

Particle statistics, frustration, and ground-state energyWenxing Nie,¹ Hosho Katsura,² and Masaki Oshikawa³¹*Center for Theoretical Physics, Department of Physics, Sichuan University, Chengdu 610064, China*²*Department of Physics, University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113-0033, Japan*³*Institute for Solid State Physics, University of Tokyo, Kashiwa 277-8581, Japan*

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We study the connections among particle statistics, frustration, and ground-state energy in quantum many-particle systems. In the absence of interaction, the influence of particle statistics on the ground-state energy is trivial: the ground-state energy of noninteracting bosons is lower than that of free fermions because of Bose-Einstein condensation and Pauli exclusion principle. In the presence of hard-core or other interaction, however, the comparison is not trivial. Nevertheless, the ground-state energy of hard-core bosons is proved to be lower than that of spinless fermions, if all the hopping amplitudes are non-negative. The condition can be understood as the absence of frustration among hoppings. By mapping the many-body Hamiltonian to a tight-binding model on a fictitious lattice, we show that the Fermi statistics of the original particles introduces an effective magnetic flux in the fictitious lattice. The latter can be effectively regarded as a kind of frustration since it leads to a destructive interference among different paths along which a single particle is propagating. If we introduce hopping frustration, the hopping frustration is expected to compete with the effective frustration due to the Fermi statistics, leading to the possibility that the ground-state energy of hard-core bosons can be higher than that of fermions. We present several examples, in which the ground-state energy of hard-core bosons is proved to be higher than that of fermions due to the hopping frustration. The basic ideas were reported in a previous paper [W.-X. Nie, H. Katsura, and M. Oshikawa, *Phys. Rev. Lett.* **111**, 100402 (2013)]; more details and several extensions, including one to the spinful case, are discussed in this paper.

DOI: [10.1103/PhysRevB.97.125153](https://doi.org/10.1103/PhysRevB.97.125153)**I. INTRODUCTION**

In this paper, we study a simple question: How do the particle statistics affect the ground-state energy of the system? More specifically, we compare the ground-state energy of bosons and fermions on an identical lattice with same parameters such as hopping amplitudes.

In noninteracting systems, the influence of particle statistics on the ground-state energy can be understood easily. The two systems in comparison are exactly equivalent to each other, and thus have exactly the same ground-state energy, when only a single particle is present. The ground-state energy of fermions is simply given by the sum of the lowest single-particle energy eigenvalues, following the Aufbau principle. In contrast, in the ground state of noninteracting bosons, all the bosons condense into the lowest single-particle state. This phenomenon is known as Bose-Einstein condensation (BEC). Therefore, the ground-state energies of noninteracting bosons and fermions satisfy the “natural” inequality

$$E_0^B \leq E_0^F. \quad (1)$$

On the other hand, the comparison of the ground-state energies of bosons and fermions is not trivial in the presence of interaction because the simple argument based on the perfect BEC breaks down. In a system of interacting bosons, it is in fact already a nontrivial question whether the BEC actually takes place. Einstein’s original argument depends on the absence of interaction. For interacting bosons, there is no general theorem that BEC always occurs [1]. A counterexample is the solid ⁴He phase, where BEC is absent even at zero temperature, under a sufficiently high pressure. Rigorously proven examples

of BEC, in the sense of the off-diagonal long-range order (ODLRO), in interacting systems are still rather limited [2–4]. Even if the occurrence of BEC or the ODLRO is proved in a system of interacting bosons, it does not necessarily restrict the ground-state energy because single-particle states with higher energies can be partially occupied. In particular, an ODLRO does not necessarily imply the inequality (1). In fact, the influence of particle statistics on the ground-state energy had not been much explored in strongly correlated systems.

The comparison of the ground-state energies is particularly appealing in the case of hard-core bosons and fermions. In both kinds of systems, each site is either empty or occupied by a single particle. Thus, the dimension of the Hilbert space is identical between them. Nevertheless, the different particle statistics generically lead to different ground-state energies, as we will see in the following.

Before discussing the issue any further, let us comment on the physical relevance of the question itself. The energy eigenvalue itself is generally unphysical in the sense that one can always redefine the energy by adding a constant. It is thus the difference of energies of two different states that matters.

We can understand the difference by defining the ground-state energy with respect to a simple reference state in each system, such as a vacuum state (in which every site is empty). This ground-state energy is the sum of energy gains in the process of filling the system with particles, and is a measurable quantity [5,6]. This is somewhat similar to the “enthalpy of formation” studied in chemistry [7], which is the total change of enthalpy (per mole) when the compound is formed from its elements under a certain condition.

Since the vacuum state is equivalent between the system of bosons and fermions, the comparison of the ground-state energies is completely well defined. Moreover, even when the energy difference itself cannot be measured, the comparison of the ground-state energies is relevant for understanding stability of various different phases. This is particularly the case with the possible realization of statistical transmutation, as we will discuss later in this paper.

Concerning the comparison of the ground-state energies between bosons and fermions, recently we found [8] a sufficient condition for the natural inequality (1) to hold, without relying on the occurrence of BEC. That is, if all the hopping amplitudes are non-negative, the ground-state energy of hard-core bosons is still lower than that of the corresponding fermions. This theorem is extended to the spinful case in this paper. Once we relax the condition of non-negative hopping amplitudes, it is possible to reverse the inequality so that the ground-state energy of bosons is higher than that of fermions. We find several concrete models in which such a reversal is realized; and in several cases it is even proved rigorously. More examples and techniques will be introduced in this paper than those discussed in Ref. [8].

Moreover, our study leads to an important physical understanding of the effects of particle statistics, in terms of *frustration* in quantal phase. This is more general than the picture based on the perfect BEC, and is indeed applicable to systems with interaction.

We can map a quantum many-particle problem to a single-particle problem on a fictitious lattice in higher dimensions. When all the hopping amplitudes are non-negative and the particles are bosons, the corresponding single-particle problem also has only non-negative hopping amplitudes. In such a case, there is no frustration in the quantal phase of the wave function. On the other hand, Fermi statistics of the original particles gives an effective magnetic flux in the corresponding single-particle problem. This implies a frustration in the phase of the wave function, induced by the Fermi statistics. When a magnetic flux is introduced in the original quantum many-particle problem, it also results in a magnetic flux in the corresponding single-particle problem, inducing a frustration. This hopping-induced frustration and the effective frustration induced by the Fermi statistics can sometimes partially cancel with each other, resulting in the reversed inequality between the ground-state energies of the hard-core bosons and fermions.

The paper is organized as follows. In Sec. II, we present the full proof of the natural inequality for the spinless case and extend the discussion to the spinful case. Based on the proof, in Sec. III, we put forward a unified understanding of the frustration for bosons and fermions in the same manner. As a by-product, a strict version of the diamagnetic inequality for a general lattice is presented. Several examples, in which the natural inequality is violated owing to the hopping frustration, are presented in Sec. IV. The examples include a simple yet instructive, exactly solvable model of particles on a one-dimensional ring, two-dimensional systems of coupled rings, systems with flux in 2D and 3D, and flat-band models. Rigorous proof of the reversed inequality is provided for most cases. Conclusions and discussions are presented in Sec. V. Detailed proofs of some of the theorems, and related technical results are presented in the Appendices.

II. NATURAL INEQUALITY

The natural inequality (1) holds trivially for noninteracting bosons and fermions with the same form of the Hamiltonian. Now, we present three theorems, which state that Eq. (1) holds even for hard-core bosons, provided that all the hopping amplitudes are non-negative. A brief overview appeared in Ref. [8], but here we give a more detailed discussion, and also an extension to the spinful case.

A. Natural inequality for spinless case

First, we consider the comparison of spinless hard-core bosons with spinless fermions. We assume the system of bosons or fermions is described by the same form of Hamiltonian

$$\mathcal{H} = - \sum_{j \neq k} (t_{jk} c_j^\dagger c_k + \text{H.c.}) - \sum_j \mu_j n_j + \sum_{j,k} V_{jk} n_j n_k, \quad (2)$$

where j is the label of a site on a finite lattice Λ and $n_j \equiv c_j^\dagger c_j$ is the number of particles on j th site. Chemical potential μ is the uniform (site-independent) part of μ_j . For a system of bosons, we identify c_j with the boson annihilation operator b_j satisfying the standard commutation relations, with the hard-core constraint $n_j = 0, 1$ at each site. The hard-core constraint may also be implemented by introducing an infinite onsite interaction $\frac{\mathcal{U}}{2} \sum_j n_j (n_j - 1)$, where $\mathcal{U} \rightarrow +\infty$. For a system of fermions, we identify c_j with the fermion annihilation operator f_j satisfying the standard anticommutation relations.

This Hamiltonian is very general. We do not make any assumption on the dimensionality or the geometry of the lattice Λ , or on the range of the hoppings. In addition, the interaction is also arbitrary, as long as it can be written in terms of V_{jk} . The interesting aspect of attractive interaction will be discussed in Appendix B. We note that the Hamiltonian (2) conserves the total particle number. Thus, the ground state can be defined for a given number of particles M (canonical ensemble) or for a given chemical potential μ (grand canonical ensemble). The comparison between bosons and fermions can be made in either circumstance.

Now, we will present a sufficient condition for the natural inequality (1). Moreover, a sufficient condition for the strict inequality $E_0^B < E_0^F$ is provided. The proof is also illuminating for physical understanding of the natural inequality in interacting systems, showing the importance of the particle statistics and exchange processes.

Theorem 1. (Natural inequality for spinless case). The inequality (1) holds for any given number of particles M on a finite lattice Λ with $N \geq M$ sites, if all the hopping amplitudes t_{jk} are real and non-negative.

Furthermore, if the lattice Λ is connected, and has a site directly connected to three or more sites, and if the number of particles satisfies $2 \leq M \leq N - 2$, the strict inequality $E_0^B < E_0^F$ holds.

Proof. To write the matrix elements of the Hamiltonian (2), we choose the occupation-number basis $|\phi^a\rangle \equiv |\{n_j^a\}\rangle$, where M is the total number of particles satisfying $\sum_j n_j^a = M$. The matrix elements of the number operator n_j are the same for hard-core bosons and spinless fermions in this basis. We begin

by defining the operator

$$\mathcal{K}^{\text{B,F}} \equiv -\mathcal{H}^{\text{B,F}} + C\mathbb{1}. \quad (3)$$

For convenience, we added an identity matrix with large enough diagonal elements C such that all the eigenvalues $\kappa^{\text{B,F}}$ of matrix $\mathcal{K}^{\text{B,F}}$ and thus all the diagonal matrix elements $\mathcal{K}_{aa}^{\text{B,F}}$ are positive. The relation of the matrix elements for bosonic and fermionic operators can be summarized as

$$\mathcal{K}_{ab}^{\text{B}} = \begin{cases} |\mathcal{K}_{ab}^{\text{F}}| & (a \neq b) \\ \mathcal{K}_{aa}^{\text{F}} & (a = b) \end{cases} = |\mathcal{K}_{ab}^{\text{F}}|. \quad (4)$$

The difference between bosons and fermions is that, given non-negative hopping amplitudes t_{jk} , the matrix elements of the bosonic operator \mathcal{K}^{B} are non-negative, while those of the fermionic operator \mathcal{K}^{F} can be negative in sign. This difference in signs generically leads to different ground-state energies between bosons and fermions.

The ground state of the Hamiltonian $\mathcal{H}^{\text{B,F}}$ corresponds to the eigenvector belonging to the largest eigenvalue $\kappa_{\text{max}}^{\text{B,F}}$ of $\mathcal{K}^{\text{B,F}}$. Let $|\Psi_0\rangle_{\text{F}} = \sum_a \psi_a |\phi^a\rangle_{\text{F}}$ be the normalized ground state for fermions. The trial state for the bosons can be assumed as $|\Psi_0\rangle_{\text{B}} = \sum_a |\psi_a| |\phi^a\rangle_{\text{B}}$, where $|\phi^a\rangle_{\text{B}}$ is the basis state for bosons corresponding to $|\phi^a\rangle_{\text{F}}$. Then, by a variational argument,

$$\begin{aligned} \kappa_{\text{max}}^{\text{B}} &\geq {}_{\text{B}}\langle\Psi_0|\mathcal{K}^{\text{B}}|\Psi_0\rangle_{\text{B}} = \sum_{ab} |\psi_a| |\psi_b| \mathcal{K}_{ab}^{\text{B}} \\ &\geq \sum_{ab} \psi_a^* \psi_b \mathcal{K}_{ab}^{\text{F}} = \kappa_{\text{max}}^{\text{F}} \end{aligned} \quad (5)$$

holds, implying $E_0^{\text{B}} \leq E_0^{\text{F}}$. The first part of Theorem 1 is thus proved. As a simple corollary, the ground-state energies for a given chemical potential μ also satisfy Eq. (1).

In order to prove the strict version of the natural inequality, let us consider $\mathcal{L}^S \equiv (\mathcal{K}^S)^n$, where $S = \text{B,F}$, for a positive integer n . In the occupation-number basis, the matrix element of \mathcal{L} is expanded as

$$\mathcal{L}_{ab}^S = \sum_{c_1, \dots, c_{n-1}} \mathcal{K}_{ac_1}^S \mathcal{K}_{c_1 c_2}^S \mathcal{K}_{c_2 c_3}^S \dots \mathcal{K}_{c_{n-1} b}^S, \quad (6)$$

in which each term in the sum represents a particle hopping process among the connected sites.

From the definition of \mathcal{L}^S and the relation (4) between \mathcal{K}^{B} and \mathcal{K}^{F} , we have the inequality for matrix elements of $\mathcal{L}^{\text{B,F}}$:

$$\begin{aligned} \mathcal{L}_{ab}^{\text{B}} &= \sum_{c_1, \dots, c_{n-1}} \mathcal{K}_{ac_1}^{\text{B}} \mathcal{K}_{c_1 c_2}^{\text{B}} \mathcal{K}_{c_2 c_3}^{\text{B}} \dots \mathcal{K}_{c_{n-1} b}^{\text{B}} \\ &= \sum_{c_1, \dots, c_{n-1}} |\mathcal{K}_{ac_1}^{\text{F}} \mathcal{K}_{c_1 c_2}^{\text{F}} \mathcal{K}_{c_2 c_3}^{\text{F}} \dots \mathcal{K}_{c_{n-1} b}^{\text{F}}| \\ &\geq \left| \sum_{c_1, \dots, c_{n-1}} \mathcal{K}_{ac_1}^{\text{F}} \mathcal{K}_{c_1 c_2}^{\text{F}} \mathcal{K}_{c_2 c_3}^{\text{F}} \dots \mathcal{K}_{c_{n-1} b}^{\text{F}} \right| = |\mathcal{L}_{ab}^{\text{F}}|. \end{aligned} \quad (8)$$

This applies, in particular, to the diagonal elements with $b = a$.

From Eq. (4), the matrix elements of \mathcal{K}^{F} and thus the amplitudes of the process in Eq. (6) can be negative for fermions, while they are non-negative for bosons. The difference between bosons and fermions shows up exactly when two particles are exchanged. To make two-particle exchange process possible,

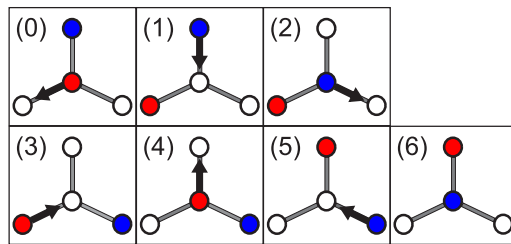


FIG. 1. A schematic example to show a two-particle exchange process in six steps, where the four-site branch cluster is a subsection of a real arbitrary lattice.

let us introduce a “branching” site directly connected to three or more sites belonging to the lattice. An example of the branching site connected to three sites is shown in Fig. 1. If the number of particles falls in the range $2 \leq M \leq N - 2$, two particles can be exchanged from an initial state $|\phi^a\rangle$ and back to the same state in six hoppings, with the aid of the branch structure. An example of particle exchange process on a lattice with a branching site is demonstrated schematically in Fig. 1. The contribution to the diagonal elements of bosons $\mathcal{L}_{aa}^{\text{B}}$ is always positive at $n = 6$, while the contribution to $\mathcal{L}_{aa}^{\text{F}}$ is negative when two particles are exchanged. On the other hand, there is always a positive contribution to $\mathcal{L}_{aa}^{\text{B}}$ and $\mathcal{L}_{aa}^{\text{F}}$ in the expansion of Eq. (6), at least from the invariant process $c_j = a$ in which no particle moves in n steps. Thus, the strict inequality $\mathcal{L}_{aa}^{\text{B}} > |\mathcal{L}_{aa}^{\text{F}}|$ holds in this case.

When the lattice Λ is connected, any basis state $|\phi^a\rangle_{\text{B}}$ can be reached by consecutive applications of the hopping term in \mathcal{K}^{B} , and thus the matrix $\mathcal{K}_{ab}^{\text{B}}$ satisfies the connectivity. Together with the property $\mathcal{K}_{ab}^{\text{B}} \geq 0$, $\mathcal{K}_{ab}^{\text{B}}$ (and thus also $\mathcal{L}_{ab}^{\text{B}}$) is a Perron-Frobenius matrix [9]. Applying a corollary of the Perron-Frobenius theorem¹ we find $\kappa_{\text{max}}^{\text{B}} > \kappa_{\text{max}}^{\text{F}}$ and hence the latter part of the theorem follows. ■

We note in passing that a consequence of the Perron-Frobenius theorem is that the ground state of bosons has a nonvanishing amplitude ${}_{\text{B}}\langle\phi^a|\Psi_0\rangle_{\text{B}}$ with a definite (say, positive) sign for every basis state $|\phi^a\rangle_{\text{B}}$. This may be understood as a lattice version of the “no-node” theorem [10,11].

B. Natural inequality for spinful case

Let us now discuss the spinful case. Here, we compare spinful hard-core bosons and spinful fermions on a finite lattice, with spin $\frac{1}{2}$. While actual bosons are known to have only integer spins, they can have pseudospin $\frac{1}{2}$, which is sufficient for the present discussion. Here, the “hard-core bosons” means that two or more particles with the *same* (pseudo)spin cannot occupy the same site: $n_{j\sigma} = 0, 1$, where $\sigma = \uparrow, \downarrow$. With this constraint, we consider the Hamiltonian

$$\begin{aligned} \mathcal{H} &= - \sum_{j \neq k} \sum_{\sigma} (t_{jk} c_{j\sigma}^{\dagger} c_{k\sigma} + \text{H.c.}) - \sum_{j\sigma} \mu_j n_{j\sigma} \\ &+ \sum_{j \neq k} \sum_{\sigma\sigma'} V_{jk} n_{j\sigma} n_{k\sigma'} + \sum_j U_j n_{j\uparrow} n_{j\downarrow}, \end{aligned} \quad (9)$$

¹See, for example, Theorem 8.4.5 of Ref. [9].

which is a generalization of Eq. (2) with the introduction of the spin degrees of freedom $\sigma = \uparrow, \downarrow$.

Let us first discuss the case in which all U_j 's are finite. Then, the following simple generalization of Theorem 1 holds:

Theorem 2. (Natural inequality for spinful case with finite U_j 's). For any set of finite U_j 's, if all the hopping amplitudes t_{jk} are real and non-negative, the inequality (1) holds for any given number of particles $M \leq 2N$ on a finite lattice Λ with N sites. Furthermore, if the lattice Λ is connected, and has a site directly connected to three or more sites, and if the number of particles satisfies $3 \leq M \leq 2N - 3$, the strict inequality holds.

The detailed proof including the restriction of filling, which is a straightforward generalization of the proof of Theorem 1, is given in Appendix A.

Now, let us discuss the case $U_j = +\infty$. The first half of Theorem 2, the nonstrict version of the inequality, remains unaffected by taking the limit $U_j = +\infty$. It is easily proved by variational principle in the same manner as in the proof of Theorem 1. However, the latter half of Theorem 2, the strict inequality, is affected by taking the limit.

The proof of the strict inequality is based on the Perron-Frobenius theorem, which requires the irreducibility of the matrix. For spinless particles and spinful particles with finite U_j 's, when the lattice is connected, any pair of occupation-number basis states $|\Phi^a\rangle$ and $|\Phi^b\rangle$ of the many-particle problem are connected by consecutive application of particle hoppings. This implies the irreducibility of the matrix representing the many-body Hamiltonian. However, in the case of spinful system with $U_j = +\infty$, connectivity of the lattice does not guarantee the irreducibility of the many-body Hamiltonian matrix. An illustrative example is the Hubbard model with $U_j = +\infty$ at half-filling. Each site is occupied by a particle with either spin up or spin down; there are many occupation-number basis states corresponding to different spin configurations. However, since there is no empty site, and double occupancy with spin-up and -down particles is forbidden, each basis state is not connected by hopping to any other basis state. Therefore, in order to prove the strict inequality, we need some additional condition which guarantees the irreducibility of the Hamiltonian matrix. In fact, the irreducibility of the Hamiltonian matrix at $U_j = +\infty$, and application of the Perron-Frobenius theorem were discussed earlier by Tasaki [12,13] in the context of Nagaoka's ferromagnetism. Nagaoka's ferromagnetism is a mechanism of ferromagnetism in the Hubbard model with a single hole doped into the half-filling with $U_j = +\infty$, and can be understood as a consequence of the Perron-Frobenius theorem. For that, the irreducibility of the Hamiltonian matrix in a certain basis is required. In Ref. [13], a sufficient condition for the irreducibility was presented: if the entire lattice is connected by exchange bonds, then the Hamiltonian matrix in the occupation-number basis is irreducible. Here, "exchange bond" [13] is defined by a pair of sites which belongs to a loop of length three or four, and the whole lattice remains connected via nonvanishing hopping amplitudes even when the two sites are removed. Thus, we obtain the following:

Theorem 3. (Natural inequality for spinful case not above half-filling). When U_j 's are either $+\infty$ or finite, if all the hopping amplitudes t_{jk} are real and non-negative, the inequality (1) holds for any given number of particles $M \leq N$ on a finite lattice Λ with N sites. Furthermore, if the entire lattice Λ is

connected by exchange bonds, and if the number of particles satisfies $3 \leq M \leq N - 1$, the strict inequality holds.

The outline of the proof of Theorem 3, including the restriction of filling, and the numerical verification of the theorems are presented in Appendix B.

In summary, in this section we have presented three theorems for the validity of the natural inequality for spinless and spinful cases, respectively. Although the proofs of the sufficient conditions for strict version of the natural inequality (see Appendices A and B) are somewhat more involved, the basic idea behind the proofs is the same as in that for Theorem 1. That is, bosons have a strictly lower ground-state energy than fermions, when the hopping amplitudes are non-negative and an exchange of particles is allowed.

III. UNIFIED UNDERSTANDING OF FRUSTRATION AND DIAMAGNETIC INEQUALITY

The role played by *frustration* is of central importance in the proofs of the theorems. The terminology "frustration" is often used for antiferromagnetically interacting spin system on geometrically frustrated lattices, such as triangular, kagome, and pyrochlore lattices. When there is no global state of the system that minimizes every antiferromagnetic interaction, there is some frustration. More generally, frustration may be applicable to a system with competing interactions, when the ground state does not minimize individual interaction simultaneously [14].

To see that the sign of hopping amplitudes t_{jk} in a many-boson system is related to frustration, it is illuminating to map the hard-core boson problem to a spin- $\frac{1}{2}$ quantum spin system [15]. The mapping is based on the equivalence between hard-core boson operators and spin- $\frac{1}{2}$ operators:

$$S_j^+ \sim b_j^\dagger, \quad S_j^- \sim b_j, \quad S_j^z \sim b_j^\dagger b_j - \frac{1}{2}. \quad (10)$$

It is then easy to see that a hopping term for hard-core bosons maps to an in-plane exchange interaction

$$-t_{jk}(b_j^\dagger b_k + b_k^\dagger b_j) \sim J_{jk}^\perp (S_j^x S_k^x + S_j^y S_k^y), \quad (11)$$

where $J_{jk}^\perp = -2t_{jk}$. Thus, the non-negative t_{jk} corresponds to ferromagnetic exchange interaction, in terms of the spin system. When all the exchange couplings are ferromagnetic, there is no frustration. Namely, every in-plane exchange interaction energy can be minimized simultaneously by aligning all the spins to the same direction in the xy plane. Going back to the original problem of quantum particles, the direction of the spins in the xy plane corresponds to the quantal phase of particles at each site. If all the hopping amplitudes are non-negative, every hopping term can be simultaneously minimized by choosing a uniform phase throughout the system. In this sense, bosons with non-negative hopping amplitudes are unfrustrated with respect to their quantal phase.

Let us now consider the case of fermions. Since Fermi statistics brings in negative signs even if all the hoppings t_{jk} are non-negative, it would be natural to expect that Fermi statistics leads to some kind of frustration. However, it is difficult to formulate this based on the above mapping to an $S = \frac{1}{2}$ spin system. To understand the frustration induced by Fermi statistics in many-particle systems, we introduce

an alternative mapping of the many-body Hamiltonian into a single-particle tight-binding model. That is, we identify each of the many-body occupation-number basis states $|\Phi^a\rangle$ with a site on a fictitious lattice. If two occupation-number basis states $|\Phi^a\rangle$ and $|\Phi^b\rangle$ are connected by Hamiltonian $\langle\Phi^b|\mathcal{H}|\Phi^a\rangle \neq 0$, there is a link connecting sites a and b in the fictitious lattice. If we can start from an initial state, and return back to the same state by successive applications of the Hamiltonian (2), there is a loop in the fictitious lattice. For bosons, there is no extra phase in the loop. In other words, the fictitious lattice for hard-core bosons is flux free. Therefore, there is no frustration for bosons because there is a constructive interference among all the paths. In contrast, for fermions, in the original many-body problem, if two particles are exchanged and the system returns back to the initial state, the system acquires an extra π phase. The minus sign introduced by Fermi statistics is relevant to sign structure [16]. Upon the mapping to the single-particle problem, this is equivalent to the presence of a π flux in the corresponding loop in the fictitious lattice. This can be interpreted as frustration, which causes destructive interferences among different paths.

For a single-particle tight-binding model, introduction of a flux always raises or does not change the ground-state energy, which is known as diamagnetic inequality [17]. The first half of Theorem 1, which states the non-strict inequality, may be then regarded as a corollary of the diamagnetic inequality. On the other hand, the latter half of Theorem 1 concerning the strict inequality does not, to our knowledge, follow from known results on the diamagnetic inequality. In fact, the arguments in the proof of Theorem 1 can be applied to a strict version of the diamagnetic inequality on general lattices. The general result can be summarized as follows.

Theorem 4. (General diamagnetic inequality and its strict version). Let us consider a single particle on a finite lattice Ξ , with the eigenequation

$$-\sum_{\beta \in \Xi} \tau_{\alpha\beta} \psi_{\beta} = E \psi_{\alpha}. \quad (12)$$

In general, $\tau_{\alpha\beta}$ is complex, with $\tau_{\alpha\beta} = \tau_{\beta\alpha}^*$. The ground-state energy E_0 for a given set of the hopping amplitudes $\{\tau_{\alpha\beta}\}$ satisfies

$$E_0(\{\tau'_{\alpha\beta} \equiv |\tau_{\alpha\beta}|\}) \leq E_0(\{\tau_{\alpha\beta}\}). \quad (13)$$

Furthermore, the strict inequality,

$$E_0(\{\tau'_{\alpha\beta} \equiv |\tau_{\alpha\beta}|\}) < E_0(\{\tau_{\alpha\beta}\}) \quad (14)$$

holds, provided that the lattice Ξ is connected and there is at least one loop which contains a nonvanishing flux. A sequence of sites $\{\alpha_0, \alpha_1, \alpha_2, \dots, \alpha_n\}$, which satisfies $\alpha_l \neq \alpha_{l+1}$, $\tau_{\alpha_l \alpha_{l+1}} \neq 0$, and $\alpha_n = \alpha_0$ is called a loop. The loop contains a nonvanishing flux when the product

$$\tau_{\alpha_0 \alpha_1} \tau_{\alpha_1 \alpha_2} \tau_{\alpha_2 \alpha_3} \dots \tau_{\alpha_{n-1} \alpha_n} \quad (15)$$

is not positive (either negative or not real).

The nonstrict version is the standard diamagnetic inequality [17,18]. However, the strict inequality obtained here appears new, also in the general context of diamagnetic inequality. The detailed proof of Theorem 4 can be found in Appendix C.

Mapping of the original quantum many-particle problem to the single-particle problem on a fictitious lattice provides a

unified understanding of frustration of quantal phase. When there is a nonvanishing flux in the original many-particle problem, we observed that there is a frustration among local quantal phases, which we call hopping frustration. On the other hand, when the particles in the original problem are fermions, there is also a frustration among quantal phases introduced by the Fermi statistics, which we name *statistical frustration*. In the original many-particle problem, the statistical frustration appears rather different from the hopping frustration. However, upon mapping to the single-particle problem on the fictitious lattice, both hopping frustration and statistical frustration are represented by a nonvanishing flux in the fictitious lattice. This provides a unified understanding of hopping and statistical frustrations.

A system of many bosons with only non-negative hopping amplitudes t_{jk} are free of frustration. Introduction of any frustration into such a system, for example magnetic flux (hopping frustration), is expected not to decrease the ground-state energy. This is a lattice version of Simon's universal diamagnetism of bosons [18]. However, in the many-fermion system, where the statistical frustration exists, the effect of introducing hopping frustration is a nontrivial problem. In such a case, the ground-state energy may or may not decrease, depending on the system in question. That is, diamagnetism is not universal in spinless fermion systems. Correspondingly, the orbital magnetism of fermions can be either paramagnetic or diamagnetic, depending on the model [19]. Considering each of the frustrations introduces a particular pattern of magnetic flux in the fictitious lattice, it is certainly possible that in some cases the hopping frustration may (partially) cancel the effect of statistical frustration, so that the introduction of the hopping frustration actually decreases the ground-state energy. This reveals the fact that the natural inequality could be violated by the introduction of hopping frustration. Some concrete examples, in which the natural inequality is violated, are demonstrated in the following section.

IV. VIOLATION OF THE NATURAL INEQUALITY

In the following, we discuss how the natural inequality can be violated. Theorems 1 and 2 leave the possibility of violation of the inequality in the presence of a hopping frustration, that is, by choosing negative or complex hopping amplitudes t_{jk} . However, the hopping frustration is a necessary but not sufficient condition to reverse the natural inequality. We will demonstrate that the violation of natural inequality indeed happens in several frustrated systems. For simplicity, we limit ourselves to the comparison between spinless fermions and hard-core bosons, with no interaction other than the hard-core constraint. The case with density-density interaction will be discussed at the end of this section.

A. Particles on a ring

We start with the best understood and solvable model in one dimension:

$$\mathcal{H} = -\sum_{j=1}^N (c_j^\dagger c_{j+1} + \text{H.c.}). \quad (16)$$

The hard-core boson version of this model, which is equivalent to the spin- $\frac{1}{2}$ XY chain, can be mapped to free fermions on a ring by Jordan-Wigner transformation [20,21]. Thus, the energy eigenvalue problems of hard-core bosons and fermions on a ring are almost the same, except for the subtle difference in the boundary condition. For the periodic or antiperiodic boundary conditions $c_{N+1} \equiv \pm c_1$, the Jordan-Wigner fermions \tilde{f}_j obey the boundary condition $\tilde{f}_{N+1} = \mp e^{i\pi M} \tilde{f}_1$, where M is the number of Jordan-Wigner fermions (equals to the number of bosons). If M is assumed as even, it implies that hard-core bosons with the periodic (antiperiodic) boundary condition are mapped to free fermions with the antiperiodic (periodic, respectively) boundary condition.

Now, let us discuss the dependence of the ground-state energy on the boundary condition. Assuming $M = N/2$ is even, the ground-state energy density (ground-state energy per site) is given as

$$\epsilon_0 = \frac{E_0}{N} = -\frac{2}{N} \sum_k \cos k, \quad (17)$$

where k is taken over all the momenta in the Fermi sea, $-\pi/2 \leq k < \pi/2$. For the periodic boundary condition (PBC), the wave number k is quantized as $k = 2\pi n/N$, while $k = \pi(2n+1)/N$ for the antiperiodic boundary condition (APBC), where n ($-N/4 \leq n < N/4$) is an integer.

The ground-state energy density asymptotically converges, in the thermodynamic limit $N \rightarrow \infty$, to the same integral for either boundary condition. Nevertheless, it does depend on the boundary condition for a finite N . The difference of ground-state energy is exactly calculated as

$$\frac{E_0^{\text{PBC}}}{N} - \frac{E_0^{\text{APBC}}}{N} = \frac{2[1 - \cos(\pi/N)]}{N \sin(\pi/N)} > 0 \quad (18)$$

for any $N > 1$. The antiperiodic boundary condition gives the lower ground-state energy. The leading order of difference can be extracted in the limit of large N as

$$\frac{E_0^{\text{PBC}}}{N} = -\frac{2}{\pi} + \frac{2\pi}{3N^2} + \frac{2\pi^3}{45N^4} + O\left(\frac{1}{N^6}\right), \quad (19)$$

$$\frac{E_0^{\text{APBC}}}{N} = -\frac{2}{\pi} - \frac{\pi}{3N^2} - \frac{7\pi^3}{180N^4} + O\left(\frac{1}{N^6}\right) \quad (20)$$

for the periodic and antiperiodic boundary conditions. The leading term of $O(1/N^2)$ is also determined by conformal field theory [22,23]. It can be seen that the noninteracting fermions on a ring have a lower ground-state energy with the antiperiodic boundary condition.

As a result, with periodic boundary condition, hard-core bosons have a lower ground-state energy than fermions, in full agreement with Theorem 1. On the other hand, the ground-state energy of hard-core bosons is higher than that of fermions with antiperiodic boundary condition. The antiperiodic boundary condition can be understood as a result of insertion of π flux inside the ring. This hopping frustration cancels the statistical frustration so that the natural inequality is violated.

This example of tight-binding model may look trivial, and indeed the calculation itself has been known for years. Nevertheless, it is very useful in highlighting the central physics of the problem, that is, the effect of the statistical

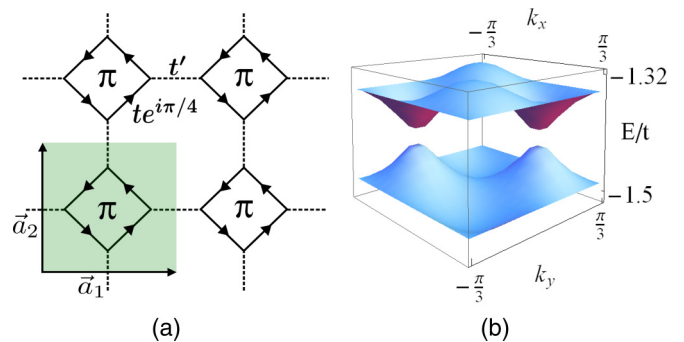


FIG. 2. (a) π -flux octagon-square lattice, in which a unit cell is shown in green. (b) The lowest two bands of Hamiltonian (21) with $t = 1$, $t' = 0.1$.

frustration of fermions can be canceled by the flux or hopping frustration. The present finding can also be applied to construction of more nontrivial examples, as we will discuss in Sec. IV B.

B. Coupled rings

Since hard-core bosons have a higher ground-state energy than fermions on a ring containing π flux inside the ring as proved in Sec. IV A, we can construct a series of systems where $E_0^{\text{B}} > E_0^{\text{F}}$, by taking many such small rings and connecting them with weak hoppings. If the inter-ring hoppings are weak enough, they are expected not to revert the inequality and $E_0^{\text{B}} > E_0^{\text{F}}$ would be kept [24].

We prove rigorously that the reversed natural inequality is indeed still kept in coupled π -flux rings, connected by weak hoppings, even in the thermodynamic limit. One example is π -flux octagon-square model. The lattice structure is shown in Fig. 2(a), where one unit cell is shown in green with basis vectors $\vec{a}_1 = (3,0)$ and $\vec{a}_2 = (0,3)$. This lattice can be deformed into the (topologically equivalent) $\frac{1}{5}$ -depleted square lattice [25,26], which is known for the model of the quasi two-dimensional compound CaV_4O_9 . Thus the octagon-square lattice is also called as deformed $\frac{1}{5}$ -depleted square lattice. It is sometimes also called as decorated square lattice [27,28]. The hopping amplitudes on thick and broken lines are denoted by t and t' , respectively. The Hamiltonian is given by

$$\mathcal{H} = -t \sum_{(i,j) \in \text{thick, oriented}} e^{i\pi/4} c_i^\dagger c_j - t' \sum_{(i,j) \in \text{broken}} c_i^\dagger c_j + \text{H.c.}, \quad (21)$$

where “thick, oriented” and “broken” refer, respectively, to the links drawn with arrows and those drawn as broken lines in Fig. 2(a). We also assume $t > t' > 0$.

By the choice of $e^{i\pi/4}$ hopping phase on the oriented thick lines, there is a π flux in every square. Therefore, it can be regarded as a model of coupled π -flux rings by weak hopping t' . In order to prove $E_0^{\text{B}} > E_0^{\text{F}}$ rigorously in the coupled rings, we seek a lower bound for E_0^{B} and an upper bound for E_0^{F} . If the former is higher than the latter, the desired inequality is proved. We introduce the positive-semidefinite

operators

$$A = t' \sum_{(i,j) \in \text{broken}} (c_i^\dagger + c_j^\dagger)(c_i + c_j) \geq 0, \quad (22)$$

$$B = t' \sum_{(i,j) \in \text{broken}} (c_i^\dagger - c_j^\dagger)(c_i - c_j) \geq 0, \quad (23)$$

where $A \geq 0$ means $\langle \Phi | A | \Phi \rangle \geq 0$ for any state $|\Phi\rangle$. Therefore, the Hamiltonian for fermions and bosons can be written as

$$\mathcal{H}^F = \tilde{\mathcal{H}}^F - A = \sum_{\diamond} h_{\diamond}^F - A, \quad (24)$$

$$\mathcal{H}^B = \tilde{\mathcal{H}}^B + B = \sum_{\diamond} h_{\diamond}^B + B, \quad (25)$$

where $h_{\diamond}^F = -t \sum_{i=1}^4 (e^{i\pi/4} c_i^\dagger c_{i+1} + \text{H.c.}) + t' \sum_{i=1}^4 c_i^\dagger c_i$ and $h_{\diamond}^B = -t \sum_{i=1}^4 (e^{i\pi/4} c_i^\dagger c_{i+1} + \text{H.c.}) - t' \sum_{i=1}^4 c_i^\dagger c_i$, the cluster Hamiltonians defined on a solid-line square for fermions and bosons, respectively. Noticing h_{\diamond} commutes with each other, the ground-state energy of $\tilde{\mathcal{H}}$ is simply given by the summation [29]

$$\tilde{E}_0 = \sum_{\diamond_i} \epsilon_{\diamond_i}, \quad (26)$$

where \tilde{E}_0 and ϵ_{\diamond_i} are the ground-state energy of $\tilde{\mathcal{H}}$ and that of h_{\diamond_i} on i th π -flux square, respectively.

Because the operator B is positive semidefinite, the ground-state energy of bosons satisfies

$$E_0^B = \langle \Phi | \mathcal{H}^B | \Phi \rangle \geq \langle \Phi | \tilde{\mathcal{H}}^B | \Phi \rangle \geq \tilde{E}_0^B = \sum_{\diamond_i} \epsilon_{\diamond_i}^B, \quad (27)$$

where $|\Phi\rangle$ is assumed as the ground state of \mathcal{H}^B .

On the other hand, an upper bound of fermions can be derived as

$$\begin{aligned} E_0^F &= \langle \Psi | \mathcal{H}^F | \Psi \rangle \leq \langle \tilde{\Psi} | \mathcal{H}^F | \tilde{\Psi} \rangle \leq \langle \tilde{\Psi} | \tilde{\mathcal{H}}^F | \tilde{\Psi} \rangle \\ &= \tilde{E}_0^F = \sum_{\diamond_i} \epsilon_{\diamond_i}^F, \end{aligned} \quad (28)$$

where $|\Psi\rangle$ and $|\tilde{\Psi}\rangle$ are the ground states of \mathcal{H}^F and $\tilde{\mathcal{H}}^F$, respectively.

By exact diagonalization, we obtain the ground-state energies $\epsilon_{\diamond}^{\text{B,F}}(m)$ in given m particle sectors, shown in Table I in Appendix D. The number of unit cells is assumed as N . From the results of exact diagonalization, a lower bound for bosons is given by $E_0^B \geq -2N(t + t')$ when $t'/t \leq 2 - \sqrt{2}$, or $E_0^B \geq -N(\sqrt{2}t + 3t')$ when $2 - \sqrt{2} < t'/t < 1$. An upper bound for fermions is given by the \tilde{E}_0^F , which is dependent on the density pattern on the whole lattice. At half-filling, an upper bound of fermions is obtained as

$$E_0^F \leq -2N(\sqrt{2}t - t'). \quad (29)$$

Thus, when the ratio falls in this range $t'/t < (\sqrt{2} - 1)/2$, we have $E_0^B > E_0^F$.

Instead of searching an upper bound of fermions, the ground-state energy of fermions can be exactly calculated at certain filling. For convenience, t is set equal to 1. In the single-particle sector, the exact dispersion relations are

obtained by Fourier transformation:

$$E_{\pm}^{(1)} = \pm \sqrt{(t')^2 + 2 - 2t' \sqrt{1 - \sin(3k_x) \sin(3k_y)}},$$

$$E_{\pm}^{(2)} = \pm \sqrt{(t')^2 + 2 + 2t' \sqrt{1 - \sin(3k_x) \sin(3k_y)}},$$

where (k_x, k_y) is the wave number which belongs to the reduced Brillouin zone $-\pi/3 \leq k_{x,y} < \pi/3$. The ground-state energy of fermions at $\mu = 0$, which corresponds to the half-filling, is given as

$$E_0^F = \sum_{k_x, k_y} [E_-^{(1)}(k_x, k_y) + E_-^{(2)}(k_x, k_y)]. \quad (30)$$

Under the assumption that the lattice is of size $9L^2$, the number of unit cells N equals L^2 . In the thermodynamic limit $L \rightarrow \infty$, the ground-state energy of fermions per unit cell at half-filling is given by the integral of the lowest two bands [shown in Fig. 2(b)] in the reduced Brillouin zone

$$\begin{aligned} \frac{E_0^F}{N} &= - \int_{-\pi}^{\pi} \frac{d\tilde{k}_x}{2\pi} \int_{-\pi}^{\pi} \frac{\tilde{k}_y}{2\pi} [\sqrt{(t')^2 + 2 + 2t' \sqrt{1 - \sin \tilde{k}_x \sin \tilde{k}_y}} \\ &\quad + \sqrt{(t')^2 + 2 - 2t' \sqrt{1 - \sin \tilde{k}_x \sin \tilde{k}_y}}]. \end{aligned} \quad (31)$$

It is easily verified that the reversed natural inequality holds with small ratio of t'/t , by comparison of the lower bound of bosons and numerical integral of Eq. (31) with given value of t' . For example, when $t = 1$ and $t' = 0.1$, $E_0^B \geq -2.2N > E_0^F = -2.831967N$. When $t' = 0.4$, $E_0^B \geq -2.8N > E_0^F = -2.885971N$. The exact result is of course consistent with the rigorous upper bound (29).

Our conjecture that the reversed inequality is kept in the coupled π -flux rings with weak enough inter-ring hopping is now verified in coupled-square lattice. Moreover, the validity of the conjecture should not depend on the specific lattice. As another example, a proof of the reversed inequality for the breathing kagome lattice at certain filling, which can be regarded as an realization of a coupled-triangle lattice, is presented in Appendix E.

C. System with flux in 2D and 3D

As we discussed in Sec. IV A, the energy difference between bosons and fermions on a ring is due to finite-size effect, and indeed vanishes in the thermodynamic limit. This is rather natural, as it is only the entire system as a ring that contains π flux. As a simple extension of the idea, here we consider the two-dimensional square lattice in a uniform magnetic field, described by the Hamiltonian

$$\mathcal{H} = - \sum_{\langle j,k \rangle} (t_{jk} c_j^\dagger c_k + \text{H.c.}), \quad (32)$$

where $t_{jk} = t \exp(i\Phi_{jk}/\Phi_0)$ and $t > 0$. The flux passing through every plaquette is $\sum_{\square} \Phi_{jk} = \Phi$. With periodic boundary condition, the total flux is quantized as an integral multiple of flux quantum ($\Phi_0 = hc/e$ is 2π in our unit). The magnetic field introduces frustration, through the existence of complex hopping amplitudes t_{jk} . To investigate all the possible values of flux per plaquette, the string gauge [30] is employed. The string gauge is constructed as follows. First, we choose (the

center of) an arbitrary plaquette S as the origin, and draw an oriented path (arrow) from the origin S to every other plaquette. Each oriented path consists of straight segments connecting the centers of neighboring plaquettes. Once such paths are constructed, the vector potential on each link is set to $2\pi mn/N$, where m is the total number of arrows cutting the edge from the left to the right with respect to the direction of hopping, and n is an arbitrary integer satisfying $0 \leq n < N$. Since one of the arrows terminates in each plaquette, the flux piercing the plaquette is then $\Phi = n\Phi_0/N$. At the origin S , where $N - 1$ arrows flow from, the flux appears to be $\Phi = -n(N - 1)\Phi_0/N$ instead. However, this is equivalent to $\Phi = n\Phi_0/N$ since the flux per plaquette is defined only modulo Φ_0 . In this way, the uniform flux $n\Phi_0/N$ is realized in every plaquette using the string gauge, although the vector potential is generally not uniform (translation invariant).

By exact diagonalization, the ground-state energies of bosons and fermions are obtained with different particle densities ($n_e = M/N$, where M is the number of particles) and various values of flux. The relative difference of the ground-state energies in the 4×7 and 5×6 lattices is shown in Fig. 3. Here, the ground-state energy density differences between bosons and fermions is shown color coded in the two-dimensional parameter space of the particle density n_e and flux density Φ/Φ_0 . The natural inequality holds in white regions, while it is violated in colored regions. It should be noted that the violation is not necessarily related to band topology. In fact, in the entire region of the parameter space except for $\Phi = 0$, each of the single-particle bands is characterized by a nonvanishing Chern number [31]. Nevertheless, the violation of the natural inequality does not happen everywhere. Instead, as shown in Fig. 3, the violation is nontrivially related to particle density or filling fraction. (Nontrivial dependence on the filling is also found in other models discussed in other sections.) To understand the physical origin of the filling dependence of the relative ground-state energy, one can recall statistical transmutation [32,33] via a flux attachment. When $\Phi/\Phi_0 = n_e$, the background magnetic field can be effectively absorbed by attaching one flux quantum to each particle, at the mean field level ignoring quantum fluctuations. The flux attachment transforms fermions into bosons and vice versa. In this picture, along the diagonal lines in the plot where $\Phi/\Phi_0 = n_e$ holds, fermions and hard-core bosons in the magnetic field are mapped, respectively, to hard-core bosons and fermions in zero field. According to Theorem 1, the hard-core bosons have a lower ground-state energy than fermions in zero field. It is thus implied that the violation of the natural inequality would occur along the diagonal lines. It should be noted that the flux attachment argument is not rigorous and its range of validity is not established. Nevertheless, it is remarkable that our numerical calculation indeed reveals the strongest violation along the diagonal lines, as expected from the naive flux attachment argument.

The effect of filling can also be understood in a different way: the energy levels of free electrons (without a lattice or a periodic potential) in a uniform magnetic field are quantized into Landau levels, which can be regarded as completely flat bands. In the presence of the lattice, each Landau level is split into dispersive subbands. Nevertheless, one may still regard them as descendants of the Landau level with small dispersion.

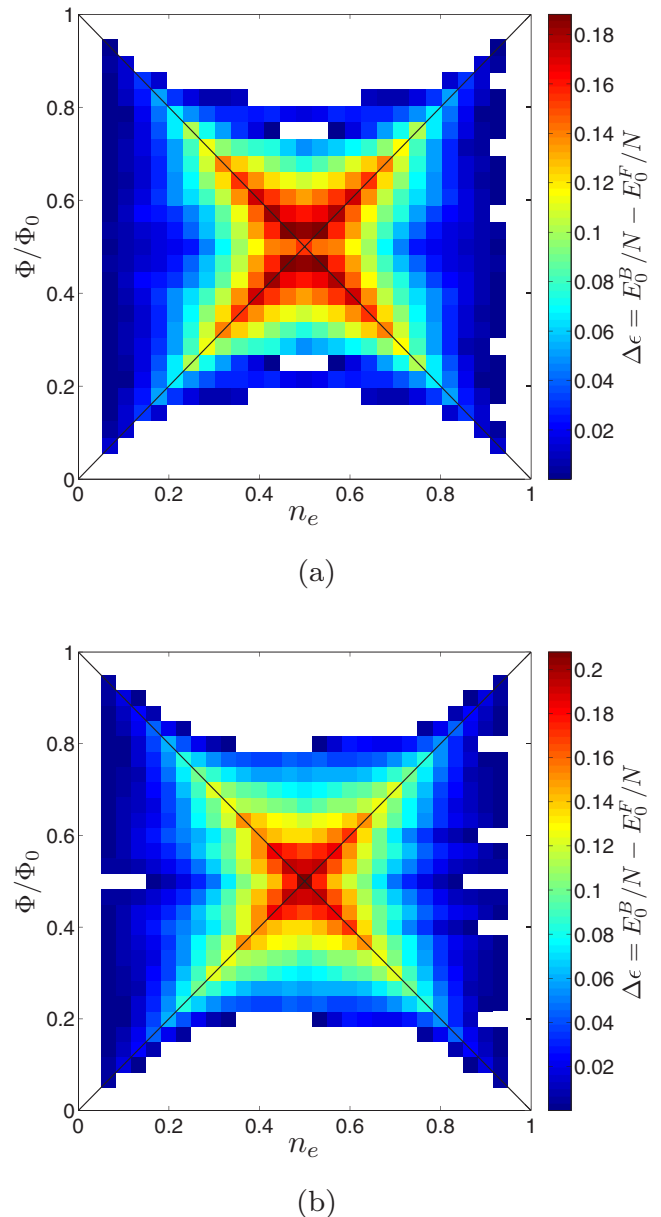


FIG. 3. The energy density difference $\Delta\epsilon = E_0^B/N - E_0^F/N$ between bosons and fermions on (a) 4×7 and (b) 5×6 square lattices, where n_e is the number of particles per site and Φ/Φ_0 is the number of the flux quanta per plaquette.

Since the main “disadvantage” of fermions for lowering the ground-state energy is the Pauli exclusion principle which forces some of the fermions to occupy higher-energy states, less dispersive bands are helpful to reverse the natural inequality. (This mechanism will be discussed more explicitly in Sec. IV D.) The filling $n_e = \Phi/\Phi_0$ corresponds to completely filling the lowest Landau level, and thus can be advantageous to reverse the natural inequality.

We note in passing that, although our numerical results in Fig. 3 appear almost particle-hole symmetric, a careful examination shows that it is not exactly particle-hole symmetric. This is because the finite-size lattices used in our calculations are not bipartite, due to the limitation of the system sizes in the exact

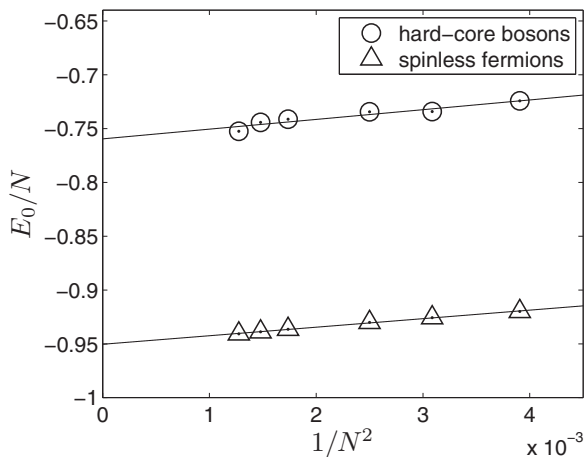


FIG. 4. Finite-size scaling of ground-state energies in two-dimensional square lattice with $(N/2 - 1)\Phi_0/N$ flux per plaquette at filling fraction $(N/2 - 1)/N$. The fitting functions are $E_0^B/N = -0.7593 + 8.973/N^2 + O(N^{-4})$ for hard-core bosons and $E_0^F/N = -0.9507 + 8.043/N^2 + O(N^{-4})$ for fermions, respectively. The extrapolated ground-state energy density for fermions matches well with the exact result $-0.958\,091$ in Eq. (33).

diagonalization calculation; the bipartiteness is needed for the fermion system on a finite lattice to possess the particle-hole symmetry.

We plotted Fig. 4 to show the finite-size scalings. Figure 4 is the finite-size scaling with $(N/2 - 1)\Phi_0/N$ flux per plaquette near half-filling $(N/2 - 1)/N$. The exact half-filling on finite-size lattices ($N/2$ particles on N sites) and the corresponding $\Phi_0/2$ flux per plaquette are avoided to reduce the strong finite-size effect (oscillatory behavior) due to commensuration, while the extrapolation corresponds to the half-filling in the thermodynamic limit. The extrapolation suggests that the fermions have a lower ground-state energy in the thermodynamic limit. Actually, we can prove [8] rigorously in the following that this is indeed the case.

As proved by Lieb [34], the optimal energy minimizing flux is π per plaquette for square lattice at half-filling. Let us discuss the square lattice with π flux per plaquette, described by the Hamiltonian (32). For convenience, we choose the gauge so that the hopping amplitude t_{jk} is $+1$ on the black links and -1 on the blue ones as shown in Fig. 5(a). By taking a 2×2 unit

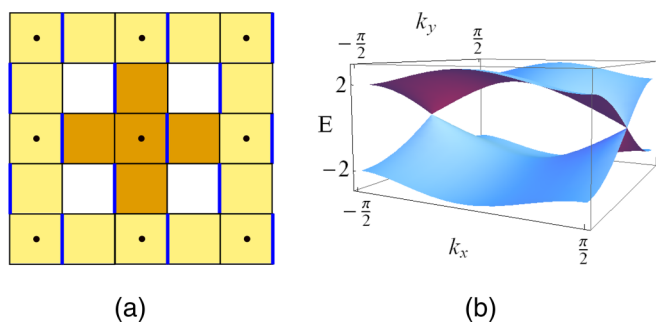


FIG. 5. (a) The square lattice with π flux in each plaquette. The brown cross represents a cluster of 12 sites. (b) The energy bands in the first Brillouin zone.

cell (which is twice as large as the minimal magnetic unit cell), the dispersion relation is $E_{\pm} = \pm\sqrt{4 + 2\cos 2k_x - 2\cos 2k_y}$, where (k_x, k_y) is the wave number which belongs to the reduced Brillouin zone $-\pi/2 \leq k_{x,y} < \pi/2$. The bands in the first Brillouin zone are shown in Fig. 5(b). Each energy level is doubly degenerate. The ground-state energy of fermions at zero chemical potential, which corresponds to the half-filling, is given as $E_0^F = \sum_{k_x, k_y} 2E_-(k_x, k_y)$, where the factor 2 comes from the double degeneracy. For the square lattice of size $L_x \times L_y$ ($N = L_x L_y$), $k_{x,y}$ is respectively quantized as integral multiples of $2\pi/L_{x,y}$. Thus, in the thermodynamic limit $L_{x,y} \rightarrow \infty$, the ground-state energy of the fermionic model at $\mu = 0$ is obtained exactly as

$$\begin{aligned} \frac{E_0^F}{N} &= -\frac{1}{2} \int_{-\pi}^{\pi} \frac{d\tilde{k}_x}{2\pi} \int_{-\pi}^{\pi} \frac{d\tilde{k}_y}{2\pi} \sqrt{4 + 2\cos \tilde{k}_x - 2\cos \tilde{k}_y} \\ &= -0.958\,091. \end{aligned} \quad (33)$$

The extrapolated ground-state energy density of fermions from finite-size scaling in Fig. 4 matches well with the exact result.

We consider the grand canonical ground-state energy of bosons at the same chemical potential ($\mu = 0$). We rewrite the Hamiltonian $\mathcal{H} = \sum_{\alpha} h_{\alpha}$, where $h_{\alpha} = -\frac{1}{2} \sum_{(j,k) \in \mathcal{C}_{\alpha}} (t_{jk} c_j^{\dagger} c_k + \text{H.c.})$ is the cluster Hamiltonian defined on a 12-site cross-shaped cluster as shown in Fig. 5(a). The whole lattice is covered by the brown cross-shaped clusters with the same pattern of hopping amplitudes within the cluster, whose centers are denoted by the black dots. Therefore, each cluster overlaps with four neighboring clusters and each link appears in two different clusters when periodic boundary conditions are imposed. The factor $\frac{1}{2}$ in h_{α} compensates this double counting. By Anderson's argument [29,35,36], the ground-state energy E_0^B of \mathcal{H}^B satisfies $E_0^B \geq \sum_{\alpha} \epsilon_{\alpha}^0$, where ϵ_{α}^0 is the ground-state energy of h_{α} . The ground-state energy of h_{α} on a cluster with a given particle number m obtained by exact diagonalization is shown in Table II in Appendix D. The grand canonical ground-state energy of the cross-shaped cluster is obtained as $\epsilon_{\alpha}^0 = -3.609\,035$. Assuming the number of sites in the square lattice is N , we obtain

$$E_0^B/N \geq -3.609\,035/4 = -0.902\,259 > E_0^F/N, \quad (34)$$

where $N/4$ is the number of clusters. Thus, hard-core bosons have a higher ground-state energy than fermions at half-filling ($\mu = 0$), even in the thermodynamic limit, as expected from extrapolation from finite-size scaling and statistical transmutation argument [8,32,33,37,38].

We note that the choice of cluster decomposition is not unique for a given model. In order to prove the reversal of the natural inequality, an appropriate choice of the cluster decomposition with a sufficiently high lower bound for the ground-state energy of bosons relative to that of fermions is necessary. Here, we have discussed the decomposition into cross-shaped clusters, which can be handled relatively easily but is still useful for proving the reversed natural inequality. Decomposition into larger clusters is expected to give a more precise estimation of a lower bound. Similar comment also applies to the cluster decompositions discussed in Sec. IV D.

For other values of flux per plaquette or filling fraction, there is no rigorous proof available at present. However, the finite-size scaling of numerical data with $\Phi_0/4$ flux per plaquette at

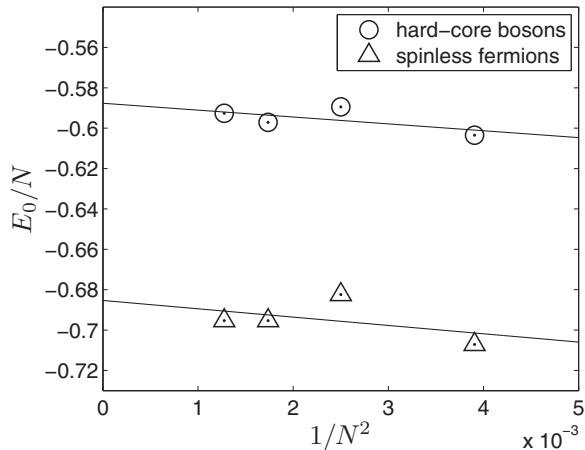


FIG. 6. Finite-size scaling of ground-state energies in two-dimensional square lattice with $\Phi_0/4$ flux per plaquette at quarter filling. The fitting functions are $E_0^B/N = -0.5877 - 3.405/N^2 + O(N^{-4})$ for hard-core bosons and $E_0^F/N = -0.6853 - 4.125/N^2 + O(N^{-4})$ for fermions, respectively.

quarter filling, shown in Fig. 6, suggests that fermions have a lower ground-state energy in the thermodynamic limit.

The violation of the natural inequality in systems with flux is not restricted to two dimensions. We have indeed proved that the natural inequality could be reversed in a tight-binding model on a three-dimensional pyrochlore lattice with flux [8].

D. Cluster decomposition in flat-band models

In this section, we present a rigorous proof that the reversed natural inequality also holds in several flat-band models, even in the thermodynamic limit. Although the existence of a flat band is neither a necessary nor sufficient condition to violate Eq. (1), it does tend to help: when the lowest flat band is occupied by the fermions, there is no extra energy gain due to Pauli exclusion principle. Therefore, the inversion of the natural inequality has a better chance to be realized in flat-band models. Here, we show that the inequality (1) is indeed violated in a few examples with flat bands, by a cluster decomposition technique.

First, we discuss the delta-chain model, for which the violation of Eq. (1) was numerically found for small clusters [39,40]. The Hamiltonian of the model can be written in the following form [41,42]:

$$\mathcal{H} = \sum_{j=1}^N a_j^\dagger a_j, \quad (35)$$

where the a operator, which acts on each triangle, is defined as $a_j = c_{2j-1} + \sqrt{2}c_{2j} + c_{2j+1}$. Periodic boundary condition is used to identify c_{2N+1} with c_1 . The Hamiltonian \mathcal{H} corresponds to a model with negative hopping amplitudes t_{jk} [as defined in Eq. (2)], which lead to frustration.

The model in the single-particle sector has two bands. The lower flat band with zero energy is spanned by states annihilated by a_j 's. We note that the Hamiltonian (35) is modified from that in Ref. [39] by a constant chemical potential, so that the flat band has exactly zero energy. Thus, the ground-state



FIG. 7. An example of decomposition of the delta-chain Hamiltonian to clusters with $p = 4$ unit cells including one decoupled site at the top of the dashed triangle.

energy of the fermionic version of the model (35) is zero as long as the filling fraction ν satisfies $\nu \leq \frac{1}{2}$.

On the other hand, in general, construction of the ground state of a system of many interacting bosons is not straightforward even if the single-particle states are known exactly. However, the flat band in the geometrically frustrated antiferromagnet also implies the existence of nonoverlapping localized zero-energy states. It was first pointed out in Ref. [43], and was later applied to various problems [44,45]. In the case of the delta chain, the ground-state energy E_0^B of bosons is zero as long as $\nu \leq \frac{1}{4}$ since each boson can occupy different nonoverlapping localized zero-energy states [43–45].

Now, let us derive a nontrivial lower bound for E_0^B for filling fractions $\nu > \frac{1}{4}$. We decompose the model into clusters, each containing p unit cells:

$$\mathcal{H} = \sum_{n=0}^{N/p-1} \mathcal{H}_n^{(p)} + \sum_{n=1}^{N/p} a_{np}^\dagger a_{np}, \quad (36)$$

where $\mathcal{H}_n^{(p)} = \sum_{j=1}^{p-1} a_{np+j}^\dagger a_{np+j}$ is the Hamiltonian for the solid triangles as in Fig. 7. Since the second term $\sum_{n=1}^{N/p} a_{np}^\dagger a_{np}$, describing hoppings on dashed triangles, is positive semidefinite, the ground-state energy \tilde{E}_0^B of the first term $\tilde{\mathcal{H}} = \sum_{n=0}^{N/p-1} \mathcal{H}_n^{(p)}$ satisfies $\tilde{E}_0^B \leq E_0^B$. $\tilde{\mathcal{H}}$ is a sum of mutually commuting cluster Hamiltonians $\mathcal{H}_n^{(p)}$. Thus, \tilde{E}_0^B is simply given by the sum of the ground-state energies of all clusters. The particle number within each cluster is also conserved separately in $\tilde{\mathcal{H}}$. Let us choose $p = 4$ as in Fig. 7, so that the cluster contains eight sites. The ground-state energy in each sector with fixed particle number m is obtained by exact diagonalization of the eight-site cluster, which is shown in Table III in Appendix D. We find $\epsilon_0^{(4)}(m) \geq \Delta_{DC}^{(4)} = 0.372605$ for $4 \leq m \leq 8$, while $\epsilon_0^{(4)}(m) = 0$ for $0 \leq m \leq 3$.

If we consider the filling fraction in the range $\frac{3}{8} < \nu \leq \frac{1}{2}$, it follows from Dirichlet's box principle that there is at least one cluster which contains four or more particles. Thus, in this range, $\tilde{E}_0^B \geq \Delta_{DC}^{(4)}$ for any system size N , while $E_0^F = 0$. Therefore, the inversion of the ground-state energies holds also in the thermodynamic limit.

The outcome of the above argument depends on the cluster size taken. In fact, the range of filling fraction ν for which we have proved the violation of Eq. (1) is not optimal. In Appendix F, using a different technique, we will extend the range to $\frac{1}{4} < \nu \leq \frac{1}{2}$; the lower bound $\frac{1}{4}$ is in fact optimal.

This method can be easily extended to other lattices. For example, the standard nearest-neighbor hopping model on the kagome lattice can be written as

$$\mathcal{H} = \sum_{\alpha} a_{\Delta_{\alpha}}^\dagger a_{\Delta_{\alpha}} + \sum_{\alpha} a_{\nabla_{\alpha}}^\dagger a_{\nabla_{\alpha}}, \quad (37)$$

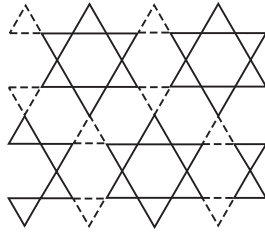


FIG. 8. The 12-site clusters of “Star of David” shape are shown in solid lines on kagome lattice.

where Δ_α and ∇_α are elementary triangles pointing up and down, respectively, of the kagome lattice, as shown in Fig. 8. We define $a_{\Delta_\alpha} \equiv c_{\alpha_1} + c_{\alpha_2} + c_{\alpha_3}$, where $\alpha_{1,2,3}$ refer to the three sites belonging to Δ_α , and likewise for a_{∇_α} . The fermionic version of the model has three bands, the lowest of which is a flat band at zero energy [42,46,47]. Thus, $E_0^F = 0$ when $\nu \leq \frac{1}{3}$.

For the ground-state energy of the bosonic version, we can use the cluster decomposition technique similar to what we have discussed above for the delta chain. Let us choose the 12-site cluster of the “Star of David” shape, which is shown by solid lines in Fig. 8. The ground-state energy of the cluster in each sector with m particles is shown in Table IV in Appendix D. The ground-state energy $\epsilon_0^{\text{cluster}}$ of each cluster is zero with $m \leq 3$, but is positive with $m \geq 4$. Thus, invoking Dirichlet’s box principle again, Eq. (1) is violated for filling fraction $\frac{1}{4} < \nu \leq \frac{1}{3}$. This conclusion also holds in the thermodynamic limit, where the system size N is taken to the infinity while keeping the filling fraction ν constant.

E. Extension to interacting systems

Throughout most of this paper, we limited the interactions to the hard-core ones for technical simplicity: fermions are then free, while bosons are subject only to the hard-core interaction. Here, we comment briefly on the effect of the other possible interactions. Theorems 1, 2, and 3 are actually valid even in the presence of density-density interactions other than the hard-core interaction. Introduction of additional density-density interactions should not essentially modify the comparison of the ground-state energies, as it would affect bosonic and fermionic models in a similar manner. For example, the interaction terms are introduced in diagonal terms in the matrix of Hamiltonian in Theorem 1, which do not affect the conclusion of the comparison. Therefore, in order to understand the essence of physics in the present problem, it would suffice to consider the hard-core interactions only.

That said, in fact, one can actually prove that the inequality (1) is violated even in the presence of an additional density-density interaction in the one-dimensional ring with π flux discussed in Sec. IV A. This can be seen by noting that Jordan-Wigner transformation applies regardless of the presence of density-density interactions, and implies

$$E_0^F(\Phi = \pi) = E_0^B(\Phi = 0), \quad (38)$$

where the number of particles is assumed to be even. Then, we see that a lattice version of Simon’s theorem [18] also applies

in the presence of the interaction

$$E_0^B(\Phi = \pi) \geq E_0^B(\Phi = 0), \quad (39)$$

giving $E_0^B(\Phi = \pi) \geq E_0^F(\Phi = \pi)$. Furthermore, under appropriate assumptions, it is possible to prove the strict inequality $E_0^B(\Phi = \pi) > E_0^F(\Phi = \pi)$ in the presence of interaction, with an argument similar to the proof of Theorems 1 and 4.

V. CONCLUSIONS AND DISCUSSIONS

In this paper, we have proved that the ground-state energy of hard-core bosons is lower than that of fermions if there is no frustration in the hopping. The effect of the statistical phase of fermions can then be understood as a frustration since it results in destructive quantum interferences among different paths. In fact, the phase introduced by Fermi statistics can be effectively described by a magnetic flux, after the mapping to the single-particle tight-binding model on a fictitious lattice which represents the Fock space. In this sense, the nonstrict version of the natural inequality is a corollary of the lattice version of the diamagnetic inequality. On the other hand, we also proved a strict version of the natural inequality, under certain conditions. The key of the proof is the contribution of an exchange process of two particles, which is exactly what demonstrates the statistics of the particles. The argument is also applied to prove the strict version of the diamagnetic inequality on the lattice.

Once a magnetic flux is introduced in the original many-particle problem, the hopping terms can be frustrated. The hopping frustration can partially cancel the statistical frustration of fermions, hinting at the possibility that the natural inequality can be reversed in the presence of hopping frustration. We proved rigorously that the natural inequality is indeed reversed in the presence of frustration, in various examples. They include one-dimensional π -flux ring, coupled rings in two dimensions, systems with flux in 2D and 3D, flat-band models by cluster decomposition technique. Finally, we demonstrated an example of the violation of natural inequality with other interactions than hard-core constraint.

In this paper, we focused on the case of hard-core bosons for simplicity. However, Theorems 1, 2, and 3 can be readily generalized to soft-core bosons. This is because hard-core bosons can be regarded as a special limit of more general interacting bosons. That is, we can introduce the onsite interaction $\frac{\mathcal{U}}{2}n_i(n_i - 1)$; the hard-core constraint can be then implemented by taking $\mathcal{U} \rightarrow +\infty$. The onsite interaction term is positive semidefinite for bosons, if $\mathcal{U} \geq 0$. Thus, the hard-core bosons have a higher ground-state energy than that of soft-core bosons at finite \mathcal{U} . This implies the applicability of Theorems 1, 2, and 3 to the soft-core bosons.

Our analysis of the hard-core boson model also suggests that the natural inequality for soft-core bosons could be reversed by introducing the hopping frustrations. However, soft-core bosons are closer to free bosons, which never violate the natural inequality because of the simple argument based on perfect BEC. Thus, the violation would be more difficult to be realized in soft-core bosons, compared to the hard-core bosons discussed in this paper. Other open problems include comparison in the presence of other degrees of freedom such as the orbital/ flavor of particles. The nonstrict version of the

theorems can be easily generalized to the case with multiple orbitals/flavors.

In this paper, we have also discussed briefly the comparison of the ground-state energies of spinful bosons and fermions. The natural inequality still holds in the absence of hopping frustration. Although we did not discuss explicitly for spinful particles, the natural inequality is expected to be violated by introducing appropriate hopping frustration.

Here, it should be recalled that physical magnetic field not only introduces phase factors in hopping terms, but is also coupled to the spin degrees of freedom via the Zeeman term. Thus, the Zeeman term should be also taken into account, in order to discuss a physical magnetic field applied to the system of charged particles. The Zeeman term acts as different chemical potentials for up-spin and down-spin particles. Thus, much of the discussion in this paper is still applicable. For example, in the absence of hopping frustration, the natural inequality still holds even in the presence of the Zeeman term. Once hopping frustration is introduced, the natural inequality can be violated. However, exactly how the violation of the natural inequality occurs does depend on the chemical potential, and on the Zeeman effect in the case of spinful particles.

On the other hand, we also note that phase factors in hopping terms and Zeeman coupling are two distinct effects, which in principle can be controlled independently. In fact, for neutral cold atoms, the phase factor in hoppings is usually introduced as “synthetic gauge field” [48] instead of the physical magnetic field. This does not produce Zeeman coupling, making it possible to study the effect of hopping frustrations separately from that of the Zeeman effect.

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APPENDIX A: PROOF OF THEOREM 2

Proof. Since the total number operator $M = \sum_{j\sigma} n_{j\sigma}$ and total magnetization $S_z = 1/2 \sum_j (n_{j\uparrow} - n_{j\downarrow})$ commute with the Hamiltonian (9), one can diagonalize the Hamiltonian in each sub-Hilbert space with fixed values of M and S_z . Each sub-Hilbert space has definite numbers of up- and down-spin particles. Let $|\phi^\mu\rangle_\uparrow \equiv |n_{j\uparrow}^\mu\rangle$ ($\mu = 1, 2, \dots, u$) be the occupation-number basis for up-spin particles, and $|\psi^v\rangle_\downarrow \equiv |n_{j\downarrow}^v\rangle$ ($v = 1, 2, \dots, v$) be the occupation-number basis for down-spin particles. Then, we can take the direct product

$|\Phi^a\rangle = |\psi^v\rangle_\downarrow \otimes |\phi^\mu\rangle_\uparrow$, where $a = 1, 2, \dots, uv$, as the basis of the sub-Hilbert space mentioned above.

The Hamiltonian can be rewritten as

$$\mathcal{H} = \mathcal{H}_t + \mathcal{H}_{\text{int}}, \quad (\text{A1})$$

$$\mathcal{H}_t = \mathbb{1}^\downarrow \otimes \mathcal{H}_t^\uparrow + \mathcal{H}_t^\downarrow \otimes \mathbb{1}^\uparrow, \quad (\text{A2})$$

where $\mathcal{H}_t^\sigma = -\sum_{j \neq k} (t_{jk} c_{j\sigma}^\dagger c_{k\sigma} + \text{H.c.})$. The matrix elements of the number operator $n_{j\sigma}$ are the same in this basis for hard-core bosons and fermions. We introduce the operator $\mathcal{K}^{\text{B,F}} \equiv -\mathcal{H}^{\text{B,F}} + C\mathbb{1}$ with a constant C . Choosing C large enough, we make all the eigenvalues and all the diagonal matrix elements of $\mathcal{K}^{\text{B,F}}$ positive. The matrix elements of bosonic and fermionic Hamiltonians obey the relation

$$\mathcal{K}_{ab}^{\text{B}} = \begin{cases} |\mathcal{K}_{ab}^{\text{F}}| & (a \neq b), \\ \mathcal{K}_{aa}^{\text{F}} & (a = b), \end{cases} \quad (\text{A3})$$

where the diagonal terms correspond to \mathcal{H}_{int} and the off-diagonal terms correspond to \mathcal{H}_t . The nonstrict inequality is easily proved by variational principle in the same manner employed in the proof of Theorem 1. Here, we focus on the discussion on strict natural inequality for spinful case with finite U_j .

With finite U_j 's, one site can be occupied by one spin-up particle and one spin-down particle. Thus, spin-up particles can move as spinless particles for any given configuration of spin-down particles, and vice versa. Of course, the interaction term \mathcal{H}_{int} , which is diagonal in this basis, is affected by the presence of particles with opposite spins. However, as far as the irreducibility (connectivity) of Hamiltonian is concerned, one can regard the system as two independent systems of hard-core particles. As a consequence, when the lattice Λ is connected, any pair of basis states $|\Phi^a\rangle_{\text{B}}$ and $|\Phi^b\rangle_{\text{B}}$ are connected to each other by successive applications of the hopping term in \mathcal{K}^{B} . Together with the property $\mathcal{K}_{ab}^{\text{B}} \geq 0$, \mathcal{K}^{B} satisfies the condition of the Perron-Frobenius theorem. When the number of particles $M \geq 3$, there are at least two particles with the same spin. The condition $M \leq 2N - 3$ guarantees that there are at least two spaces which can accommodate two particles with the same spin. Thus, when the number of particles falls in the range $3 \leq M \leq 2N - 3$, we can exchange two identical particles and return back to the same state, based on the branch structure as in Fig. 1. Therefore, when U_j 's are finite, the lattice is connected and has a branch structure, and $3 \leq M \leq 2N - 3$, two-particle exchange always happens. As in the proof of Theorem 1 for the spinless case, the strict inequality $E_0^{\text{B}} < E_0^{\text{F}}$ follows from the Perron-Frobenius theorem. ■

APPENDIX B: REMARKS ABOUT THE PROOF OF THEOREM 3 AND DISCUSSIONS

The nonstrict inequality remains unaffected by taking $U_j = +\infty$. Here, we focus on a sufficient condition for strict natural inequality with infinite repulsion for spinful case.

With infinite onsite repulsion, the maximum number of particles is N . The condition $M \geq 3$ is to guarantee there are at least two particles with the same spin such that they can be exchanged. For a lattice connected by exchange bonds, two particles on an exchange bond can be exchanged without

changing the configuration outside, by hopping a hole around the loop on which both the exchange bond and the hole lie [13]. Hence, when the number of particles M satisfies $3 \leq M \leq N - 1$, two particles with the same spin can be exchanged on an exchange-bond lattice by successive particle hoppings.

The property that the entire lattice is connected by exchange bonds can be verified [13] in various common lattices, such as triangular, square, simple cubic, fcc, or bcc lattices, in which nearest-neighbor sites are connected by nonvanishing hopping amplitudes. Thus, the above theorem holds for these lattices.

We also note that Nagaoka's ferromagnetism only applies to the system with single hole with respect to half-filling. However, this restriction is only necessary to guarantee that all the matrix elements are non-negative. The irreducibility of the Hamiltonian matrix does not require that there is only one hole. In fact, the breakdown of the positivity in the presence of more than one hole in the Hubbard model with $U_j = +\infty$ is precisely due to the Fermi statistics of the electrons. If we consider the "Bose-Hubbard model" with spin- $\frac{1}{2}$ bosons instead of electrons, all the matrix elements are non-negative in the occupation-number basis, for any number of holes. Thus, the Bose-Hubbard model with spin- $\frac{1}{2}$ bosons exhibit ferromagnetism for any filling fraction [49]. This non-negativity of the matrix elements for bosons is also essential for Theorem 3, which holds for any filling fraction.

The proofs of Theorems 1 and 2 are insensitive to the signs of the interaction terms V_{jk} and U_j . Namely, the natural inequality holds no matter the interaction is repulsive or attractive. The interesting aspect of the attractive interaction is that it will induce the Cooper pair of fermions. In the case of spinless fermions, the orbital part of the Cooper pair wave function must be antisymmetric with respect to the exchange of two fermions. This results in an extra cost in the kinetic energy. Such a fermionic BEC state thus has a higher ground-state energy than its bosonic counterpart, in full agreement of Theorem 1.

In contrast, in the case of spinful fermions, with attractive interaction, fermions could pair up in the nodeless s channel. In this case, there is no obvious reason why the fermions have a higher ground-state energy than bosons. Nevertheless, according to Theorem 2, spinful fermions still have strictly higher ground-state energy than corresponding bosons, even when the pairing is in the nodeless s channel.

This can be interpreted physically in the following way. If the pairing of two particles is completely robust, the problem is reduced to the identical problem of bosonic "molecules," whether the original particles are fermions or bosons. Then, the ground-state energies should be the same for fermions and bosons. However, in general, the pairing is not completely robust, and two pairs can (virtually) exchange each one of their constituent particles. The amplitude for such a process has negative sign only for fermions, leading to the nonvanishing energy difference between fermions and bosons. The exception occurs when the onsite attractive interaction between up- and down-spin particles is infinite ($U_j = -\infty$). Then, the pairs are completely robust, and no virtual exchange of constituent particles occurs; the ground-state energies for fermions and bosons become identical in this limit. On the other hand, with the infinite attraction, the irreducibility can not be satisfied. Because a hopping of a molecule requires its breaking, which

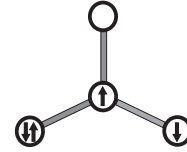


FIG. 9. A four-site lattice with four spins at half-filling and $S_z=0$.

costs an infinite energy and is thus prohibited. This implies that the bosonic molecules are completely localized in the model (9). Thus, the natural inequality is reduced to the trivial equality $E_0^B = E_0^F$ in the limit $U_j \rightarrow -\infty$.

In the following, as an example, we numerically demonstrate the above observations in spinful hard-core Bose-Hubbard and Fermi-Hubbard models on a four-site lattice as shown in Fig. 9. The Hamiltonian is given by

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} \sum_{\sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + \text{H.c.}) + U \sum_j n_{j\uparrow} n_{j\downarrow}, \quad (\text{B1})$$

where $t > 0$, $\langle i,j \rangle$ denotes a pair of neighboring sites, and the hard-core constraint $n_{j\sigma} = 0, 1$ is again imposed for the bosons. We consider the spin- $\frac{1}{2}$ bosons and fermions at half-filling (the total number of particles per site $\nu = 1$) and $S^z = 0$. That is, on this four-site cluster, there are two up-spin particles and two down-spin particles. The energy difference between spinful bosons and spinful fermions ($\Delta E = E_0^B - E_0^F$) is shown as a function of $U = U_j$ in Fig. 10.

Conforming to Theorem 2, $E_0^B \leq E_0^F$ holds for all range of U , independent of the sign of U . Moreover, $\Delta E(U)$ is symmetric along $U = 0$ due to particle-hole symmetry of Hubbard model at half-filling $\nu = 1$ [50].

When U is finite, fermions have strictly higher ground-state energy than bosons, again in agreement with the latter half of Theorem 2. When $U = +\infty$, on the other hand, the particles are completely immobile at half-filling and thus no particle exchange occurs. The ground-state energy is indeed exactly the same for fermions and for bosons in this limit. Likewise, in the limit of $U = -\infty$, either bosons or fermions form completely robust (and immobile) pairs, and the ground-state energies

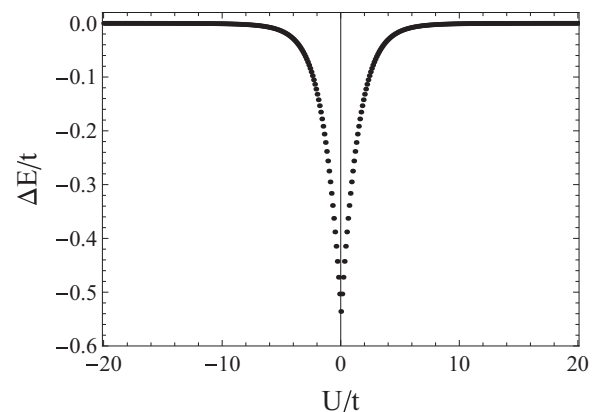


FIG. 10. Difference of ground-state energy ($\Delta E = E_0^B - E_0^F$) between hard-core bosons and fermions on the four-site lattice with a branch in $S_z = 0$ sector with four spins. The absolute value of energy difference decreases down to $\sim 10^{-8}t$ around $|U|/t = 100$.

TABLE I. The ground-state energies of fermions and hard-core bosons on a thick-line square as shown in Fig. 2(a), where m is the number of particles on a π -flux square. The results are used in the proof of π -flux octagon-square model in Sec. IV B.

m	$\epsilon_{\diamond}^F(m)$	$\epsilon_{\diamond}^B(m)$
1	$-\sqrt{2}t + t'$	$-\sqrt{2}t - t'$
2	$-2\sqrt{2}t + 2t'$	$-2t - 2t'$
3	$-\sqrt{2}t + 3t'$	$-\sqrt{2}t - 3t'$
4	$4t'$	$-4t'$

are exactly the same. In the present case, this can also be understood as a consequence of the particle-hole symmetry at half-filling [50], which maps $U \rightarrow -U$.

APPENDIX C: PROOF OF THEOREM 4

Proof. The proof is similar to that of Theorem 1. We can define the matrices $\mathcal{K}, \mathcal{K}'$ by

$$\mathcal{K}_{\alpha\beta} \equiv \tau_{\alpha\beta} + C\delta_{\alpha\beta}, \quad (C1)$$

$$\mathcal{K}'_{\alpha\beta} \equiv \tau'_{\alpha\beta} + C\delta_{\alpha\beta}, \quad (C2)$$

with a sufficiently large constant C so that \mathcal{K} and \mathcal{K}' are positive definite. We then define $\mathcal{L} \equiv \mathcal{K}^n$ and $\mathcal{L}' \equiv \mathcal{K}'^n$ for the length n of the loop with a nonvanishing flux. The positive definiteness of \mathcal{K} and \mathcal{K}' implies that \mathcal{L} and \mathcal{L}' are also positive definite, and thus all the diagonal matrix elements $\mathcal{L}_{\alpha\alpha}$ and $\mathcal{L}'_{\alpha\alpha}$ are strictly positive. Similarly to the proof of Theorem 1, $\mathcal{L}'_{\alpha\beta} \geq |\mathcal{L}_{\alpha\beta}|$ holds for any α, β . In particular, the diagonal matrix elements of \mathcal{L}' and \mathcal{L} are expanded as

$$\mathcal{L}'_{\alpha_0\alpha_0} = \sum_{\alpha_1, \dots, \alpha_{n-1}} \mathcal{K}'_{\alpha_0\alpha_1} \mathcal{K}'_{\alpha_1\alpha_2} \dots \mathcal{K}'_{\alpha_{n-1}\alpha_0}, \quad (C3)$$

$$\mathcal{L}_{\alpha_0\alpha_0} = \sum_{\alpha_1, \dots, \alpha_{n-1}} \mathcal{K}_{\alpha_0\alpha_1} \mathcal{K}_{\alpha_1\alpha_2} \dots \mathcal{K}_{\alpha_{n-1}\alpha_0}. \quad (C4)$$

TABLE II. The lowest energies of π -flux model on a 12-site cross-shaped cluster, as shown in Fig. 5(a). Here, m is the number of particles on the cluster. It shows that $\epsilon_0^\alpha(m=6)$ is the lowest ground-state energy. The results are used in the proof in Sec. IV C.

m	$\epsilon_0^\alpha(m)$
0	0
1	-1.096997
2	-2.013783
3	-2.629382
4	-3.086229
5	-3.415430
6	-3.609035
7	-3.415430
8	-3.086229
9	-2.629382
10	-2.013783
11	-1.096997
12	0

TABLE III. Ground-state energy $\epsilon_0^{(4)}(m)$ of the cluster Hamiltonian $\mathcal{H}_n^{(4)}$ for delta-chain model, as shown in Fig. 7, with m particles in a cluster. It shows the ground-state energy of the eight-site cluster is strictly positive when there are no less than four particles on this cluster. The results are used in Sec. IV D.

m	1	2	3	4	5	6	7	8
$\epsilon_0^{(4)}(m)$	0	0	0	0.372605	1.838145	4.323487	8	12

Each term in the expansion satisfies

$$\mathcal{K}'_{\alpha_0\alpha_1} \mathcal{K}'_{\alpha_1\alpha_2} \dots \mathcal{K}'_{\alpha_{n-1}\alpha_0} \geq |\mathcal{K}_{\alpha_0\alpha_1} \mathcal{K}_{\alpha_1\alpha_2} \dots \mathcal{K}_{\alpha_{n-1}\alpha_0}|, \quad (C5)$$

thanks to $\mathcal{K}'_{\alpha\beta} \geq |\mathcal{K}_{\alpha\beta}|$. By assumption, there is a nonvanishing contribution to $\mathcal{L}_{\alpha_0\alpha_0}$ from the loop of length n ,

$$\mathcal{K}_{\alpha_0\alpha_1} \mathcal{K}_{\alpha_1\alpha_2} \dots \mathcal{K}_{\alpha_{n-1}\alpha_0} = \tau_{\alpha_0\alpha_1} \tau_{\alpha_1\alpha_2} \dots \tau_{\alpha_{n-1}\alpha_0}, \quad (C6)$$

which is not positive. Here, we used the fact that the off-diagonal elements of \mathcal{K} and τ are identical. Combining with the contribution from its reverse loop

$$\mathcal{K}_{\alpha_0\alpha_{n-1}} \mathcal{K}_{\alpha_{n-1}\alpha_{n-2}} \dots \mathcal{K}_{\alpha_1\alpha_0}, \quad (C7)$$

which is the complex conjugate of Eq. (C6), we find the strict inequality

$$\begin{aligned} & \mathcal{K}'_{\alpha_0\alpha_1} \mathcal{K}'_{\alpha_1\alpha_2} \dots \mathcal{K}'_{\alpha_{n-1}\alpha_0} + \text{c.c.} \\ & > \mathcal{K}_{\alpha_0\alpha_1} \mathcal{K}_{\alpha_1\alpha_2} \dots \mathcal{K}_{\alpha_{n-1}\alpha_0} + \text{c.c.} \end{aligned} \quad (C8)$$

Thus, $\mathcal{L}'_{\alpha_0\alpha_0} > \mathcal{L}_{\alpha_0\alpha_0} > 0$. Invoking the Perron-Frobenius theorem again, the strict diamagnetic inequality (14) is proved. ■

APPENDIX D: SUPPORTING RESULTS OF DIAGONALIZATION INVOLVED IN THIS WORK

The results of numerical exact diagonalization on finite lattices are presented here in Tables I–V to assist the proofs in the main text.

TABLE IV. The lowest energies of cluster Hamiltonian $\mathcal{H}^{\text{cluster}}$ on 12-site ‘‘Star of David’’ shape as shown in Fig. 8, in sectors with different numbers of particles m . It shows the ground-state energy of one cluster is strictly positive when the number of particles on this cluster $m \geq 4$. The results are used in Sec. IV D.

m	$\epsilon_0^{\text{cluster}}(m)$
1	0
2	0
3	0
4	0.311475
5	0.937767
6	1.706509
7	3.365207
8	5.196963
9	7.456468
10	10.393543
11	14
12	18

TABLE V. The ground-state energies of fermions and hard-core bosons on a thick-line up triangle as shown in Fig. 11(a), where m is the number of particles on a triangle. The results are used in the proof of π -flux hexagon-triangle model in Appendix E.

m	$\epsilon_{\Delta}^F(m)$	$\epsilon_{\Delta}^B(m)$
1	$-t + 2t'$	$-t - 2t'$
2	$-2t + 4t'$	$-t - 4t'$
3	$6t'$	$-6t'$

APPENDIX E: COUPLED TRIANGLES

The second example to show the natural inequality is reversed in coupled rings as in Sec. IV B is the π -flux hexagon-triangle lattice, which is shown in Fig. 11(a). This is actually a breathing kagome lattice. In the vanadium oxyfluoride compound $(\text{NH}_4)_2[\text{C}_7\text{H}_{14}\text{N}][\text{V}_7\text{O}_6\text{F}_{18}](\text{DQVOF})$, the V^{4+} ions realize a breathing kagome lattice [51], topological equivalent to the hexagon triangle as we discussed here. One unit cell is shown in green in Fig. 11(a), with basis vectors $\vec{a}_1 = (0, 1)$ and $\vec{a}_2 = (1/2, \sqrt{3}/2)$. The Hamiltonian is defined as

$$\mathcal{H} = -t \sum_{(i,j) \in \text{thick, oriented}} e^{i\pi/3} c_i^\dagger c_j - t' \sum_{(i,j) \in \text{broken}} c_i^\dagger c_j + \text{H.c.}, \quad (\text{E1})$$

where ‘‘thick, oriented’’ and ‘‘broken’’ links are specified in Fig. 11(a). This model can be regarded as triangles with π flux, coupled by weak hopping t' . To obtain a lower bound for the ground-state energy of bosons and an upper bound for that of fermions, the Hamiltonians are written as $\mathcal{H}^F = \sum_{\Delta} h_{\Delta}^F - A$ and $\mathcal{H}^B = \sum_{\Delta} h_{\Delta}^B + B$ with the same definitions of A and B in Eqs. (22) and (23), where $h_{\Delta}^F = -t \sum_{i=1}^3 (e^{i\pi/3} c_i^\dagger c_{i+1} + \text{H.c.}) + 2t' \sum_{i=1}^3 c_i^\dagger c_i$

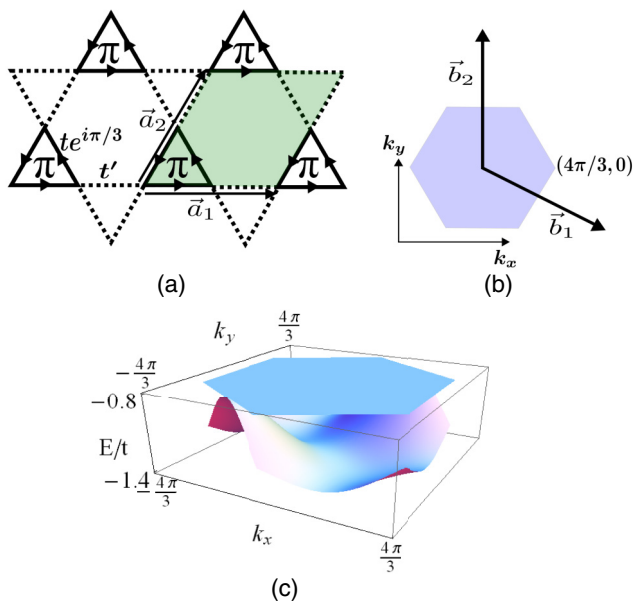


FIG. 11. (a) π -flux hexagon-triangle lattice, in which a unit cell is shown in green. (b) The first Brillouin zone. The basis vectors are denoted by \vec{b}_1 and \vec{b}_2 . (c) Dispersions of the lowest two bands with $t = 1$, $t' = 0.2$.

and $h_{\Delta}^B = -t \sum_{i=1}^3 (e^{i\pi/3} c_i^\dagger c_{i+1} + \text{H.c.}) - 2t' \sum_{i=1}^3 c_i^\dagger c_i$, the cluster Hamiltonians defined on a solid-line pointing up triangle. Therefore, we have $E_0^B \geq \sum_{\Delta_i} \epsilon_{\Delta_i}^B$, $E_0^F \leq \sum_{\Delta_i} \epsilon_{\Delta_i}^F$. The ground-state energies in given m -particle sectors are displayed in Table V in Appendix D. A lower bound for bosons is now given by $E_0^B \geq -N(t + 4t')$ when $t'/t \leq \frac{1}{2}$ or $E_0^B \geq -6Nt'$ when $\frac{1}{2} < t'/t < 1$, where N is the number of unit cells. An upper bound for fermions is given by \tilde{E}_0^F , which also depends on the density pattern on the whole lattice. At $\frac{2}{3}$ filling, we find $E_0^F \leq -2N(t - 2t')$. According to the results of exact diagonalization on a cluster, we find when $t'/t < \frac{1}{8}$, $E_0^B \geq -N(t + 4t') > -2N(t - 2t') \geq E_0^F$. Thus, the reversal of the inequality is proved.

The second approach for the ground-state energy of fermions is based on an exact evaluation. The dispersion relations are ($t = 1$ is assumed)

$$\begin{aligned} E^{(1)} &= \frac{1}{2}(1 - t' - \sqrt{9(t')^2 + 6t' + 9 + 8t'\Lambda(\vec{k})}), \\ E^{(2)} &= t' - 1, \\ E^{(3)} &= \frac{1}{2}(1 - t' + \sqrt{9(t')^2 + 6t' + 9 + 8t'\Lambda(\vec{k})}), \end{aligned}$$

where $\Lambda(\vec{k}) = \cos k_1 + \cos k_2 - \cos k_3$, $k_{1,2} = \vec{k} \cdot \vec{a}_{1,2}$ and $k_3 = k_1 - k_2$. The ground-state energy of fermions at $\frac{2}{3}$ filling is given by the integral of the lowest two bands in the Brillouin zone, which is shown in Fig. 11(c):

$$\begin{aligned} E_0^F &= \sum_{k_x, k_y} [E^{(1)}(k_x, k_y) + E^{(2)}] \\ &= \frac{\sqrt{3}N}{2} \iint_{\text{BZ}} \frac{dk_x}{2\pi} \frac{dk_y}{2\pi} [E^{(1)}(k_x, k_y) + E^{(2)}], \quad (\text{E2}) \end{aligned}$$

where $k_{x,y} \in \text{BZ}$ as shown in Fig. 11(b). The basis vectors \vec{b}_1 and \vec{b}_2 are chosen accordingly as $2\pi(1, -1/\sqrt{3})$ and $2\pi(0, 2/\sqrt{3})$, respectively. The reversed natural inequality holds when $t' \ll t$. For example, when $t = 1$ and $t' = 0.1$, $E_0^B \geq -1.4N > E_0^F = -2.004349N$; when $t' = 0.2$, $E_0^B \geq -1.8N > E_0^F = -2.017037N$.

APPENDIX F: OPTIMAL LOWER BOUND OF FILLING FRACTION OF THE VIOLATION IN DELTA-CHAIN MODEL

Let us improve the estimate of the range of the filling fraction, for which the violation of Eq. (1) occurs on the delta-chain model, as discussed in Sec. IV D. Our result is that the violation occurs, namely the reversed inequality $E_0^B > E_0^F$ holds, for $\frac{1}{4} < v \leq \frac{1}{2}$. In fact, in this range of filling, the ground-state energy of bosons is strictly positive while the ground-state energy of fermions is zero.

To prove this, consider the Bose-Hubbard model (without hard-core constraint) with finite onsite $\mathcal{U} > 0$ in the enlarged Hilbert space first:

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_{\text{hop}} + \mathcal{H}_{\text{int}}, \\ \mathcal{H}_{\text{hop}} &= \sum_{j=1}^N a_j^\dagger a_j, \\ \mathcal{H}_{\text{int}} &= \frac{\mathcal{U}}{2} \sum_{i=1}^{2N} n_i(n_i - 1), \end{aligned}$$

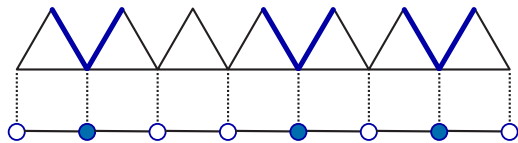


FIG. 12. Schematic figure of mapping to particle configurations in one-dimensional chain with nearest-neighbor exclusion. Localized zero-energy states (valley states) are shown in blue lines.

where $n_i = c_i^\dagger c_i$, and $[c_i, c_j^\dagger] = \delta_{ij}$ for bosons. The definition of a operator is the same as $a_j = c_{2j-1} + \sqrt{2}c_{2j} + c_{2j+1}$. The hard-core constraint can be implemented by taking $\mathcal{U} \rightarrow \infty$, and this problem is reduced to Eq. (35) in this limit.

Obviously, the hopping term \mathcal{H}_{hop} is positive semidefinite. The onsite interaction, \mathcal{U} term, is also positive semidefinite because $\frac{\mathcal{U}}{2}n_i(n_i - 1) = \frac{\mathcal{U}}{2}c_i^\dagger c_i^\dagger c_i c_i$ for bosons. As a consequence, none of the eigenvalues can be negative. Therefore, any state with $E^{\text{B}} = 0$ is a ground state. If such a ground state $|\Phi_{\text{GS}}^{\text{B}}\rangle$ exists, it satisfies

$$\mathcal{H}_{\text{hop}}|\Phi_{\text{GS}}^{\text{B}}\rangle = \mathcal{H}_{\text{int}}|\Phi_{\text{GS}}^{\text{B}}\rangle = 0, \quad (\text{F1})$$

namely, $|\Phi_{\text{GS}}^{\text{B}}\rangle$ a simultaneous zero-energy ground state of \mathcal{H}_{hop} and \mathcal{H}_{int} . Therefore, we first seek zero-energy ground states of \mathcal{H}_{hop} and \mathcal{H}_{int} , separately.

Localized-electron states are discussed in the field of flat-band ferromagnet of Fermi-Hubbard model [41,42,46,52]. We can construct the localized state for bosons in a similar way. Consider the zero-energy ground state of \mathcal{H}_{hop} first. Define the b operator as $b_j = c_{2j} - \sqrt{2}c_{2j+1} + c_{2j+2}$. Because b operators commute with any a operator, $[a_i, b_j^\dagger] = 0$ for any i and j , the single-particle flat band with E_0^{B} is spanned by $b_j^\dagger|0\rangle$. Note that these states $b_j^\dagger|0\rangle$ are linearly independent but not orthogonal to each other. The zero-energy state (valley state) $b_j^\dagger|0\rangle$ is shown in Fig. 12 by blue lines. It is the first excited state of spin- $\frac{1}{2}$ antiferromagnetic Heisenberg model near saturation field, with single magnon trapped in the valley of the delta chain [43–45]. The current setup corresponds to the magnetic field exactly at the saturation field, so that these trapped magnons are exactly at zero energy. The ground state of \mathcal{H}_{hop} can be constructed out of b operators as

$$|\Phi_0^{\text{B}}\rangle = \sum_{\{n_1, \dots, n_N\}} f(n_1, \dots, n_N) (b_1^\dagger)^{n_1} (b_2^\dagger)^{n_2} \dots (b_N^\dagger)^{n_N} |0\rangle, \quad (\text{F2})$$

where $n_j = 0, 1, 2, \dots$ and $f(n_1, \dots, n_N)$ is the coefficient. It is easy to confirm $\mathcal{H}_{\text{hop}}|\Phi_0^{\text{B}}\rangle = 0$, by using the commutation relation $[a_i, b_j^\dagger] = 0$.

Now, we require those zero-energy ground states (F2) of \mathcal{H}_{hop} to satisfy $\mathcal{H}_{\text{int}}|\Phi_0^{\text{B}}\rangle = 0$. This is equivalent to require $c_i c_i |\Phi_0^{\text{B}}\rangle = 0$, which imposes restrictions on the coefficients $f(n_1, \dots, n_N)$. We first note that

$$c_{2j+1}^2 |\Phi_0^{\text{B}}\rangle = \sum_{\{n_1, \dots, n_N\}} 2n_j(n_j - 1) f(n_1, \dots, n_N) \times (b_1^\dagger)^{n_1} \dots (b_j^\dagger)^{n_j-2} \dots (b_N^\dagger)^{n_N} |0\rangle. \quad (\text{F3})$$

Then, the linear independence of b operators, together with $c_{2j+1}^2 |\Phi_0^{\text{B}}\rangle = 0$, implies that $f(n_1, \dots, n_N) = 0$ if there exists j such that $n_j > 1$. We thus restrict our attention to the case where $n_j = 0$ or 1 for all j in the sum. We successively find

$$c_{2j}^2 |\Phi_0^{\text{B}}\rangle = \sum_{\{n_1, \dots, n_N\}} 2n_{j-1}n_j f(n_1, \dots, n_N) \times (b_1^\dagger)^{n_1} \dots (b_{j-1}^\dagger)^{n_{j-1}-1} (b_j^\dagger)^{n_j-1} \dots (b_N^\dagger)^{n_N} |0\rangle, \quad (\text{F4})$$

where $n_j = 0$ or 1 has been applied. From the linear independence of b operators and $c_{2j}^2 |\Phi_0^{\text{B}}\rangle = 0$, we see that $f(n_1, \dots, n_N) = 0$ if there exists j such that $n_j n_{j-1} \neq 0$. This implies that, for bosons, in the construction of the zero-energy ground state, b^\dagger operators on adjacent valleys cannot be applied on the vacuum $|0\rangle$. Thus, the zero-energy ground states are in one-to-one correspondence with particle configurations in one-dimensional chain with nearest-neighbor exclusion. This mapping is schematically shown in Fig. 12. In the range $\nu \leq \frac{1}{4}$, we can find a particle configuration that satisfies the exclusion rule. However, in the case $\nu > \frac{1}{4}$ we cannot find such configuration, implying the absence of zero-energy state.

The zero-energy ground states remain as ground states for any $\mathcal{U} > 0$, and hence in the limit $\mathcal{U} \rightarrow \infty$. Since the onsite \mathcal{U} term is positive semidefinite, no state joins the zero-energy sector with increasing \mathcal{U} . Therefore, the ground-state energy of hard-core bosons (corresponding to infinite \mathcal{U}) is strictly positive in the range of filling $\nu > \frac{1}{4}$.

On the other hand, for fermions, $\{a_i, b_j^\dagger\} = 0$ holds for any i and j . The zero-energy state for fermions in the range of filling fraction $\nu \leq \frac{1}{2}$ can also be constructed by b operators,

$$|\Phi_0^{\text{F}}\rangle = \sum_{\{n_1, \dots, n_N\}} f(n_1, \dots, n_N) (b_1^\dagger)^{n_1} (b_2^\dagger)^{n_2} \dots (b_N^\dagger)^{n_N} |0\rangle, \quad (\text{F5})$$

where $n_j = 0, 1$. It is easy to confirm that this is the zero-energy state of \mathcal{H} because $\mathcal{H}_{\text{hop}}|\Phi_0^{\text{F}}\rangle = 0$, and \mathcal{H}_{int} vanishes. We conclude the reversed inequality $E_0^{\text{B}} > E_0^{\text{F}}$ holds in the range $\frac{1}{4} < \nu \leq \frac{1}{2}$.

From the above analysis, it also follows that both bosonic and fermionic systems have exactly zero-energy ground states for $\nu \leq \frac{1}{4}$. Thus, the lower bound of the range of the filling

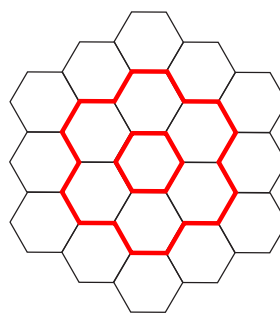


FIG. 13. One example of uncontractible cycle sets on honeycomb lattice, which is constituted by two uncontractible cycles.

fraction for the reversed inequality to hold, $\frac{1}{4}$, is in fact optimal.

An argument similar to the above for the delta-chain model can be employed for the kagome lattice, to extend the range of filling fraction where the natural inequality is violated. The zero-energy states for the kagome lattice (the line graph of honeycomb lattice) are in one-to-one correspondence with *uncontractible cycle sets* on the honeycomb lattice, as

defined in Ref. [53] in terms of graph theory. An example of uncontractible cycle sets is shown in Fig. 13. It can then be deduced that the zero-energy states exist for $\nu \leq \frac{1}{9}$. The uncontractible cycle sets are given by close-packed hard hexagons [43,44,53] at the critical value $\nu = \frac{1}{9}$, and do not exist for $\nu > \frac{1}{9}$. Therefore, the range of filling fraction in which $E_0^B > E_0^F$ holds on the kagome lattice, is extended to $\frac{1}{9} < \nu \leq \frac{1}{3}$.

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