}, \hat{B}) \geqslant \tfrac{1}{2} E_0(\hat{A}, \overline{\theta(\hat{A})}) + \tfrac{1}{2} E_0(\overline{\theta(\hat{B})}, \hat{B}). \tag{19}$$

Both Theorems 3.1 and 3.2 have been applied to study the localized spin models. Some of these results are summarized in ref. 48. However, we shall skip their proofs here. Instead, we prove them by studying some concrete examples in the following sections. In this way, the implications of these theorems can be seen more clearly. In fact, after reading the proofs of Theorem 6.1 and Lemma 7.1, the readers should have no difficulty to establish the general proofs of these theorems.

In general, the Hamiltonian of a specific many-body system, such as the Hubbard model, does not possess the reflection positive form of Theorem 3.1. Therefore, we cannot directly show whether this Hamiltonian is reflection positive. However, in many cases, we can find a unitary transformation which maps $\hat{H}$ into an equivalent Hamiltonian $\tilde{H}$ and the latter has the required form. That allows us to uncover some properties of the ground state of $\tilde{H}$ by using Theorem 3.1. On the other hand, since $\tilde{H}$ is unitarily equivalent to $\hat{H}$, they must have the same spectrum. In particular, their ground states are mapped into each other by the unitary transformation and its inverse. Therefore, it is possible for us to understand the behavior of the ground state of $\hat{H}$ by studying its counterpart.

For instance, by applying the so-called partial particle-hole transformation

$$\tilde{U}_H = \left[\prod_{\mathbf{i} \in \Lambda} (\hat{c}^\dagger_{\mathbf{i}\uparrow} + \hat{c}_{\mathbf{i}\uparrow}) \prod_{\mathbf{i} \in \Lambda} (2\hat{n}_{\mathbf{i}\uparrow} - 1) \right] \tag{20}$$

which only transforms the up-spin fermion operators according to Eq. (11), the Hubbard Hamiltonian is mapped into

$$\begin{aligned} \tilde{H}_H = \tilde{U}^\dagger_H H_H \tilde{U}_H &= \hat{T}_\uparrow \otimes \hat{I}_\downarrow + \hat{I}_\uparrow \otimes \hat{T}_\downarrow \\ &\quad - U \sum_{\mathbf{i} \in \Lambda} (n_{\mathbf{i}\uparrow} - \tfrac{1}{2}) \otimes (n_{\mathbf{i}\downarrow} - \tfrac{1}{2}) - \mu(N_\Lambda - \hat{N}_\uparrow) - \mu \hat{N}_\downarrow . \end{aligned} \tag{21}$$

Notice that all the operators in $\tilde{H}$ are real and the coupling constant $-U$ is negative. Consequently, when $\mu = 0$, $\tilde{H}_H$ can be written into the spin-reflection positive form of Theorem 3.1 by letting $\hat{D}_\mathbf{i} = \sqrt{U}\,(\hat{n}_\mathbf{i} - 1/2)$.

Similarly, the partial particle-hole transformation $\tilde{U}_\Lambda$ can be also defined for the periodic Anderson model.[25] Under this transformation, we have (with $\mu = 0$)

$$\begin{aligned} \tilde{H}_\Lambda = \tilde{U}^\dagger_\Lambda H_\Lambda \tilde{U}_\Lambda &= \hat{T}_\uparrow \otimes \hat{I}_\downarrow + \hat{I}_\uparrow \otimes \hat{T}_\downarrow \\ &\quad + V \sum_{\mathbf{i} \in \Lambda} (\hat{C}^\dagger_{\mathbf{i}\uparrow} \hat{D}_{\mathbf{i}\uparrow} + \hat{D}^\dagger_{\mathbf{i}\uparrow} \hat{C}_{\mathbf{i}\uparrow}) \otimes \hat{I}_\downarrow + \hat{I}_\uparrow \otimes V \sum_{\mathbf{i} \in \Lambda} (\hat{C}^\dagger_{\mathbf{i}\downarrow} \hat{D}_{\mathbf{i}\downarrow} + \hat{D}^\dagger_{\mathbf{i}\downarrow} \hat{C}_{\mathbf{i}\downarrow}) \\ &\quad - U \sum_{\mathbf{i} \in \Lambda} (n^D_{\mathbf{i}\uparrow} - \tfrac{1}{2}) \otimes (n^D_{\mathbf{i}\downarrow} - \tfrac{1}{2}) . \end{aligned} \tag{22}$$

Obviously, $\tilde{H}_\Lambda$ is spin-reflection positive.

By following the example of the periodic Anderson model, one can easily introduce the partial particle-hole transformation $\tilde{U}_K$ for the Kondo lattice model.[26] Under this transformation, the Hamiltonian $\hat{H}_K$ becomes

$$\begin{aligned}\tilde{H}_K = \tilde{U}_K^{\dagger} H_K \tilde{U}_K = \hat{T}_\uparrow \otimes \hat{I}_\downarrow + \hat{I}_\uparrow \otimes \hat{T}_\downarrow \\ -\frac{J}{2}\sum_{i\in\Lambda}[\hat{C}_{i\uparrow}^{\dagger}\hat{F}_{i\uparrow}\otimes\hat{C}_{i\downarrow}^{\dagger}\hat{F}_{i\downarrow} + \hat{F}_{i\uparrow}^{\dagger}\hat{C}_{i\uparrow}\otimes\hat{F}_{i\downarrow}^{\dagger}\hat{C}_{i\downarrow}] \\ +\frac{J}{4}\sum_{i\in\Lambda}(\hat{n}_{i\uparrow}^{C}+\hat{n}_{i\downarrow}^{C}-1)(\hat{n}_{i\uparrow}^{F}+\hat{n}_{i\downarrow}^{F}-1).\end{aligned} \tag{23}$$

However, it is not spin-reflection positive. Fortunately, this situation can be saved by taking the constraint condition (7), which now reads

$$\hat{F}_{i\uparrow}^{\dagger}\hat{F}_{i\uparrow} = \hat{F}_{i\downarrow}^{\dagger}\hat{F}_{i\downarrow}, \tag{24}$$

into consideration. This equation requires that a localized orbital must be either empty or occupied simultaneously by a pair of F-quasifermions. Substituting this condition into the expression of the Hamiltonian $\tilde{H}_K$ and dropping an unimportant constant $JN_\Lambda/4$, we obtain

$$\begin{aligned}\tilde{H}_K = \left(\hat{T}_\uparrow + \frac{J}{2}\sum_{i\in\Lambda}\hat{n}_{i\uparrow}^{C}\hat{n}_{i\uparrow}^{F} - \frac{J}{4}\hat{N}_\uparrow\right)\otimes\hat{I}_\downarrow + \hat{I}_\uparrow\otimes\left(\hat{T}_\downarrow + \frac{J}{2}\sum_{i\in\Lambda}\hat{n}_{i\downarrow}^{C}\hat{n}_{i\downarrow}^{F} - \frac{J}{4}\hat{N}_\downarrow\right) \\ -\frac{J}{2}\sum_{i\in\Lambda}(\hat{C}_{i\uparrow}^{\dagger}\hat{F}_{i\uparrow})\otimes(\hat{C}_{i\downarrow}^{\dagger}\hat{F}_{i\downarrow}) - \frac{J}{2}\sum_{i\in\Lambda}(\hat{F}_{i\uparrow}^{\dagger}\hat{C}_{i\uparrow})\otimes(\hat{F}_{i\downarrow}^{\dagger}\hat{C}_{i\downarrow}),\end{aligned} \tag{25}$$

which is in the spin-reflection positive form.

We are now ready to explore the consequences of the spin-reflection positivity method.

4. SIMPLE SIGN RULE FOR THE GROUND-STATE WAVE FUNCTION AND ITS CONSEQUENCES

As stated in Introduction, a direct application of the spin-reflection-positivity method is to overcome the difficulties caused by the fermion sign problem of the itinerant electron systems. To make our explanation more readable, we shall follow a golden rule for the chroniclers and start from where the last story ends. Let us first recall some facts which we learnt from the elementary quantum mechanics.[49]

It is well known that, in many cases, the ground-state wave function of the Schrödinger equation can be chosen to be real. Furthermore, it has no

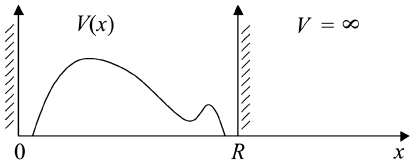

Fig. 1. The potential function of a one-dimensional quantum well.

node inside of the region in which particles move. Consequently, one can choose a ground-state wave function which is positive in the region. A corollary of this sign rule is that the ground state is nondegenerate. In this section, we show that this type of sign rule can be also established for the ground states of some localized fermion models, such as the Heisenberg model on a bipartite lattice.

As a warm-up exercise, let us first recall how to prove the sign rule for the ground-state wave function of a simple system: One particle moving in the one-dimensional potential well shown in Fig. 1. According to the elementary quantum mechanics, the ground-state wave function $\Psi_0(x)$ of this system is determined by the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi_0(x)}{dx^2}+V(x)\,\Psi_0(x)=E_0\Psi_0(x), \tag{26}$$

with E_0 being the lowest eigenvalue of the differential equation. For simplicity, we assume that the potential function $V(x)$ is continuous and bounded in the interval $(0, R)$.

When $V(x)=0$, Eq. (26) can be explicitly solved. For any $x\in(0, R)$, we have $\Psi_0(x)=\sqrt{2/R}\sin(\pi x/R)>0$ and hence, the sign rule is true. To show that the rule still holds for the ground-state wave function $\Psi_0(x)$ when $V(x)\neq 0$, we apply both the variational principle and the Harnack theorem for the second order elliptical differential equations.[50] While the variational principle argument provides a global picture of the ground-state wave function, differential equation (26) determines its local behavior.

First, we notice that, by the variational principle, $\Psi_0(x)$ is a ground-state solution of Eq. (26), if and only if it is also a minimizing function of the following energy functional

$$\mathscr{E}(\psi)=\frac{\hbar^2}{2m}\int_0^R\left|\frac{d\psi(x)}{dx}\right|^2 dx+\int_0^R|\psi(x)|^2\,V(x)\,dx \tag{27}$$

in the function space $H^1(0, R)$, requiring that both $|\psi|^2$ and $|d\psi/dx|^2$ be integrable over $(0, R)$. Suppose that the sign of $\Psi_0(x)$ is indefinite in $(0, R)$, as shown in Fig. 2.

We construct a new wave function $\Psi(x)$ by taking the absolute value of $\Psi_0(x)$, i.e., $\Psi(x) = |\Psi_0|(x)$. Notice that the replacement of $\Psi_0(x)$ by its absolute value does not change the value of the second term in Eq. (27). On the other hand, it can be shown that inequality

$$\int_0^R \left| \frac{d\Psi_0(x)}{dx} \right|^2 dx \geqslant \int_0^R \left| \frac{d\,|\Psi_0|(x)}{dx} \right|^2 dx \tag{28}$$

holds (See the appendix of ref. 27). Therefore, we have

$$\min_{\psi \in H^1} \mathscr{E}(\psi) = \mathscr{E}(\Psi_0) \geqslant \mathscr{E}(\Psi). \tag{29}$$

In other words, $\Psi(x)$ must be also a minimizing function of energy functional (27) and hence, a solution of Eq. (26).

Next, we show that the ground state wave function $\Psi_0(x)$ cannot have zero point in $(0, R)$. If this is not true, then, there must be, at least, one point $x_0 \in (0, R)$ such that $\Psi(x_0) = |\Psi_0|(x_0) = 0$. However, as a nonnegative solution of a second order elliptical differential equation, $\Psi(x)$ satisfies the so-called Harnack theorem.[50] It tells us that, on any open interval $(a, b) \subset (0, R)$, there is a constant $C_{(a,b)}$ such that

$$\max_{x \in (a,b)} \Psi(x) \leqslant C_{(a,b)} \min_{x \in (a,b)} \Psi(x). \tag{30}$$

Let us take an open interval containing x_0. Then, the Harnack theorem implies that $\Psi(x) \equiv 0$ in this interval. Repeating this argument an appropriate number of times, we find that $\Psi(x)$ as well as $\Psi_0(x)$ must be identically zero in $(0, R)$. This is certainly absurd. Therefore, $\Psi_0(x)$ cannot have zero point in $(0, R)$ and must be nondegenerate. It enables us to take $\Psi_0(x) = \Psi(x)$, which is positive in the interval.

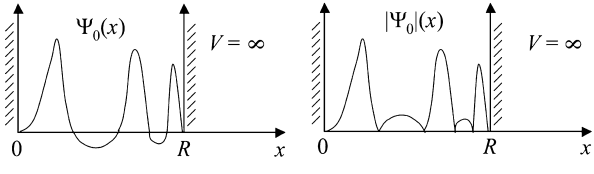

Fig. 2. The ground state wave functions $\Psi_0(x)$ and $|\Psi_0|(x)$.

It is worthwhile to emphasize that, in the above proof, the connectivity of the interval $(0, R)$ by the particle motion is essential to exclude the zero points of $\Psi_0(x)$ inside it. For the strongly correlated electron systems, we shall show that electron hopping on the lattice plays a similar role.

With this example in mind, we proceed to establish the similar sign rule for some localized electron models, such as the antiferromagnetic Heisenberg model. On a finite lattice Λ, the Hamiltonian of this well-known model is of the following form

$$H_{\mathrm{AF}} = \sum_{\langle \mathbf{ij} \rangle} J_{\mathbf{ij}} \vec{S}_{\mathbf{i}} \cdot \vec{S}_{\mathbf{j}} = \tfrac{1}{2} \sum_{\langle \mathbf{ij} \rangle} J_{\mathbf{ij}} (\hat{S}_{\mathbf{i}+} \hat{S}_{\mathbf{j}-} + \hat{S}_{\mathbf{i}-} \hat{S}_{\mathbf{j}+}) + \sum_{\langle \mathbf{ij} \rangle} J_{\mathbf{ij}} \hat{S}_{\mathbf{iz}} \hat{S}_{\mathbf{jz}}, \tag{31}$$

where $J_{\mathbf{ij}} \geqslant 0$ are the superexchange couplings between the localized spins $\vec{S}_{\mathbf{i}}$ and $\vec{S}_{\mathbf{j}}$. The lattice Λ is assumed to be connected by these couplings and bipartite, i.e., $J_{\mathbf{ij}} \neq 0$ only connect lattice sites $\mathbf{i}$ and $\mathbf{j}$ belonging to different sublattices.

Since the Heisenberg Hamiltonian commutes with the total spin operators $\hat{S}^2$ and $\hat{S}_z$, both S and S_z are good quantum numbers of the system. Therefore, the Hilbert space of this model is a direct sum of subspaces $\{V(S_z = M)\}$. A natural basis of subspace $V(M)$ is given by

$$\chi_\alpha(M) = |m_1, m_2, \ldots, m_{N_\Lambda}\rangle, \tag{32}$$

where $m_{\mathbf{i}}$ represents the eigenvalue of operator $\hat{S}_{\mathbf{iz}}$ at site $\mathbf{i}$ and they are subject to the condition $m_1 + m_2 + \cdots + m_{N_\Lambda} = M$. In terms of this basis, the ground-state wave function $\Psi_0(M)$ of H_{AF} can be written as

$$\Psi_0(M) = \sum_\alpha C_\alpha \chi_\alpha(M), \tag{33}$$

where the sum is over all the possible configurations $\{\chi_\alpha(M)\}$.

However, due to the positive sign of the coupling constants $\{J_{\mathbf{ij}}\}$, it is difficult to uncover directly the sign rule satisfied by these expansion coefficients $\{C_\alpha\}$. To remedy this problem, we follow ref. 24 and introduce a unitary transformation $\hat{U}_{\mathrm{AF}} = \exp(i\pi \sum_{\mathbf{i} \in B} \hat{S}_{\mathbf{iz}})$, which rotates each spin in sublattice B by an angle π about its S_z-axis. Under $\hat{U}_{\mathrm{AF}}$, the spin operators are transformed by

$$\hat{U}^\dagger_{\mathrm{AF}} \hat{S}_{\mathbf{ix}} \hat{U}_{\mathrm{AF}} = \epsilon(\mathbf{i})\, \hat{S}_{\mathbf{ix}}, \qquad \hat{U}^\dagger_{\mathrm{AF}} \hat{S}_{\mathbf{iy}} \hat{U}_{\mathrm{AF}} = \epsilon(\mathbf{i})\, \hat{S}_{\mathbf{iy}}, \qquad \hat{U}^\dagger_{\mathrm{AF}} \hat{S}_{\mathbf{iz}} \hat{U}_{\mathrm{AF}} = \hat{S}_{\mathbf{iz}}. \tag{34}$$

Obviously, this transformation does not change S_z of each configuration $\chi_\alpha(M)$. In other words, it maps $V(M)$ into itself. Consequently, the Heisenberg Hamiltonian H_{AF} is mapped into

$$\tilde{H}_{\mathrm{AF}} = \hat{U}_{\mathrm{AF}}^{\dagger} H_{\mathrm{AF}} \hat{U}_{\mathrm{AF}} = \sum_{\langle \mathbf{ij} \rangle} (-J_{\mathbf{ij}}/2)(\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}-} + \hat{S}_{\mathbf{i}-}\hat{S}_{\mathbf{j}+}) + \sum_{\langle \mathbf{ij} \rangle} J_{\mathbf{ij}} \hat{S}_{\mathbf{iz}} \hat{S}_{\mathbf{jz}}. \tag{35}$$

In the meantime, its ground state $\Psi_0(M)$ in the subspace $V(M)$ becomes

$$\tilde{\Psi}_0(M) = \sum_{\alpha} \tilde{C}_\alpha \chi_\alpha(M). \tag{36}$$

For $\tilde{\Psi}_0(M)$, we have the following sign rule.

Theorem 4.1. Let $\tilde{\Psi}_0(M)$ be the ground state of $\tilde{H}_{\mathrm{AF}}$ in the subspace $V(S_z = M)$. Then, its expansion coefficients $\{\tilde{C}_\alpha\}$ in Eq. (36) can be chosen to be strictly positive. Therefore, $\tilde{\Psi}_0(M)$ is nondegenerate.

Proof. Following the above procedure described for the one-dimensional quantum mechanical system, we rewrite first the ground-state energy $E_0(M)$ of the Hamiltonian $\tilde{H}_{\mathrm{AF}}$ into an expectation (energy functional) form.

$$\begin{aligned} E_0(M) &= \langle \tilde{\Psi}_0(M) |\, \tilde{H}_{\mathrm{AF}} \,| \tilde{\Psi}_0(M) \rangle \\ &= \sum_{\langle \mathbf{ij} \rangle} \left(-\frac{J_{\mathbf{ij}}}{2} \right) \langle \tilde{\Psi}_0(M) |\, \hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}-} + \hat{S}_{\mathbf{i}-}\hat{S}_{\mathbf{j}+} \,| \tilde{\Psi}_0(M) \rangle \\ &\quad + \sum_{\langle \mathbf{ij} \rangle} J_{\mathbf{ij}} \langle \tilde{\Psi}_0(M) |\, \hat{S}_{\mathbf{iz}}\hat{S}_{\mathbf{jz}} \,| \tilde{\Psi}_0(M) \rangle \\ &= \sum_{\alpha,\alpha'} \sum_{\langle \mathbf{ij} \rangle} \left(-\frac{J_{\mathbf{ij}}}{2} \right) \tilde{C}_\alpha^* \tilde{C}_{\alpha'} \langle \chi_\alpha(M) |\, \hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}-} + \hat{S}_{\mathbf{i}-}\hat{S}_{\mathbf{j}+} \,| \chi_{\alpha'}(M) \rangle \\ &\quad + \sum_{\alpha} \sum_{\langle \mathbf{ij} \rangle} J_{\mathbf{ij}} |\tilde{C}_\alpha|^2 \langle \chi_\alpha(M) |\, \hat{S}_{\mathbf{iz}}\hat{S}_{\mathbf{jz}} \,| \chi_\alpha(M) \rangle. \end{aligned} \tag{37}$$

Notice that the operators $\hat{S}_{\mathbf{i}+}$ and $\hat{S}_{\mathbf{i}-}$ are defined by

$$\begin{aligned} \hat{S}_{\mathbf{i}+} \,|S_{\mathbf{i}}, m_{\mathbf{i}}\rangle &= \sqrt{S_{\mathbf{i}}(S_{\mathbf{i}}+1) - m_{\mathbf{i}}(m_{\mathbf{i}}+1)}\, |S_{\mathbf{i}}, m_{\mathbf{i}}+1\rangle, \\ \hat{S}_{\mathbf{i}-} \,|S_{\mathbf{i}}, m_{\mathbf{i}}\rangle &= \sqrt{S_{\mathbf{i}}(S_{\mathbf{i}}+1) - m_{\mathbf{i}}(m_{\mathbf{i}}-1)}\, |S_{\mathbf{i}}, m_{\mathbf{i}}-1\rangle. \end{aligned} \tag{38}$$

Therefore, we have inequality

$$\langle \chi_\alpha(M) |\, \hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}-} + \hat{S}_{\mathbf{i}-}\hat{S}_{\mathbf{j}+} \,| \chi_{\alpha'}(M) \rangle \geqslant 0 \tag{39}$$

for any admissible pair of indices α and α'. It implies that, if we replace each coefficient $\tilde{C}_\alpha$ with its absolute value $|\tilde{C}_\alpha|$ in Eq. (37), the quantity on the right-hand side of the equation becomes less. In other words, the new wave function $\tilde{\Psi}(M)$ defined by

$$\tilde{\Psi}(M) \equiv \sum_\alpha |\tilde{C}_\alpha| \, \chi_\alpha(M) \tag{40}$$

has a lower energy than $E_0(M)$. By the variational principle, $\tilde{\Psi}(M)$ must be a ground state of the Hamiltonian $\tilde{H}_{\mathrm{AF}}$ in the same subspace $V(M)$, too. Therefore, we reach the conclusion that, for any given ground state $\tilde{\Psi}_0(M)$ of $\tilde{H}_{\mathrm{AF}}$ in $V(M)$, there exists another one whose expansion coefficients are nonnegative.

In the second step, we show that none of the expansion coefficients $\{\tilde{C}_\alpha\}$ in Eq. (36) can be zero. As emphasized above, this fact is determined by the connectivity of lattice Λ by the spin flipping, which may be thought of as the hopping of hard-core bosons on the lattice.[51]

Assume that one coefficient $\tilde{C}_\beta = 0$. Then, the corresponding coefficient $|\tilde{C}_\beta|$ in the ground-state wave function $\tilde{\Psi}(M)$ is also absent. Multiplying the Schrödinger equation $\tilde{H}_{\mathrm{AF}}\tilde{\Psi}(M) = E_0(M)\,\tilde{\Psi}(M)$ from the left by $\langle\chi_\beta(M)|$, we obtain

$$\begin{aligned} E_0(M)\,|\tilde{C}_\beta| = &-\sum_\gamma \langle\chi_\beta(M)| \sum_{\langle \mathbf{ij}\rangle} \frac{J_{\mathbf{ij}}}{2} (\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}-} + \hat{S}_{\mathbf{i}-}\hat{S}_{\mathbf{j}+}) \, |\chi_\gamma(M)\rangle \, |\tilde{C}_\gamma| \\ &+ \sum_{\langle \mathbf{ij}\rangle} J_{\mathbf{ij}} \langle\chi_\beta(M)| \, \hat{S}_{\mathbf{i}z}\hat{S}_{\mathbf{j}z} \, |\chi_\beta(M)\rangle \, |\tilde{C}_\beta|. \end{aligned} \tag{41}$$

Substituting $|\tilde{C}_\beta| = 0$ into this equation yields

$$\sum_\gamma \langle\chi_\beta(M)| \sum_{\langle \mathbf{ij}\rangle} \left(\frac{J_{\mathbf{ij}}}{2}\right) (\hat{S}_{\mathbf{i}+}\hat{S}_{\mathbf{j}-} + \hat{S}_{\mathbf{i}-}\hat{S}_{\mathbf{j}+}) \, |\chi_\gamma(M)\rangle \, |\tilde{C}_\gamma| = 0. \tag{42}$$

On the other hand, as shown by Eq. (39), all the matrix elements in Eq. (42) are nonnegative. Therefore, any coefficient $|\tilde{C}_\gamma|$, representing a state $\chi_\gamma(M)$ which is connected to $\chi_\beta(M)$ by a spin-flipping exchange, must be identically zero.

By repeating this process an appropriate number of times, we can show that all the coefficients $|\tilde{C}_\alpha|$ in Eq. (36) must be identically zero because lattice Λ is connected by the spin-flipping interaction. However, this is not possible. Therefore, $\tilde{C}_\alpha \neq 0$ must hold for each admissible index α. ▌

In literature, this sign rule is called the Marshall rule, although it is rather different from the original one discovered by Marshall for the antiferromagnetic Heisenberg Hamiltonian.[52] It leads to the nondegeneracy of the ground state of the Hamiltonian $\tilde{H}_{\mathrm{AF}}$ in each subspace $V(M)$. On the other hand, since $\tilde{H}_{\mathrm{AF}}$ is unitarily equivalent to the original antiferromagnetic Heisenberg Hamiltonian H_{AF}, the ground state $\Psi_0(M)$ of H_{AF} must be also nondegenerate in $V(M)$.

Interestingly, the sign rule established for the ground-state wave function of a many-body model provides generally more information on the system. For instance, in their original paper,[24] based on Theorem 4.1, Lieb and Mattis also proved

Theorem 4.2. The global ground state of the antiferromagnetic Heisenberg model on a bipartite lattice has spin number

$$S = |S_A - S_B|. \tag{43}$$

Here, $S_A = \sum_{\mathrm{i} \in A} S_{\mathrm{i}}$ and $S_B = \sum_{\mathrm{i} \in B} S_{\mathrm{i}}$ are the algebraic sums of the spins on sublattices A and B, respectively.

Proof. To prove this theorem, Lieb and Mattis introduced an auxiliary Hamiltonian

$$H_{\mathrm{LM}} = \sum_{\mathrm{i} \in A} \sum_{\mathrm{j} \in B} \vec{S}_{\mathrm{i}} \cdot \vec{S}_{\mathrm{j}}. \tag{44}$$

Obviously, for this Hamiltonian, we can repeat the proof of Theorem 4.1. Therefore, all the coefficients $\{\tilde{C}_\alpha^{\mathrm{LM}}\}$ in the ground-state wave function $\tilde{\Psi}_0^{\mathrm{LM}}(M)$ of the transformed Hamiltonian $\tilde{H}_{\mathrm{LM}} = \hat{U}_{\mathrm{AF}}^\dagger H_{\mathrm{LM}} \hat{U}_{\mathrm{AF}}$ are positive. Consequently, $\tilde{\Psi}_0^{\mathrm{LM}}(M)$ has a nonzero overlap with the ground state $\tilde{\Psi}_0(M)$. By applying the inverse of $\hat{U}_{\mathrm{AF}}$ to both ground states, we obtain

$$\langle \Psi_0(M) \,|\, \Psi_0^{\mathrm{LM}}(M) \rangle \neq 0. \tag{45}$$

It implies that $\Psi_0(M)$ and $\Psi_0^{\mathrm{LM}}(M)$ must have the same spin number S. On the other hand, the energy levels of H_{LM} can be explicitly calculated and are given by

$$E(S) = \tfrac{1}{2}\,[S(S+1) - S_A(S_A+1) - S_B(S_B+1)]. \tag{46}$$

Therefore, if $|M| \geqslant |S_A - S_B|$, its ground state $\Psi_0^{\mathrm{LM}}(M)$ in subspace $V(M)$ must have $S = |M|$ and its global ground state has spin number $S = |S_A - S_B|$. So does the global ground state of the antiferromagnetic Heisenberg Hamiltonian. ▌

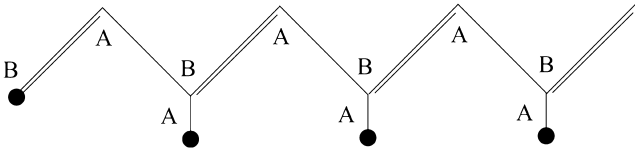

Fig. 3. The lattice structure of organic conjugated polymers.

Theorem 4.2 shows that the Marshall rule for the ground state of the antiferromagnetic Heisenberg model can be exploited to discover more interesting properties of the system. In fact, it is not the whole story yet. By using the Marshall rule and the Lieb–Mattis theorem, we can further prove the following theorem.[36, 53]

Theorem 4.3. The ground state of the antiferromagnetic Heisenberg model on a bipartite lattice has both the ferromagnetic and the antiferromagnetic long-range orders, if n_A, the number of sites belonging to sublattice A in each unit cell, is not equal to n_B. In other words, it is ferrimagnetically ordered.

One example of such a lattice is shown in Fig. 3. For this lattice, we have $n_A = 2$ and $n_B = 1$.

Proof of Theorem 4.3. First, let us consider the transverse spin correlation in the ground state $\tilde{\Psi}_0(M)$ of the transformed Hamiltonian $\tilde{H}_{\mathrm{AF}}$. Take an arbitrary pair of lattice sites $\mathbf{h}$ and $\mathbf{k}$. The transverse spin correlation in the ground state is defined by

$$\langle \tilde{\Psi}_0(M)|\, \hat{S}_{\mathbf{h}-} \hat{S}_{\mathbf{k}+}\, |\tilde{\Psi}_0(M)\rangle = \sum_{\alpha,\,\beta} \tilde{C}_\alpha \tilde{C}_\beta \langle \chi_\alpha(M)|\, \hat{S}_{\mathbf{h}-} \hat{S}_{\mathbf{k}+}\, |\chi_\beta(M)\rangle. \quad (47)$$

As shown above, the matrix element $\langle \chi_\alpha|\, \hat{S}_{\mathbf{h}+} \hat{S}_{\mathbf{k}-}\, |\chi_\beta\rangle$ is nonnegative for any pair of basis vectors χ_α and χ_β. On the other hand, by Theorem 4.1, all the expansion coefficients $\tilde{C}_\alpha$ are positive. Therefore, we have

$$\langle \tilde{\Psi}_0(M)|\, \hat{S}_{\mathbf{h}-} \hat{S}_{\mathbf{k}+}\, |\tilde{\Psi}_0(M)\rangle \geqslant 0. \quad (48)$$

Next, by applying the inverse of the unitary transformation $\hat{U}_{\mathrm{AF}}$ to this inequality, we map $\tilde{\Psi}_0(M)$ onto $\Psi_0(M)$, the ground state of the antiferromagnetic Heisenberg model in the same subspace $V(M)$. Consequently, we obtain

$$\begin{aligned} &\langle \tilde{\Psi}_0(M)|\, \hat{S}_{\mathbf{h}-} \hat{S}_{\mathbf{k}+}\, |\tilde{\Psi}_0(M)\rangle \\ &\quad = \langle \tilde{\Psi}_0(M)|\, \hat{U}_{\mathrm{AF}} (\hat{U}^\dagger_{\mathrm{AF}} \hat{S}_{\mathbf{h}-} \hat{U}_{\mathrm{AF}}) (\hat{U}^\dagger_{\mathrm{AF}} \hat{S}_{\mathbf{k}+} \hat{U}_{\mathrm{AF}})\, \hat{U}^\dagger_{\mathrm{AF}}\, |\tilde{\Psi}_0(M)\rangle \\ &\quad = \epsilon(\mathbf{h})\, \epsilon(\mathbf{k}) \langle \Psi_0(M)|\, \hat{S}_{\mathbf{h}-} \hat{S}_{\mathbf{k}+}\, |\Psi_0(M)\rangle \geqslant 0. \end{aligned} \quad (49)$$

It tells us that the transverse spin correlation of $\Psi_0(M)$ is antiferromagnetic. A direct consequence of Eq. (49) is the following inequality

$$\frac{1}{N_\Lambda}\sum_{\mathbf{k},\mathbf{h}} \epsilon(\mathbf{h})\,\epsilon(\mathbf{k})\langle\Psi_0(M)|\,\hat{S}_{\mathbf{h}-}\hat{S}_{\mathbf{k}+}\,|\Psi_0(M)\rangle$$
$$\geqslant \frac{1}{N_\Lambda}\sum_{\mathbf{k},\mathbf{h}} \langle\Psi_0(M)|\,\hat{S}_{\mathbf{h}-}\hat{S}_{\mathbf{k}+}\,|\Psi_0(M)\rangle = \frac{1}{N_\Lambda}\langle\Psi_0(M)|\,\hat{S}_-\hat{S}_+\,|\Psi_0(M)\rangle, \tag{50}$$

which holds in each admissible subspace $V(M)$.

On the other hand, by the Lieb–Mattis theorem, when $n_A \neq n_B$, the total spin of the global ground state of H_{AF} is

$$S = |S_A - S_B| = s\,|N_A - N_B| = sN_c\,|n_A - n_B|, \tag{51}$$

where s is the value of spin at each lattice site and N_c is the number of unit cells in the lattice. Therefore, the global ground state is $(2S+1)$-fold degenerate and each representative $\Psi_0(M)$ of it has a spin number $S_z = M$ with $-S \leqslant M \leqslant S$. Take an arbitrary complex function $f(\mathbf{i})$ on lattice Λ with $|f(\mathbf{i})| = 1$. We define the averaged transverse and longitudinal spin correlation functions of Ψ_0 by

$$\begin{aligned} G_T(f) &\equiv \frac{1}{2S+1}\sum_{M=-S}^{S} \langle\Psi_0(M)|\,\hat{S}_-(\bar{f})\,\hat{S}_+(f)\,|\Psi_0(M)\rangle, \\ G_L(f) &\equiv \frac{1}{2S+1}\sum_{M=-S}^{S} \langle\Psi_0(M)|\,\hat{S}_z(\bar{f})\,\hat{S}_z(f)\,|\Psi_0(M)\rangle, \end{aligned} \tag{52}$$

where $\hat{S}_\alpha(f) \equiv N_\Lambda^{-1/2}\sum_{\mathbf{i}\in\Lambda} f(\mathbf{i})\,\hat{S}_{\mathbf{i}\alpha}$ with $\alpha = +, -, z$, is the "Fourier transformation" of these spin operators. In particular, the functions $v(\mathbf{i}) = 1$ and $\epsilon(\mathbf{i})$ give the ferromagnetic and the antiferromagnetic components of the spin-wave excitations in the system, respectively. With these definitions, inequality (50) is reduced to

$$G_T(\epsilon) \geqslant G_T(v). \tag{53}$$

Furthermore, by the spin $SU(2)$ symmetry of the Heisenberg Hamiltonian, we have also

$$G_T(f) = 2G_L(f). \tag{54}$$

Therefore, inequality

$$G_L(\epsilon) = \tfrac{1}{2} G_T(\epsilon) \geqslant \tfrac{1}{2} G_T(v) = G_L(v) \tag{55}$$

holds. The longitudinal spin correlation function $G_L(v)$ on the right-hand side of Eq. (55) can be directly calculated. A little algebra yields

$$\begin{aligned} G_L(v) &= \frac{1}{(2S+1)\, N_A} \sum_{M=-S}^{S} \langle \Psi_0(M) |\, \hat{S}_z \hat{S}_z \,| \Psi_0(M) \rangle \\ &= \frac{2}{(2S+1)\, N_A} (S^2 + (S-1)^2 + \cdots + 1^2) \geqslant \frac{S^2}{3N_A}. \end{aligned} \tag{56}$$

Therefore, when $S = N_c s\, |n_A - n_B|$, we have

$$G_L(\epsilon) \geqslant G_L(v) \cong O(N_c^2 / N_A) \cong O(N_A), \tag{57}$$

as $N_A \to \infty$. This equation shows that the global ground state of the Heisenberg model on the lattice has both the longitudinal ferromagnetic and antiferromagnetic long-range orders. Therefore, the model represents a ferrimagnet. ▮

Theorem 4.3 was first proven for the Hubbard model[36] (see Theorems 5.2–5.5 in the next section) and then, was generalized to the antiferromagnetic Heisenberg model.[53] It can be also proven for the so-called alternative spin models.[54] The simplest example of these systems is the antiferromagnetic Heisenberg model on a one-dimensional (bipartite) chain. However, unlike the usual spin chain, we have different spins on different sublattices in such a system. For example, the materials with spins of $S = 1$ on sublattice A and $S = 1/2$ on the sublattice B have been made in experiments.[55] Naturally, their properties attract many physicists' interest.[56–61] To these systems, the Lieb–Mattis theorem applies. For instance, the global ground state of the alternative spin chain has spin

$$S = |S_A - S_B| = \frac{N_A}{2} \left| 1 - \frac{1}{2} \right| = \frac{N_A}{4}. \tag{58}$$

Therefore, by repeating the proof of Theorem 4.3, we can easily show that this system has also a ferrimagnetic long-range order.[54]

5. APPLICATION OF THE SPIN-REFLECTION-POSITIVITY METHOD TO ITINERANT ELECTRON MODELS

Now, we return to the itinerant electron models. As stated in Introduction, the fermion sign problem in these models makes their rigorous

analysis extremely difficult. Consequently, in general, it is even hard to prove the nondegeneracy of their ground states, let alone the existence of various long-range orders in these states.

This situation has been greatly improved by introduction of the spin-reflection-positivity method.[23] With this method, Lieb showed that, if the Hamiltonian of a strongly correlated electron system is spin-reflection positive, then the expansion coefficients of its ground-state wave function can be written into a matrix and *this matrix is positive (or negative) definite*. Obviously, this result is a generalized sign rule for the itinerant electron models. It implies the nondegeneracy the ground states of these models. More importantly, it also enables us to employ the techniques developed in Section 4 to study the correlation functions of these itinerant electron systems, as we shall explain in the following.

As usual, we take the negative-U Hubbard Hamiltonian (21) for example. Formally, with $\mu = 0$, it is already in the spin-reflection positive form of Theorem 3.1. However, there is a subtle point which is worth mentioning. The reflection positivity of the Hamiltonian in Theorem 3.1 implies that the subspaces, in which the operators $\hat{B}$ and $\overline{\theta(\hat{B})}$ act respectively, are isomorphic to each other. For the negative-U Hubbard model, it requires that both the subspaces $V_\uparrow$ and $V_\downarrow$ have the same dimension. Fortunately, this requirement can be easily satisfied by taking an even integer $N = 2L$ for the electron number in the system. As noticed in Section 2, the (negative-U) Hubbard Hamiltonian commutes with the spin operators $\hat{S}_+$ and $\hat{S}_-$ when the trivial chemical potential term is ignored. Consequently, one of its ground states has spin number $S_z = (1/2)(N_\uparrow - N_\downarrow) = 0$ in the subspace $V(L, L)$. Moreover, in terms of the quasi-fermion operators, we have $V(L, L) = V_\uparrow(L) \otimes V_\downarrow(L)$ and a natural basis of $V_\sigma(L)$ is given by

$$\psi_\alpha^\sigma(L) = \hat{C}^\dagger_{\mathbf{i}_1\sigma}\hat{C}^\dagger_{\mathbf{i}_2\sigma}\cdots\hat{C}^\dagger_{\mathbf{i}_L\sigma}|0\rangle, \tag{59}$$

where $(\mathbf{i}_1, \mathbf{i}_2, ..., \mathbf{i}_L)$ denotes the lattice sites occupied by electrons of spin σ. $|0\rangle$ is the vacuum state. Obviously, $V_\uparrow(L)$ is isomorphic to $V_\downarrow(L)$ and both of them have the same dimension $D = C^L_{N_A}$. Therefore, the ground-state wave function of the negative-U Hubbard Hamiltonian in $V(L, L)$ can be written as

$$\tilde{\Psi}_0(2L) = \sum_{\alpha,\beta} W_{\alpha\beta}\psi^\uparrow_\alpha(L) \otimes \psi^\downarrow_\beta(L). \tag{60}$$

By taking α for the row index and β for the column index, the expansion coefficients $\{W_{\alpha\beta}\}$ in Eq. (60) can be put into a $C^L_{N_A} \times C^L_{N_A}$ square matrix $\mathscr{W}$. For this matrix, we have

Theorem 5.1 (Lieb). Assume that $0 \leqslant L \leqslant N_\Lambda$. Then, the coefficient matrix $\mathscr{W}$ of the ground-state wave function $\tilde{\Psi}_0(2L)$ of the negative-U Hubbard Hamiltonian on an arbitrary (not necessarily bipartite) lattice can be chosen to be positive definite.

Proof. Following the procedure described in Section 4, we first write the energy of the ground state $\tilde{\Psi}_0(2L)$ as

$$\begin{aligned} E_0(2L) &= \langle \tilde{\Psi}_0(2L)| \, \tilde{H}_H \, |\tilde{\Psi}_0(2L)\rangle \\ &= \sum_{\alpha,\beta} \sum_{\gamma,\delta} \bar{W}_{\gamma\delta} W_{\alpha\beta} \langle \psi_\gamma^\uparrow | \, \hat{T}_\uparrow \, |\psi_\alpha^\uparrow\rangle \, \delta_{\delta\beta} + \sum_{\alpha,\beta} \sum_{\gamma,\delta} \bar{W}_{\gamma\delta} W_{\alpha\beta} \delta_{\gamma\alpha} \langle \psi_\delta^\downarrow | \, \hat{T}_\downarrow \, |\psi_\beta^\downarrow\rangle \\ &\quad - U \sum_{\mathbf{i}\in\Lambda} \sum_{\alpha,\beta} \sum_{\gamma,\delta} \bar{W}_{\gamma\delta} W_{\alpha\beta} \langle \psi_\gamma^\uparrow | \, \hat{n}_{\mathbf{i}\uparrow} - \tfrac{1}{2} \, |\psi_\alpha^\uparrow\rangle \langle \psi_\delta^\downarrow | \, \hat{n}_{\mathbf{i}\downarrow} - \tfrac{1}{2} \, |\psi_\beta^\downarrow\rangle, \end{aligned} \tag{61}$$

with $\mathrm{Tr}\, \mathscr{W}^\dagger \mathscr{W} = 1$. Without causing confusion, we shall drop the spin indices in Eq. (61) and write it into a more compact form

$$E_0(2L) = \mathrm{Tr}(T\mathscr{W}\mathscr{W}^\dagger) + \mathrm{Tr}(T\mathscr{W}^\dagger\mathscr{W}) - U \sum_{\mathbf{i}\in\Lambda} \mathrm{Tr}(\mathscr{W}^\dagger N_\mathbf{i} \mathscr{W} N_\mathbf{i}), \tag{62}$$

where T is the matrix of the electron hopping operator $\hat{T}$ and $N_\mathbf{i}$ stands for the matrix of $\hat{N}_\mathbf{i} = (\hat{n}_\mathbf{i} - 1/2)$.

On the other hand, since all the operators and the basis vectors are real and the Hamiltonian is symmetric in the spin indices, we see that, if $\mathscr{W}$ corresponds to a ground state, so does $\mathscr{W}^\dagger$. By linearity, it implies that both $\mathscr{W} + \mathscr{W}^\dagger$ and $i(\mathscr{W} - \mathscr{W}^\dagger)$ also represent ground states of the negative-U Hubbard model. Therefore, we may choose an Hermitian coefficient matrix $\mathscr{W}$ and diagonalize it by a unitary matrix V. Let $\{|m\rangle\}$ be the column vectors of V and $\{r_m\}$ be the diagonal elements of $V^\dagger \mathscr{W} V = \mathscr{R}$. Then, the ground-state energy $E_0(2L)$ can be further written as

$$E_0(2L) = 2 \sum_m \langle m| \, T \, |m\rangle \, r_m^2 - U \sum_{\mathbf{i}\in\Lambda} \sum_{m,n} r_m r_n \, |\langle n| \, N_\mathbf{i} \, |m\rangle|^2. \tag{63}$$

Obviously, if we replace r_m with $|r_m|$, the first sum on the right-hand side of this equation keeps unchanged but the second sum becomes less. Therefore, if the coefficient matrix $\mathscr{W}$ is indefinite, we can construct a new state $\tilde{\Psi}(2L)$ by replacing $\mathscr{W}$ with $|\mathscr{W}| \equiv V \, |\mathscr{R}| \, V^\dagger$ in Eq. (60) and this state has a lower energy (Notice that $\mathrm{Tr}\, |\mathscr{W}|^2 = \mathrm{Tr}\, \mathscr{W}^2 = 1$). By the variational principle, $\tilde{\Psi}(2L)$ must be also a ground state.

Next, we show that $\mathscr{W}$ does not have zero eigenvalue. Suppose that it is not true. Then, by the definition of matrix $|\mathscr{W}|$, there is, at least, a nonzero vector $\vec{u}$ such that $|\mathscr{W}| \, \vec{u} = 0$. In other words, the kernel space Q of matrix $|\mathscr{W}|$ is not trivial. We prove that, under this assumption, Q actually

coincides with the whole space in which $|\mathscr{W}|$ acts. Therefore, $|\mathscr{W}|$ must be identically zero. However, this is impossible. Consequently, $\mathscr{W}$ cannot have zero eigenvalue at all. It implies that the ground state of the negative-U Hubbard model in the subspace $V(L, L)$ is nondegenerate. Therefore, $\mathscr{W}$ equals $|\mathscr{W}|$ (or $-|\mathscr{W}|$).

We start from the Schrödinger equation of the ground-state wave function $\tilde{\Psi}(2L)$. Taking the inner product of this equation with vectors $\{\langle\psi_\delta^\downarrow| \otimes \langle\psi_\gamma^\downarrow|\}$, it can be written into an equation of matrices

$$T\,|\mathscr{W}|+|\mathscr{W}|\,T-U\sum_{\mathbf{i}\in\Lambda} N_{\mathbf{i}}\,|\mathscr{W}|\,N_{\mathbf{i}}=E_0(2L)\,|\mathscr{W}|. \tag{64}$$

Picking up an arbitrary vector $\vec{v}\in Q$ and calculating the expectation of Eq. (64) in it, we obtain

$$\langle\vec{v}|\,T\,|\mathscr{W}|\,|\vec{v}\rangle+\langle\vec{v}|\,|\mathscr{W}|\,T\,|\vec{v}\rangle-U\sum_{\mathbf{i}\in\Lambda}\langle\vec{v}|\,N_{\mathbf{i}}\,|\mathscr{W}|\,N_{\mathbf{i}}\,|\vec{v}\rangle=E_0(2L)\langle\vec{v}|\,|\mathscr{W}|\,|\vec{v}\rangle. \tag{65}$$

Since $|\mathscr{W}|\vec{v}=0$ by definition, this equation is reduced to

$$\sum_{\mathbf{i}\in\Lambda}\langle\vec{v}|\,N_{\mathbf{i}}\,|\mathscr{W}|\,N_{\mathbf{i}}\,|\vec{v}\rangle=0. \tag{66}$$

On the other hand, since $|\mathscr{W}|$ is semipositive definite, we conclude that $N_{\mathbf{i}}\vec{v}\in Q$ for each $\mathbf{i}\in\Lambda$. In other words, $N_{\mathbf{i}}$ maps Q into itself. Now, let equation (64) act on $\vec{v}$. Because $|\mathscr{W}|\,\vec{v}=0$ and $|\mathscr{W}|\,N_{\mathbf{i}}\vec{v}=0$, we have $|\mathscr{W}|\,T\vec{v}=0$. Thus T, which is the matrix of the electron hopping term, also maps Q into Q.

With these facts in mind, we finish the proof of Theorem 5.1. Notice that a vector $\vec{v}\in Q$ actually represents the set of coefficients $\{v_\lambda\}$ in the state $|v\rangle=\sum_\lambda v_\lambda\psi_\lambda^\downarrow$. Therefore, $\vec{v}\neq 0$ indicates that there is, at least, one index μ such that $v_\mu\neq 0$. Let I_μ be the set of lattice sites which are occupied by electrons in the configuration $\psi_\mu^\downarrow$. Obviously, we can project out vector

$$\vec{v}_\mu\equiv(0,0,\ldots,v_\mu,\ldots,0)\equiv v_\mu\vec{e}_\mu \tag{67}$$

by multiplying $\vec{v}$ with the matrix $N_\mu=\prod_{\mathbf{i}\in I_\mu}(N_{\mathbf{i}}+1/2)$ from left. On the other hand, since each matrix $N_{\mathbf{i}}+1/2$ maps the kernel space Q into itself, $\vec{v}_\mu=N_\mu\vec{v}$ must be also a vector in Q. Next, we multiply $\vec{v}_\mu$ again by matrix T, which represents the electron hopping operator $\hat{T}_\downarrow$ and also maps Q into Q, from left. It yields another nonzero vector $\vec{v}'$, which belongs to Q

and does not have component in $\vec{e}_\mu$. That enables us to project out a different basis vector $\vec{e}_\nu$ by multiplying $\vec{v}'$ with a proper matrix $N_\nu = \prod_{i \in I_\nu}(N_i + 1/2)$ and then, dividing the result by v'_ν. Since lattice Λ is connected by the electron hopping operator $\hat{T}_\downarrow$, one can easily see that, starting from $\vec{v}_\mu$, any basis vector $\vec{e}_\epsilon$ can be reached by repeating the above operations an appropriate number of times. Because these operations map Q into Q, we conclude that all the basis vectors $\{\vec{e}_\alpha\}$ must be contained in Q. In other words, $|\mathscr{W}| \equiv 0$. This is impossible. Therefore, $\mathscr{W}$ cannot have zero eigenvalue and Theorem 5.1 is proven. ▮

A direct corollary of Theorem 5.1 is ref. 23

Corollary 5.1. The ground state $\tilde{\Psi}_0(2L)$ of the negative-U Hubbard model in the subspace $V(L, L)$ has total spin $S = 0$. Therefore, it is the unique ground state of $\tilde{H}_H$ in the subspace $V(2L) = \sum_{l=-L}^{L} \oplus V(L-l, L+l)$.

Proof. Since the expansion coefficient matrix $\mathscr{W}$ of the ground state $\tilde{\Psi}_0(2L)$ is positive definite, one of its diagonal elements $W_{\alpha\alpha} \neq 0$. Therefore, $\tilde{\Psi}_0(2L)$ has a nonzero overlap with state $|\psi_\alpha^\uparrow\rangle \otimes |\psi_\alpha^\downarrow\rangle$, which has total spin $S = 0$. So does $\tilde{\Psi}_0(2L)$. ▮

Theorem 5.1 can be thought of as a weaker sign rule for the ground state of the negative-U Hubbard model. Indeed, although the coefficient matrix $\mathscr{W}$ is positive definite, these coefficients have actually different signs. However, this result is sufficient for people to reveal some interesting properties of the strongly correlated electron systems. For instance, based on Theorem 5.1, Lieb further proved the following theorem in ref. 23.

Theorem 5.2. The ground state of the original Hubbard Hamiltonian (with positive U) in the half-filled subspace has total spin $S = |N_A - N_B|/2$.

To prove Theorem 5.2, Lieb used the fact that the half-filled Hubbard Hamiltonian is reduced to an antiferromagnetic Heisenberg Hamiltonian on the same lattice when U is large.[10] Consequently, Theorem 4.2 of Section 4 applies. Here, we shall take a different approach, which was independently proposed in the second and third papers of ref. 26.

Proof of Theorem 5.2. Applying the partial particle-hole transformation $\tilde{U}_H$ to the Lieb–Mattis Hamiltonian defined in Eq. (44), we obtain a unitarily equivalent Hamiltonian

$$\tilde{H}_{\mathrm{LM}} = -\tfrac{1}{2} \sum_{i \in A} \sum_{j \in B} (\hat{C}_{i\uparrow}\hat{C}_{i\downarrow}\hat{C}^\dagger_{j\downarrow}\hat{C}^\dagger_{j\uparrow} + \hat{C}^\dagger_{i\downarrow}\hat{C}^\dagger_{i\uparrow}\hat{C}_{j\uparrow}\hat{C}_{j\downarrow}) + \tfrac{1}{4} \sum_{i \in A} \sum_{j \in B} (\hat{C}^\dagger_{i\uparrow}\hat{C}_{i\uparrow} + \hat{C}^\dagger_{i\downarrow}\hat{C}_{i\downarrow} - 1)(\hat{C}^\dagger_{j\uparrow}\hat{C}_{j\uparrow} + \hat{C}^\dagger_{j\downarrow}\hat{C}_{j\downarrow} - 1). \quad (68)$$

However, this Hamiltonian is not spin-reflection positive. Fortunately, in the Lieb–Mattis Hamiltonian, all the electrons are localized. Therefore, like the transformed Kondo lattice Hamiltonian $\tilde{H}_K$, the quasi-fermion operators $\hat{C}_{i\sigma}$ and $\hat{C}^\dagger_{i\sigma}$ in $\tilde{H}_{\mathrm{LM}}$ are subject to the condition $\hat{C}^\dagger_{i\uparrow}\hat{C}_{i\uparrow} = \hat{C}^\dagger_{i\downarrow}\hat{C}_{i\downarrow}$. Substituting this condition into $\tilde{H}_{\mathrm{LM}}$ and neglecting a constant $N_A N_B/4$, it can be further rewritten as

$$\begin{aligned}\tilde{H}_{\mathrm{LM}} = {} & \tfrac{1}{4}\left(2\sum_{i\in A}\sum_{j\in B}\hat{n}_{i\uparrow}\hat{n}_{j\uparrow} - N_A\sum_{j\in B}\hat{n}_{j\uparrow} - N_B\sum_{i\in A}\hat{n}_{i\uparrow}\right) \\ & + \tfrac{1}{4}\left(2\sum_{i\in A}\sum_{j\in B}\hat{n}_{i\downarrow}\hat{n}_{j\downarrow} - N_A\sum_{j\in B}\hat{n}_{j\downarrow} - N_B\sum_{i\in A}\hat{n}_{i\downarrow}\right) \\ & - \tfrac{1}{2}\sum_{i\in A}\sum_{j\in B}(\hat{C}^\dagger_{j\uparrow}\hat{C}_{i\uparrow})\otimes(\hat{C}^\dagger_{j\downarrow}\hat{C}_{i\downarrow}) - \tfrac{1}{2}\sum_{i\in A}\sum_{j\in B}(\hat{C}^\dagger_{i\uparrow}\hat{C}_{j\uparrow})\otimes(\hat{C}^\dagger_{i\downarrow}\hat{C}_{j\downarrow}),\end{aligned} \tag{69}$$

which is spin-reflection positive. By repeating the proof of Theorem 5.1, we conclude that the expansion coefficient matrix of the ground-state wave function $\tilde{\Psi}^{\mathrm{LM}}_0(2L)$ is also positive definite. (In fact, it is a diagonal matrix according to the constraint condition imposed on the quasi-fermion operators). Therefore, the ground-state wave function $\tilde{\Psi}_0(2L) = \tilde{\Psi}_0(L, L)$ of the negative-U Hubbard model has a nonzero overlap with $\tilde{\Psi}^{\mathrm{LM}}_0(2L) = \tilde{\Psi}^{\mathrm{LM}}_0(L, L)$. By applying the inverse of the partial particle-hole transformation to both the wave functions, we map them onto $\Psi_0(N_A - L, L)$ and $\Psi^{\mathrm{LM}}_0(N_A - L, L)$, which are the ground state of the positive-U Hubbard Hamiltonian and the Lieb–Mattis Hamiltonian in the same subspace $V(N_A - L, L)$, respectively, and obtain

$$\langle \Psi_0(N_A - L, L) \,|\, \Psi^{\mathrm{LM}}_0(N_A - L, L)\rangle \neq 0. \tag{70}$$

Consequently, these states must have the same spin number S. On the other hand, as shown in Theorem 4.2, the spin of the ground state $\Psi^{\mathrm{LM}}_0(N_A - L, L) \equiv \Psi^{\mathrm{LM}}_0(M = N_A/2 - L)$ can be directly calculated. Therefore, by repeating the proof of Theorem 4.2, we reach the conclusion of Theorem 5.2. ▌

As another application of Theorem 5.1, we shall now prove Theorem 3.1 for the negative-U Hubbard model. More precisely, we show

Theorem 5.3. For any local operator $\hat{K}_\uparrow$, inequality

$$\langle\tilde{\Psi}_0(2L)|\,\hat{K}_\uparrow\overline{\theta(\hat{K}_\uparrow)}\,|\tilde{\Psi}_0(2L)\rangle = \langle\tilde{\Psi}_0(2L)|\,\hat{K}_\uparrow\overline{\hat{K}_\downarrow}\,|\tilde{\Psi}_0(2L)\rangle \geqslant 0 \tag{71}$$

holds for the ground state $\tilde{\Psi}_0(2L)$ of the negative-U Hubbard Hamiltonian in each subspace $V(2L)$ with $0 \leqslant L \leqslant N_A$.

Proof. To establish Theorem 5.3, we shall follow the proof of Theorem 1 in our paper.[34] Substituting the wave function of $\tilde{\Psi}_0(L, L)$ into the right-hand side of Eq. (71), we obtain

$$\langle\tilde{\Psi}_0(2L)|\,\hat{K}_\uparrow\overline{\hat{K}_\downarrow}\,|\tilde{\Psi}_0(2L)\rangle = \sum_{\alpha,\,\beta}\sum_{\gamma,\,\delta}\bar{W}_{\gamma\delta}W_{\alpha\beta}\langle\psi_\gamma^\uparrow|\,\hat{K}_\uparrow\,|\psi_\alpha^\uparrow\rangle\langle\psi_\delta^\downarrow|\,\overline{\hat{K}_\downarrow}\,|\psi_\beta^\downarrow\rangle. \tag{72}$$

Notice that the vectors $\{\psi_\mu^\sigma\}$ are real by their definition (See Eq. (59)). Therefore, we have

$$\langle\psi_\delta^\downarrow|\,\overline{\hat{K}_\downarrow}\,|\psi_\beta^\downarrow\rangle = \overline{\langle\psi_\delta^\downarrow|\,\hat{K}_\downarrow\,|\psi_\beta^\downarrow\rangle} = \langle\psi_\beta^\downarrow|\,\hat{K}_\downarrow^\dagger\,|\psi_\delta^\downarrow\rangle. \tag{73}$$

It enables us to rewrite Eq. (72) into

$$\langle\tilde{\Psi}_0(2L)|\,\hat{K}_\uparrow\overline{\hat{K}_\downarrow}\,|\tilde{\Psi}_0(2L)\rangle = \mathrm{Tr}(\mathscr{W}^\dagger\mathscr{K}\mathscr{W}\mathscr{K}^\dagger) = \mathrm{Tr}(\mathscr{W}\mathscr{K}\mathscr{W}\mathscr{K}^\dagger), \tag{74}$$

where $\mathscr{K}$ is the matrix of the operator $\hat{K}$ in terms of the basis vectors $\{\psi_\mu^\sigma\}$.

On the other hand, since the coefficient matrix $\mathscr{W}$ of $\tilde{\Psi}_0(2L)$ is positive definite by Theorem 5.1, its square root $\sqrt{\mathscr{W}}$ is well defined. Therefore, the right-hand side of the above equation can be further rewritten as

$$\mathrm{Tr}(\mathscr{W}\mathscr{K}\mathscr{W}\mathscr{K}^\dagger) = \mathrm{Tr}[(\sqrt{\mathscr{W}}\,\mathscr{K}\,\sqrt{\mathscr{W}})(\sqrt{\mathscr{W}}\,\mathscr{K}\,\sqrt{\mathscr{W}})^\dagger], \tag{75}$$

which is certainly a nonnegative quantity. ∎

Theorem 5.3 can be thought of as a special case of Theorem 3.1 at temperature $T = 0$. In fact, its proof demands more strict conditions on the Hubbard Hamiltonian. For instance, in establishing the positive definiteness of the coefficient matrix $\mathscr{W}$ of $\tilde{\Psi}_0(2L)$, we used implicitly the condition that the Coulomb repulsion $U > 0$ at each site $\mathbf{i} \in \Lambda$. However, to prove Theorem 3.1 at nonzero temperature, such conditions are not necessary, as we shall show in Section 7 (See the proof of Lemma 7.1).

Theorem 5.3 was later used to explore the correlation functions in the ground states of the itinerant electron models.[34–36] First, by applying this theorem, we proved the following theorem on the pairing correlation function of the negative-U Hubbard model.[34]

Theorem 5.4. The on-site pairing correlation of electrons in the ground state $\tilde{\Psi}_0(2L)$ of the negative-U Hubbard model on an arbitrary (not necessarily bipartite) lattice is nonnegative. More precisely, inequality

$$\langle\tilde{\Psi}_0(2L)|\,(\hat{C}_{\mathbf{h}\uparrow}^\dagger\hat{C}_{\mathbf{h}\downarrow}^\dagger)(\hat{C}_{\mathbf{k}\downarrow}\hat{C}_{\mathbf{k}\uparrow})\,|\tilde{\Psi}_0(2L)\rangle \geqslant 0 \tag{76}$$

holds for any pair of lattice sites $\mathbf{h}$ and $\mathbf{k}$.

Proof. The above correlation function can be rewritten as

$$\langle\tilde{\Psi}_0(2L)|\,(\hat{C}^\dagger_{\mathbf{h}\uparrow}\hat{C}^\dagger_{\mathbf{h}\downarrow})(\hat{C}_{\mathbf{k}\downarrow}\hat{C}_{\mathbf{k}\uparrow})\,|\tilde{\Psi}_0(2L)\rangle$$
$$= \langle\tilde{\Psi}_0(2L)|\,(\hat{C}^\dagger_{\mathbf{h}\uparrow}\hat{C}_{\mathbf{k}\uparrow})(\hat{C}^\dagger_{\mathbf{h}\downarrow}\hat{C}_{\mathbf{k}\downarrow})\,|\tilde{\Psi}_0(2L)\rangle. \tag{77}$$

Let $\hat{K}_\uparrow = \hat{C}^\dagger_{\mathbf{h}\uparrow}\hat{C}_{\mathbf{k}\uparrow}$ and $\hat{K}_\downarrow = \hat{C}^\dagger_{\mathbf{h}\downarrow}\hat{C}_{\mathbf{k}\downarrow}$. Then, the right-hand side of this equation has the form of $\langle\tilde{\Psi}_0(2L)|\,\hat{K}_\uparrow\overline{\hat{K}_\downarrow}\,|\tilde{\Psi}_0(2L)\rangle$. Therefore, by Theorem 5.3, it is nonnegative. ∎

In physics, the operator $\hat{C}^\dagger_{\mathbf{i}\uparrow}\hat{C}^\dagger_{\mathbf{i}\downarrow}$ represents the creation operator of an on-site Cooper pair of electrons at site $\mathbf{i}$. Therefore, the correlation function of Theorem 5.4 characterizes the superconducting off-diagonal order in the ground state $\tilde{\Psi}_0(2L)$ (see ref. 62 for the definition of the off-diagonal correlation function in a fermion system), if we take the negative-U Hubbard model as a phenomenological model of superconductivity.[63] Theorem 5.4 actually tells us that, for any unimodular complex function $f(\mathbf{i})$ on lattice Λ, inequality

$$\frac{1}{N_\Lambda}\sum_{\mathbf{h},\,\mathbf{k}}\langle\tilde{\Psi}_0(2L)|\,\hat{C}^\dagger_{\mathbf{h}\uparrow}\hat{C}^\dagger_{\mathbf{h}\downarrow}\hat{C}_{\mathbf{k}\downarrow}\hat{C}_{\mathbf{k}\uparrow}\,|\tilde{\Psi}_0(2L)\rangle$$
$$\geqslant \frac{1}{N_\Lambda}\sum_{\mathbf{h},\,\mathbf{k}}\overline{f(\mathbf{h})}\,f(\mathbf{k})\langle\tilde{\Psi}_0(2L)|\,\hat{C}^\dagger_{\mathbf{h}\uparrow}\hat{C}^\dagger_{\mathbf{h}\downarrow}\hat{C}_{\mathbf{k}\downarrow}\hat{C}_{\mathbf{k}\uparrow}\,|\tilde{\Psi}_0(2L)\rangle \tag{78}$$

must hold. Therefore, in the ground state of the negative-U Hubbard model, the on-site Cooper pair correlation has maximum at momentum $\mathbf{p}=0$. This conclusion supports the intuitive picture of the tightly-bound electron pairs behaving like hard-core bosons in the negative-U Hubbard model.[63]

Another implication of Theorem 5.4 was pointed out by Professor C. N. Yang in his referee report to ref. 34: Under the inverse transformation of $\tilde{U}_H$, $\tilde{\Psi}_0(2L)$ is mapped onto $\Psi_0(N_\Lambda - L, L)$, the ground state of the original Hubbard Hamiltonian in the subspace $V(N_\Lambda - L, L)$. In the meantime, the on-site pairing operator $\hat{C}^\dagger_{\mathbf{i}\uparrow}\hat{C}^\dagger_{\mathbf{i}\downarrow}$ (resp. $\hat{C}_{\mathbf{i}\downarrow}\hat{C}_{\mathbf{i}\uparrow}$) is transformed into operator $\epsilon(\mathbf{i})\,\hat{C}_{\mathbf{i}\uparrow}\hat{C}^\dagger_{\mathbf{i}\downarrow} \equiv -\epsilon(\mathbf{i})\,\hat{S}_{\mathbf{i}-}$. (resp. $\epsilon(\mathbf{i})\,\hat{C}_{\mathbf{i}\downarrow}\hat{C}^\dagger_{\mathbf{i}\uparrow} \equiv -\epsilon(\mathbf{i})\,\hat{S}_{\mathbf{i}+}$). Therefore, Eq. (76) becomes

$$\langle\tilde{\Psi}_0(2L)|\,\tilde{U}^\dagger_H\tilde{U}_H(\hat{C}^\dagger_{\mathbf{h}\uparrow}\hat{C}^\dagger_{\mathbf{h}\downarrow})\,\tilde{U}^\dagger_H\tilde{U}_H(\hat{C}_{\mathbf{k}\downarrow}\hat{C}_{\mathbf{k}\uparrow})\,\tilde{U}^\dagger_H\tilde{U}_H\,|\tilde{\Psi}_0(2L)\rangle$$
$$= \epsilon(\mathbf{h})\,\epsilon(\mathbf{k})\langle\Psi_0(N_\Lambda - L, L)|\,\hat{S}_{\mathbf{h}-}\hat{S}_{\mathbf{k}+}\,|\Psi_0(N_\Lambda - L, L)\rangle \geqslant 0. \tag{79}$$

Formally, this inequality is identical to inequality (49) and hence, implies that the transverse spin correlation in the ground state of the Hubbard model in each half-filled subspace $V(N_A - L, L)$ is antiferromagnetic. It leads to the following result.[36]

Theorem 5.5. The global ground state of the half-filled Hubbard model on a bipartite lattice has both the ferromagnetic and the antiferromagnetic long-range orders, if n_A, the number of sites belonging to sublattice A in each unit cell, is not equal to n_B.

Proof. We proved first this theorem for the half-filled Hubbard model in ref. 36 and then, extended it to the antiferromagnetic Heisenberg model.[53] Therefore, the proofs of this theorem and Theorem 4.3 in Section 4 are similar. We shall not repeat it here. In fact, the main difference between their proofs is in the ways to establish inequalities (49) and (79), as discussed above. ▌

The systems discussed in Theorem 5.5 have been actually realized in experiments. For example, the organic conjugated polymers shown in Fig. 3 were manufactured by several groups[64] a decade ago. Their properties are investigated by many groups.[65–69] In fact, ESR and the magnetic susceptibility measurements showed evidence of the ferrimagnetic long-range order between unpaired π electrons in these systems. Our rigorous result indicates that the electronic states of these polymers can be theoretically described by the half-filled Hubbard model. However, it is also worthwhile to point out that, in the Hubbard Hamiltonian (1), both parameters t and U are chosen to be site-independent for simplicity. However, in the real materials such as the organic polymers shown in Fig. 3, they are generally site-dependent real constants. Fortunately, in these cases, one can easily check that all the theorems established in this section still hold as long as the Coulomb interaction intensity $U_{\mathbf{i}} > 0$ is nonzero at any site $\mathbf{i} \in \Lambda$. Therefore, the ferrimagnetic long-range order in these systems is very robust.

Theorem 5.1 has been extended to the half-filled periodic Anderson model[25] and the Kondo lattice model.[26] As a result, Eq. (79) can be easily proven for these strongly correlated electron models and the spin correlation in their ground states are also antiferromagnetic.[35] Interestingly, the constraint condition (24) on the wave functions of the transformed Hamiltonian $\tilde{H}_K$ does not cause any technical difficulty in handling the system with an even number of electrons. Instead, as shown in section III, it helps actually to write $\tilde{H}_K$ into a spin-reflection positive form.

6. APPLICATION OF THE DYSON–LIEB–SIMON THEOREM TO THE STRONGLY CORRELATED ELECTRON SYSTEMS

In Section 5, we studied the properties of the strongly correlated electron models with an even number of particles. In the following, we shall consider the opposite case: The same models with an odd number of electrons.

In this case, although the hopping operators $\hat{T}_\uparrow$ and $\hat{T}_\downarrow$ have the same form, they are actually not isomorphic to each other. This is due to fact that the spaces $V_\uparrow$ and $V_\downarrow$, in which $\hat{T}_\uparrow$ and $\hat{T}_\downarrow$ act respectively, have different dimensions. To see this point, let us assume that there are $2L+1$ electrons in the system and denote the ground state of the Hubbard Hamiltonian by $\Psi_0(2L+1)$. Obviously, this state has spin $S \geqslant 1/2$ and one of its representatives has $S_z = (N_\uparrow - N_\downarrow)/2 = 1/2$. In other words, it is a state in the subspace $V(L+1, L)$. On the other hand, in terms of the quasi-fermion operators, $V(L+1, L)$ can be written as $V_\uparrow(L+1) \otimes V_\downarrow(L)$ and a natural basis of $V_\sigma(J)$ is given by

$$\psi_\alpha^\sigma \equiv \hat{C}_{i_1\sigma}^\dagger \cdots \hat{C}_{i_J\sigma}^\dagger |0\rangle, \tag{80}$$

where $J = L+1$ for $\sigma = \uparrow$ and $J = L$ for $\sigma = \downarrow$. Therefore, $V_\uparrow(L+1)$ has dimension $D_\uparrow = C_{N_\Lambda}^{L+1}$ while the dimension of $V_\downarrow(L)$ is $C_{N_\Lambda}^{L}$. In general, they are not equal. As a result, $\hat{T}_\downarrow$ is not isomorphic to $\overline{\theta \hat{T}_\uparrow}$ since the latter acts in $V_\downarrow(L+1)$ rather than $V_\downarrow(L)$.

Fortunately, although the spin-reflection positivity is violated in this case, the Dyson–Lieb–Simon theorem (Theorem 3.2) still applies. It enables us to prove the following inequality for the negative-U Hubbard model.[70]

Theorem 6.1. Let Λ be an arbitrary (not necessarily bipartite) finite lattice. Then, for any integer $0 < L < N_\Lambda$, the ground state energies of the negative-U Hubbard Hamiltonian in subspaces $V(2L), V(2L+1)$ and $V(2L+2)$ satisfy inequality

$$E_0(2L+1) > \tfrac{1}{2} E_0(2L) + \tfrac{1}{2} E_0(2L+2). \tag{81}$$

Proof. In terms of the basis vectors defined in Eq. (80), the wave function $\tilde{\Psi}_0(2L+1)$ can be written as

$$\tilde{\Psi}_0(2L+1) = \sum_{\alpha,\beta} W_{\alpha\beta} \psi_\alpha^\uparrow \otimes \psi_\beta^\downarrow. \tag{82}$$

However, unlike the previous case studied in Section 5, the coefficient matrix $\mathscr{W} = (W_{\alpha\beta})$ in Eq. (82) is an $C_{N_\Lambda}^{L+1} \times C_{N_\Lambda}^{L}$ matrix, which is not square.

To deal with such a matrix, we employ the singular polar decomposition theorem in matrix theory.

Lemma 6.1 (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 R_1, and an $m \times n$ matrix V_1 such that

$$A = U_1 R_1 V_1. \tag{83}$$

Moreover, the 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 R_2, and an $n \times n$ unitary matrix U_2 such that

$$A = V_2 R_2 U_2 \tag{84}$$

with the columns of V_2 being orthonormal.

The proof of this lemma can be found in any standard textbook on matrix theory.[71] For the reader's convenience, we shall give a simplified proof of it in the appendix of this paper.

For definiteness, let us assume that the coefficient matrix $\mathscr{W}$ has more rows than columns. In this case, the singular polar decomposition theorem tells us that there are three matrices $U_{\mathscr{W}}$, $V_{\mathscr{W}}$, and $R_{\mathscr{W}}$ such that

$$\mathscr{W} = V_{\mathscr{W}} R_{\mathscr{W}} U_{\mathscr{W}}, \tag{85}$$

where $V_{\mathscr{W}}$ is an $C_{N_A}^{L+1} \times C_{N_A}^{L}$ matrix with orthonormal columns and $U_{\mathscr{W}}$ is an $C_{N_A}^{L} \times C_{N_A}^{L}$ unitary matrix. $R_{\mathscr{W}}$ is an $C_{N_A}^{L} \times C_{N_A}^{L}$ diagonal matrix with elements $r_\gamma \geqslant 0$. Consequently, the ground state wave function $\tilde{\Psi}_0(2L+1)$ can be rewritten as

$$\begin{aligned} \tilde{\Psi}_0(2L+1) &= \sum_{\alpha,\beta} W_{\alpha\beta} \psi_\alpha^\uparrow \otimes \psi_\beta^\downarrow = \sum_{\alpha,\beta} (V_{\mathscr{W}} R_{\mathscr{W}} U_{\mathscr{W}})_{\alpha\beta} \psi_\alpha^\uparrow \otimes \psi_\beta^\downarrow \\ &= \sum_{\gamma=1}^{D} r_\gamma \xi_\gamma^\uparrow \otimes \phi_\gamma^\downarrow \end{aligned} \tag{86}$$

with $D = C_{N_A}^{L}$. In Eq. (86), $\xi_\gamma^\uparrow$ and $\phi_\gamma^\downarrow$ are defined by

$$\xi_\gamma^\uparrow = \sum_\alpha (V_{\mathscr{W}})_{\alpha\gamma} \psi_\alpha^\uparrow, \qquad \phi_\gamma^\downarrow = \sum_\beta (U_{\mathscr{W}})_{\gamma\beta} \psi_\beta^\downarrow. \tag{87}$$

On the other hand, since $U_{\mathscr{W}}$ is unitary and the columns of $V_{\mathscr{W}}$ are orthonormal, the new sets of vectors $\{\xi_\gamma^\uparrow\}$ and $\{\phi_\gamma^\downarrow\}$ are orthonormal, too. More

importantly, these new vectors $\{\xi_\gamma^\uparrow\}$ and $\{\phi_\gamma^\downarrow\}$ are also the eigenvectors of the particle number operators $\hat{N}_\uparrow$ and $\hat{N}_\downarrow$ with eigenvalues of $L+1$ and L, respectively. The normalization condition of $\tilde{\Psi}_0(2L+1)$ now reads

$$\langle\tilde{\Psi}_0(2L+1)\,|\,\tilde{\Psi}_0(2L+1)\rangle = \mathrm{Tr}\,\mathscr{W}^\dagger\mathscr{W} = \sum_{\gamma=1}^{D} r_\gamma^2 = 1. \tag{88}$$

With the simple form (86) of $\tilde{\Psi}_0(2L+1)$, its energy $E_0(2L+1)$ is given by

$$\begin{aligned} E_0(2L+1) &= \langle\tilde{\Psi}_0(2L+1)|\,\tilde{H}_H\,|\tilde{\Psi}_0(2L+1)\rangle \\ &= \sum_{\gamma=1}^{D} r_\gamma^2[\langle\xi_\gamma^\uparrow|\,\hat{T}_\uparrow\,|\xi_\gamma^\uparrow\rangle + \langle\phi_\gamma^\downarrow|\,\hat{T}_\downarrow\,|\phi_\gamma^\downarrow\rangle] \\ &\quad - U\sum_{\mathbf{i}\in\Lambda}\left(\sum_{\gamma_1,\gamma_2} r_{\gamma_1}r_{\gamma_2}\langle\xi_{\gamma_2}^\uparrow|\,\hat{n}_{\mathbf{i}\uparrow} - \tfrac{1}{2}\,|\xi_{\gamma_1}^\uparrow\rangle\langle\phi_{\gamma_2}^\downarrow|\,\hat{n}_{\mathbf{i}\downarrow} - \tfrac{1}{2}\,|\phi_{\gamma_1}^\downarrow\rangle\right). \end{aligned} \tag{89}$$

By dropping the spin indices in Eq. (89) and applying inequality $|ab| \leqslant \frac{1}{2}(|a|^2+|b|^2)$ to each term in the last line, we obtain

$$\begin{aligned} E_0(2L+1) \geqslant{}& \frac{1}{2}\sum_{\gamma=1}^{D} r_\gamma^2[\langle\xi_\gamma|\,\hat{T}\,|\xi_\gamma\rangle + \langle\xi_\gamma|\,\hat{T}\,|\xi_\gamma\rangle] \\ &+ \frac{1}{2}\sum_{\gamma=1}^{D} r_\gamma^2[\langle\phi_\gamma|\,\hat{T}\,|\phi_\gamma\rangle + \langle\phi_\gamma|\,\hat{T}\,|\phi_\gamma\rangle] \\ &- \frac{U}{2}\sum_{\mathbf{i}\in\Lambda}\left(\sum_{\gamma_1,\gamma_2} r_{\gamma_1}r_{\gamma_2}\,\langle\xi_{\gamma_2}|\,\hat{n}_{\mathbf{i}} - \frac{1}{2}\,|\xi_{\gamma_1}\rangle\overline{\langle\xi_{\gamma_2}|\,\hat{n}_{\mathbf{i}} - \frac{1}{2}\,|\xi_{\gamma_1}\rangle}\right) \\ &- \frac{U}{2}\sum_{\mathbf{i}\in\Lambda}\left(\sum_{\gamma_1,\gamma_2} r_{\gamma_1}r_{\gamma_2}\langle\phi_{\gamma_2}|\,\hat{n}_{\mathbf{i}} - \frac{1}{2}\,|\phi_{\gamma_1}\rangle\overline{\langle\phi_{\gamma_2}|\,\hat{n}_{\mathbf{i}} - \frac{1}{2}\,|\phi_{\gamma_1}\rangle}\right). \end{aligned} \tag{90}$$

In the above derivation, inequality $r_\gamma \geqslant 0$ is used.

The right-hand side of Eq. (90) can be further simplified by introducing new wave functions

$$\Psi_1(2L+2) = \sum_{\gamma=1}^{D} r_\gamma\xi_\gamma^\uparrow \otimes \bar{\xi}_\gamma^\downarrow, \qquad \Psi_2(2L) = \sum_{\gamma=1}^{D} r_\gamma\phi_\gamma^\uparrow \otimes \bar{\phi}_\gamma^\downarrow, \tag{91}$$

where $\bar{\xi}_\gamma^\sigma$ and $\bar{\phi}_\gamma^\sigma$ are the complex conjugates of ξ_γ^σ and ϕ_γ^σ, respectively. In terms of Ψ_1 and Ψ_2, inequality (90) is reduced to

$$E_0(2L+1) \geqslant \tfrac{1}{2}\langle\Psi_1(2L+2)|\,\tilde{H}_H\,|\Psi_1(2L+2)\rangle + \tfrac{1}{2}\langle\Psi_2(2L)|\,\tilde{H}_H\,|\Psi_2(2L)\rangle. \tag{92}$$

Notice that, by their constructions, $\Psi_1(2L+2)$ and $\Psi_2(2L)$ are actually wave functions in the subspaces $V(2L+2)$ and $V(2L)$, respectively. Therefore, by the variational principle, inequality (92) implies that

$$E_0(2L+1) \geqslant \tfrac{1}{2} E_0(2L+2) + \tfrac{1}{2} E_0(2L). \tag{93}$$

To finish the proof of Theorem 6.1, we still need to show that inequality (93) is actually strict. For this purpose, we replace inequality $|ab| \leqslant \frac{1}{2}|a|^2 + \frac{1}{2}|b|^2$ with identity

$$a\bar{b} + \bar{a}b = |a|^2 + |b|^2 - |a-b|^2. \tag{94}$$

Consequently, we are able to rewrite Eq. (90) into

$$E_0(2L+1) = \frac{1}{2}\langle \Psi_1(2L+2)|\, \tilde{H}_H\, |\Psi_1(2L+2)\rangle + \frac{1}{2}\langle \Psi_2(2L)|\, \tilde{H}_H\, |\Psi_2(2L)\rangle$$
$$+ \frac{U}{2} \sum_{\mathbf{i}\in\Lambda} \sum_{\gamma_1,\gamma_2} r_{\gamma_1} r_{\gamma_2} \left| \langle \xi_{\gamma_2}|\, \hat{n}_{\mathbf{i}\uparrow} - \frac{1}{2}|\xi_{\gamma_1}\rangle - \overline{\langle \phi_{\gamma_2}|\, \hat{n}_{\mathbf{i}\downarrow} - \frac{1}{2}|\phi_{\gamma_1}\rangle} \right|^2. \tag{95}$$

Now, by applying the variational principle, we obtain an improved inequality

$$\begin{aligned} & E_0(2L+1) - \frac{1}{2} E_0(2L+2) - \frac{1}{2} E_0(2L) \\ & \geqslant \frac{U}{2} \sum_{\mathbf{i}\in\Lambda} \sum_{\gamma_1,\gamma_2} r_{\gamma_1} r_{\gamma_2} \left| \langle \xi_{\gamma_2}|\, \hat{n}_{\mathbf{i}} - \frac{1}{2}|\xi_{\gamma_1}\rangle - \overline{\langle \phi_{\gamma_2}|\, \hat{n}_{\mathbf{i}} - \frac{1}{2}|\phi_{\gamma_1}\rangle} \right|^2 \\ & \geqslant \frac{U}{2} \sum_{\mathbf{i}\in\Lambda} \sum_{\gamma} r_{\gamma}^2 \left(\langle \xi_{\gamma}|\, \hat{n}_{\mathbf{i}} - \frac{1}{2}|\xi_{\gamma}\rangle - \langle \phi_{\gamma}|\, \hat{n}_{\mathbf{i}} - \frac{1}{2}|\phi_{\gamma}\rangle \right)^2. \end{aligned} \tag{96}$$

Furthermore, by applying the Cauchy–Schwartz inequality, we find that the right-hand side of Eq. (96) is bounded below by

$$\begin{aligned} & \frac{U}{2} \sum_{\mathbf{i}\in\Lambda} \sum_{\gamma} r_{\gamma}^2 \left(\langle \xi_{\gamma}|\, \hat{n}_{\mathbf{i}} - \frac{1}{2}|\xi_{\gamma}\rangle - \langle \phi_{\gamma}|\, \hat{n}_{\mathbf{i}} - \frac{1}{2}|\phi_{\gamma}\rangle \right)^2 \\ & \geqslant \frac{U}{2} \left[\sum_{\mathbf{i}\in\Lambda} \sum_{\gamma} r_{\gamma}^2 \right]^{-1} \left[\sum_{\mathbf{i}\in\Lambda} \sum_{\gamma} r_{\gamma}^2 \left(\langle \xi_{\gamma}|\, \hat{n}_{\mathbf{i}} - \frac{1}{2}|\xi_{\gamma}\rangle - \langle \phi_{\gamma}|\, \hat{n}_{\mathbf{i}} - \tfrac{1}{2}|\phi_{\gamma}\rangle \right) \right]^2 \\ & = \frac{U}{2N_\Lambda} \langle \Psi_0(2L+1)|\, (\hat{N}_\uparrow - \hat{N}_\downarrow)\, |\Psi_0(2L+1)\rangle^2 = \frac{U}{2N_\Lambda}. \end{aligned} \tag{97}$$

Therefore, we have

$$E_0(2L+1)-\frac{1}{2}E_0(2L+2)-\frac{1}{2}E_0(2L)\geqslant\frac{U}{2N_A}. \tag{98}$$

That ends the proof of Theorem 6.1. ▌

As a special case of the Dyson–Lieb–Simon theorem, the proof of Theorem 6.1 contains all the essential ingredients to establish Theorem 3.2. Mathematically minded readers can find a more abstract proof of the DLS theorem in the appendix of ref. 43.

Theorem 6.1 can be easily extended to the transformed periodic Anderson Hamiltonian $\tilde{H}_A$ without further ado. However, for the Hamiltonian $\tilde{H}_K$, more careful consideration is needed. In particular, we should check whether both the wave functions $\tilde{\Psi}_1(2L+2)$ and $\tilde{\Psi}_2(2L)$ constructed in Eq. (91) satisfy the constraint condition (24).

For this purpose, we first write the ground-state wave function $\tilde{\Psi}_0(2L+1)$ of $\tilde{H}_K$ as a summation of "partial" wave functions

$$\tilde{\Psi}_0(2L+1)=\sum_{\alpha,\beta}^{(1)} W_{\alpha\beta}^{(1)}\psi_\alpha^{(1)\uparrow}\otimes\psi_\beta^{(1)\downarrow}+\cdots+\sum_{\alpha,\beta}^{(k)} W_{\alpha\beta}^{(k)}\psi_\alpha^{(k)\uparrow}\otimes\psi_\beta^{(k)\downarrow}+\cdots. \tag{99}$$

In each partial sum, the distribution of $\hat{F}$-quasifermions is specified and satisfies the constraint condition (24). Therefore, the coefficient matrix $\mathscr{W}$ of the ground-state wave function has the following block diagonal form

$$\mathscr{W}=\mathrm{diag}(\mathscr{W}^{(1)},\ldots,\mathscr{W}^{(k)},\ldots). \tag{100}$$

For definiteness, let us take the submatrix $\mathscr{W}^{(k)}$ for example. Assume that the number of $\hat{F}$-quasifermion pairs in this sector is n_F. Then, in this sector, there are $n_\uparrow^c=L+1-n_F$ up-spin and $n_\downarrow^c=L-n_F$ down-spin itinerant electrons. Consequently, the coefficients of this partial sum can be organized into a $C_{N_A}^{n_\uparrow^c}\times C_{N_A}^{n_\downarrow^c}$ submatrix. By applying the singular polar decomposition theorem to $\mathscr{W}^{(k)}$, we find orthonormal matrices U_k and V_k such that $U_k\mathscr{W}^{(k)}V_k=\mathscr{R}^{(k)}$. Obviously, the new bases of vectors $\{\psi_l^{(k)\uparrow}\}$ and $\{\phi_l^{(k)\downarrow}\}$ constructed according to Eq. (87) have also the same distribution of $\hat{F}$-quasifermions.

Next, we introduce unitary matrices U and V with the same block diagonal form

$$U=\mathrm{diag}(U_1,\ldots,U_k,\ldots),\qquad V=\mathrm{diag}(V_1,\ldots,V_k,\ldots), \tag{101}$$

which gives $\mathscr{R}=U\mathscr{W}V=\mathrm{diag}(\mathscr{R}^{(1)},\ldots,\mathscr{R}^{(k)},\ldots)$. It is easy to check that the trial wave functions $\tilde{\Psi}_1$ and $\tilde{\Psi}_2$ constructed by coefficient matrix $\mathscr{R}$ are subject to the constraint condition (24).

In condensed matter physics, the quantity

$$\Delta_B(L) \equiv E_0(2L+1) - \tfrac{1}{2} E_0(2L) - \tfrac{1}{2} E_0(2L+2) \tag{102}$$

is called the binding energy of electrons. Theorem 6.1 shows that, for the negative-U Hubbard model on a finite lattice, the binding energy of electrons is always nonzero. Consequently, they will be bound into the Cooper pairs. The same method was also used to study the superconducting crossover in the ultrasmall metallic grains.[72] As is well known, the BCS theory gives a very accurate description of superconductivity in large metallic samples.[73] Then, a natural question is whether such a description is still valid as the sample size shrinks to the nanometer scale. Anderson addressed this problem in a paper published in 1959.[74] He argued that, when the average single-particle energy level spacing δ, which is inversely proportional to the volume of a metallic grain, becomes of the order of the BCS gap, superconductivity will disappear. Recently, theoretical interest on this topics is rekindled by the experimental observations of the parity dependent spectroscopic gaps in nanometer-scale Al grains.[75] The important issue is that, in these experiments, the Coulomb charging effects actually allows one to fix the number of electrons in the grain. Consequently, in dealing with these systems, the particle number conservation law must be strictly observed. In other words, the description of superconductivity in ultrasmall metallic grains calls for a canonical ensemble formalism. The interested readers can find a detailed review on the latest numerical and analytical developments in this field in ref. 76. One of the important conclusions is that the superconducting crossover in the metallic grains is actually a smooth process. In our works,[72] based on Theorem 6.1, we studied the parity effect parameter[77] and the pair-mixing correlation function[78] of these superconducting grains. Our rigorous results support the above mentioned conclusion.

Theorem 6.1 can also be applied to establish a general relation between the quasi-particle gap and the spin excitation gap in the strongly correlated electron models. It is summarized in the following theorem.

Theorem 6.2. Define the quasi-particle gap Δ_{QP} and the spin excitation gap Δ_S of the half-filled Hubbard model, the periodic Anderson model, and the Kondo lattice model by

$$\Delta_{QP} \equiv E_0(\tilde{N}+1) + E_0(\tilde{N}-1) - 2E_0(\tilde{N}),$$

$$\Delta_S \equiv E_0(\tilde{N}, S=1) - E_0(\tilde{N}, S=0), \tag{103}$$

where $\tilde{N} = N_\Lambda$ for the Hubbard model and $\tilde{N} = 2N_\Lambda$ for both the periodic Anderson model and the Kondo lattice model. For these models on a simple cubic lattice, Δ_{QP} and Δ_S satisfy inequality

$$\Delta_{QP} \geqslant \Delta_S. \tag{104}$$

Originally, this relation was observed by the numerical calculations on small size samples.[79] Based on Theorem 6.1, we proved it rigorously in ref. 37.

Proof. By applying respectively the inverse of the partial particle-hole transformations $\tilde{U}_H$, $\tilde{U}_A$, and $\tilde{U}_K$ to the "negative coupling" Hamiltonians $\tilde{H}_H$, $\tilde{H}_A$, and $\tilde{H}_K$, we obtain the original Hamiltonians H_H, H_A, and H_K. Here, we are interested in the change of inequality (81) under these transformations, with $2L = \tilde{N}$. In the following, to distinguish the ground-state energies of the "negative coupling" Hamiltonians from their counterparts of the original Hamiltonians, we shall use $\tilde{E}_0$ for the former and and E_0 for the latter.

First, we have identity $\tilde{E}_0(\tilde{N}) = E_0(\tilde{N})$. That is due to fact that, under the unitary partial particle-hole transformation, the global ground states $\tilde{\Psi}_0$ of the negative coupling Hamiltonians are respectively mapped onto Ψ_0, the global ground states of the original Hamiltonians. As discussed in Section 2, these states are in the same half-filled subspace $V(\tilde{N})$ since the strongly correlated electron models possess the particle-hole symmetry at half-filling. Furthermore, by Corollary 5.1 and Theorem 5.2, both $\tilde{\Psi}_0(\tilde{N})$ and $\Psi_0(\tilde{N})$ have spin number $S = 0$ when Λ is a simple cubic lattice. Therefore, we shall denote this global ground state energy by $E_0(\tilde{N}, S = 0)$ in the following.

Next, we show that

$$\tilde{E}_0(\tilde{N}+1) = E_0(\tilde{N}+1) \tag{105}$$

also holds. In fact, since the partial particle-hole transformations only change the particle number $N_\uparrow$ from $\tilde{N}/2+1$ to $\tilde{N}/2-1$ and keep $N_\downarrow$ unchanged, the ground-state energy $\tilde{E}_0(\tilde{N}+1) = \tilde{E}_0(\tilde{N}/2+1, \tilde{N}/2)$ of the "negative coupling" Hamiltonians equals the ground-state energy $E_0(\tilde{N}/2-1, \tilde{N}/2) = E_0(\tilde{N}-1)$ of the original Hamiltonians. Furthermore, by the particle-hole symmetry of these Hamiltonians, we have identity $E_0(\tilde{N}-1) = E_0(\tilde{N}+1)$. Therefore, Eq. (105) holds true.

The change of $\tilde{E}_0(\tilde{N}+2)$ under the partial particle-hole transformations demands a careful thinking. By Corollary 5.1 in Section 5, we know that the ground state $\tilde{\Psi}_0(\tilde{N}+2)$ of the "negative coupling" Hamiltonians

has spin $S=0$. In other words, it is a state in the subspace $V(\tilde{N}/2+1, \tilde{N}/2+1)$. Under the partial particle-hole transformations, this subspace is mapped into $V(\tilde{N}/2-1, \tilde{N}/2+1)$, in which each state has quantum number $S_z=-1/2$. Therefore, $\tilde{\Psi}_0(\tilde{N}+2)$ is mapped onto $\Psi_0(\tilde{N}/2-1, \tilde{N}/2+1)$, the ground state of the original Hamiltonians in this subspace. As shown in Theorem 5.2, this state has spin $S=1/2$ and hence, $\tilde{E}_0(\tilde{N}+2)=E_0(\tilde{N}, S=1)$ holds.

In summary, under the inverse of the partial particle-hole transformations, inequality (81) becomes

$$E_0(\tilde{N}+1) \geqslant \tfrac{1}{2} E_0(\tilde{N}, S=0)+\tfrac{1}{2} E_0(\tilde{N}, S=1). \tag{106}$$

By subtracting the global ground-state energy $E_0(\tilde{N}, S=0)$ from both sides of Eq. (106) and multiplying it by a factor 2, we obtain

$$2[E_0(\tilde{N}+1)-E_0(\tilde{N})] \geqslant E_0(\tilde{N}, S=1)-E_0(\tilde{N}, S=0). \tag{107}$$

Equation (104) is finally proven by substituting identity $E_0(\tilde{N}+1)=E_0(\tilde{N}-1)$ into the left-hand side of Eq. (107). That ends our proof of Theorem 6.2. ▮

A similar relation $\Delta_C \geqslant \Delta_S$ can be also proven for the charged gap $\Delta_C \equiv E_0(\tilde{N}+2)-E_0(\tilde{N})$ and the spin excitation Δ_S of the strongly correlated electron models on a simple cubic lattice. Its detailed proof is given in the second paper of ref. 37.

7. THE SPIN-REFLECTION-POSITIVITY METHOD AT NONZERO TEMPERATURE

In the previous sections, we mainly concentrated on the case of temperature $T=0$. In fact, both Theorems 3.1 and 3.2 were originally proven for the cases of nonzero temperature. In this section, we shall explain briefly how to extend some of the results established in the previous sections to nonzero temperature cases.

In a paper published in 1990,[33] Kubo and Kishi introduced the finite-temperature version of spin-reflection-positivity method and applied it to derive some upper bounds to the spin susceptibility and the on-site pairing susceptibility of the Hubbard model. Their results can be summarized in the following theorem.

Theorem 7.1. Define the Duhamel two-point function by

$$(\hat{A}, \hat{B}) \equiv \int_0^1 dx \langle \exp^{\beta x \hat{H}} \hat{A} \exp^{-\beta x \hat{H}} \hat{B} \rangle_{\hat{H}}. \tag{108}$$

Then, for the negative-U Hubbard Hamiltonian on an arbitrary lattice Λ, its spin susceptibility satisfies inequality

$$(\hat{S}^z_{\mathbf{q}}, \hat{S}^z_{-\mathbf{q}}) \equiv \left(\frac{1}{N_\Lambda} \sum_{\mathbf{i} \in \Lambda} \hat{S}_{\mathbf{i}z} e^{-i\mathbf{q}\cdot\mathbf{i}}, \frac{1}{N_\Lambda} \sum_{\mathbf{i} \in \Lambda} \hat{S}_{\mathbf{i}z} e^{i\mathbf{q}\cdot\mathbf{i}} \right) \leqslant \frac{1}{4\beta |U|}. \tag{109}$$

Moreover, if lattice Λ is bipartite, the on-site pairing susceptibility function

$$(\hat{P}_{\mathbf{q}}, \hat{P}_{-\mathbf{q}}) \equiv \left(\frac{1}{\sqrt{N_\Lambda}} \sum_{\mathbf{i} \in \Lambda} \hat{C}^\dagger_{\mathbf{i}\uparrow} \hat{C}^\dagger_{\mathbf{i}\downarrow} \exp^{-i\mathbf{q}\cdot\mathbf{i}}, \frac{1}{\sqrt{N_\Lambda}} \sum_{\mathbf{i} \in \Lambda} \hat{C}_{\mathbf{i}\downarrow} \hat{C}_{\mathbf{i}\uparrow} e^{i\mathbf{q}\cdot\mathbf{i}} \right) \tag{110}$$

of the half-filled Hubbard model satisfies the same inequality.

The general properties of the Duhamel function and, in particular, its relation to the more familiar symmetric correlation function $\langle \hat{A}\hat{B} + \hat{B}\hat{A} \rangle_{\hat{H}}$ are discussed in ref. 46.

Theorem 7.1 implies the absence of the magnetic order in the negative-U Hubbard model and the on-site pairing off-diagonal order in the half-filled Hubbard model. Since its proof demands some technical preparations, we shall not discuss it here. Instead, we consider another example whose proof requires little more than what we have explained above and can be thought of as an application of Theorem 3.1.

Theorem 7.2. Take any pair of lattice sites $\mathbf{h}$ and $\mathbf{k}$. Then, at $T \neq 0$, the transverse spin correlation functions of the Hubbard model, the periodic Anderson model, and the Kondo lattice model on a bipartite lattice are antiferromagnetic. More precisely, the following inequality

$$\langle \hat{S}_{\mathbf{h}-} \hat{S}_{\mathbf{k}+} \rangle_{\hat{H}} \begin{cases} \geqslant 0, & \text{if both } \mathbf{h} \text{ and } \mathbf{k} \in A \text{ or } B; \\ \leqslant 0, & \text{otherwise.} \end{cases} \tag{111}$$

holds for these models at half-filling.

In Section 5, we proved inequality (111) for the ground states of these models at half-filling. Here, by using the finite-temperature version of the spin-reflection-positivity method, we re-establish it at nonzero temperature. Therefore, the antiferromagnetic spin correlation is always dominant in these models, even if their magnetic long-range orders have been destroyed by thermal fluctuations at sufficiently high temperature.

Proof of Theorem 7.2. We take the Hubbard model for example. Since $Z_{\hat{H}} \equiv \mathrm{Tr}\, e^{-\beta \hat{H}}$ is a positive quantity, Theorem 7.2 is proven if we can show that inequality (111) is satisfied by the numerator $\mathrm{Tr}_{V(N_\Lambda)}[\hat{S}_{\mathbf{h}-} \hat{S}_{\mathbf{k}+} \exp(-\beta H_H)]$. Furthermore, because the subspace $V(N_\Lambda)$ is

a direct sum of subspaces $\{V(N_\Lambda - L, L)\}$, this task is further reduced to establish inequality (111) for each trace $\mathrm{Tr}_{V(N_\Lambda - L, L)}[\hat{S}_{\mathbf{h}-}\hat{S}_{\mathbf{k}+}\exp(-\beta H_H)]$.

Under the partial particle-hole transformation, the Hubbard Hamiltonian is mapped into the negative-U Hubbard Hamiltonian. In the meantime, $V(N_\Lambda - L, L)$ is mapped into the subspace $V(L, L)$ and the spin operators $\hat{S}_{\mathbf{h}-}$ and $\hat{S}_{\mathbf{k}+}$ become the pairing operators $\epsilon(\mathbf{h})\,\hat{C}^\dagger_{\mathbf{h}\downarrow}\hat{C}^\dagger_{\mathbf{h}\uparrow}$ and $\epsilon(\mathbf{k})\,\hat{C}_{\mathbf{k}\uparrow}\hat{C}_{\mathbf{k}\downarrow}$, respectively. Therefore, Theorem 7.2 is actually a corollary of the following lemma.

Lemma 7.1. At $T \neq 0$, the on-site Cooper-pairing correlation function of the *negative-U* Hubbard Hamiltonian in any symmetric subspace $V(L, L)$ with $0 \leqslant L \leqslant N_\Lambda$ is nonnegative, i.e., inequality

$$\mathrm{Tr}_{V(L,L)}(\hat{C}^\dagger_{\mathbf{h}\downarrow}\hat{C}^\dagger_{\mathbf{h}\uparrow}\hat{C}_{\mathbf{k}\uparrow}\hat{C}_{\mathbf{k}\downarrow}e^{-\beta\tilde{H}_H}) \geqslant 0 \tag{112}$$

holds for any pair of lattice sites $\mathbf{h}$ and $\mathbf{k}$.

In Section 5, we proved inequality (112) for the ground state of the negative-U Hubbard model. We would like to emphasize that, in the proofs of Theorems 5.3 and 5.4, the positive definiteness of the coefficient matrix $\mathscr{W}$ of the ground-state wave function $\tilde{\Psi}_0(2L)$ plays a pivotal role. However, as temperature T increases, one expects that more and more excited states of the system are activated. On the other hand, these states must have indefinite coefficient matrices because they are orthogonal to the ground state. Therefore, it is reasonable to question the validity of inequality (112) when temperature is sufficiently high. Lemma 7.1 tells us that the influence of the ground state in the negative-U Hubbard model is actually robust against thermal fluctuations. In other words, the dominance of the on-site pairing correlation at $\mathbf{q} = 0$ is protected by the spin-reflection positivity of the Hamiltonian at nonzero temperature.

Now, let us turn to the proof of Lemma 7.1.

Proof of Lemma 7.1. First, we rewrite the trace in Eq. (112) as

$$\begin{aligned}
&\mathrm{Tr}_{V(L,L)}[\hat{C}^\dagger_{\mathbf{h}\downarrow}\hat{C}^\dagger_{\mathbf{h}\uparrow}\hat{C}_{\mathbf{k}\uparrow}\hat{C}_{\mathbf{k}\downarrow}\exp(-\beta\tilde{H}_H)] \\
&\quad = \mathrm{Tr}_{V(L,L)}\Bigg[(\hat{C}^\dagger_{\mathbf{h}\uparrow}\hat{C}_{\mathbf{k}\uparrow})(\hat{C}^\dagger_{\mathbf{h}\downarrow}\hat{C}_{\mathbf{k}\downarrow})\exp\Bigg(-\beta\Bigg(\hat{T}_\uparrow - \frac{U}{2}\sum_{\mathbf{i}}\left(\hat{n}_{\mathbf{i}\uparrow} - \frac{1}{2}\right)^2 \\
&\qquad + \hat{T}_\downarrow - \frac{U}{2}\sum_{\mathbf{i}}\left(\hat{n}_{\mathbf{i}\downarrow} - \frac{1}{2}\right)^2\Bigg) - \frac{\beta U}{2}\sum_{\mathbf{i}\in\Lambda}(\hat{n}_{\mathbf{i}\uparrow} - \hat{n}_{\mathbf{i}\downarrow})^2\Bigg)\Bigg],
\end{aligned} \tag{113}$$

where $\hat{T}_\sigma$ represents the hopping term of the fermions with spin σ. In the derivation of Eq. (113), we used identity $\hat{n}_{\mathbf{i}\sigma}^2 = \hat{n}_{\mathbf{i}\sigma}$. To go further, we need to decouple operators $\hat{n}_{\mathbf{i}\uparrow}$ from $\hat{n}_{\mathbf{i}\downarrow}$ in the interaction terms. It can be achieved in two steps. First, by using the Trotter formula,[80] we decompose $\exp(-\beta\tilde{H}_H)$ into a product of exponential operators

$$\exp(-\beta\tilde{H}_H) = \lim_{M\to\infty}\left[\exp(-\beta\hat{K}_\uparrow/M)\exp(-\beta\hat{K}_\downarrow/M) \times\exp\left(-\frac{\beta U}{2M}\sum_{\mathbf{i}\in\Lambda}(\hat{n}_{\mathbf{i}\uparrow}-\hat{n}_{\mathbf{i}\downarrow})^2\right)\right]^M, \tag{114}$$

where operator $\hat{K}_\sigma$ stands for $\hat{T}_\sigma - (U/2)\sum_{\mathbf{i}\in\Lambda}(\hat{n}_{\mathbf{i}\sigma}-1/2)^2$. Then, we apply the well-known Hubbard–Stratonovich transformation

$$\exp(-\hat{A}^2) = \frac{1}{2\sqrt{\pi}}\int_{-\infty}^{\infty} dk\,\exp(-k^2/4 + ik\hat{A}) \tag{115}$$

to each exponential operator containing interaction terms. A detailed discussion of this well-established procedure can be found in any standard textbook on the quantum field theory.[13]

After carrying on the above-mentioned procedure, we obtain

$$\begin{aligned}
&\mathrm{Tr}_{V(L,L)}[\hat{C}_{\mathbf{h}\downarrow}^\dagger\hat{C}_{\mathbf{h}\uparrow}^\dagger\hat{C}_{\mathbf{k}\uparrow}\hat{C}_{\mathbf{k}\downarrow}\exp(-\beta\tilde{H}_H)]\\
&\quad= \lim_{M\to\infty}\frac{1}{(2\sqrt{\pi})^{MN_\Lambda}}\int\prod_{m,\mathbf{i}} dk_{\mathbf{i},m}\exp\left(-\sum_{m,\mathbf{i}}\frac{k_{\mathbf{i},m}^2}{4}\right)\\
&\qquad\times\mathrm{Tr}_{V(N_\uparrow=L)}\left\{(\hat{C}_{\mathbf{h}\uparrow}^\dagger\hat{C}_{\mathbf{k}\uparrow})\prod_{m=1}^{M}\left[\exp\left(-\frac{\beta}{M}\hat{K}_\uparrow\right)\right.\right.\\
&\qquad\left.\left.\times\exp\left(i\sqrt{\beta U/2M}\sum_{\mathbf{i}\in\Lambda}k_{\mathbf{i},m}\hat{n}_{\mathbf{i}\uparrow}\right)\right]\right\}\\
&\qquad\times\mathrm{Tr}_{V(N_\downarrow=L)}\left\{(\hat{C}_{\mathbf{h}\downarrow}^\dagger\hat{C}_{\mathbf{k}\downarrow})\prod_{m=1}^{M}\left[\exp\left(-\frac{\beta}{M}\hat{K}_\downarrow\right)\right.\right.\\
&\qquad\left.\left.\times\exp\left(-i\sqrt{\beta/2M}\sum_{\mathbf{i}\in\Lambda}k_{\mathbf{i},m}\hat{n}_{\mathbf{i}\downarrow}\right)\right]\right\}.
\end{aligned} \tag{116}$$

In Eq. (116), $\mathrm{Tr}_{V(N_\sigma=L)}$ denotes the sum over all the possible configurations of L fermions with spin σ in the lattice. Obviously, the traces on the right-hand side of Eq. (116) are complex conjugate to each other. Therefore,

their product is a positive quantity. Moreover, other factors in the integrand are also positive. Consequently, the whole expression in Eq. (116) is a positive quantity. ▌

After establishing Lemma 7.1, we immediately obtain

$$\epsilon(\mathbf{h})\,\epsilon(\mathbf{k})\,\mathrm{Tr}_{V(N_A-L,\,L)}(\hat{S}_{\mathbf{h}-}\hat{S}_{\mathbf{k}+}e^{-\beta H_H}) \geqslant 0 \tag{117}$$

for the (positive-U) Hubbard Hamiltonian, by applying the inverse of the partial particle-hole transformation $\tilde{U}_H$ to Eq. (112). Therefore, $\mathrm{Tr}_{V(N_A-L,\,L)}(\hat{S}_{\mathbf{h}-}\hat{S}_{\mathbf{k}+}e^{-\beta H_H})$ is antiferromagnetic. So does the spin correlation function $\langle \hat{S}_{\mathbf{h}-}\hat{S}_{\mathbf{k}+}\rangle_{\hat{H}}$.

That ends the proof of Theorem 7.2. ▌

Since the Hubbard Hamiltonian is invariant under the rotation in the spin space, we further conclude that, at half-filling, the longitudinal spin correlation functions $\langle \hat{S}_{\mathbf{hz}}\hat{S}_{\mathbf{kz}}\rangle_{\hat{H}}$ of these strongly correlated electron models are antiferromagnetic at $T \neq 0$.

As usual, in proving Lemma 7.1 and Theorem 7.2 for the Kondo lattice model, we need to take the constraint condition (24) into consideration. For this purpose, we introduce a subspace

$$\tilde{V}(L,L) \equiv \sum_{n_f=0}^{L} \sum_{\{n_F\}} \oplus V(n_\uparrow^c = L-n_F,\, n_\downarrow^c = L-n_F,\, \{n_F\}), \tag{118}$$

where $\{n_F\}$ represents a specific configuration of n_F paired F-quasifermions in the lattice. Obviously, $\tilde{V}(L,L)$ is a subspace of $V(L,L)$ and the constraint condition (24) is automatically satisfied in it. Then, by replacing the trace $\mathrm{Tr}_{V(L,L)}$ in Eq. (112) with $\mathrm{Tr}_{\tilde{V}(L,L)}$ and repeating the rest of the proof, one can easily re-establish Lemma 7.1 and Theorem 7.2 for the Kondo lattice model.

An interesting implication of Theorem 7.2 is that, in one- and two-dimensions, the ferromagnetic spin-wave excitations of the itinerant electron ferrimagnets discussed in Section 5 are gapless. The detailed discussion on this issue can be found in the second paper of refs. 35.

8. SUMMARY: SOME RELATED ISSUE AND OPEN PROBLEMS

Before summarizing this paper, we would like to say a few words on some related approach to the strongly correlated electron systems and mention several open problems, which attract recently many condensed matter physicists' interest.

8.1. The Space-Reflection Approach and the Flux Phase Conjecture

When we talk about "reflection" in a lattice system, most of us would immediately have the "space reflection" in mind. More precisely, by imposing the periodic boundary condition on lattice Λ, we cut it into two equal halves, the left and the right half sublattices, by a perpendicular plane P to Λ. As a result, algebra $\mathscr{U}$ of the relevant observables can be naturally written as a direct product of $\mathscr{U}_L$, the subalgebra on the left sublattice Λ_L, and $\mathscr{U}_R$ on the right sublattice Λ_R. With this decomposition, we shall look for the Hamiltonians with the reflection positive form of Theorem 3.1 and then, carry on our further investigation. Comparing with the spin reflection, this approach is so natural and straightforward. People would ask why it was not taken.

Indeed, for the localized spin models, this strategy was effectively used to establish the magnetic long-range orders in both nonzero[46, 47] and zero temperature cases.[81, 82] However, it achieves only limited success in exploring the properties of the itinerant electron systems. The main difficulty is caused by the fermion characteristics of the electron hopping terms in these models. To make this point more clear, let us take a spinless electron tight-binding Hamiltonian for example. In terms of the division $\Lambda = \Lambda_L \cup \Lambda_R$ of the lattice, this Hamiltonian is of the following form

$$\hat{H} = -t \sum_{\langle \mathbf{ij} \rangle} \hat{c}_{\mathbf{i}}^{\dagger} \hat{c}_{\mathbf{j}} = -t \sum_{\langle \mathbf{ij} \rangle \in L} \hat{c}_{\mathbf{i}}^{\dagger} \hat{c}_{\mathbf{j}} - t \sum_{\langle \mathbf{ij} \rangle \in R} \hat{c}_{\mathbf{i}}^{\dagger} \hat{c}_{\mathbf{j}} - t \sum_{\langle \mathbf{ij} \rangle \in M} \hat{c}_{\mathbf{i}}^{\dagger} \hat{c}_{\mathbf{j}}, \tag{119}$$

where $t > 0$ is a real parameter. In Eq. (119), the third term describes the electron hopping between the left and the right halves of the lattice.

To rewrite Hamiltonian (119) into a direct product form of the operators in $\mathscr{U}_L$ and $\mathscr{U}_R$, we follow ref. 83 and introduce a new set of quasifermion perators $\hat{C}_{\mathbf{i}}$ by

$$\hat{C}_{\mathbf{i}} = (-1)^{\hat{N}_L} \hat{c}_{\mathbf{i}}, \qquad \hat{C}_{\mathbf{i}}^{\dagger} = \hat{c}_{\mathbf{i}}^{\dagger} (-1)^{\hat{N}_L}, \tag{120}$$

where $\hat{N}_L$ is the particle number operator in the left half of the lattice, i.e., $\hat{N}_L = \sum_{\mathbf{i} \in L} \hat{c}_{\mathbf{i}}^{\dagger} \hat{c}_{\mathbf{i}}$. It is easy to check that the operators $\hat{C}_{\mathbf{i}}$ and $\hat{C}_{\mathbf{j}}$ satisfy the conventional anticommutation relations if $\mathbf{i}, \mathbf{j} \in L$ or $\mathbf{i}, \mathbf{j} \in R$, but commute with each other if $\mathbf{i} \in L, \mathbf{j} \in R$ or $\mathbf{i} \in R, \mathbf{j} \in L$. That allows us to rewrite Hamiltonian $\hat{H}$ as

$$\hat{H} = \hat{T}_L \otimes \hat{I}_R + \hat{I}_L \otimes \hat{T}_R - t \sum_{\langle \mathbf{ij} \rangle \in M} (\hat{C}_{\mathbf{i}}^{\dagger} \otimes \hat{C}_{\mathbf{j}} + \hat{C}_{\mathbf{i}} \otimes \hat{C}_{\mathbf{j}}^{\dagger}). \tag{121}$$

Then, we make the simple particle-hole transformation on the right half of the lattice and obtain

$$\hat{U}^{\dagger}\hat{C}_{\mathbf{i}}\hat{U}=\hat{C}_{\mathbf{i}}^{\dagger},\qquad \hat{U}^{\dagger}\hat{C}_{\mathbf{i}}^{\dagger}\hat{U}=\hat{C}_{\mathbf{i}}, \tag{122}$$

for all $\mathbf{i}\in R$ while the operators $\hat{C}_{\mathbf{i}}$ with $\mathbf{i}\in L$ remain unchanged. Under this transformation, the Hamiltonian becomes

$$\tilde{H}=\hat{U}^{\dagger}\hat{H}\hat{U}=-t\sum_{\langle\mathbf{ij}\rangle\in L}\hat{C}_{\mathbf{i}}^{\dagger}\hat{C}_{\mathbf{j}}+t\sum_{\langle\mathbf{ij}\rangle\in R}\hat{C}_{\mathbf{i}}^{\dagger}\hat{C}_{\mathbf{j}}-t \times\sum_{\mathbf{i}\in L,\mathbf{j}\in R}\hat{C}_{\mathbf{i}}^{\dagger}\otimes\hat{C}_{\mathbf{j}}^{\dagger}-t\sum_{\mathbf{i}\in R,\mathbf{j}\in L}\hat{C}_{\mathbf{i}}\otimes\hat{C}_{\mathbf{j}}. \tag{123}$$

In the transformed Hamiltonian $\tilde{H}$, although the last two terms are in the form required by the reflection positivity, the change of sign in the second term violates it. That explains why the simple space-reflection approach does not apply to the itinerant electron models.

However, as the ancient Chinese philosopher Lao-tzu would like to say when he was in trouble, a bad luck may be an omen for good fortune. Interestingly, it is this violation of the space reflection positivity in the itinerant electron systems which makes it possible to prove rigorously the so-called flux phase conjecture. This conjecture states that the ground-state energy of a half-filled itinerant electron model in an external magnetic field is minimized when the magnetic flux equals π (in unit hc/e) per plaquette[84] (Zeeman terms are excluded). This conjecture, along with extensions to positive temperature, higher dimensional geometries, and allowance for some electron-electron interactions was rigorously proven by Lieb, using the space-reflection approach.[85] Later, a simplified proof was given by Macris and Nachtergaele.[83]

Here, we sketch its proof as another application of Theorem 3.2 to the strongly correlated electron models. For simplicity, we consider the spinless electron tight-binding Hamiltonian (119) on a two-dimensional square lattice.

In an external magnetic field, the hopping constants become, in general, site-dependent complex parameters by the so-called Peierls substitution.[86] In terms of the quasi-fermion operators, the Hamiltonian of this system has the following form

$$H=\sum_{\langle\mathbf{ij}\rangle\in L}t_{\mathbf{ij}}\hat{C}_{\mathbf{i}}^{\dagger}\hat{C}_{\mathbf{j}}+\sum_{\langle\mathbf{ij}\rangle\in R}t_{\mathbf{ij}}\hat{C}_{\mathbf{i}}^{\dagger}\hat{C}_{\mathbf{j}}+\sum_{\mathbf{ij}\in M}t_{\mathbf{ij}}\hat{C}_{\mathbf{i}}^{\dagger}\hat{C}_{\mathbf{j}}, \tag{124}$$

where $\langle \mathbf{ij} \rangle$ denotes a pair of nearest-neighbor sites and $t_{\mathbf{ij}} = -t \exp(i\phi_{\mathbf{ij}})$ is the hopping amplitude of electron from site $\mathbf{j}$ to site $\mathbf{i}$ in the magnetic field.

Let $\gamma = (\mathbf{i}_1, \ldots, \mathbf{i}_k)$ be a set of distinct lattice sites such that $\langle \mathbf{i}_i, \mathbf{i}_{i+1} \rangle$ for $i = 1, \ldots, k-1$, and $\langle \mathbf{i}_k, \mathbf{i}_1 \rangle$ are pairs of nearest-neighbor sites. It is called a circuit in the following. By representing the circuit as an ordered sequence, we have implicitly given it one of the two possible orientations (for $k > 2$).

It can be shown[87] that the ground-state energy of Hamiltonian (124) depends on the hopping constants $\{t_{\mathbf{ij}} = t \exp(i\phi_{\mathbf{ij}})\}$ only through their absolute value t and the flux variables Φ_γ for circuits $\{\gamma\}$, which are defined by

$$\Phi_\gamma = \sum_{k=1}^{n} \phi_{\mathbf{i}_k, \mathbf{i}_{k+1}}, \qquad \mod 2\pi. \tag{125}$$

This follows from the fact that, for any two phases $\{\phi_{\mathbf{ij}}\}$ and $\{\phi'_{\mathbf{ij}}\}$ which give the same fluxes Φ_γ for all the possible circuits γ, there is a unitary transformation of the following form

$$\hat{C}^\dagger_{\mathbf{i}} \to e^{i\theta_{\mathbf{i}}} \hat{C}^\dagger_{\mathbf{i}}, \qquad \hat{C}_{\mathbf{i}} \to e^{-i\theta_{\mathbf{i}}} \hat{C}_{\mathbf{i}}, \tag{126}$$

which changes phase $\{\phi_{\mathbf{ij}}\}$ into $\{\phi'_{\mathbf{ij}}\}$. This transformation is called a gauge transformation. In particular, a phase $\{\phi^c_{\mathbf{ij}}\}$ is called canonical if it yields a uniform flux π for each unit cell.

Under the particle-hole transformation defined in Eq. (122), the Hamiltonian is changed into

$$\tilde{H} = \sum_{\langle \mathbf{ij} \rangle \in L} t_{\mathbf{ij}} \hat{C}^\dagger_{\mathbf{i}} \hat{C}_{\mathbf{j}} + \sum_{\langle \mathbf{ij} \rangle \in R} (-\overline{t_{\mathbf{ij}}})\, \hat{C}^\dagger_{\mathbf{i}} \hat{C}_{\mathbf{j}} + \sum_{\mathbf{i} \in L, \mathbf{j} \in R} t_{\mathbf{ij}} \hat{C}^\dagger_{\mathbf{i}} \otimes \hat{C}^\dagger_{\mathbf{j}} + \sum_{\mathbf{i} \in R, \mathbf{j} \in L} t_{\mathbf{ij}} \hat{C}_{\mathbf{i}} \otimes \hat{C}_{\mathbf{j}}. \tag{127}$$

For a specific phase $\{\phi_{\mathbf{ij}}\}$, we perform gauge transformation

$$\hat{C}^\dagger_{\mathbf{i}} \to -e^{-i\phi_{\mathbf{ij}}} \hat{C}^\dagger_{\mathbf{i}}, \qquad \hat{C}_{\mathbf{i}} \to -e^{i\phi_{\mathbf{ij}}} \hat{C}_{\mathbf{i}} \tag{128}$$

for sites $\mathbf{i} \in R$ which are connected to a site $\mathbf{j} \in L$ by a nonzero hopping constant $t_{\mathbf{ij}}$. Under this transformation, all the hopping matrix elements across the reflection plane in Hamiltonian (127) become negative, i.e., we have

$$\tilde{H} = \sum_{\langle \mathbf{ij} \rangle \in L} t'_{\mathbf{ij}} \hat{C}^\dagger_{\mathbf{i}} \hat{C}_{\mathbf{j}} + \sum_{\langle \mathbf{ij} \rangle \in R} (-\overline{t'_{\mathbf{ij}}})\, \hat{C}^\dagger_{\mathbf{i}} \hat{C}_{\mathbf{j}} - \sum_{\mathbf{i} \in L, \mathbf{j} \in R} t \hat{C}^\dagger_{\mathbf{i}} \otimes \hat{C}^\dagger_{\mathbf{j}} - \sum_{\mathbf{i} \in R, \mathbf{j} \in L} t \hat{C}_{\mathbf{i}} \otimes \hat{C}_{\mathbf{j}}. \tag{129}$$

To this Hamiltonian, Theorem 3.2 applies. Consequently, we obtain the following lemma for the ground-state energy of the tight-binding Hamiltonian (124) (not $\tilde{H}$).

Lemma 8.1. Let Φ_L (resp. Φ_R) be the set of fluxes through the unit cells which are entirely in Λ_L (resp. Λ_R) and Φ_M be the flux configuration for the unit cells which are cut in middle by the reflection plane P. Then, the ground-state energy $E_0(\Phi_L, \Phi_M, \Phi_R)$ of the tight-binding Hamiltonian at half-filling satisfies

$$E_0(\Phi_L, \Phi_M, \Phi_R) \geqslant \tfrac{1}{2} E_0(-\Phi_R, \Phi_M^{(c)}, \Phi_R) + \tfrac{1}{2} E_0(\Phi_L, \Phi_M^{(c)}, -\Phi_L), \quad (130)$$

where $\Phi_M^{(c)}$ is the canonical flux configuration through the unit cells intersecting P.

Lemma 8.1 implies that one of the two energies, say $E_0(-\Phi_R, \Phi_M^{(c)}, \Phi_R)$ must be less than $E_0(\Phi_L, \Phi_M, \Phi_R)$. Therefore, by repeating this argument with respect to a properly-chosen sequence of reflection planes $(P_1, P_2, \ldots, P_N)$, we reach the following conclusion

Theorem 8.1. The ground-state energy of the tight-binding Hamiltonian $\hat{H}$ is minimized by the canonical phase. More precisely, we have

$$\inf_{\{\phi_{ij}\}} E_0(H(\{\phi_{ij}\}) \geqslant E_0(H(\{\phi_{ij}^{(c)}\})). \quad (131)$$

Following the above steps, one see easily that the effect of the extra magnetic flux π per unit cell is actually to cancel out the unwanted change of sign in the hopping constants under the particle-hole transformation. Therefore, Theorem 8.1 is a result of the Pauli principle which interferes with the electron orbital motion in a magnetic field.

8.2. Some Open Problems

Currently, the strongly correlated electron systems are still under intensive investigations by condensed matter physicists. The whole field is in rapid development. Here, we would like to mention two open problems which attract recently many condensed matter physicists' interest.

In this paper, we explained the spin-reflection-positivity method and its applications to strongly correlated electron systems. However, the readers may find that all the results established for the (positive-U) Hubbard model are mainly restricted to the half-filled case. In fact, few

rigorous results have been proven for the doped cases with $N \neq N_A$.[88] This is due to the fact that the partial particle-hole transformation, which is needed to make the sign of interaction between up- and down-spin electrons negative, maps also the subspace $V(L/2, L/2)$ into $V(N_A - L/2, L/2)$. However, when the system is doped, $N_A - L/2 \neq L/2$. Consequently, although the transformed Hamiltonian $\tilde{H}_H$ has seemingly the spin-reflection positive form, the relevant subspaces $V_\uparrow(N_A - L/2)$ and $V_\downarrow(L/2)$, in which the operators $\hat{T}_\uparrow$ and $\hat{T}_\downarrow$ act respectively, are not isomorphic. Therefore, the spin-reflection-positivity method does not apply. It is still an open problem to treat the doped strongly correlated electron models on a mathematically rigorous basis.

Another open problem is how to apply the spin-reflection-positivity method to the frustrated strongly correlated electron models. A well-known example is the so-called $t-t'-U$ Hubbard model on a simple cubic lattice. In this model, except the nearest-neighbor hopping, electrons are also allowed to hop between the next-nearest-neighbor sites with amplitude t'.[89] To this model, the simple cubic lattice is no longer bipartite. Consequently, under the partial particle-hole transformation, the hopping energy terms $\hat{T}_\uparrow$ and $\hat{T}_\downarrow$ do not even have the same form and hence, Theorem 3.1 cannot be applied. Up to now, no rigorous results have been established for this model.

8.3. Summary

In summary, in the present paper, we discuss the spin-reflection-positivity method and its applications to the strongly correlated electron systems in a pedagogical way. In many cases, this method can be successfully used to deal with the technical difficulties caused by the fermion sign problem plagued in the itinerant electron models. Consequently, it enables us to prove rigorously some interesting properties of the strongly correlated electron systems. In particular, by applying this method, we are able to explore the electron pairing correlation and the magnetic correlation in the Hubbard model, the periodic Anderson model, and the Kondo lattice model at either zero or nonzero temperatures.

APPENDIX

In this appendix, for reader's convenience, we shall give a simplified proof of the singular polar decomposition theorem, which we applied to prove Theorem 6.1 in Section 6. One can find a more detailed proof of this theorem in ref. 71.

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 $(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_m)$, which satisfy equations

$$AA^\dagger \mathbf{x}_i = \lambda_i^2 \mathbf{x}_i, \qquad 1 \leqslant i \leqslant m. \tag{132}$$

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

$$\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_k > \lambda_{k+1} = \cdots = \lambda_m = 0, \tag{133}$$

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

$$\Lambda_1 = \begin{pmatrix} \lambda_1 \cdots 0 \\ \cdots\cdots \\ 0 \cdots \lambda_m \end{pmatrix} \tag{134}$$

and

$$U_1 = (\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_m), \tag{135}$$

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

$$V_1^i = \frac{1}{\lambda_i} (A^\dagger \mathbf{x}_i)^\dagger. \tag{136}$$

Since $\lambda_i \neq 0$ for $1 \leqslant i \leqslant k$, 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. (136) are orthonormal to each other*. Actually, we have

$$\overline{\langle V_1^i \mid V_1^j \rangle} = \frac{1}{\lambda_i \lambda_j} \langle A^\dagger \mathbf{x}_i \mid A^\dagger \mathbf{x}_j \rangle = \frac{1}{\lambda_i \lambda_j} \mathbf{x}_i^\dagger AA^\dagger \mathbf{x}_j = \frac{1}{\lambda_i \lambda_j} \lambda_j^2 \mathbf{x}_i^\dagger \mathbf{x}_j = \delta_{ij}. \tag{137}$$

In the last step of the above-derivation, we used the definition of the 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 $\mathbf{z}_1^\dagger, \mathbf{z}_2^\dagger, ..., \mathbf{z}_{m-k}^\dagger$, which are orthogonal to each V_1^i with $1 \leqslant i \leqslant k$. 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

$$U_1^\dagger A = \Lambda_1 V_1 \tag{138}$$

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 $k+1 \leqslant l \leqslant m$ and calculate its norm.

$$\begin{aligned}
\langle \mathbf{x}_l^\dagger A \mid \mathbf{x}_l^\dagger A \rangle &= \sum_{\alpha=1}^{n} \overline{\left(\sum_{\beta=1}^{m} \overline{(\mathbf{x}_l)_\beta}\, A_{\beta\alpha} \right)} \left(\sum_{\gamma=1}^{m} \overline{(\mathbf{x}_l)_\gamma}\, A_{\gamma\alpha} \right) \\
&= \sum_{\alpha=1}^{n} \left[\sum_{\beta=1}^{m} \sum_{\gamma=1}^{m} \overline{A_{\beta\alpha}} (\mathbf{x}_l)_\beta\, A_{\gamma\alpha} \overline{(\mathbf{x}_l)_\gamma} \right] \\
&= \sum_{\alpha=1}^{n} \left[\sum_{\beta=1}^{m} \sum_{\gamma=1}^{m} \overline{(\mathbf{x}_l)_\gamma}\, A_{\gamma\alpha} A_{\alpha\beta}^\dagger (\mathbf{x}_l)_\beta \right] \\
&= \mathbf{x}_l^\dagger A A^\dagger \mathbf{x}_l = \lambda_l^2 \mathbf{x}_l^\dagger \mathbf{x}_l = 0. \qquad (139)
\end{aligned}$$

Therefore, $\mathbf{x}_l^\dagger A = 0$ and Eq. (138) 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 $AA^\dagger$. ∎

ACKNOWLEDGMENTS

This paper is dedicated to Professor Elliott Lieb for his 70th birthday. I would like to take this chance to express my deep gratitude to Professor Lieb for everything which he has done for me, as my former thesis supervisor. Since that time on, he is always my example to follow in my own career. I would also like to thank Professor Joel Lebowitz for inviting me to participate in the 88th Statistical Mechanics Meeting. I also thank Professor Hai-Qing Lin and Professor Michael Ma for many interesting discussions and conversations during my stay at the Chinese University of Hong Kong from the February to May of Year 2003. It is their friendship which made this difficult period of time not only endurable but also very enjoyable. This work is partially supported by the Chinese National Science Foundation under Grant No. 10174002.

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