学位論文

Effect of Particle Statistics and Frustration on Ground-State Energy

（粒子統計とフラストレーションの基底状態

エネルギーに対する影響）

平成 25 年 12 月博士（理学）申請

東京大学大学院理学系研究科

物理学専攻

聶　文星

（NIE Wenxing）

Abstract

We study the connections among particle statistics, frustration, and ground-state energy, in many-particle systems. Statistics of identical particles is one of the most fundamental concepts, which pervades all of quantum mechanics. A consequence of the particle statistics appears in the ground-state energy. We compare the ground-state energies of bosons and fermions with the same Hamiltonian. In noninteracting systems, 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 (BEC) and Pauli exclusion principle. The relation that bosons have a lower ground-state energy than fermions is described as natural inequality in this thesis. However, 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. In strongly correlated systems, the influence of particle statistics on the ground-state energy is still a relatively unexplored area.

We have found a sufficient condition for the natural inequality to hold for spinless and spinful cases respectively, without relying on the occurrence of BEC. That is, if all the hopping amplitudes are nonnegative, the ground-state energy of hard-core bosons is still lower than that of fermions. The same argument implies that, once we relax the condition of nonnegative hopping amplitudes, it is possible to reverse the inequality so that the ground-state energy of bosons could be higher than that of fermions. By relaxing the condition, we indeed have found several concrete examples in which the ground-state energy of hard-core bosons is proved to be higher than that of fermions. Many of the examples are even proved rigorously in the thermodynamic limit.

Our study leads to a novel 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 nonnegative and the particles are bosons, the corresponding single-particle problem also has only nonnegative hopping amplitudes. In such a case, there is no frustration in the quantal phase of the wavefunction. On the other hand, Fermi statistics of the original particles gives an effective magnetic flux in the corre-

sponding single-particle problem. This implies a frustration in the phase of the wavefunction, which can be regarded as "statistical frustration": it is induced by the Fermi statistics and it leads to a destructive interference among propagation along different paths.

In the presence of a non-vanishing flux in the original many-body problem, we observe that there is also a magnetic flux in the corresponding single-particle problem, inducing a frustration among quantal phases, which we name hopping frustration. In the original many-particle problem, the statistical frustration appears rather differently 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 non-vanishing flux in the fictitious lattice. This provides a unified understanding of frustration. Based on the unified understanding, we find the mechanism as to why the ground-state energy of hard-core bosons can be higher than that of fermions. For many-body bosonic systems, in which there is no statistical frustration, introduction of hopping frustration will not decrease the ground-state energy. This is known as Simon's universal diamagnetism of bosons. On the other hand, in many-body fermionic systems, where statistical frustration already exists, hopping frustration if introduced, is expected to compete with statistical frustration and sometimes partially cancel with each other, resulting in the reversed inequality between the ground-state energies of the hard-core bosons and fermions.

Contents

Chapter 1

Introduction

“Quantum many-body problem”, the study of intriguing phenomena and properties of a large number of quantum mechanically interacting particles, for example interacting electrons in a solid, is still challenging in modern condensed matter physics. Motion of a single particle is described by the Schrödinger equation in quantum mechanics. Even a many-body system can still be described, in principle, by the Schrödinger equation as well, in terms of many-body wavefunctions. However, the problem confronted by condensed matter physicists is much more complicated than what is expected from these formulations. On one hand, the degrees of freedom grows exponentially with the number of particles. Thus, in order to just represent the many-body wavefunction faithfully, the required memory for storage grows exponentially with system size. This quickly becomes impractical, even with the aid of a supercomputer. On the other hand, new phenomena, new physics and new principles appear in many-body problems, which are far beyond a mere technical problem of solving the Schrödinger equation. This is what called as “emergence” or stated as “more is different” by Anderson [1].

The difficulty mentioned above calls for new frameworks to understand the physics of many-body systems. One of the approaches to quantum many-body physics is approximation, for example mean field approximation. In the frame of mean-field theory, the correlations between two particles are neglected. Mean-field theory is often successful in giving a qualitative description of the phase diagram. It is quantitatively accurate in some cases where the fluctuations are suppressed. However, it generally fails to give a prediction near the critical point, where the correlations are so strong and cannot be neglected. Therefore, the limitation of approximation is obvious. Apart from approximation, another approach to the quantum many-body system is numerical calculation with the aid of computers. Exact diagonalization of a Hamiltonian is a direct and precise method, with very high precession. However, due to the computation cost of storage, which grows exponentially with system size, exact diagonalization only works for small systems. Density matrix renormalization group (DMRG) [2] is powerful and reliable in one dimension. Recently proposed infinite time evolving block decimation (iTEBD) [3] and multiscale entanglement renormalization ansatz (MERA) [4] are becoming widely used in the calculation of strongly correlated systems in one dimension. However, the latter three methods are still difficult to be utilized in systems with dimensions higher than one. Quantum Monte-Carlo can be implemented for relatively large size systems, but it has the sign problem in frustrated systems.

Mathematically rigorous approach is another important route to quantum many-body systems. Two well known solvable models are the Lieb-Liniger model [5] and the spin-1/2 XXZ Heisenberg chain [6, 7, 8], which can be exactly solved by the Bethe ansatz method. Although the solvable cases that we encountered are so rare, the results can be used to compare with experiments in detail. Investigation of the solvability of the models is one of the branch of mathematically rigorous approach. We notice that there are many mathematical rigorous theorems about the properties of the ground state and low-lying excited states [9]. Nagaoka's theorem is the first rigorous result of ferromagnetism in the Hubbard model, which states the unique ferromagnetic ground state with the maximum total spin [10]. The Lieb-Mattis theorem excludes the possibility of ferromagnetism of the Hubbard model with only nearest neighbor hoppings in one dimension with open boundary conditions [11]. Lieb's theorem proves the absence of ferromagnetism on bipartite lattices at half filling for any repulsive interaction [12]. Koma and Tasaki's theorem proves upper bounds for correlation functions at finite temperatures [13]. The Yamanaka-Oshikawa-Affleck theorem describes the low-lying excitations in general electron systems on one-dimensional lattice [14]. These theorems do not focus on specific calculation of certain physical quantity. Instead, they give qualitative estimate or prediction by mathematically rigorous proof. The importance of mathematically rigorous theorems is that it usually sheds light on the possibility or impossibility of some physical phenomena. For example, if one knows Lieb's theorem [12], he/she can avoid spending effort for ferromagnetism on a bipartite lattice at half filling by approximation or numerical calculation. Although rigorous theorems are limited to some cases, they are very useful and sometimes they give guidelines on concrete calculations. We can check the correctness of the results from approximations and numerical calculations with the rigorous theorems. Therefore, the mathematically rigorous theorems provide many physical insights and play important roles for concrete calculation.

In this thesis, we investigate a very fundamental and significant problem: the effect of particle statistics and frustration on the ground-state energy of quantum many-body systems, by mathematically rigorous approach. In condensed matter physics, it is fundamental to understand the ground state and its energy. The ground state of a quantum system is its state with the lowest energy. The interest in the ground state is partially due to its simplicity, compared with the properties of excited states. The ground state is in principle realized in the limit of zero temperature. In reality, the absolute zero temperature can never be achieved in any experiment. Nevertheless, elucidation of the ground state is important for understanding of physics at sufficiently low temperatures. Moreover, quantum phase transitions, which occur in the ground state, sometimes govern physics up to rather high temperatures. In addition, some ordered states are expected in the ground state, such as antiferromagnetic (Néel) order and crystalline order. Consequently, the investigation on the properties of the ground state and low-lying excitations is an indispensable part in physics. Three rigorous theorems are put forward, in which a sufficient condition when the ground-state energy of bosons is (strictly) lower than that of corresponding fermions is proved. A strict diamagnetic inequality is proved in the fourth theorem.

To address the effect of particle statistics and frustration on the ground-state energy, we compare the ground-state energies of hard-core bosons and fermions with the same Hamiltonian. The hard-core boson is introduced as a model of boson behaving like impenetrable hard sphere, with infinite on-site repulsion (or infinite Dirac δ-function repulsive interaction), which allows the number of bosons at the same place to be 0 or 1. Bosons with large repulsive interaction at close range such as Helium-4 can be regarded as a hard-core bosons model. The hard-core boson is of great interest in condensed matter physics because it is mathematically equivalent to a spin-1/2 magnet. On the other hand, the hard-core boson is not a purely theoretical model. Hard-core bosons confined to one dimension are also known as the Tonk-Girardeau gas [15, 16], which has been realized in a one-dimensional optical lattice experimentally [17]. With the hard-core constraint of bosons, the dimension of the Hilbert space is the same as fermions. On the same site, hard-core bosons obey the anticommutation relation, which is typical for fermions. Therefore, hard-core bosons are expected to have some "fermionic-like" behaviors. However, hard-core bosons are still statistically different from fermions because on different sites they satisfy the commutation relation as usual bosons. The wavefunction of N hard-core bosons does not have the antisymmetry property with respect to exchange of two particles. This essential and fundamental difference makes the hard-core bosons statistically distinct from fermions, and the difference can be shown in the ground-state energy.

This thesis is organized as follows. In Chap. 2, the background of our research is presented. To focus on the discussion on physics in the main body, four frequently involved theorems are presented in Chap. 3. In Chap. 4, we explain why the comparison is trivial for noninteracting systems, that the ground-state energy of bosons is always lower than fermions (natural inequality). We also explain why it becomes non-trivial in the presence of hard-core and other interactions. We proved if all the hopping amplitudes are nonnegative, the ground-state energy of hard-core bosons is still lower than that of the corresponding fermions, which is summarized in Theorem 1, Theorem 2 and Theorem 3 for spinless and spinful cases respectively. Proof of strict diamagnetic inequality is presented in Theorem 4. Based on the proofs, we propose a unified understanding of frustration in Chap. 5. The quantal phase introduced by Fermi statistics is understood as statistical frustration, in terms of a fictitious lattice. Hopping frustration and statistical frustration are understood in a unified way. We find the mechanism that the reversion of the natural inequality is possible. In Chap. 6 and Chap. 7, we present the natural inequality is indeed reversed in various systems due to hopping frustration, by rigorous proof assisted by exact diagonalization. The examples include particles on a ring, coupled rings from one dimension to two dimensions, the two-dimensional square lattice with uniform flux, and flat band models. Many of the examples are rigorous in the thermodynamic limit. Finally, conclusions and discussions are presented in Chap. 8.

Chapter 2

Background

In this chapter, I will present the background of the research in this thesis. Some known results of previous research are reviewed: Simon's universal diamagnetism of bosons [18] and optimal phase problem of fermions [19]. These two studies focus on the influence of magnetic field or flux on the ground-state energies of bosons and fermions, respectively. They did not deal directly with our main question of the comparison between bosons and fermions. Nevertheless, the response to magnetic flux reveals the differences between bosons and fermions. These results hint some of our findings, and are also useful for developing a more systematic, unified approach in the present thesis. In Sec. 2.3, the rigorously solved Lieb-Liniger model at infinite repulsion limit is reviewed, which is also known as Tonk-Giradeau gas. The similarities and differences between Tonks-Girardeau gas and one-dimensional spinless free fermion gas will also be reviewed. Although we are working on lattice systems, review of one-dimensional continuous system gives us some physical insights. For example, bosons with hard-core constraint have some "fermionic-like" behaviors, but they are still bosons for statistical reason. One-dimensional gas is the continuous analog of particles on a lattice ring in Chap. 6. Bose-Fermi mapping on one-dimensional Tonks-Giradeau gas is analogous to Jordan-Wigner transformation on one-dimensional lattice hard-core bosons. The relation between the ground-state energy of one-dimensional bosonic gas and that of fermionic gas is analogous to the one between bosons and fermions on a lattice. The discussion of momentum distribution of Tonks-Giradeau gas is a good example to show why perfect Bose-Einstein condensation breaks down in bosonic gas with hard-core interaction.

2.1 Universal diamagnetism of bosons

The terminology of "diamagnetism" was introduced by Michael Faraday to describe the fact that all the materials in natures possessed some form of diamagnetic response to external magnetic field. Generally speaking, diamagnetism is the property of an object to prevent the external magnetic filed inside itself, signatured by the negative magnetic susceptibility. Diamagnetism is a quantum mechanical effect, since Bohr-van Leeuwen theory states that a classical gas of charged particle is nonmagnetic [20].

There are some known theorems associated with diamagnetism [20]. Langevin (Larmor) theory of diamagnetism applies to isolated magnetic moments: atoms with localized electrons. For itinerant electrons (free electron gas), the theory of diamagnetism is attributed to Landau, which is a result of total energy change of the system due to the presence of Landau levels, when the system is subject to a magnetic field.

Diamagnetism of spinless bosons is rigorously proved by Barry Simon [18]. He proved that the ground-state energy of nonrelativistic spinless Bose particles in any arbitrary magnetic filed is greater than corresponding bosons without magnetic filed. Namely, arbitrary magnetic filed increases the ground-state energy of nonrelativistic spinless bosons. The terminology of "diamagnetism" for bosons here is consistent with those associated with negative magnetic susceptibility in above theorems. Negative magnetic susceptibility is consistent with minimal ground-state energy at zero magnetic field. This is because at zero temperature, $F = E - TS = E$, $\chi = \partial M/\partial H = -\partial^2 F/\partial H^2$, and $\partial E/\partial H|_{H\to 0} = 0$ due to time reversal symmetry at $H = 0$. I will present Simon's theorem and the outline of the proof here.

Consider N interacting nonrelativistic spinless Bose particles. The many-body Hamiltonian is assumed as

$$\mathcal{H}(\vec{A}) = -\sum_{j=1}^{N} \frac{1}{2m_j}[\nabla_j - ie_j\vec{A}(\vec{r}_j)]^2 + \sum_{j<k} v_{jk}(\vec{r}_j - \vec{r}_k) + \sum_j v_j(\vec{r}_j), \tag{2.1}$$

where e_j is the charge carried by jth particle, $\vec{A}(\vec{r}_j)$ is an arbitrary magnetic field vector potential (no assumption of uniform magnetic field here), v_{jk} is the interaction potential between two bosons which are located at $\vec{r}_j$ and $\vec{r}_k$ in coordinate space, and $v_j(\vec{r}_j)$ is the scalar potential. For example, the site independent part of $v_j(\vec{r}_j)$ is the chemical potential. All the functions $\vec{A}$, v_{jk} and v_j are assumed to take real values.

Theorem. (Simon's diamagnetism in [18])

As an operator $\mathcal{H}(\vec{A})$ [1] on functions with Bose statistics on all of the particles, the ground-state energy $\mathcal{H}(0)$ cannot be greater than $\mathcal{H}(\vec{A})$.

The foundation of Simon's diamagnetism is based on the inequality

$$\int d\tau\ |\psi|^*\mathcal{H}(0)|\psi| \leq \int d\tau\ \psi^*\mathcal{H}(\vec{A})\psi \tag{2.2}$$

for any ψ, which follows from a more general inequality of Kato [21]. The details of the proof of Eq. (2.2) is presented in Appendix.

Assume ϕ is the orthonormalized ground state of $\mathcal{H}(0)$ with energy $E(0)$, and assume ψ is the orthonormalized ground state of $\mathcal{H}(\vec{A})$ with energy $E(\vec{A})$. Therefore $E(0) = \int d\tau\phi^*\mathcal{H}(0)\phi$ and $E(\vec{A}) = \int d\tau\psi^*\mathcal{H}(\vec{A})\psi$, where the wave functions ϕ and ψ satisfy Bose statistics. By variational principle and Eq. (2.2),

$$\int d\tau\phi^*\mathcal{H}(0)\phi \leq \int d\tau|\psi|^*\mathcal{H}(0)|\psi| \leq \int d\tau\psi^*\mathcal{H}(\vec{A})\psi, \tag{2.3}$$

leading to Simon's diamagnetism,

$$E(0) \leq E(\vec{A}), \tag{2.4}$$

where $|\psi|$ plays as a trial wavefunction of $\mathcal{H}(0)$ in the first inequality in Eq. (2.3).

There are some remarks of this theorem:

- This theorem describes the property of many-body bosonic system. It is different with diamagnetic inequality in Sec. 2.2.1, which is restricted to single particle case.

- This theorem can only apply to compare the ground-state energies of $\mathcal{H}(0)$ and $\mathcal{H}(\vec{A})$. It implies nothing about excited states. This is because the ground-state wavefunction of bosons in coordinate space has "no node" [22, 23], namely $\psi_0(\vec{r}) > 0$. Assume the excited state is $\psi_1(\vec{r})$, which must satisfy the orthogonality $\langle\psi_1(\vec{r})\big|\psi_0(\vec{r})\rangle = \int d\vec{r}\ \psi_1^*(\vec{r})\psi_0(\vec{r}) = 0$. If $\psi_1(\vec{r}) =$

[1] $\mathcal{H}(\vec{A})$ is defined in equation (2.1).

$|\psi_0(\vec{r})|$, the orthogonality $\langle|\psi_0(\vec{r})||\psi_0(\vec{r})\rangle = \int d\vec{r}\ |\psi_0(\vec{r})|^*\psi_0(\vec{r}) = 0$ cannot be satisfied, considering $\psi_0(\vec{r}) > 0$. Therefore, $|\psi_0(\vec{r})|$ cannot be the trial wavefunction of excited states and this theorem gives no information about excited states.

- This theorem only applies to bosonic systems since no-node wave function $|\psi|$ cannot be used as a trial wavefunction for fermions, where $|\psi|$ destroys the Fermi statistics.

- Simon's original proof is for bosonic gas. An argument similar to the proof of the Theorem can be used to prove a lattice version of Simon's theorem on diamagnetism of bosons.

2.2 Flux phase problem of fermions

The influence of magnetic field on the ground-state energy of fermions is in the context of "flux phase" problem. The flux phase problem in condensed matter physics is to find the real phase flux distribution which optimally minimizes the ground-state energy of fermions. Some history of this problem is reviewed in the literature [19].

2.2.1 Diamagnetic inequality

Diamagnetic inequality [19] is one of the significant conclusions of flux phase problem. It holds for single-particle tight-binding Hamiltonian. Consider a given planar graph $\Lambda(V, E)$. The number of vertices is $|\Lambda|$. The Hamiltonian for single electron is $-\mathcal{L}$, where $\mathcal{L}$ is Laplacian. Associated with the graph $\Lambda(V, E)$, the matrix of $\mathcal{L}$ is known as adjacency matrix in the context of graph theory, which is a $|\Lambda| \times |\Lambda|$ matrix. Namely, $\mathcal{L}_{xx} = 0$, and $\mathcal{L}_{xy} = 1$ $(x \neq y)$ if sites x and y are connected by an edge, otherwise $\mathcal{L}_{xy} = 0$. Assume the eigenvalues of $\mathcal{L}$ are arranged in a non-ascending order, namely $\lambda_1(\mathcal{L}) \geq \lambda_2(\mathcal{L}) \geq \cdots \geq \lambda_{|\Lambda|}(\mathcal{L})$, such that the ground-state energy of Hamiltonian $-\mathcal{L}$ is equivalent to $-\lambda_1(\mathcal{L})$.

In the presence of a spatially dependent magnetic field, the matrix element $\mathcal{L}_{xy}$ is replaced by $T_{xy} = \mathcal{L}_{xy}e^{i\theta(x,y)}$. The functions θ's are real and satisfy $\theta(x, y) = -\theta(y, x)$ such that T is a Hermitian matrix. Physically, the phase $\theta(x, y)$ can be interpreted as the integral of the vector potential $\vec{A}$ along the edge connecting site x and site y in an magnetic filed: $\theta(x,y) = \int_x^y \vec{A}\cdot d\vec{l}$. The order of the eigenvalues of T is also assumed in a non-ascending way: $\lambda_1(T) \geq \lambda_2(T) \geq \cdots \geq \lambda_{|\Lambda|}(T)$. Therefore, the ground-state energy of fermions in such a magnetic filed with Hamiltonian $-T$ corresponds to $-\lambda_1(T)$.

Take the single-particle basis $\{|\phi_x\rangle\}$, which means the site x is occupied by the electron. Assume ϕ is the normalized eigenvector belonging to the largest eigenvalue $\lambda_1(T)$ of T. Thus the ground state can be expanded as $|\phi\rangle = \sum_x \phi_x|\phi^x\rangle$. By variational principle,

$$\begin{aligned}\lambda_1(T) = \langle\phi|T|\phi\rangle &= \sum_{xy}\phi_x^*\phi_y\langle\phi^x|T|\phi^y\rangle = \sum_{xy}\phi_x^*\phi_y T_{xy} = \sum_{xy}\phi_x^*\phi_y\mathcal{L}_{xy}e^{i\theta(x,y)}\\ &\leq \sum_{xy}|\phi_x||\phi_y|\mathcal{L}_{xy} \leq \lambda_1(\mathcal{L}).\end{aligned} \tag{2.5}$$

It directly leads to the diamagnetic inequality,

$$E_0(\{\theta(x,y)\}) \geq E_0(\{\theta = 0\}) \tag{2.6}$$

for any distribution of $\{\theta(x,y)\}$. Thus $\{\theta = 0\}$ is the optimal distribution of phase to minimize the ground-state energy of single particle.

This conclusion is easily extended to "t-V" model $\mathcal{H} = -T + V$, since V is a real and diagonal matrix. In addition, in the limit of continuous systems $\mathbb{R}^n$, where $\mathcal{H} = -[\nabla - i\vec{A}(\vec{r})]^2 + V(\vec{r})$, $\vec{A}(\vec{r}) = 0$ minimizes the ground-state energy of $\mathcal{H}$. The physical meaning of diamagnetic inequality can be represented as "a magnetic field increases the ground-state energy of one particle" intuitively.

Different with Simon's diamagnetism of bosons, the Eq. (2.6) holds only for single particle tight-binding problem. It can be extended to hold in the limit of low electron density. Because at low electron density, it is the lattice analog to Landau's diamagnetism for free electron gas. However, at high electron density, diamagnetic inequality cannot be applied, because the analogy to Landau's diamagnetism breaks down at high electron density. The actual case of high electron density will be discussed in the following section.

2.2.2 Optimal phase at half filling

For an arbitrary filling fraction especially at high electron density, it is a highly nontrivial problem to determine the optimal flux distribution. The reason can be explained in terms of the well known Hofstadter's butterfly [24] with the uniform flux distribution.

Hofstadter considers single electron on a two-dimensional square lattice with periodic boundary condition, immersed in a uniform magnetic field perpendicular to the lattice plane. By tight-binding approximation, the energy spectrum as a function of flux density α is obtained by solving a one-dimensional difference equation associated with Harper, where $\alpha = \Phi/\Phi_0$ is the number of flux quanta passing through every plaquette. The beauty of this problem is highly captured in the energy spectrum $E(\alpha)$, which is continuous with α and full of gaps with a remarkable fractal structure as shown in Figure 2.1. For fixed number of free electrons, the ground-state energy of many-body fermions in a uniform magnetic filed is obtained by particle filling to the Hofstadter's butterfly up to the Fermi level. Due to the complicity of the energy spectrum as functions of α, it is not a trivial question to find the phase that optimally minimizes the ground-state energy for given number of particles.

However, the optimal phase is found in the most special case at half filling $\nu = 1$, where ν is filing fraction, the number of particles per site. The term "flux phase" was introduced firstly in I. Affleck and J. B. Marston's paper on large-n limit of the Heisenberg-Hubbard model for high temperature superconductivity, when they needed to describe the state with minimal ground-state energy as a function of the hopping phase [25]. Contrary to diamagnetic inequality that the ground-state energy is raised by magnetic field [19], they found that a state arrives at the minimum of the ground-state energy with π flux per plaquette near half filling. Great interests and intensive studies have casted on the investigation of the optimal phase in various lattice and more values of particle filling fraction [26, 27, 28]. Based on numerical calculations, the original flux phase conjecture is that for a tight-binding model on a square planar lattice at half filling, the optimal flux that minimizes the ground-state energy of fermions is π per plaquette [25, 26, 27, 29]. In addition, the conjecture is rigorously proved later by E. H. Lieb and M. Loss in several cases [19]. And later it is proved to be beyond the original conjecture in several ways, where only refection symmetry is needed and it works for extended Hubbard model (with any sign of on-site interaction and long range interactions) for any lattice with dimensions $D \geq 2$ (periodicity in $D - 1$ is needed) at any temperature [30].

The conclusion that π flux is the optimal phase for square lattice is very useful in

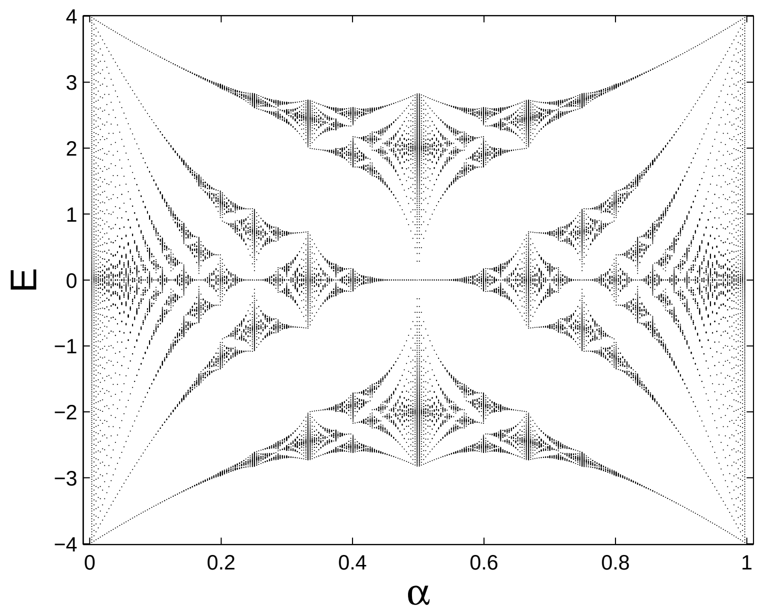


Figure 2.1: Hofstadter's butterfly: the energy spectrum of single electron on a two-dimensional square lattice in a uniform magnetic field, which is perpendicular to the lattice. Vertical variable is energy E and horizontal variable is flux density per plaquette α, whose value is given by the number of flux quanta per plaquette Φ/Φ_0.

the following discussion in the Sec. 7.3.1. Considering π flux greatly minimizes the ground-state energy of fermions, and on the other hand any arbitrary magnetic filed increases the ground-state energy of spinless bosons according to Simon's universal diamagnetism of bosons, these two conclusions shed light on the possibility that the ground-state energy of bosons can be higher than that of corresponding fermions with π flux per plaquette.

2.3 1D interacting Bose gas

In this section, I present some results of previous studies of one-dimensional interacting Bose gas. There are some exactly solved interacting boson models in one dimension. For instance, a model of Bose gas via $1/(r_i - r_j)^2$ type interaction introduced by Calogero is solvable [31]. Another instance is the Lieb-Liniger model [5]; a model of Bose gas via a two-body δ-function interaction is exactly solved by Bethe ansatz.

The limit of infinite repulsion in the Lieb-Liniger model, is also called as the Tonks-Girardeau or hard-core limit [15, 32]. One of the main subjects in this thesis is the ground-state energy of hard-core bosons. Although we are working on lattice systems, reviewing the properties of the Tonks-Girardeau gas, which is the continuous analog of lattice hard-core bosons, is able to give us many physical insights for discrete lattice systems. In addition, the "fermionic-like" behaviors possessed by hard-core bosons can be shown in the discussion of Tonks-Girardeau gas. Since we are also working on the effect of particle statistics on the ground-state energy, the studies of Tonks-Girardeau gas will tell us the differences between hard-core bosons and spinless free fermions in one dimension.

2.3.1 Ground-state energy of Tonks-Girardeau gas

The simplest and nontrivial model of interacting bosons in the continuum is Lieb-Liniger model [5]. They consider N bosons in one dimension interacting via a two-body δ-function potential (assume $\hbar = 1$, $2m = 1$),

$$\mathcal{H} = -\sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} + 2c \sum_{1\leq i<j\leq N} \delta(x_i - x_j), \tag{2.7}$$

where $2c > 0$ is the amplitude of the repulsive δ interaction.

In the limit of $c \to \infty$, we obtain the Tonks-Girardeau limit, since the particles are interacting with an impenetrable point potential. The infinite repulsion enforces the constraint that the eigenfunction of Hamiltonian (2.7) in the limit of $c \to \infty$ must vanish when two particles meet at the same point,

$$\Psi(x_1, \cdots, x_i, \cdots, x_i, \cdots, x_N) = 0. \tag{2.8}$$

This constraint can be implemented by assuming the symmetric wave function of N particle Bose gas [15, 32],

$$\Psi^B(x_1, \cdots, x_N) = S(x_1, \cdots, x_N)\Psi^F(x_1, \cdots, x_N), \tag{2.9}$$

where $S(x_1, \cdots, x_N) = \prod_{1\leq i<j\leq N} \mathrm{sign}(x_i - x_j)$ and $\Psi^F(x_1, \cdots, x_N)$ is the wavefunction of N spinless free fermions. The sign change of $\Psi^F(x_1, \cdots, x_N)$ when two particles are exchanged is compensated by the function $S(x_1, \cdots, x_N)$, therefore the wavefunction in Eq. (2.9) obeys Bose statistics. And at the same time $\Psi^B(x_1, \cdots, x_i, \cdots, x_j, \cdots, x_N) = 0$ is satisfied automatically if $x_i = x_j$.

The many-body wavefunction of spinless free fermion is given by

$$\Psi^F(x_1, \cdots, x_N) \propto \det[\phi_j(x_l)],$$

where det denotes the Slater determinant and $\phi_j(x)$ is the jth eigenfunction of the single-particle Hamiltonian. For free fermion, the single particle wavefunction is of plane-wave type $\phi_j(x_l) \propto e^{ik_j x_l}$. Therefore, the wavefunction of Tonks-Giradeau gas is

$$\Psi^B(x_1, \cdots, x_N | k_1, \cdots, k_N) \propto \det[e^{ik_j x_l}] \prod_{1 \leq j < l \leq N} \mathrm{sign}(x_j - x_l). \tag{2.10}$$

The wavefunction (2.10) is the eigenfunction of the Hamiltonian in (2.7) with the corresponding eigenvalues [33]

$$E = \sum_{j=1}^{N} k_j^2. \tag{2.11}$$

Assume the system is a ring of circumference L with periodic boundary condition,

$$\Psi^B(x_1, \cdots, x_j = 0, \cdots, x_N | k_1, \cdots, k_N) = \Psi^B(x_1, \cdots, x_j = L, \cdots, x_N | k_1, \cdots, k_N),$$

leading to the condition $e^{ik_j L} = (-1)^{N-1}$. The quantization condition brought by periodic boundary can be written as

$$k_j = \frac{2\pi n_j}{L}, \qquad j = 1, \cdots, N, \tag{2.12}$$

where n_j are arbitrary odd number for even N and arbitrary even for odd N. Assume the total number of particle is odd. The ground-state energy of Tonks-Girardeau gas is obtained by choosing the values of n_j lying within the Fermi surface [15],

$$-\frac{1}{2}(N-1) \leq n_j \leq \frac{1}{2}(N-1).$$

The ground-state energy is given by

$$E_0 = \sum_{n_j = -\frac{1}{2}(N-1)}^{\frac{1}{2}(N-1)} (\frac{2\pi n_j}{L})^2.$$

In the thermodynamic limit ($N, L \to \infty$, N/L is finite), the ground-state energy is obtained by integral

$$E_0 = \frac{L}{2\pi} \int_{-\pi N/L}^{\pi N/L} dk\, k^2 = \frac{L\pi^2\rho^3}{3}, \tag{2.13}$$

where $\rho = N/L$ is the particle density. This is consistent with Lieb and Liniger's results by Bethe ansatz [5].

The ground-state energy of Tonks-Girardeau or one-dimensional hard-core boson gas is exactly the same as that of one-dimensional spinless free fermion gas in the thermodynamic limit. This is the result in continuum limit, due to Bose-Fermi mapping (see Sec. 2.3.2). In one-dimensional lattice system, the ground-state energies of free fermions and hard-core bosons are the same as well in the thermodynamic limit, by Jordan-Wigner transformation. The latter of discrete lattice system will be discussed in Chap. 6: Particles on a ring.

2.3.2 Bose-Fermi mapping

The Bose-Fermi mapping denoted by Eq. (2.9), is first put forward by M. Girardeau in 1960, which demonstrates the connections between one-dimensional hard-core bosonic gas and spinless free fermionic gas. It maps a strongly interacting many-body bosonic problem into a noninteracting many-body fermionic problem! This is an astonishing mapping, since the distinction between bosons and fermions looks as if being blurred by this mapping. In this section, more discussion of the similarities and differences will be presented.

Bose-Fermi mapping is even simplified in the case of the ground state. Notice the function $S(x_1, \cdots, x_N) = \prod_{1\le i<j\le N} \mathrm{sign}(x_i - x_j)$ can only takes the value $+1$ or -1. And consider the ground-state wave function of bosons is positive definite according to Feynman's "no-node" theorem [22, 23]. The relation (2.9) is reduced to [15]

$$\Psi_0^B = \left|\Psi_0^F\right|. \tag{2.14}$$

The hard-core constraint or Tonks-Girardeau limit has some similar effect on bosons as that of Pauli principle on a gas of spinless fermions, since any two bosons cannot occupy the same site in real space. To minimize their mutual repulsion, the bosons are avoided to occupy the same position, which mimics the Pauli exclusion principle for fermion. Therefore, some "fermion-like" behaviors are expected in hard-core bosons. The relation $\left|\Psi_0^B\right|^2 = \left|\Psi_0^F\right|^2$ results the fundamental similarities between one-dimensional hard-core boson and spinless free fermions. M. Girardeau proved that not only the energy spectra of one-dimensional hard-core bosons and spinless free fermions are identical, but also all configurational probability distributions are the same [15].

However, as denoted by Bose-Fermi mapping (2.9), the wavefunction of hard-core bosons is symmetric, which is statistically different from fermions. Due to the different symmetries of the wavefunctions, the momentum distribution of Tonks-Girardeau gas is very different from that of free fermions system [15]. The difference is also signatured by the one-particle density matrix [34]. This difference can be understood qualitatively by the Heisenberg uncertainty relation. Since hard-core bosons cannot occupy the same position in real space, they will distribute in a wider region in momentum space, compared with weakly interacting bosons. This also lends help to explain why perfect Bose-Einstein condensation (all the bosons condense into the same lowest energy state) breaks down in interacting bosons. On the other hand, hard-core bosons do not have to be in different momentum states, this is the fundamental difference from fermions.

All of the observations reveal that hard-core bosons do not exhibit completely fermionic or bosonic quantum behaviors. However, hard-core bosons are still bosons, satisfying Bose statistics that is the fundamental property, even if they possess some "fermionic-like" behaviors. The distinction of statistics is not blurred by hard-core interaction. And a consequence of statistics appears on the ground-state energy, which is the main subject in this thesis. Although in the thermodynamic limit, Tonk-Girardeau gas has the same ground-state energy as free fermion gas, the energy difference indeed exists in finite system. To see this, consider the case when the number of particles is even, then after Bose-Fermi mapping, "new" free fermions satisfies anti-periodic boundary condition. Free fermions with anti-periodic boundary condition has a lower ground-state energy than that with periodic boundary condition in finite system. The detailed discussion of the energy difference on one-dimensional lattice will be presented in Chap. 6.

Chapter 3

Frequently used theorems

To focus on the discussion of physics instead of being distracted by mathematical theorems or techniques involved in the main part of this thesis, I present some frequently used theorems in this chapter. All of them play important roles for our proof for natural inequality (in Chap. 4) and rigorous proofs for a lower or an upper bound of the ground-state energy in infinite system (in Chap. 7), based on the results obtained from finite clusters by exact diagonalization.

3.1 Min-max principle

Min-max principle (or min-max theorem, Courant-Fischer-Weyl min-max principle) is a standard theorem in linear algebra and matrix analysis. It variationally characterizes eigenvalues of a Hermitian operator in the Hilbert space.

The theorem that we use frequently is one of the important applications of the Courant-Fischer theorem (see Chap. 4.2.11 in [35] and Chap. 4.3.1 in [36]), associated with Weyl.

Theorem. (Weyl (see Chap. 4.3.1 in [36]))

Let A and B be $n \times n$ Hermitian matrices and let the eigenvalues $\lambda_i(A)$, $\lambda_i(B)$ and $\lambda_i(A{+}B)$ be arranged in non-decreasing order ($\lambda_1(X) \leq \lambda_2(X) \leq \cdots \leq \lambda_n(X)$, where $X = A, B, A+B$). For each $k = 1, 2, \cdots, n$, we have

$$\lambda_k(A) + \lambda_1(B) \leq \lambda_k(A+B) \leq \lambda_k(A) + \lambda_n(B). \tag{3.1}$$

Weyl's theorem can be used to compare the eigenvalues of matrix $A + B$ and those of matrix A. One important application of Weyl's theorem is the case with $k = 1$ for the lowest eigenvalues:

$$\lambda_1(A) + \lambda_1(B) \leq \lambda_1(A+B) \leq \lambda_1(A) + \lambda_n(B). \tag{3.2}$$

When the Hermitian matrices A, B and $A+B$ are associated with Hamiltonians, the Eq. (3.2) gives an upper bound and a lower bound of the ground-state energy of the Hamiltonian $A+B$.

One extension of the Eq. (3.2) is that if all the eigenvalues of B is positive semi-definite ($\lambda_i(B) \geq 0$ for any i), a lower bound of $A+B$ is simply given by the lowest eigenvalue of A:

$$\lambda_1(A) \leq \lambda_1(A+B), \tag{3.3}$$

which will be frequently used for positive semi-definite Hamiltonian in Chap. 7.

3.2 Anderson's argument

Mathematically speaking, Anderson's argument [37] is a corollary and special case of Weyl's min-max principle as in Eq. (3.2). It gives more insights from the aspects of physics.

Theorem. (Anderson (see [37]))

The lowest eigenvalues of the total Hamiltonian must be greater than the sum of the lowest eigenvalues of its parts.

Anderson's argument is easily proved by variational principle.

Proof. Assume E_0^A, E_0^B and E_0^{A+B} are the ground-state energies for $\mathcal{H}^A$, $\mathcal{H}^B$, and $\mathcal{H}^A + \mathcal{H}^B$, respectively. And assume $|\psi\rangle$ is the ground state of total Hamiltonian $\mathcal{H}^A + \mathcal{H}^B$. By variational principle, We have

$$E_0^{A+B} = \langle\psi|H^A + H^B|\psi\rangle = \langle\psi|H^A|\psi\rangle + \langle\psi|H^B|\psi\rangle \geq E_0^A + E_0^B, \tag{3.4}$$

where $|\psi\rangle$ plays as the trial wave function of ground states for $\mathcal{H}^A$ and $\mathcal{H}^B$. $\square$

From above proof, the lower bound of E_0^{A+B} holds when $\mathcal{H}^A|\psi\rangle = E_0^A|\psi\rangle$ and $\mathcal{H}^B|\psi\rangle = E_0^B|\psi\rangle$. Namely, the ground-state energy of $\mathcal{H}^A + \mathcal{H}^B$ is $E_0^A + E_0^B$ when

Figure 3.1: A cartoon to show Pigeonhole principle. There are ten pigeons but only nine holes. If all the pigeons are put in holes, there is at least one hole accommodating more than one pigeon. This figure is taken from Wikimedia Commons (http://en.wikipedia.org/wiki/File:TooManyPigeons.jpg). The copy right belongs to BenFrantzDale, licensed under the Creative Commons Attribution-Share Alike 3.0 Unported license.

the ground state of $\mathcal{H}^A + \mathcal{H}^B$ is simultaneously the ground state of $\mathcal{H}^A$ and $\mathcal{H}^B$. One sufficient condition of the lower bound is $[\mathcal{H}^A, \mathcal{H}^B] = 0$, which means when the cluster Hamiltonian commutes with each other, the ground-state energy of total Hamiltonian is simply given by the summation of the ground-state energy of cluster Hamiltonians.

Anderson's argument will be frequently used in cluster decomposition technique in Chap. 7.

3.3 Dirichlet's box principle

In mathematics, Dirichlet's box principle is also known as pigeonhole principle and drawer principle. It starts with the observation that when ten pigeons are put in nine holes, there is at least one hole containing more than one pigeon as shown in Fig 3.1. It is first formalized by Peter Gustav Lejeune Dirichlet in 1834 in the proof of a theorem in diophantine approximation. Dirichlet's box principle is a very basis counting argument, and it has very important applications in number theory.

Theorem. (Dirichlet Box Principle (see [38]))

If more than N objects are placed in N boxes, at least one box contains two or more objects.

A generalized version of this principle states as follows,

Theorem. (generalization of Dirichlet Box Principle (see Chap. 2 in [39]))

Let S be a finite set containing n elements, and let $S_1, S_2, \cdots, S_k$ be a partition of S into k subsects. Then at lest one subset S_i, $1 \leq i \leq k$, contains at least $[n/k]$ elements.

The notation $[n/k]$ in above theorem means the ceiling function, denoting the smallest integer which is larger than or equal to n/k.

Dirichlet's box principle will be used in Sec. 7.4 for filling fraction of reversed natural inequality in flat band models.

3.4 Perron-Frobenius theorem

The Perron-Frobenius theorem is standard in linear algebra [40, 35, 36], which states the properties of eigenvalues and eigenvectors of nonnegative matrices. It is firstly proved by O. Perron and G. Frobenius for positive matrices, and is extended by G. Frobenius for nonnegative irreducible matrices.

Perron-Frobenius theorem plays a significant role and is broadly applicable in the research of physics. It is widely used in different ares, for example in the study of Markov chains in stochastic process [41], and in the study of the ground state in condensed matter physics [42, 43, 44, 45]. One reason why Perron-Frobenius theorem is so useful is that it shows the properties of the dominant eigenvalue, whose absolute value is the largest.

The Perron-Frobenius theorem used in this thesis is the one for nonnegative irreducible matrix. Let me present the general notations used in mathematics first. Assuming A is an n by n matrix, if the matrix element a_{ij} of A satisfies $a_{ij} \geq 0$ for any i and j, matrix A is said to be nonnegative and is denoted by writing $A \geq 0$. If every matrix element a_{ij} is not smaller than corresponding b_{ij} of matrix B ($a_{ij} \geq b_{ij}$ for any i, j), it is denoted by $A \geq B$. The notation of $|B|$ is for a matrix whose matrix element is $|b_{ij}|$. The largest eigenvalue of matrix A is assumed as λ_A. The spectral radius of A is defined as $\rho(A) \equiv \max_{1\leq i\leq n}(|\lambda_i|)$.

With these notations, the Perron-Frobenius is presented below:

Theorem. (Perron-Frobenius theorem for nonnegative irreducible matrix (see Theorem 7.7 in [40]))

If $A \geq |B|$, where A is an $n \times n$ nonnegative irreducible matrix and B is an $n \times n$ real or complex matrix, then:
(1) *any eigenvalue β of B satisfies $|\beta| \leq \lambda_A = \rho(A)$;*
(2) *the condition to have the equal sign in the equality in (1) is $|B| = A$.*

In mathematics, matrix A is said to be reducible when there exists a permutation matrix P (a product of elementary interchange matrices which interchanges two rows) such that $P^T AP = \begin{pmatrix} X & Y \\ O & Z \end{pmatrix}$, where X and Z are square matrices [36]. Otherwise A is said to be an irreducible matrix. This definition is not directly useful when we want to make sure if one matrix is irreducible or not. One necessary and sufficient condition of the irreducibility of A is that if and only if $(I+A)^{n-1} > 0$ [36, 35], where I is identity matrix and n is the dimension of matrix A. It can be used as a criterion if A is known.

Actually, in the context of graph theory, the irreducibility is more physically meaningful. As is known in graph theory, a matrix can be constructed from a graph. It is also possible to reverse the process by starting with a matrix to build an associated graph. The graph of $A_{n\times n}$ (denoted by $G(A)$) is defined on a directed graph with n nodes $\{V_1, V_2, \cdots, V_n\}$ in this way: there is a directed edge from node V_i to V_j if and only if $a_{ij} \neq 0$. The directed graph $G(A)$ is said to be strongly connected if there is a sequence of directed edges leading from V_i to V_j for any pair of nodes (V_i, V_j). Matrix A is said to be irreducible if and only if $G(A)$ is strongly connected [36].

However, in our work, we do not need such a strong condition that the graph $G(A)$ is strongly connected, because the matrix of Hamiltonian is not a general one but Hermitian with the property that $H_{ij} = H^*_{ji}$. This property leads to the fact that graph $G(H)$ is undirected. The requirement of irreducibility of a Hermitian or symmetric matrix is reduced to the connectivity of the undirected graph. Namely, any two different vertices V_i and V_j are connected by a path, or connected by nonvanishing matrix elements of H. More precisely, for any $i \neq j$, there is a sequence $(i_1, \cdots, i_K)$ such that $i_1 = i$, $i_K = j$ and $a_{i_k,i_{k+1}} \neq 0$ for all $k < K$. Therefore, the terminology of "connectivity" is widely used in the physical literatures instead of "irreducibility".

By the mapping to the graph, irreducibility can be regarded as the property of a tight-binding model defined on a "lattice" ($G(H)$) in "single-particle" basis. Considering a tight-binding model, if the lattice (graph $G(H)$ is the lattice) is connected, a particle can get from any site to any other site by successive hoppings, with nonvanishing nearest neighbor hopping amplitudes. Therefore, in single particle basis, the matrix of tight-binding Hamiltonian is irreducible (or connected) on a connected lattice, no matter the particle is spinless or spinful. However, the irreducibility of the matrix of tight binding Hamiltonian in single particle basis does not necessarily leads to the irreducibility or connectivity of the matrix of Hamiltonian in many-body basis for spinful particles. A care need to be taken on the connectivity of Hamiltonian in many-body basis. The application of Perron-Frobenius theorem and a care of connectivity of Hamiltonian in many-body basis will be presented in Chap. 4.

Chapter 4

Natural inequality

In quantum many-body problem, understanding of the ground state and corresponding energy is fundamental. The ground-state energy is a physical quantity which governs the stability of the system, and in principle it is measurable by measuring the exchange of the energy with the outside, during a process starting from a known initial state. The ground-state energy also reflects the statistics of identical particles, which pervades all of quantum physics. We study the effect of particle statistics and frustration on the ground-state energy, by comparing bosons and fermions subject to the same lattice Hamiltonian.

In this chapter, we will explain why in the absence of interaction, the comparison is trivial in Sec. 4.1: the ground-state energy of noninteracting bosons is always lower than that of free fermions (natural inequality). And we will demonstrate why the comparison is not trivial in the presence of hard-core interaction among bosons in Sec. 4.2. We prove that the ground-state energy of hard-core bosons is still lower than that of fermions if all the hopping amplitudes are nonnegative, for spinless case (Theorem 1) and spinful case (Theorem 2 and Theorem 3) respectively.

4.1 In noninteracting systems

In noninteracting systems, the influence of particle statistics on the ground-state energy is quite trivial, because we can do particle filling to the single particle states.

For a system of free fermions, the ground state of fermions is obtained by filling the individual single-particle states up to the Fermi level, due to Pauli

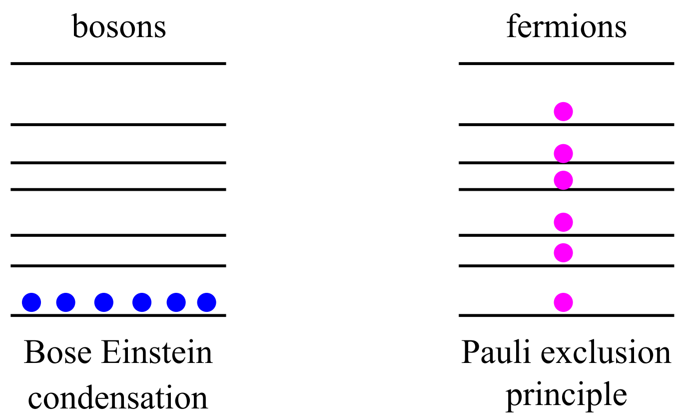


Figure 4.1: An illustration of particle filling to the single-particle states in noninteracting systems for bosons and fermions, respectively.

exclusion principle [46] and the Aufbau principle. In contrast, in the ground state of noninteracting bosons, all the bosons condense into the lowest single-particle state, as known as Bose-Einstein condensation (BEC) [47, 48]. (At zero temperature, the condensation is perfect for free bosons.) Therefore, the ground state of bosons is obtained by putting all the particles in the lowest-energy state of the single-particle Hamiltonian. Thus, the ground-state energy of bosons E_0^{B} and that of fermions E_0^{F}, for the same form of the Hamiltonian, satisfy

$$E_0^{\mathrm{B}} \leq E_0^{\mathrm{F}}, \tag{4.1}$$

if the particles are noninteracting.

A schematic illustration of particle filling is shown in Fig. 4.1. The Eq. (4.1) is called as *"natural" inequality* in this thesis.

4.2 In interacting systems

In the presence of interaction, the comparison of the ground-state energies of bosons and fermions is not trivial, because the simple argument based on the perfect BEC breaks down. Einstein's original literature assumes the absence of interaction and it is restricted to the thermal equilibrium [48, 49]. Namely, the original argument only tells us that below a critical temperature, BEC will occur in a noninteracting system in thermal equilibrium. But how about the case in interacting many-body bosonic system? In a system of interacting bosons, it is in fact already a nontrivial question whether the BEC actually takes place. It is obvious that there can not be any general theorem that BEC always occur in interacting bosonic system, because the crystalline solid phase of ^{4}He is a counterexample, where BEC (in the sense of off-diagonal long range order) is absent even at zero temperature, under a sufficiently high pressure. To our knowledge, the only rigorously proven example of BEC (in the sense of the off-diagonal long-range order) in an interacting system is the hard-core bosons on hypercubic lattice at half-filling and at zero temperature, in two or higher dimensions, proved by Kennedy et al. [50]. Even if the occurrence of BEC or the off-diagonal long-range order 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.

On the other hand, the "no-go" theorem associated with Mermin-Wagner-Hohenberg states that there can not be any long-range order in any system with short range interactions in $d \leq 2$ dimensions at finite temperature [51, 52, 53]. It excludes the possibility of BEC in such systems, since the presence of off-diagonal long-range order is the criterion of BEC. (In literatures, the Mermin-Wagner-Hohenberg theorem is also equivalently represented as the statement that there cannot be any spontaneous breaking of a continuous symmetry in $d \leq 2$ dimensions [54], such as $U(1)$ symmetry. By this statement, it also rules out the existence of BEC in interacting bosons in such systems, since $U(1)$ symmetry is preserved [32].)

With the reasons given above, the BEC (even if it happens) is no longer perfect in interacting bosons. The simple argument based on perfect BEC can not be used to compare the ground-state energies of interacting bosons and fermions. In the strongly correlated system, the influence of particle statistics on the ground-state energy is still a relatively unexplored area. Even in the simplest and extreme interacting case only hard-core interaction among bosons, the issue was note clarified. Therefore, we need investigate if the natural inequality (4.1) still holds in interacting systems. Intuitively, it would be still natural to expect that Eq. (4.1) holds. This is the reason why the Eq. (4.1) is called as the natural inequality in this thesis.

However, recently an apparent counterexample was found numerically in small cluster [55, 56], in which the ground-state energy of hard-core bosons is higher than that of fermions on delta-chain and kagome lattice with flat band. This motivates us to examine the fundamental question: how general is the "natural" inequality (4.1) and when can it be actually violated?

In the following, we focus on the comparison of the ground-state energies of hard-core bosons and fermions with the same Hamiltonian. In fact, we can give [57] a sufficient condition for the natural inequality (4.1). That is, if all the hopping amplitudes are nonnegative, 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.

4.2.1 Hard-core bosons

In the frame of second quantization, the Schrödinger wavefunction is raised to the operator, which satisfies commutation or anticommutation algebras. For fermions, the field operators satisfy anticommutation relation:

$$\{c_i, c_j^\dagger\} = \delta_{ij}, \qquad \{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0, \tag{4.2}$$

where c_i ($c_i^\dagger$) is the annihilation (creation) operator of fermion at site i. Pauli exclusion principle is represented as $c_i^2 = 0$, and $(c_i^\dagger)^2 = 0$. For bosons, the field operators satisfy commutation relation:

$$[b_i, b_j^\dagger] = \delta_{ij}, \qquad [b_i, b_j] = [b_i^\dagger, b_j^\dagger] = 0. \tag{4.3}$$

With Dirac δ repulsive interaction (on-site repulsion goes to infinity), bosons behave like impenetrable particles, which is called as hard-core boson. For hard-core boson, double occupancy is not allowed. Thus, the hard-core constraint can be applied by $n_i = b_i^\dagger b_i = 0$ or 1. On different sites, the hard-core bosons commute as usual bosons, obeying the commutation relation in Eq. (4.3). However, on the same site these operators satisfy anticommutation relations typical for fermions:

$$\{b_i, b_i^\dagger\} = 1, \qquad \{b_i, b_i\} = \{b_i^\dagger, b_i^\dagger\} = 0,$$

which is clear after the Matsubara-Matsuda mapping [58] as shown below.

Hard-core boson is of great interest in condensed matter physics, since it is mathematically equivalent to quantum spin-1/2 magnet. By the Matsubara-Matsuda transformation, hard-core bosons can be mapped to spin 1/2 magnets:

$$S_j^+ = b_j^\dagger, \qquad S_j^- = b_j, \qquad S_j^z = b_j^\dagger b_j - 1/2 \tag{4.4}$$

where $S_j^+ = (\sigma_j^x + i\sigma_j^y)/2$, spin raising operator. And $\sigma_j^{x,y,z}$ is the Pauli matrix, satisfying $[\sigma^a, \sigma^b] = 2i\sum_c \epsilon_{abc}\sigma^c$. A more general mapping from hard-core boson to spin is Holstein-Primakoff transformation [59, 60]

$$S_j^+ = b_j^\dagger\sqrt{1-n_j}, \qquad S_j^- = \sqrt{1-n_j}\,b_j, \qquad S_j^z = n_j - 1/2, \tag{4.5}$$

which can be used for higher S spins and any dimension.

Apart from the mathematical equivalence to spin-1/2 magnet, hard-core boson is of great interest because of the experimental realization. One dimensional hard-core boson, also known as Tonks-Giradeau gas [15, 16], is not a toy model, which has already been realized in experiment by optical trap [17].

With hard-core constraint of bosons, the dimension of Hilbert space is the same compared with fermions. On the same site, hard-core bosons obey anticommutation relation, which is typical for fermions. In this sense, the behavior of hard-core boson has some similarity as fermions. (The "fermionic-like" behaviors of one-dimensional hard-core bosonic gas is discussed in Sec. 2.3.2.) But still they are distinctly different because on different sites hard-core bosons satisfy commutation relation as usual bosons. The wavefunction of N hard-core bosons does not have the antisymmetry property with respect to exchange of two particles. This essential, and also distinguished difference, makes hard-core bosons obey Bose statistics and statistically different with fermions. The difference of statistics can be shown in the ground-state energy.

4.2.2 Spinless case

The "natural" inequality (4.1) holds trivially for noninteracting bosons and fermions with the same form of the Hamiltonian. Now we present three theorems (one theorem for spinless case in this section, and two theorems for spinful case in Sec. 4.2.3), which state that Eq. (4.1) holds even for hard-core bosons, provided that all the hopping amplitudes are nonnegative.

To simplify this matter, in this section we focus on the comparison of spinless hard-core bosons with spinless fermions. (See also Refs. [61, 62].) "Spinless boson" can be understood as there is no internal degree of freedom, for example liquid ^{4}He. "Spinless fermions" means the spin orientation or spin degrees of freedom could be ignored, or it can be understood as fully polarized. The discussion of spinful version is presented in Sec. 4.2.3.

The Hamiltonian is given by

$$\mathcal{H} = -\sum_{j,k} \left(t_{jk} c_j^\dagger c_k + \text{H.c.} \right) - \sum_j \mu_j n_j + \sum_{j,k} V_{jk} n_j n_k, \tag{4.6}$$

where each site j belongs to a finite lattice Λ, $n_j \equiv c_j^\dagger c_j$, and $t_{jk} = 0$ is assumed for

$j = k$. The uniform (site independent) part of μ_j is the chemical potential μ. 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 ($n_j = 0, 1$) may also be implemented by introducing the on-site interaction $U \sum_j n_j(n_j - 1)$ and then taking $U \to +\infty$. For a system of fermions, we identify c_j with the fermion annihilation operator f_j satisfying the standard anticommutation relations.

This generic 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 Sec. 4.2.3. We note that the Hamiltonian (4.6) 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.

First we present a sufficient condition for the "natural" inequality (4.1) to hold. Furthermore, we find sufficient conditions for the strict inequality $E_0^{\mathrm{B}} < E_0^{\mathrm{F}}$ to hold. The proof also gives us a physical insight into the reason why the inequality still holds even in interacting systems, where the simple argument based on the perfect Bose-Einstein condensation of bosons breaks down.

Theorem 1. (Natural inequality for spinless case)

The inequality (4.1) 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 nonnegative.

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 $E_0^{\mathrm{B}} < E_0^{\mathrm{F}}$ holds.

Proof. Let us take 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 number operator n_j has the same matrix elements in this basis, for hard-core bosons and spinless fermions. It is convenient to introduce the operator,

$$\mathcal{K}^{\mathrm{B,F}} \equiv -\mathcal{H}^{\mathrm{B,F}} + C\mathbb{1}, \tag{4.7}$$

with a sufficiently large real number C so that all the eigenvalues $\kappa^{\mathrm{B,F}}$ of matrix $\mathcal{K}^{\mathrm{B,F}}$ and thus all the diagonal matrix elements $\mathcal{K}_{aa}^{\mathrm{B,F}}$ are positive. The matrix elements of each hopping term in the bosonic operator $\mathcal{K}^{\mathrm{B}}$ is nonnegative (see also Feynman's "no-node" theorem [22, 23]). While the corresponding matrix element for the fermionic operator must have the same absolute value but could differ in signs. Thus the matrix elements for bosonic and fermionic operators satisfy

$$\mathcal{K}^{\mathrm{B}}_{ab} = \begin{cases} |\mathcal{K}^{\mathrm{F}}_{ab}| & (a \neq b) \\ \mathcal{K}^{\mathrm{F}}_{aa} & (a = b) \end{cases} = |\mathcal{K}^{\mathrm{F}}_{ab}| \tag{4.8}$$

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

$$\kappa^{\mathrm{B}}_{\max} \geq {}_{\mathrm{B}}\langle\Psi_0|\mathcal{K}^{\mathrm{B}}|\Psi_0\rangle_{\mathrm{B}} = \sum_{ab} |\psi_a||\psi_b|\mathcal{K}^{\mathrm{B}}_{ab} \geq \sum_{ab} \psi^*_a\psi_b\mathcal{K}^{\mathrm{F}}_{ab} = \kappa^{\mathrm{F}}_{\max}, \tag{4.9}$$

implying $E^{\mathrm{B}}_0 \leq E^{\mathrm{F}}_0$. The first part of Theorem 1 is proved. As a simple corollary, the ground-state energies for a given chemical potential μ also satisfy Eq. (4.1).

For strict natural inequality, let us now consider $\mathcal{L}^S \equiv \left(\mathcal{K}^S\right)^n$, where $S = \mathrm{B}, \mathrm{F}$, for a positive integer n. Its matrix elements in the occupation number basis can be expanded as

$$\mathcal{L}^S_{ab} = \sum_{c_1,\ldots,c_{n-1}} \mathcal{K}^S_{ac_1}\mathcal{K}^S_{c_1c_2}\mathcal{K}^S_{c_2c_3}\ldots\mathcal{K}^S_{c_{n-1}b}. \tag{4.10}$$

Each term in the sum represents a process in which a particle can hop among connected sites.

We will derive two useful relations first. From the definition of $\mathcal{L}^S$ and the relation between $\mathcal{K}^{\mathrm{B}}$ and $\mathcal{K}^{\mathrm{F}}$ denoted by Eq. (4.8), we have following useful inequality:

$$\begin{aligned} \mathcal{L}^{\mathrm{B}}_{ab} &= \sum_{c_1,\ldots,c_{n-1}} \mathcal{K}^{\mathrm{B}}_{ac_1}\mathcal{K}^{\mathrm{B}}_{c_1c_2}\mathcal{K}^{\mathrm{B}}_{c_2c_3}\ldots\mathcal{K}^{\mathrm{B}}_{c_{n-1}b} = \sum_{c_1,\ldots,c_{n-1}} |\mathcal{K}^{\mathrm{F}}_{ac_1}\mathcal{K}^{\mathrm{F}}_{c_1c_2}\mathcal{K}^{\mathrm{F}}_{c_2c_3}\ldots\mathcal{K}^{\mathrm{F}}_{c_{n-1}b}| \\ &\geq \Big|\sum_{c_1,\ldots,c_{n-1}} \mathcal{K}^{\mathrm{F}}_{ac_1}\mathcal{K}^{\mathrm{F}}_{c_1c_2}\mathcal{K}^{\mathrm{F}}_{c_2c_3}\ldots\mathcal{K}^{\mathrm{F}}_{c_{n-1}b}\Big| = |\mathcal{L}^{\mathrm{F}}_{ab}|. \end{aligned} \tag{4.11}$$

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

Another important relation is the property of diagonal terms in $\mathcal{L}^S$. Since $\mathcal{K}$ is a Hermitian matrix, $\mathcal{K}$ is diagonalizable. The eigenvalues of $\mathcal{K}$ are real and corresponding eigenvectors can be chosen to be mutually orthogonal. Let κ_i and $\vec{u}_i$ are the eigenvalues and orthonormal eigenvectors of $\mathcal{K}$, where $\kappa_i \geq 0$ by taking

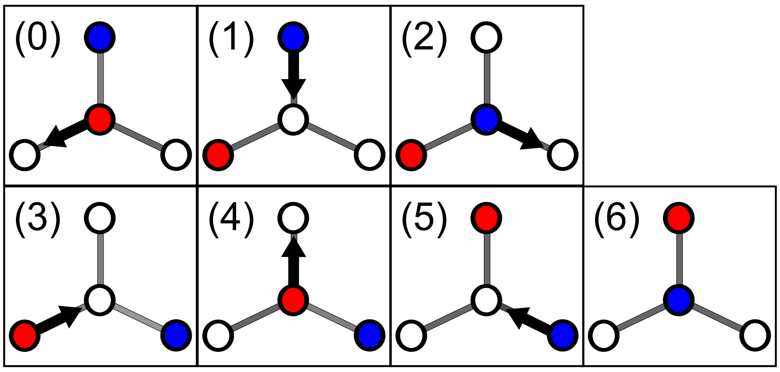


Figure 4.2: An illustration of two-particle exchange process in six steps.

sufficient large C in equation (4.7). By spectral decomposition of Hermitian matrix $\mathcal{K}$ [1], we have

$$\mathcal{K} = \sum_{i=1}^{m} \kappa_i \vec{u}_i \vec{u}_i^T = \sum_{i}^{m} \kappa_i P_{\kappa_i}, \tag{4.12}$$

where P_{κ_i} is the projection operator to κ_i satisfying $P_{\kappa_i} P_{\kappa_j} = P_{\kappa_i} \delta_{ij}$. Therefore, the diagonal elements of $\mathcal{L}$ is nonnegative,

$$\mathcal{L}_{aa} = (\mathcal{K}^n)_{aa} = (\sum_i \kappa_i P_i)^n_{aa} = (\sum_i \kappa_i^n P_{\kappa_i})_{aa} > 0, \tag{4.13}$$

leading to $\mathcal{L}^{\mathrm{B}}_{aa} \geq \mathcal{L}^{\mathrm{F}}_{aa} > 0$.

From Eq. (4.8), it follows that the matrix elements of $\mathcal{K}^{\mathrm{F}}$ and thus the amplitudes of the process in Eq. (4.10) can be negative for fermions, while they are positive for bosons. The difference between bosons and fermions shows up exactly when two particles are exchanged. To make two-particle exchange process possible, let us consider a lattice with a "branching" site directly connected to three or more sites. If the number of particle 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 6 hoppings. An example of particle exchange on a lattice with a branching site is demonstrated schematically in Fig. 4.2. The contribution to the diagonal elements of bosons $\mathcal{L}^{\mathrm{B}}_{aa}$ is always positive at $n = 6$, while the contribution to $\mathcal{L}^{\mathrm{F}}_{aa}$ is negative when two particles are exchanged. This implies the strict inequality $\mathcal{L}^{\mathrm{B}}_{aa} > \mathcal{L}^{\mathrm{F}}_{aa} > 0$ for the particular diagonal element. In other words, $\mathcal{L}^{\mathrm{B}}_{aa} > |\mathcal{L}^{\mathrm{F}}_{aa}|$ holds if two particles are exchanged in this process.

When the lattice Λ is connected, any basis state $|\phi^a\rangle_{\mathrm{B}}$ can be reached by a consecutive application of the hopping term in $\mathcal{K}^{\mathrm{B}}$, and thus the matrix $\mathcal{K}^{\mathrm{B}}_{ab}$

[1]See Theorem 2.5.6 of Ref. [35].

satisfies the connectivity. Together with the property $\mathcal{K}^{\mathrm{B}}_{ab} \geq 0$, $\mathcal{K}^{\mathrm{B}}_{ab}$ (and thus also $\mathcal{L}^{\mathrm{B}}_{ab}$) is a Perron-Frobenius matrix [35].

Applying a corollary of Perron-Frobenius theorem [2] we find $\kappa^{\mathrm{B}}_{\max} > \kappa^{\mathrm{F}}_{\max}$ and hence the latter part of the theorem follows. □

A distinct property of bosons, described by the Hamiltonian (4.6) is that the matrix element of $\mathcal{K}$ is positive semi-definite as denoted by Eq. (4.8). This property is consistent with Feynman's "no-node" theorem (see Sec. 11.3 of [22]). According to Feynman's discussion in ^{4}He system, it is stated that the many-body ground-state wavefunction of bosons are positive-definite in the coordinate representation, if there is no external rotation applied. External rotation will introduce effective flux, which can be understood as frustration in a unified manner (see the discussion in Chap. 5). Therefore, "no-node" theorem applies to the ground state of flux free bosons. This strong argument reduces the general complex-valued many-body wavefunctions to be positive definite. This theorem also paves the way for the study of the ground-state properties of bosonic systems (such as ^{4}He) by quantum Monte Carlo simulation, in which case it is free of sign problem. The distinct property of bosons in unfrustrated system leads to the natural inequality (4.1).

Of course, the fact that the matrix element of $\mathcal{K}^{\mathrm{B}}$ in occupation number basis is positive semi-definite is a different thing from the "no-node" theorem that the ground-state wavefunction is positive definite in coordinate space. The relation can be explained in the following way. Under the assumption that the connectivity is satisfied, the positive semi-definite matrix $\mathcal{K}^{\mathrm{B}}$ is a Perron-Frobenius matrix. According to the Perron-Frobenius theorem in [63], the largest eigenvalue of $\mathcal{K}^{\mathrm{B}}$ is nondegenerate and the corresponding eigenvector $\vec{v} = (v_i)_{i=1,\cdots,N}$ can be taken to satisfy $v_i > 0$ for all i, which corresponds to the ground state of $\mathcal{H}^{\mathrm{B}}$. Feynman's theorem tells us that this eigenvector can be taken in coordinate space, which is positive definite.

The essence of the proof is that a state without "no node" has low energy, which is quite familiar in quantum mechanics (for example, see Sec. 20 of [64]). The unconventional boson systems beyond Feynman's paradigm (i.e. meta-stable state of bosons in the high orbital bands in optical lattice, and spinful bosons with spin-orbital coupling), whose wavefunction is complex, is discussed by C. Wu et al. [23, 65, 66]. The unconventional bosons beyond Feynman's diagram is not the

[2] See Theorem 8.4.5 of Ref. [35] and Theorem in the review section 3.4.

subject investigated in this chapter.

Another point need noticed is that for spinless case, the connectivity of the matrix of Hamiltonian in many-body basis is satisfied when the hopping matrix in single-particle basis is irreducible. Irreducibility of a symmetric matrix $M = (m_{ij})$ means for any $i \neq j$, we can take a sequence $\{i_1, i_2, \cdots, i_n\}$ with $i_1 = i$ and $i_n = j$ such that $m_{i_k, i_{k+1}} \neq 0$ for all $k < n$. Intuitively, the irreducibility simply means that one can bring a particle from site j to i by successive applications of the hopping term. Namely, if the lattice is not decoupled into disconnected pieces. Therefore, for spinless particles, the irreducibility of the hopping matrix in single-particle basis (or connectivity of the lattice) leads to the irreducibility of the matrix of Hamiltonian in many-body basis, making the Perron-Frobenius theorem applicable. The connectivity for spinful case with infinite on-site repulsion is quite involved, and will be presented in Sec. 4.2.3.

Theorem 1 gives a qualitative estimate of the comparison between the ground-state energies of hard-core bosons and spinless fermions. It is obvious that the magnitude of energy difference depends on the models in the question. Therefore, there cannot be any general or mathematically rigorous theorem about the order of the energy difference. For a given concrete model, a lower bound of the energy difference may be obtained quantitatively. For example, consider the tight-binding model on a two dimensional square lattice $\mathcal{H} = -\sum_{\langle j,k \rangle}(c_j^\dagger c_k + \text{H.c.})$. The dispersion relation is easily obtained as $\epsilon(k_x, k_y) = -2(\cos k_x + \cos k_y)$. The ground-state energy at half filling is obtained by filling up the Fermi sea,

$$E_0^{\mathrm{F}}/N = \frac{1}{N} \sum_{k_x, k_y \in FS} \epsilon(k_x, k_y) = \frac{4}{(2\pi)^2} \int_0^{\pi} dk_x \int_0^{-k_x+\pi} dk_y \; \epsilon(k_x, k_y) = -0.81057, \tag{4.14}$$

where the Fermi sea is shown by the dark region in Fig. 4.3. An upper bound of the ground-state energy of hard-core bosons can be obtained by variational method. Due to the hard-core constraint, we can use the spin-1/2 notation to represent a site which is occupied by one particle or empty: $|\uparrow\rangle = b^\dagger|0\rangle$, $|\downarrow\rangle = |0\rangle$. The trial wavefunction of hard-core bosons is assumed as a direct product of the wavefunction on every site: $|\Psi\rangle = (\frac{1}{\sqrt{2}}|\uparrow\rangle_1 + \frac{1}{\sqrt{2}}|\downarrow\rangle_1) \otimes (\frac{1}{\sqrt{2}}|\uparrow\rangle_2 + \frac{1}{\sqrt{2}}|\downarrow\rangle_2) \otimes \cdots$, where $\frac{1}{\sqrt{2}}|\uparrow\rangle_i + \frac{1}{\sqrt{2}}|\downarrow\rangle_i$ is the wavefunction of ith spin-1/2 pointing to the x axis. By variational principle, $E_0^{\mathrm{B}} \geq \langle\Psi|\mathcal{H}|\Psi\rangle = -\frac{1}{4} \times 4N = -N$. Therefore, a lower bound of the energy density difference is obtained

$$\Delta\epsilon = E_0^{\mathrm{F}}/N - E_0^{\mathrm{B}}/N \geq 0.18943. \tag{4.15}$$

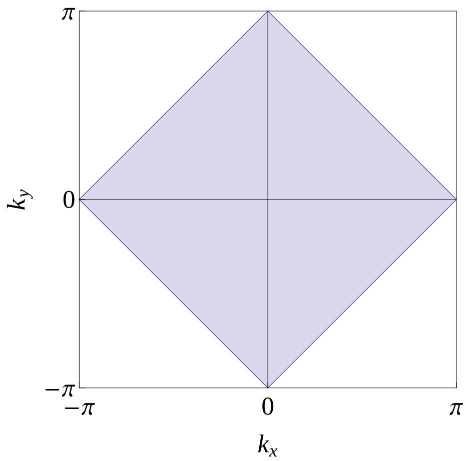


Figure 4.3: Fermi sea for two-dimensional tight-binding model.

The discussion of the estimation on the magnitude of the ground-state energy density difference can be extended to other two-dimensional lattices and also to higher dimensions by the same method. In a generic system in two or higher dimensions, we expect that the energy difference scales linearly in the system size (or equivalently, the difference in the ground-state energy density approaches a constant).

4.2.3 Spinful case

In Sec. 4.2.2, we have proved a sufficient condition of (strict) natural inequality for spinless case. In this section, we extend the discussion of natural inequality for spinful case. (See Ref. [67] for a similar inequality for spinful fermions.)

We consider the comparison between spin-1/2 hard-core bosons and spin-1/2 fermions. The pseudospin-1/2 bosons can be regards as bosons with two internal degrees of freedom, for example two-component bosons [32]. The Hamiltonian is:

$$\mathcal{H} = -\sum_{j\neq k}\sum_{\sigma}\left(t_{jk}c^{\dagger}_{j\sigma}c_{k\sigma} + \text{H.c.}\right) - \sum_{j\sigma}\mu_j n_{j\sigma} + \sum_{j\neq k}\sum_{\sigma,\sigma'}V_{jk}n_{j\sigma}n_{k\sigma'} + \sum_{j}U_j n_{j\uparrow}n_{j\downarrow}, \tag{4.16}$$

where $n_j = \sum_\sigma c^{\dagger}_{j\sigma}c_{j\sigma}$, the number of particles on site j of the finite lattice Λ, and $\sigma =\uparrow,\downarrow$, the spin index for fermions and bosons. This Hamiltonian is a generalization of Eq. (4.6) with the introduction of the spin degrees of freedom $\sigma =\uparrow,\downarrow$. For a system of fermions, $c_{j\sigma}$ is identified with the fermion annihilation operator $f_{j\sigma}$, satisfying anticommutation relation $\{f_{j\sigma}, f^{\dagger}_{k\sigma'}\} = \delta_{jk}\delta_{\sigma\sigma'}$. For a system of bosons,

$c_{j\sigma}$ is identified with the boson annihilation operator $b_{j\sigma}$, satisfying commutation relation $[b_{j\sigma}, b^\dagger_{k\sigma'}] = \delta_{jk}\delta_{\sigma\sigma'}$. The hard-core constrain ($n^{\mathrm{B}}_{j\sigma} = b^\dagger_{j\sigma} b_{j\sigma} = 0, 1$ without summation over σ and j) is applied to each site; two or more particles with the same spin cannot occupy the same site. Similarly to the Hamiltonian for spinless case (4.6), the generic Hamiltonian is also very general. The interesting point of attractive on-site interaction ($U_j < 0$) will be discussed in section 4.2.3.3.

4.2.3.1 Finite U_j's

Let us first discuss the case in which all U_j's are finite. We present sufficient conditions for the natural inequality and strict natural inequality $E^{\mathrm{B}}_0 < E^{\mathrm{F}}_0$ for spinful case with finite U_j's first. The discussion of infinite U_j's is presented in section 4.2.3.2 and 4.2.3.3.

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 (4.1) 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 connecting to three or more site, and if the number of particles satisfies $3 \leq M \leq 2N - 3$, the strict inequality holds.

The proof of the Theorem 2 is a straightforward generation of that for spinless case in Theorem 1 in section 4.2.2.

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 (4.16), 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-spin and down-spin particles. Let $|\phi^\mu\rangle_\uparrow \equiv |\{n^\mu_{j\uparrow}\}\rangle$ ($\mu = 1, 2, \cdots, u$) be the occupation number basis for up-spin particles, and $|\psi^\nu\rangle_\downarrow \equiv |\{n^\nu_{j\downarrow}\}\rangle$ ($\nu = 1, 2, \cdots, v$) be the occupation number basis for down-spin particles. Then, we can take the direct product $|\Phi^a\rangle = |\psi^\nu\rangle_\downarrow \otimes |\phi^\mu\rangle_\uparrow$, where $a = 1, 2, \cdots, uv$, as the basis of the sub-Hilbert space mentioned above.

The Hamiltonian can be rewritten as:

$$\mathcal{H} = \mathcal{H}_{\mathrm{t}} + \mathcal{H}_{\mathrm{int}}, \tag{4.17}$$

$$\mathcal{H}_{\mathrm{t}} = \mathbb{1}^{\downarrow} \otimes \mathcal{H}_{\mathrm{t}}^{\uparrow} + \mathcal{H}_{\mathrm{t}}^{\downarrow} \otimes \mathbb{1}^{\uparrow}, \tag{4.18}$$

where $\mathcal{H}_{\mathrm{t}}^{\sigma} = -\sum_{j\neq k}(t_{jk}c_{j\sigma}^{\dagger}c_{k\sigma}+\mathrm{H.c.})$. 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 $\mathcal{K}^{\mathrm{B,F}} \equiv -\mathcal{H}^{\mathrm{B,F}} + C\mathbb{1}$ with a constant C. Choosing C large enough, we make all the eigenvalues and all the diagonal matrix elements of $\mathcal{K}^{\mathrm{B,F}}$ positive. The matrix elements of bosonic and fermionic Hamiltonians obey the relation:

$$\mathcal{K}_{ab}^{\mathrm{B}} = \begin{cases} |\mathcal{K}_{ab}^{\mathrm{F}}| & (a \neq b) \\ \mathcal{K}_{aa}^{\mathrm{F}} & (a = b), \end{cases} \tag{4.19}$$

where the diagonal terms correspond to $\mathcal{H}_{\mathrm{int}}$ and the off-diagonal terms correspond to $\mathcal{H}_{\mathrm{t}}$. 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 $\mathcal{H}_{\mathrm{int}}$, 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 a combination of two independent systems of hard-core particles. As a consequence, when the lattice Λ is connected, any pair of basis states $|\Phi^a\rangle_{\mathrm{B}}$ and $|\Phi^b\rangle_{\mathrm{B}}$ are connected to each other by a successive applications of the hopping terms in $\mathcal{K}^{\mathrm{B}}$. Together with the property $\mathcal{K}_{ab}^{\mathrm{B}} \geq 0$, $\mathcal{K}^{\mathrm{B}}$ 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 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. 4.2. 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 spinless case, the strict inequality $E_0^{\mathrm{B}} < E_0^{\mathrm{F}}$ follows from the Perron-Frobenius theorem [3]. □

4.2.3.2 $U_j = +\infty$

Now let us discuss the case $U_j = +\infty$. The first half of Theorem 2, the non-strict version of the inequality, is not affected by taking $U_j = +\infty$. However,

[3] See Theorem 8.4.5 of Ref. [35].

the latter half of Theorem 2, the strict inequality, is affected. 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 applications of particle hoppings. This implies the irreducibility of the matrix representing the many-body Hamiltonian.

However, in the case of spinful system with $U_j = +\infty$, the connectivity of the lattice does not guarantee the irreducibility of the many-body Hamiltonian matrix. A special care should be taken on the irreducibility. 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. 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 many-body basis.

In fact, the irreducibility of the Hamiltonian matrix at $U_j = +\infty$, and application of the Perron-Frobenius theorem were discussed earlier by Tasaki in the context of Nagaoka's ferromagnetism [63]. Nagaoka's ferromagnetism is a mechanism of ferromagnetism in the Hubbard model with a single hole 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. [63], 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" 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

Theorem 3. (Natural inequality for spinful case)

When U_j's are either $+\infty$ or finite, if all the hopping amplitudes t_{jk} are real and nonnegative, the inequality (4.1) 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.

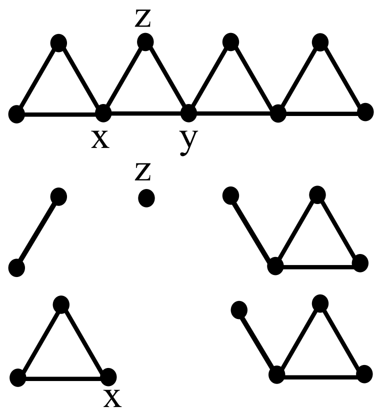


Figure 4.4: An example of exchange-bond lattice. The horizontal bond $\{x, y\}$ is not an exchange bond, because the site z is disconnected when the two sites x and y are removed. However, the $\{y, z\}$ bond is an exchange bond, because the lattice is still connected with periodic boundary condition when sites y and z are removed. The delta-chain is an exchange-bond lattice, since the whole lattice is connected via non-horizontal exchange bonds.

The property that the entire lattice is connected by exchange bonds can be verified [63] in various common lattices, such as triangular, square, simple cubic, fcc, or bcc lattices, in which nearest neighbor sites are connected by non-vanishing 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 nonnegative. 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 holes 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-1/2 bosons instead of electrons, all the matrix elements are nonnegative in the occupation number basis, for any number of holes. Thus the Bose-Hubbard model with spin-1/2 bosons exhibit ferromagnetism for any filling fraction [68]. This non-negativity of the matrix elements for bosons is also essential for Theorem 3, which holds for any filling fraction.

4.2.3.3 $U_j = -\infty$

The proofs of Theorems 1, 2 and 3 are insensitive to the signs of the interaction V_{jk} or 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, orbital part of the Cooper pair wavefunction must be antisymmetric with respect to the exchange of two fermions. This results in an extra cost in the kinetic energy. Such fermionic BEC state thus has a higher ground-state energy than its bosonic counterpart, in full agreement of the 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 and Theorem 3, 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 paring 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 on-site 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 breaking such a pair costs infinite energy U_j, resulting a completely localized ground state. Thus the natural inequality is reduced to the trivial equality $E_0^{\mathrm{B}} = E_0^{\mathrm{F}}$ in the limit $U_j \to -\infty$.

4.2.3.4 Spinful Hubbard model

In the following, we numerically demonstrate the above observations in a spinful Bose-Hubbard model and Fermi-Hubbard model on a 4-site cluster as shown in Fig. 4.5. Here the bosons in the "Bose-Hubbard" model still obey a particular hard-core condition $n_{j\sigma}^{\mathrm{B}} = 0, 1$. The Hamiltonian is given by

$$\mathcal{H} = -t \sum_{\langle i,j\rangle\sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + \mathrm{H.c.}) + U \sum_{j} n_{j\uparrow} n_{j\downarrow}, \tag{4.20}$$

where $t > 0$, and $\langle i, j \rangle$ denotes the nearest hopping. We consider the spin-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 4-site cluster, there are two up-spin particles and two down-spin particles. The energy difference between spinful bosons and spinful fermions ($\Delta E = E_0^{\mathrm{B}} - E_0^{\mathrm{F}}$) is shown as a function of $U = U_j$ in Fig. 4.6.

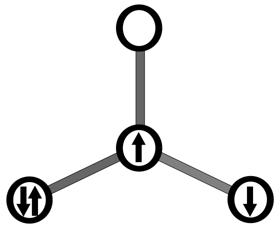


Figure 4.5: Four-site branch lattice with four spins at half filling and $S_z = 0$.

Conforming to Theorem 2, $E_0^{\mathrm{B}} \leq E_0^{\mathrm{F}}$ holds for all range of U, independent of the signs of U. Moreover, $\Delta E(U)$ is symmetric with respect to $U = 0$ due to the particle-hole symmetry of the Hubbard model at half filling $\nu = 1$ [69].

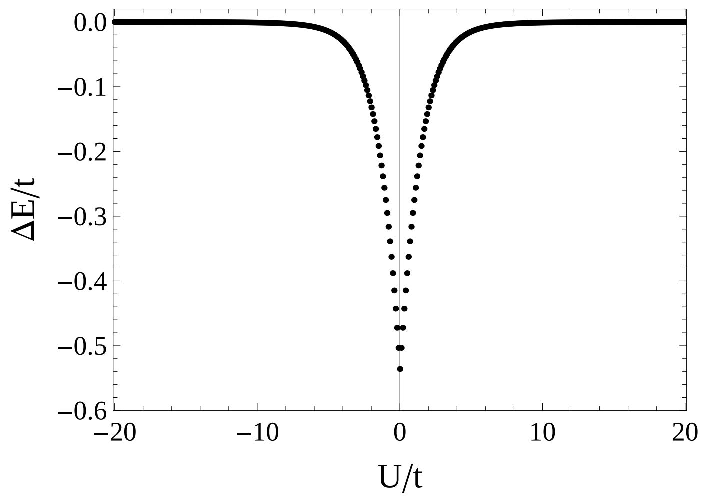


Figure 4.6: Difference of ground-state energy ($\Delta E = E_0^{\mathrm{B}} - E_0^{\mathrm{F}}$) between hard-core bosons and fermions on the 4-site lattice with a branch, in $S_z = 0$ sector with 4 spins.

When U is finite, fermions have strictly higher ground-state energy than bosons, again in agreement with the latter half of Theorem 2. When $U = +\infty$, the present 4-site cluster does not contain any exchange bond, and thus the strict inequality cannot be proven. In fact, in this limit, it is easy to see that the particles are completely immobile and no exchange of identical particles 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 are exactly the same. In the present case, this can also be understood as a consequence of the particle-hole symmetry which maps $U \to -U$ at specific filling [69].

The asymptotical behavior of $\Delta E(|U|)$ can be estimated by the expansion in terms of $t/|U|$ in the strong-coupling limit ($t \ll |U|$). In the strong-coupling limit at half filling, the Hubbard model is mapped to spin-1/2 Heisenberg model $\mathcal{H} = J \sum_{\langle j,k \rangle} \vec{S}_j \cdot \vec{S}_k$, where $J = 2t^2/|U|$ (for example, see texture book [70]). The energy difference induced by statistics in the strong-coupling limit should appear in the order of $O(t(t/|U|)^2)$. The numerical fitting for strong-coupling limit is shown in Fig. 4.7. The leading term in the energy difference is in the order of $t(t/|U|)^5$, where 5 is the minimum number of intermediate states when two particles are exchanged on such a branch lattice. In the weak-coupling limit ($t \gg |U|$), the mean-field Hamiltonian for fermions can be derived by Hartree-Fock approximation [70]. However, with hard-core constraint, perturbation theory is invalid for hard-core bosons in the limit of weak coupling. Hence, perturbation theory could not give any information of the magnitude of the energy difference in weak-coupling limit. Anyway, we can numerically show the asymptotical behavior of $\Delta E(|U|)$ in the weak-coupling limit, which is shown in Fig. 4.8.

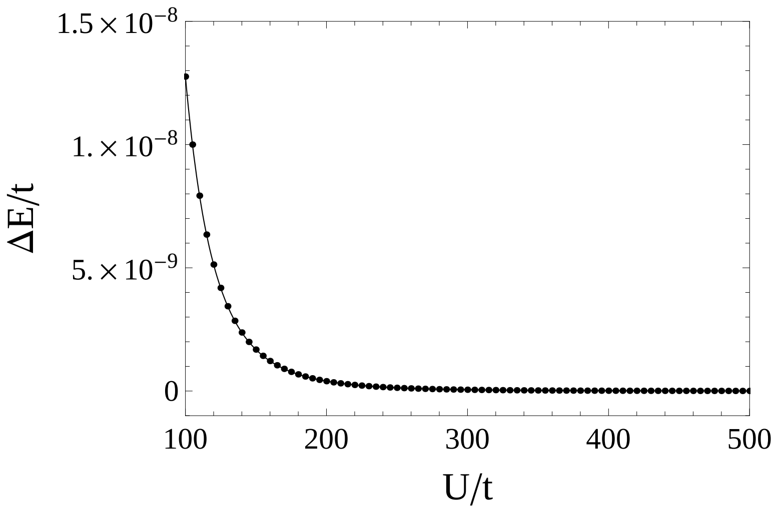


Figure 4.7: Numerical fitting of $\Delta E(|U|)$ in the limit of strong coupling at half filling. The fitting function is $\Delta E/t = 5.022946^{-13} + 127.639773(t/|U|)^5$.

In summary, in this chapter, we mathematically prove a sufficient condition for the natural inequality (4.1) to hold for interacting systems without relying on the occurrence of BEC, where the simple argument based on perfect BEC breaks down.

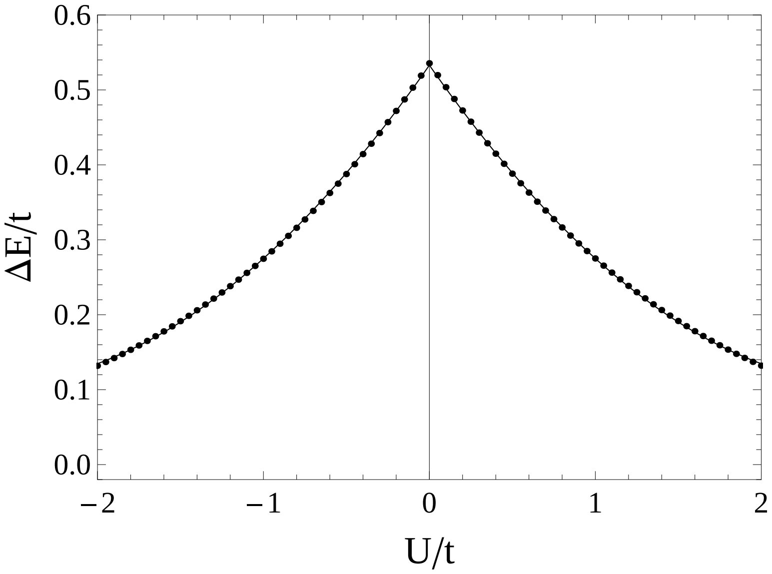


Figure 4.8: Numerical fitting of $\Delta E(|U|)$ in the limit of weak coupling at half filling. The fitting function is $\Delta E/t = 0.058859 - 0.316873|U|/t + 0.532999(|U|/t)^2$.

That is, if all the hopping amplitudes are nonnegative, the ground-state energy of hard-core bosons is still lower than that of the corresponding fermions. Theorem 1 is proved for spinless case, and Theorems 2, 3 are proved for spinful case. The physical understanding of the condition "nonnegative" hopping amplitudes will be discussed in the next chapter.

Chapter 5

Unified understanding of frustration

In Chap. 4, we prove that when all the hopping amplitudes are nonnegative, hard-core bosons still have a lower ground-state energy than corresponding fermions. What is the physical understanding of this condition? In this chapter, we will reveal the physics behind the condition. Our study leads to a novel understanding of the effects of particle statistics, in terms of *frustration* of quantal phase. From this understanding, we will see the role played by *frustration* is of central importance in the proof of these theorems.

In this chapter, we will review previous definition of frustration and then present our understanding of the effects of particle statistics. Namely, Fermi statistics introduces "statistical frustration" in terms of a fictitious lattice. This is more general than the picture based on the perfect BEC, and is indeed applicable to systems with interaction. Based on the fictitious lattice, a strict version of the diamagnetic inequality for general lattice is presented and proved as a by-product. Finally, we put forward the unified understanding of hopping frustration and statistical frustration, pointing out a mechanism to reverse the natural inequality.

5.1 Previous definition

Narrowly speaking, when not every bond of a lattice is able to achieve the lowest bond energy simultaneously, there is some frustration. Namely, the minimum total energy is not given by the the summation of the minimum of each bound energy.

Frustration is often associated with antiferromagnetically interacting spin systems on geometrically frustrated lattices, such as triangle, kagome and pyrochlore lattice. This is also called as geometric frustration, which originates from the incompatibility between magnetic degree of freedom and crystal geometry [71]. The origin can be simply illustrated by as few as three spins on a triangle (shown in Fig. 5.1).

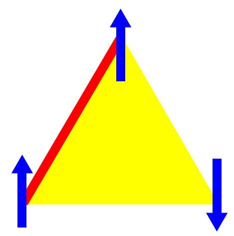


Figure 5.1: An illustration of geometry frustration of three antiferromagnets on a triangle.

Besides the geometric frustration, another frequently involved frustration is introduced by magnetic filed or gauge potential, which is independent of the fact that the lattice is geometrically frustrated or not. For example, consider a Bose-Hubbard model subjected to a magnetic field. The Hamiltonian is give by: $\mathcal{H} = -J\sum_{ij}(a_i^\dagger a_j e^{iA_{ij}} + \text{H.c.}) + \frac{U}{2}\sum_i n_i(n_i - 1)$. In the limit of $U \gg J$ and $S \to \infty$, spin vector can be parameterized as [72]: $\vec{s} = S(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\phi)$. The Bose-Hubbard Hamiltonian becomes $H = -2JS^2\sum_{\langle i,j\rangle}\sin\theta_i\sin\theta_j\cos(\phi_i - \phi_j + A_{ij})$ [72]. Consider a plaquette from a lattice shown in Fig. 5.2. Every bond energy cannot be simultaneously minimized if the flux passing through the plaquette is not zero. This is because for a given phase ϕ_1 at site 1, we can choose ϕ_2, ϕ_3 and ϕ_4 (the values are labeled in Fig. 5.2) to minimize the bound energy on three of the four bounds. If the total flux of this plaquette $A_{12} + A_{23} + A_{34} + A_{41}$ is not zero, the fourth bond cannot be minimized simultaneously.

More generally, the concept of frustration may be applicable to a system with competing interactions, when the ground state does not minimize individual interaction simultaneously [73].

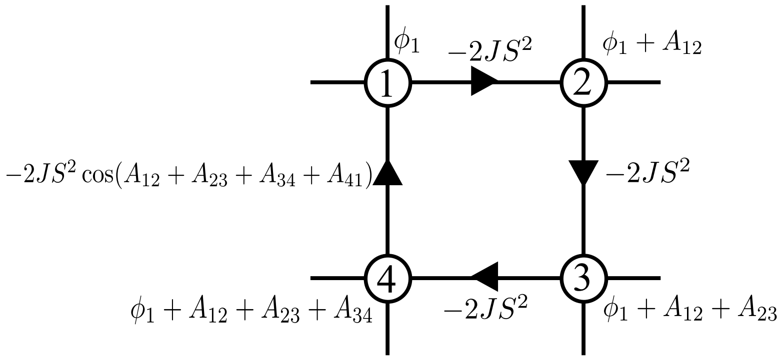


Figure 5.2: An illustration of frustration introduced by gauge field.

5.2 Unified frustration and diamagnetic inequality

The frustration of hard-core bosons in Hamiltonians (4.6) can be figured out by the previous definition of frustration in Sec. 5.1.

To see the sign of hopping amplitudes t_{jk} in a many-boson system is related to frustration, we can map the hard-core boson problem to spin-1/2 quantum spin system [58]. The mapping is based on the equivalence between hard-core boson operators and spin-1/2 operators:

$$S_j^+ \sim b_j^\dagger, \qquad S_j^- \sim b_j, \qquad S_j^z \sim b_j^\dagger b_j - \frac{1}{2}. \tag{5.1}$$

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

$$-t_{jk}\left(b_j^\dagger b_k + b_k^\dagger b_j\right) \sim J_{jk}^\perp \left(S_j^x S_k^x + S_j^y S_k^y\right), \tag{5.2}$$

where $J_{jk}^\perp = -2t_{jk}$. Thus the nonnegative t_{jk} corresponds to ferromagnetic interaction, in terms of 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 nonnegative, every hopping term can be simultaneously minimized by choosing a uniform phase throughout the system. In this sense, bosons with nonnegative hopping amplitudes are unfrustrated with respect to their quantal phase.

5.2.1 Statistical frustration

Let us now consider the case of fermions. Since Fermi statistics brings in negative signs even if all the hoppings t_{jk} are nonnegative, 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 $S = 1/2$ spin system. To understand the frustration induced by Fermi statistics in many-particle system, 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 basis states $|\Phi^a\rangle$ with a site on a fictitious lattice.

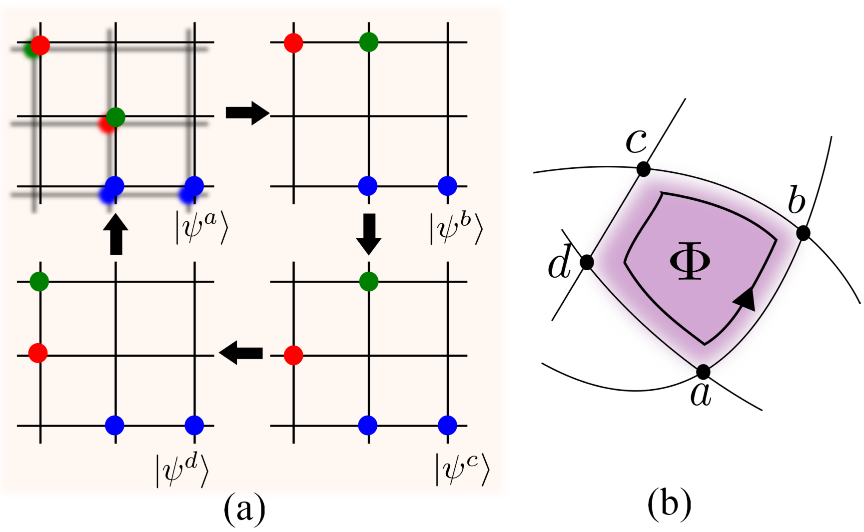


Figure 5.3: A schematic figure to explain the relation between original many-body problem and the tight binding model on a fictitious lattice. Figure 5.3 (a) demonstrates the process to exchange two particles in real lattice. Figure 5.3 (b) shows the corresponding loop in a fictitious lattice, where site a is identified with the many-body basis state $|\psi^a\rangle$. The flux Φ in Fig. 5.3 (b) is π for fermions but zero for bosons.

The relation of original many-body problem and the tight-binding model on a lattice can be summarized as:

- If two 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 (4.6), there is a loop in the fictitious lattice.

One schematic figure of the fictitious lattice and the relation to the original many-body problem is shown in Fig. 5.3. All the particles in this figure are identical. The different colors are only for the purpose to show the process of particle exchange.

For the boson problem, all the hopping amplitudes in this single-particle problem are again nonnegative. Hence there is no extra phase in the loop for bosons. In other words, the fictitious lattice for hard-core boson 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. 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 a frustration, which causes destructive interferences among different paths. The π phase introduced by fermi statistics cannot be gauged out by gauge transformation, and it can be interpreted as an effective magnetic flux. In this thesis, we call the effective magnetic flux as "statistical frustration" because it is introduced by Fermi statistics, which is unique for fermions.

5.2.2 Strict diamagnetic inequality

For a single-particle tight-binding model, introduction of any flux always raises or does not change the energy, which is known as diamagnetic inequality [19]. By the mapping to the single-particle problem on the fictitious lattice, the first half of Theorem 1, which states the non-strict inequality, may be then regarded as a corollary of the diamagnetic inequality (see Ref. [19] and references therein). On the other hand, the latter half of the 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 lattice. The general result can be presented 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

$$-\sum_{\beta\in\Xi}\tau_{\alpha\beta}\psi_\beta = E\psi_\alpha. \tag{5.3}$$

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

$$E_0(\{\tau'_{\alpha\beta} \equiv |\tau_{\alpha\beta}|\}) \leq E_0(\{\tau_{\alpha\beta}\}). \tag{5.4}$$

Furthermore, the strict inequality,

$$E_0(\{\tau'_{\alpha\beta} \equiv |\tau_{\alpha\beta}|\}) < E_0(\{\tau_{\alpha\beta}\}) \tag{5.5}$$

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

$$\tau_{\alpha_0\alpha_1}\tau_{\alpha_1\alpha_2}\tau_{\alpha_2\alpha_3}\dots\tau_{\alpha_{n-1}\alpha_n} \tag{5.6}$$

is not positive (either negative or not real).

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

$$\mathcal{K}_{\alpha\beta} \equiv \tau_{\alpha\beta} + C\delta_{\alpha\beta}, \tag{5.7}$$
$$\mathcal{K}'_{\alpha\beta} \equiv \tau'_{\alpha\beta} + C\delta_{\alpha\beta}, \tag{5.8}$$

with a sufficiently large constant C so that $\mathcal{K}$ and $\mathcal{K}'$ is positive definite. We then define $\mathcal{L} \equiv \mathcal{K}^n$ and $\mathcal{L}' \equiv \mathcal{K}'^n$, for the length l 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 element of $\mathcal{L}'$ is expanded as

$$\mathcal{L}'_{\alpha_0\alpha_0} = \sum_{\alpha_1,\cdots,\alpha_{n-1}} \mathcal{K}'_{\alpha_0\alpha_1}\mathcal{K}'_{\alpha_1\alpha_2}\dots\mathcal{K}'_{\alpha_{n-1}\alpha_0}, \tag{5.9}$$
$$\mathcal{L}_{\alpha_0\alpha_0} = \sum_{\alpha_1,\cdots,\alpha_{n-1}} \mathcal{K}_{\alpha_0\alpha_1}\mathcal{K}_{\alpha_1\alpha_2}\dots\mathcal{K}_{\alpha_{n-1}\alpha_0}, \tag{5.10}$$

Each term in the expansion satisfies $\mathcal{K}'_{\alpha_0\alpha_1}\mathcal{K}'_{\alpha_1\alpha_2}\dots\mathcal{K}'_{\alpha_{n-1}\alpha_0} \geq |\mathcal{K}_{\alpha_0\alpha_1}\mathcal{K}_{\alpha_1\alpha_2}\dots\mathcal{K}_{\alpha_{n-1}\alpha_0}|$, 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

$$\mathcal{K}_{\alpha_0\alpha_1}\mathcal{K}_{\alpha_1\alpha_2}\dots\mathcal{K}_{\alpha_{n-1}\alpha_0} = \tau_{\alpha_0\alpha_1}\tau_{\alpha_1\alpha_2}\dots\tau_{\alpha_{n-1}\alpha_0}, \tag{5.11}$$

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

$$\mathcal{K}_{\alpha_0\alpha_{n-1}}\mathcal{K}_{\alpha_{n-1}\alpha_{n-2}}\dots\mathcal{K}_{\alpha_1\alpha_0}, \tag{5.12}$$

which is complex conjugate of Eq. (5.11), we find the strict inequality

$$\mathcal{K}'_{\alpha_0\alpha_1}\mathcal{K}'_{\alpha_1\alpha_2}\dots\mathcal{K}'_{\alpha_{n-1}\alpha_0} + \text{c.c.} > \mathcal{K}_{\alpha_0\alpha_1}\mathcal{K}_{\alpha_1\alpha_2}\dots\mathcal{K}_{\alpha_{n-1}\alpha_0} + \text{c.c.}. \tag{5.13}$$

Thus $\mathcal{L}'_{\alpha_0\alpha_0} > \mathcal{L}_{\alpha_0\alpha_0} > 0$. Invoking the Perron-Frobenius theorem again, the strict diamagnetic inequality in equation (5.5) is proved. The non-strict version is the standard diamagnetic inequality [19]. However, the strict inequality obtained here appears new, also in the general context of diamagnetic inequality.

5.2.3 Unified understanding of frustration

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 non-vanishing flux in the original many-particle problem, we observed that there is a frustration among local quantal phases, which we may call hopping frustration. On the other hand, when the particles in the original problem are fermions, there is also a frustration among quantal phases, which we name statistical frustration. In the original many-particle problem, the statistical frustration appears rather differently 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 non-vanishing flux in the fictitious lattice. This provides a unified understanding of hopping frustration and statistical frustration.

A system of many bosons with only nonnegative hopping amplitudes t_{jk} represents a frustration-free system. Introduction of any frustration into such a system is expected not to decrease the ground-state energy. For example, introduction of magnetic flux (hopping frustration) does not decrease the ground-state energy. This is a lattice version of Simon's universal diamagnetism in bosonic systems [18].

On the other hand, when one type of frustration already exists, the effect of introducing another type of frustration is a non-trivial problem. For example, in a system of fermions, the statistical frustration exists. What happens if one further introduces hopping frustration (magnetic flux)? In such a case, there cannot be a general statement: the ground-state energy may or may not decrease, depending on the system in the question. That is, diamagnetism is not universal in spinless fermions systems. Correspondingly, the orbital magnetism of fermions can be either paramagnetic or diamagnetic, depending on the model.

This means 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. The possibility of partial cancelation between the two kinds of frustration can be again naturally understood by the mapping to the single-particle problem on a fictitious lattice. Each of the frustrations introduces a particular pattern of magnetic flux in the fictitious lattice. It is certainly possible that these two magnetic flux (partially) cancel with each other.

In summary, in this chapter, we discuss the physical understanding of the sufficient condition of natural inequality. For bosons with nonnegative hopping amplitudes are unfrustrated with respect to their quantal phase. Fermi statistics has the effect to introduce statistical frustration. The natural inequality is nontrivially explained by diamagnetic inequality. As a by-product, the proof of strict natural inequality leads to a strict diamagnetic inequality. In terms of the fictitious lattice, the hopping frustration and statistical frustration can be understood in a unified manner. The latter is unique for fermions. The unified understanding of frustration hints us the possibility that the ground-state energy of hard-core bosons could be higher than fermions due to hopping frustration. The exact examples of the reversed natural inequality will be presented in Chaps. 6 and 7.

Chapter 6

One enlightening example: particles on a ring

In the following, we discuss how the natural inequality can be violated. Theorem 1, Theorems 2 and 3 leave the possibility of violation of the inequality by introducing 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. Intuitively, this means that we can cancel the effect of the statistical phases by that of hopping amplitudes, so that the fermions have a lower energy than the corresponding bosons. For simplicity, we limit ourselves to the comparison between spinless fermions and hard-core bosons, with no interaction other than the hard-core constraint, setting $V_{jk} = 0$. The case with other interactions will be discussed at the end of Chap. 7.

In this chapter, we discuss the best understood and solvable model in one dimension: the ground-state energy of hard-core bosons and spinless fermions on a ring. In the thermodynamic limit, the ground-state energy of hard-core bosons and fermions are the same, which is consistent with the discussion in continuum limit in Sec.2.3.1. However, the energy difference does exist in finite systems. And the ground-state energy density (ground-state energy per site) of bosons is found to be higher than that of fermions in finite systems. We believe it is a very useful model in highlighting the central physics of the problem, namely the effect of the statistical frustration introduced by Fermi statistics can be canceled by the flux or hopping frustration.

6.1 Boundary conditions and Jordan-Wigner transformation

We begin with a simple but instructive example in one dimension: the tight-binding model on a ring,

$$\mathcal{H} = -\sum_{j=1}^{N}(c_j^\dagger c_{j+1} + \text{H.c.}). \tag{6.1}$$

The hard-core boson version of this model is equivalent to the $S = 1/2$ XY chain. Because of the hard-core constraint, bosonic creation and annihilation operators ($b_j^\dagger$ and b_j) are mapped to S_j^+ and S_j^- exactly [58]. After this mapping, the Hamiltonian is mapped into one-dimensional $S = 1/2$ XY model,

$$\mathcal{H}^{\text{B}} = -\sum_{j=1}^{N}(S_j^+ S_{j+1}^- + \text{H.c.}). \tag{6.2}$$

To diagonalize the Hamiltonian (6.2), we use the Jordan-Wigner transformation [74, 75],

$$S_j^+ = \exp\Big(-\pi i \sum_{l=1}^{j-1} n_l\Big) f_i^\dagger, \qquad S_j^- = f_i \exp\Big(\pi i \sum_{l=1}^{j-1} n_l\Big), \qquad S_j^z = n_j - 1/2, \tag{6.3}$$

which maps the spin-1/2 magnet into noninteracting fermions on the ring. Thus the hard-core bosons and fermions are almost equivalent in this case. And this is the discrete analog of Bose-Fermi mapping for Tonks-Giradeau gas (see Sec. 2.3.2).

However, a care should be taken on the boundary condition when we discuss the ring of finite length. For simplicity, we assume the number of sites N is an integral multiple of 4, and the number of particles $M = N/2$. The number of particles is assumed as even. For the periodic or antiperiodic boundary condition $c_{N+1} \equiv \pm c_1$, 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), which has been assumed as even. It implies that hard-core bosons with the periodic (antiperiodic) boundary condition are mapped to noninteracting fermions with the antiperiodic (periodic, respectively) boundary condition:

$$E_0^{\text{B}}(\text{PBC}) = E_0^{\text{F}}(\text{APCB}), \qquad E_0^{\text{B}}(\text{APBC}) = E_0^{\text{F}}(\text{PCB}). \tag{6.4}$$

6.2 Dependence of E_0^{F} on boundary conditions

Now let us discuss the dependence of the ground-state energy of free fermions on the boundary conditions. The ground-state energy density is obtained by Fourier transformation,

$$\epsilon_0 = \frac{E_0}{N} = -\frac{2}{N}\sum_k \cos k, \tag{6.5}$$

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

The ground-state energy density asymptotically converges, in the thermodynamic limit $N \to \infty$, 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

$$\frac{E_0^{\mathrm{PBC}}}{N} - \frac{E_0^{\mathrm{APBC}}}{N} = \frac{2[1-\cos(\pi/N)]}{N\sin(\pi/N)} > 0, \tag{6.6}$$

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,

$$\begin{aligned} \frac{E_0^{\mathrm{PBC}}}{N} &= -\frac{2}{\pi} + \frac{2\pi}{3N^2} + \frac{2\pi^3}{45N^4} + O(\frac{1}{N^6}) \\ \frac{E_0^{\mathrm{APBC}}}{N} &= -\frac{2}{\pi} - \frac{\pi}{3N^2} - \frac{7\pi^3}{180N^4} + O(\frac{1}{N^6}), \end{aligned} \tag{6.7}$$

for the periodic (PBC) and antiperiodic (APBC) boundary conditions.

It can be seen that the noninteracting fermions on a ring have a lower energy with the antiperiodic boundary condition. The leading term of $O(1/N^2)$ is also determined by conformal field theory[76, 77], the detail of which will be presented in Sec. 6.3.

Considering the relation of boundary condition in Eq. (6.4), this implies that the hard-core bosons have a lower energy than fermions on a ring with the periodic boundary condition, conforming to Theorem 1 since all the hopping amplitudes are nonnegative. On the other hand, the same result implies that, under the antiperiodic boundary condition, the hard-core bosons have a higher energy than fermions. The anti-periodic boundary condition can be understood as a result of insertion of π-flux inside the ring. This hopping frustration cancels the statistical phase so that the natural inequality is violated.

6.3 Calculation by conformal field theory

The leading term of $O(1/N^2)$ is also determined by conformal field theory[76, 77].

For one dimensional quantum XXZ model:

$$\mathcal{H}_{XXZ} = -\frac{\gamma}{2\pi \sin\gamma}\sum_{i=1}^{L}(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \Delta\sigma_i^z\sigma_{i+1}^z), \tag{6.8}$$

where $\Delta = -\cos\gamma$, $0 \leq \gamma \leq \pi$. The ground state energy density of XXZ chain is given by[77, 78]

$$E_0(\Delta, L, \psi) = e_\infty - \frac{\pi}{6L^2}c(\psi) + O(L^{-2}), \tag{6.9}$$

where the central charge $c(\psi)$ is given by $1 - \frac{3\psi^2}{2\pi(\pi-\gamma)}$ and ψ is the angle of twisted boundary condition

$$\sigma_{L+1}^x \pm i\sigma_{L+1}^y = e^{\pm i\psi}(\sigma_1^x \pm i\sigma_1^y), \qquad \sigma_{L+1}^z = \sigma_1^z.$$

Consider $\gamma = \pi/2$, in which case the Hamiltonian (6.8) turns into one dimensional XY model

$$\mathcal{H} = -\frac{1}{2}\sum_{j=1}^{N}(S_j^+S_{j+1}^- + \text{H.c.}).$$

Periodic boundary condition corresponds to $\psi = 0$, and antiperiodic boundary condition corresponds to $\psi = \pi$. Therefore

$$\begin{aligned} E_0(\Delta = 0, L, \psi = 0) &= e_\infty - \frac{\pi}{6L^2} + O(L^{-2}), \\ E_0(\Delta = 0, L, \psi = \pi) &= e_\infty + \frac{\pi}{3L^2} + O(L^{-2}). \end{aligned} \tag{6.10}$$

The results obtained by conformal field theory is exactly the same as Eq. (6.7). Since the XY chain with PBC ($\psi = 0$) is equivalent to the fermions with APBC, when the number of particles is even, as shown in Sec. 6.1. And the XY chain with APBC ($\psi = \pi$) is equivalent to the hard-core bosons with APBC. Therefore, with APBC, hard-core bosons have a higher ground-state energy density than fermions, with leading term of $O(1/N^2)$.

In summary, hard-core bosons has a higher ground-state energy density than free fermions on a ring of finite length, with antiperiodic boundary condition. Imposing the antiperiodic boundary condition is equivalent to introducing a π-flux inside the ring, which can cancel the effect of the statistical phase so that the inequality (4.1) is indeed inverted. This 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, namely the effect of the statistical frustration introduced by Fermi statistics can be canceled by the flux or hopping frustration, in terms of a fictitious lattice.

However, the energy difference on the ring vanishes asymptotically in the thermodynamic limit $N \to \infty$. Thus, we shall seek for the examples where the hard-core bosons have a higher energy than fermions in the thermodynamic limit. The application of particles on a ring and nonvanishing energy density difference in the thermodynamic limit will be discussed in the next chapter.

Chapter 7

More examples of reversed natural inequality

As demonstrated in the last chapter, hard-core bosons have a higher ground-state energy density than fermions on a finite ring with π flux inside the ring. It is the best example to highlight the central physics of the problem. Hopping frustration and statistical frustration can be understood in a unified manner in terms of a fictitious lattice. Introduction of hopping frustration is expected to compete with (and cancel) statistical frustration introduced by Fermi statistics. Therefore, the ground-state energy of fermions may or may not decrease. On the other hand, frustration always increases the ground-state energy of bosons. This is the mechanism that it is possible to reverse the natural inequality by introducing hopping frustration. And this reversal is indeed found in one-dimensional ring in the last chapter.

In this chapter, we will present more examples in which such a reversal is realized, and in several cases it is proved rigorously in the thermodynamic limit, with rigorous proof and techniques assisted by exact diagonalization.

7.1 Coupled rings

Since hard-core bosons have a higher ground-state energy than fermions on a ring with π flux inside the ring as demonstrated in Chap. 6, we can construct a series of systems where $E_0^{\mathrm{B}} \geq E_0^{\mathrm{F}}$, by taking many such small rings and connecting them with weak hoppings. The conjecture is that if the inter-ring hoppings are weak

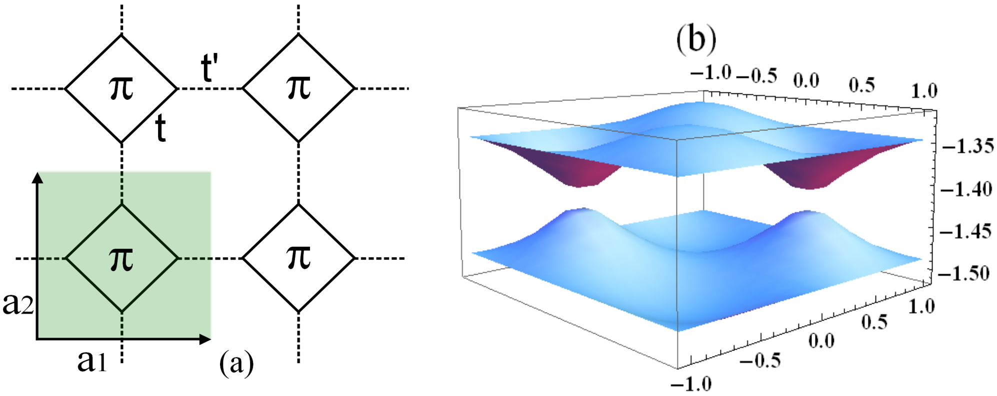


Figure 7.1: Figure 7.1(a) is π-flux octagon-square lattice, and Figure 7.1(b) is the plot of lowest two bands of Hamiltonian (7.1) with $t = 1$, $t' = 0.1$.

enough, they would be expected not to revert the inequality and $E_0^{\mathrm{B}} \geq E_0^{\mathrm{F}}$ would be kept [79].

7.1.1 π-flux octagon-square lattice

We prove rigorously that the reversed natural inequality is still kept in coupled π-flux rings, connected by weak hoppings, even in the thermodynamic limit. The first example is π-flux octagon-square model. The lattice structure is shown in Fig. 7.1 (a), where one unit cell is shown in green with basis vectors $\vec{a}_1 = (3, 0)$ and $\vec{a}_2 = (0, 3)$. The hopping amplitudes on thick and broken lines are denoted by t and t' respectively. The Hamiltonian is given by

$$\mathcal{H} = -t \sum_{\langle i,j\rangle \in \text{thick,oriented}} e^{i\pi/4} c_i^\dagger c_j - t' \sum_{\langle i,j\rangle \in \text{broken}} c_i^\dagger c_j + \text{H.c.}, \tag{7.1}$$

where $t > t' > 0$. 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'.

7.1.1.1 Lower bound of bosons and upper bound of fermions

In order to prove $E_0^{\mathrm{B}} > E_0^{\mathrm{F}}$ 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 semi-definite operators,

$$A = t' \sum_{\langle i,j\rangle \in \mathrm{Broken}} (c_i^\dagger + c_j^\dagger)(c_i + c_j) \geq 0, \tag{7.2}$$

$$B = t' \sum_{\langle i,j\rangle \in \mathrm{Broken}} (c_i^\dagger - c_j^\dagger)(c_i - c_j) \geq 0, \tag{7.3}$$

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

$$\mathcal{H}^{\mathrm{F}} = \tilde{\mathcal{H}}^{\mathrm{F}} - A = \sum_{\diamond} h_\diamond^{\mathrm{F}} - A, \tag{7.4}$$

$$\mathcal{H}^{\mathrm{B}} = \tilde{\mathcal{H}}^{\mathrm{B}} + B = \sum_{\diamond} h_\diamond^{\mathrm{B}} + B, \tag{7.5}$$

where $h_\diamond^{\mathrm{F}} = -t\sum_{i=1}^{4}(e^{i\pi/4}c_i^\dagger c_{i+1} + \mathrm{H.c.}) + t'\sum_{i=1}^{4} c_i^\dagger c_i$ and $h_\diamond^{\mathrm{B}} = -t\sum_{i=1}^{4}(e^{i\pi/4}c_i^\dagger c_{i+1} + \mathrm{H.c.}) - t'\sum_{i=1}^{4} c_i^\dagger c_i$, the cluster Hamiltonians defined on a solid-line square for fermions and bosons, respectively. Noticing $h_\diamond$ commutes with each other, we can give the ground-state energy of $\tilde{\mathcal{H}}$ simply by the summation [37]:

$$\tilde{E}_0 = \sum_{\diamond_i} \epsilon_{\diamond_i}, \tag{7.6}$$

where $\tilde{E}_0$ and $\epsilon_{\diamond_i}$ are the ground-state energy of $\tilde{\mathcal{H}}$ and $h_{\diamond_i}$ on ith π-flux square respectively.

Because the operators B is positive semi-definite, the ground-state energy of bosons satisfies

$$E_0^{\mathrm{B}} = \langle\Phi|\mathcal{H}^{\mathrm{B}}|\Phi\rangle \geq \langle\Phi|\tilde{\mathcal{H}}^{\mathrm{B}}|\Phi\rangle \geq \tilde{E}_0^{\mathrm{B}} = \sum_{\diamond_i} \epsilon_{\diamond_i}^{\mathrm{B}}, \tag{7.7}$$

where Φ is assumed as the ground state of $\mathcal{H}^{\mathrm{B}}$. The min-max principle [1] has been applied in the first inequality in Eq. (7.7).

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

$$E_0^{\mathrm{F}} = \langle\Psi|\mathcal{H}^{\mathrm{F}}|\Psi\rangle \leq \langle\tilde{\Psi}|\mathcal{H}^{\mathrm{F}}|\tilde{\Psi}\rangle \leq \langle\tilde{\Psi}|\tilde{\mathcal{H}}^{\mathrm{F}}|\tilde{\Psi}\rangle = \tilde{E}_0^{\mathrm{F}} = \sum_{\diamond_i} \epsilon_{\diamond_i}^{\mathrm{F}}, \tag{7.8}$$

[1] See Theorem 4.3.1 of Ref. [35].

m_i	$\epsilon^{\mathrm{F}}_{\diamond_i}(m_i)$	$\epsilon^{\mathrm{B}}_{\diamond_i}(m_i)$
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	$4t'$	$-4t'$

Table 7.1: The ground-state energies of fermions and hard-core bosons on a thick-line square, where m_i is the number of particles on i-th cluster.

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

By exact diagonalization, we obtain the ground-state energies $\epsilon^{\mathrm{B,F}}_{\diamond_i}(m_i)$ in given m_i particles sectors, shown in Table 7.1.

Assuming the number of unit cells is N, from the results of exact diagonalization, we have one lower bound of bosons as $E_0^{\mathrm{B}} \geq -2N(t+t')$ when $t'/t \leq 2-\sqrt{2}$, or $E_0^{\mathrm{B}} \geq -N(\sqrt{2}t+3t')$ when $2-\sqrt{2} < t'/t < 1$. An upper bound of fermions is given by the $\tilde{E}_0^{\mathrm{F}}$, which is dependent on the density pattern on the whole lattice. At half filling, an upper bound of fermions is obtained as $E_0^{\mathrm{F}} \leq -2N(\sqrt{2}t-t')$. Thus, when the ratio falls in this range $t'/t \leq (\sqrt{2}-1)/2$, we have $E_0^{\mathrm{B}} \geq E_0^{\mathrm{F}}$.

7.1.1.2 E_0^{F} by exact calculation of dispersion

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 chosen as 1. It is useful to introduce the vector notation,

$$\vec{c}_i = \begin{pmatrix} c_{i,A} \\ c_{i,B} \\ c_{i,C} \\ c_{i,D} \end{pmatrix} \text{ and } \vec{c}_{\vec{k}} = \begin{pmatrix} c_{\vec{k},A} \\ c_{\vec{k},B} \\ c_{\vec{k},C} \\ c_{\vec{k},D} \end{pmatrix} = \frac{1}{\sqrt{N}} \sum_i e^{i\vec{k}\cdot\vec{R}_i} \vec{c}_i.$$

The unit cells i are at positions $\vec{R}_i = m_i\vec{a}_i + n_i\vec{a}_2$, $m_i, n_i \in \mathbb{Z}$ with $\vec{a}_1 = (0,3)$, $\vec{a}_2 = (3,0)$. One unit cell is shown in Fig. 7.1 (a). After the Fourier transformation, the Hamiltonian (7.1) now reads (for convenience, t is chosen as 1)

$$\mathcal{H} = \vec{c}^{\dagger}_{\vec{k}} \sum_{\vec{k}} \begin{pmatrix} 0 & -e^{i(k_x+k_y)} & -t'e^{-ik_y} & -e^{-i(k_x-k_y)} \\ -e^{-i(k_x+k_y)} & 0 & e^{-i(k_x-k_y)} & -t'e^{ik_x} \\ -t'e^{ik_y} & e^{i(k_x-k_y)} & 0 & -e^{-i(k_x+k_y)} \\ -e^{i(k_x-k_y)} & -t'e^{-ik_x} & -e^{i(k_x+k_y)} & 0 \end{pmatrix} \vec{c}_{\vec{k}}, \tag{7.9}$$

where the sum is over the first Brillouin zone. Diagonalizing this matrix gives the four bands,

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

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

$$E_0^{\mathrm{F}} = \sum_{k_x,k_y} \left[E_{-}^{(1)}(k_x, k_y) + E_{-}^{(2)}(k_x, k_y)\right]. \tag{7.10}$$

For the lattice of size $9L^2$, the number of unit cells N equals L^2. In the thermodynamic limit $L \to \infty$, the ground-state energy per unit cell of fermions at half filling is given by the integral of the lowest two bands (shown in Fig. 7.1(b)) in the reduced Brillouin zone,

$$\frac{E_0^{\mathrm{F}}}{N} = -\int_{-\pi}^{\pi} \frac{d\tilde{k}_x}{2\pi} \int_{-\pi}^{\pi} \frac{\tilde{k}_y}{2\pi} \Bigg[\sqrt{(t')^2 + 2 + 2t'\sqrt{1 - \sin\tilde{k}_x \sin\tilde{k}_y}} + \sqrt{(t')^2 + 2 - 2t'\sqrt{1 - \sin\tilde{k}_x \sin\tilde{k}_y}} \Bigg]. \tag{7.11}$$

It is easily verified that the reversed natural inequality holds with small ratio of t'/t, by comparison of the lower bond of bosons and numerical integral of Eq. (7.11) with given value of t'. For example when $t = 1$ and $t' = 0.1$, $E_0^{\mathrm{B}} \ge -2.2N > E_0^{\mathrm{F}} = -2.831967N$, where N is the number of unit cells. When $t' = 0.4$, $E_0^{\mathrm{B}} \ge -2.8N > E_0^{\mathrm{F}} = -2.885971N$.

7.1.2 π-flux hexagon-square lattice

The second example is the π-flux hexagon-triangle lattice, which is shown in Fig. 7.2(a). One unit cell is shown in green in Fig. 7.2(a), with basis vectors $\vec{a}_1 = (0, 1)$ and $\vec{a}_2 = (1/2, \sqrt{3}/2)$. The Hamiltonian is defined as

$$\mathcal{H} = -t \sum_{\langle i,j\rangle \in \text{thick, orinted}} e^{i\pi/3} c_i^\dagger c_j - t' \sum_{\langle i,j\rangle \in \text{broken}} c_i^\dagger c_j + \text{H.c.}, \tag{7.12}$$

which can be regarded as π-flux triangles coupled by weak hopping t'. To obtain a lower bound of bosons and an upper bound of fermions, the Hamiltonian is written

m	$\epsilon^{\mathrm{F}}_{\Delta_i}(m_i)$	$\epsilon^{\mathrm{B}}_{\Delta_i}(m_i)$
1	$-t+2t'$	$-t-2t'$
2	$-2t+4t'$	$-t-4t'$
3	$6t'$	$-6t'$

Table 7.2: The ground-state energies of fermions and hard-core bosons on a thick-line up triangle, where m_i is the number of particles on i-th cluster.

as $\mathcal{H}^{\mathrm{F}} = \sum_{\Delta} h^{\mathrm{F}}_{\Delta} - A$ and $\mathcal{H}^{\mathrm{B}} = \sum_{\Delta} h^{\mathrm{B}}_{\Delta} + B$ with the same definitions of A and B in equations (7.2)(7.3), where $h^{\mathrm{F}}_{\Delta} = -t\sum_{i=1}^{3}(e^{i\pi/3}c_i^{\dagger}c_{i+1} + \mathrm{H.c.}) + 2t'\sum_{i=1}^{3} c_i^{\dagger}c_i$ and $h^{\mathrm{B}}_{\Delta} = -t\sum_{i=1}^{3}(e^{i\pi/3}c_i^{\dagger}c_{i+1} + \mathrm{H.c.}) - 2t'\sum_{i=1}^{3} c_i^{\dagger}c_i$ are the cluster Hamiltonians defined on a solid-line pointing up triangle. Therefore, we have $E^{\mathrm{B}}_0 \geq \sum_{\Delta_i} \epsilon^{\mathrm{B}}_{\Delta_i}$ and $E^{\mathrm{F}}_0 \leq \sum_{\Delta_i} \epsilon^{\mathrm{F}}_{\Delta_i}$. The ground-state energies in sectors of m_i's particles are demonstrated in Table 7.2. Also the number of unit cells is N, we obtain a lower bound of bosons as $E^{\mathrm{B}}_0 \geq -N(t+4t')$ when $t'/t \leq 1/2$ or $E^{\mathrm{B}}_0 \geq -6Nt'$ when $1/2 < t'/t < 1$. One upper bound of fermions is given by $\tilde{E}^{\mathrm{F}}_0$, which also depends on the density pattern on the whole lattice. At 2/3 filling, we find $E^{\mathrm{F}}_0 \leq -2N(t-2t')N$. According to the results of exact diagonalization on a cluster, we find when $t'/t \leq 1/8$, $E^{\mathrm{B}}_0 \geq -N(t+4t') \geq -2N(t-2t') \geq E^{\mathrm{F}}_0$.

The second approach for the ground-state energy of fermion is calculating the dispersion. 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 2/3 filling is given by the integral of the lowest two bands in Brillouin zone, which is shown in Fig. 7.2 (c),

$$
\begin{aligned}
E^{\mathrm{F}}_0 &= \sum_{k_x,k_y} \left[E^{(1)}(k_x,k_y) + E^{(2)}\right] \\
&= \frac{\sqrt{3}N}{2}\iint_{BZ} \frac{dk_x}{2\pi}\frac{dk_y}{2\pi}\left[E^{(1)}(k_x,k_y) + E^{(2)}\right], \qquad (7.13)
\end{aligned}
$$

where $k_{x,y} \in BZ$ as shown in Fig. 7.2 (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 $t' = 0.1$, $E^{\mathrm{B}}_0 \geq$

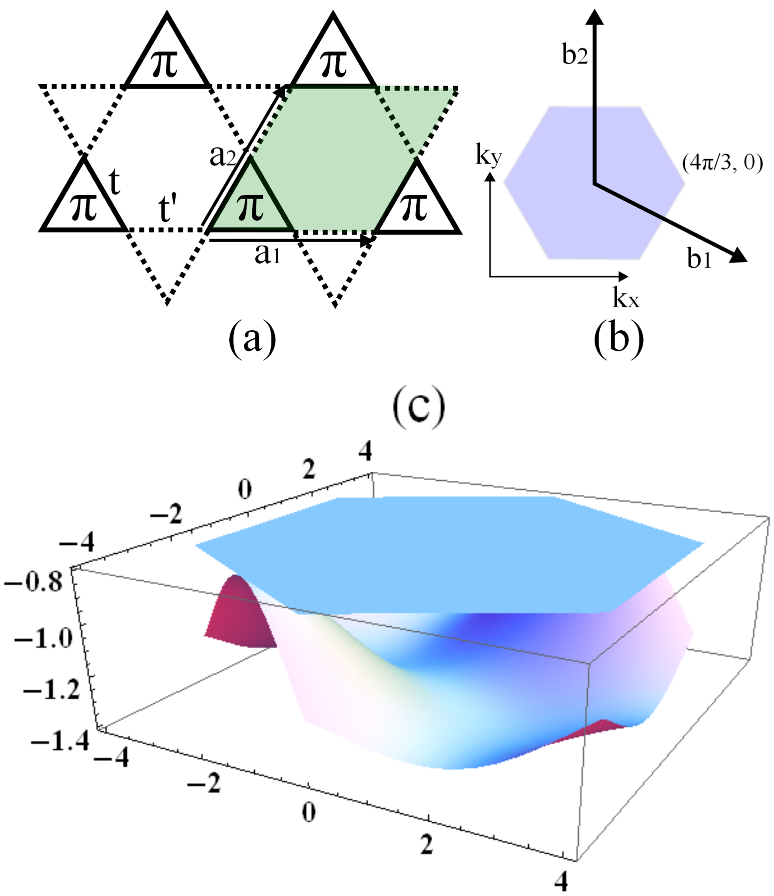


Figure 7.2: The lattice structure of π-flux hexagon-triangle is shown in Fig. 7.2 (a), in which the unit cell is labeled in green. The first Brillouin zone is shown in Fig. 7.2 (b), where the basis vectors are shown by $\vec{b}_1$ and $\vec{b}_2$. Figure 7.2 (c) is the lowest two bands with $t = 1$, $t' = 0.2$.

$-1.4N > E_0^{\mathrm{F}} = -2.004349N$; when $t' = 0.2$, $E_0^{\mathrm{B}} \geq -1.8N > E_0^{\mathrm{F}} = -2.017037N$, in which case the inequality $E_0^{\mathrm{B}} \geq E_0^{\mathrm{F}}$ is not reverted by the weak inter-ring coupling t' as expected.

In both examples, we find the reversed natural inequality still holds when the inter-ring hopping is sufficiently weak.

7.2 2D square lattice with flux

As we discussed in Chap. 6, the energy difference between bosons and fermions on a ring is a finite size effect, and indeed vanishes in the thermodynamic limit.

This is rather natural, because it is only the entire system as a ring that contains π flux. As a simple extension of the idea, here we consider two-dimensional square lattice in a uniform magnetic field.

7.2.1 Electrons in 2D magnetic field

A natural system to consider would be a two-dimensional lattice with flux. Continuing relaxation of the condition of nonnegative hopping amplitudes, we change the real negative hopping factor t_{jk} into complex one. One possible exact expression of complex hopping terms is:

$$t_{jk} = te^{iA_{jk}}, \qquad (t \geq 0, t \in \mathbb{R}, A_{jk} \in \mathbb{R}). \tag{7.14}$$

The meaning of this substitution from the physical point of view can be explained in terms of vector potential in electromagnetic field. Consider a 2D square lattice with unit spacing, immersed in an uniform magnetic field $\vec{B}$, which is perpendicular to the plane. The magnetic flux passing through surface S can be calculated by a surface integral,

$$\Phi = \int_S \vec{B} \cdot d\vec{S} = \int_S \vec{\nabla} \times \vec{A} \cdot d\vec{S} = \oint_L \vec{A} \cdot d\vec{l} = \sum_{\text{plaquette}} A_{jk},$$

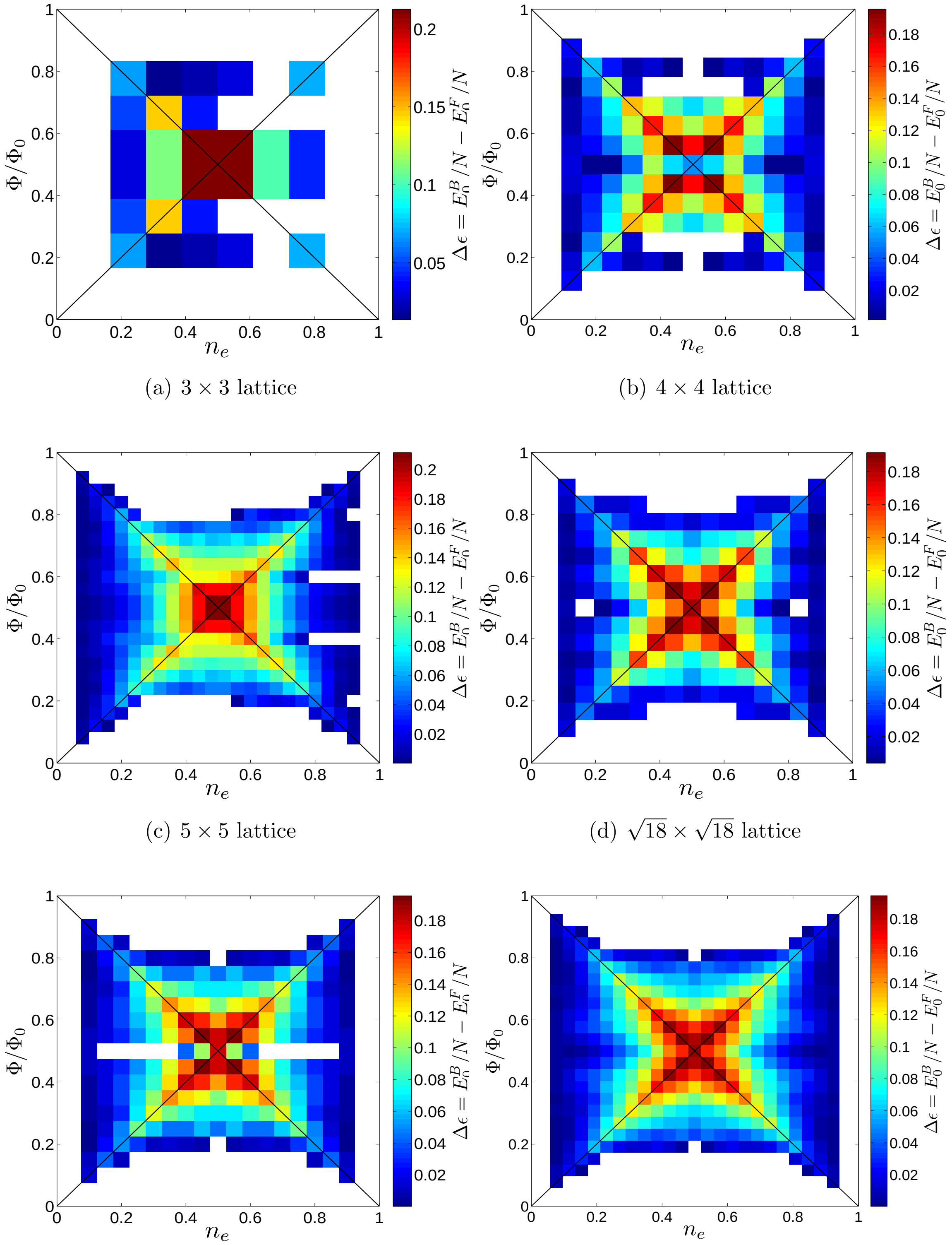
where Stokes theorem have been applied. For every plaquette, the magnetic flux passing through is given by $\sum_{\text{plaquette}} A_{jk}$, from which we have seen that the complex hopping term is relevant to the problem of particles in a magnetic field. D. R. Hofstadter's butterfly is a famous problem of single Bloch electron in an uniform magnetic field with rational value of Φ [24], which has been intensively studied in past decades.

7.2.2 Energy spectra

We consider two-dimensional square lattice in a uniform magnetic field, described by the Hamiltonian,

$$\mathcal{H} = -\sum_{\langle j,k \rangle} \big(t_{jk} c_j^\dagger c_k + \text{H.c.} \big), \tag{7.15}$$

where $t_{jk} = t \exp(i\Phi_{jk}/\Phi_0)$ and $t > 0$. The flux passing through every plaquette is uniform as $\sum_\square \Phi_{jk} = \Phi$. With periodic boundary condition, the total flux is quantized to integer numbers of flux quanta (the unit flux quantum $\Phi_0 = hc/e$ is 2π



(a) 3×3 lattice

(b) 4×4 lattice

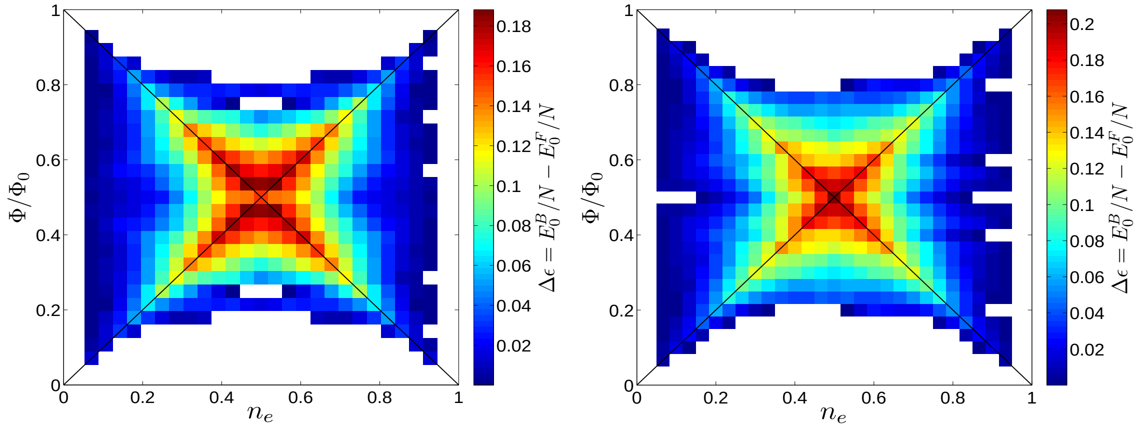
(c) 5×5 lattice

(d) $\sqrt{18} \times \sqrt{18}$ lattice

(e) $\sqrt{20} \times \sqrt{20}$ lattice

(f) $\sqrt{26} \times \sqrt{26}$ lattice

Figure 7.3: Differences of ground-state energy density $\Delta\epsilon$ between hard-core bosons and fermions on the square lattices with Φ flux per plaquette and n_e particle per site. The natural inequality (4.1) holds in white region, while its violation is color coded. Statistical transmutation is expected along the two solid diagonal lines $\Phi/\Phi_0 = n_e$ and $\Phi/\Phi_0 = 1 - n_e$.



(a) 4×7 lattice (b) 5×6 lattice

Figure 7.4: Differences of ground-state energy density $\Delta\epsilon$ between hard-core bosons and fermions on the rectangle lattices with Φ flux per plaquette and n_e particle per site.

in our unit). For the finite square lattice with N plaquettes, the flux per plaquette Φ is quantized in unit of $2\pi/N$. The magnetic field introduces frustration, through the existence of complex hopping amplitudes t_{jk}. The choice of gauge fixing to determine Φ_{jk} does not affect the energy eigenvalues. To investigate all possible value of flux per plaquette, we choose the string gauge [80]. Starting from one arbitrary plaquette S, we draw $N-1$ outgoing arrows (strings) from S with periodic boundary condition, where N is the number of sites (plaquettes). The value of Φ_{jk} is given by $\Phi\mathcal{N}_{jk}$, where $\mathcal{N}_{jk}$ is the number of strings cutting the link jk. Due to the condition of uniformity, the possible value of the number of flux quanta per plaquette is restricted as discrete: $\Phi = 2\pi n/N$, $(n = 0, 1, \cdots, N)$.

Exact diagonalization for 3×3, 4×4, 5×5, $\sqrt{18}\times\sqrt{18}$, $\sqrt{20}\times\sqrt{20}$ and $\sqrt{26}\times\sqrt{26}$ square lattices [81] is employed in our work. We obtained the ground-state energy of hard-core bosons and fermions with various densities of particles n_e and various values of flux Φ using exact numerical diagonalization, for square lattices up to 26 sites with periodic boundary conditions. The energy spectra are shown in Fig 7.3. We use colors as quantities of the third dimension to demonstrate the differences of ground-state energy densities between two kinds of particles. The quantity in the third dimension is defined as $\Delta\epsilon_0 = E_0^{\mathrm{B}}/N - E_0^{\mathrm{F}}/N$, If $\Delta\epsilon_0$ is positive, which we are interested in, the value of it is shown in color bar. Otherwise, it is filled in white. The column along $n_e = 1/N$ is the result of single-particle problem, in which we can not distinguish boson from fermion. The row along $\Phi = 0$ is the case described by the Theorem 1, in which the ground-state energy of bosons is proved to be lower. From above figures, we can see large parts in every figure are filled in colors. We find that the "natural" inequality (4.1) is violated in a wide region of the phase diagram, in various lattice sizes, particle densities and flux densities.

The energy spectra of 4×7 and 5×6 lattices are shown in Fig 7.4. The natural inequality holds in white plaquettes and it is violated in colored regions. The energy spectra with our choice of geometry are not of particle-hole symmetry, because these lattices are not bipartite so that particle-hole symmetry is absent for fermions.

7.2.3 Statistical transmutation

In particular, the inversion is significant along the diagonal lines $\Phi/\Phi_0 = n_e$ and $\Phi/\Phi_0 = 1 - n_e$, where the particle densities are equivalent to flux density. These lines are precisely where the statistical transmutation between the hard-core boson and the fermion is expected to occur [82, 83]. Namely, in the mean-field level, one flux quantum can be attached to each particle to form a composite particle, transforming fermions into bosons and vice versa, at the same time eliminating the background field. At zero field, the frustration is absent and hard-core bosons have a lower energy than fermions. Thus, the statistical transmutation implies that, hard-core bosons have a higher energy than fermions on two diagonal lines. While this argument is not rigorous and the actual physics is presumably more involved [84], our numerical result supports the statistical transmutation scenario. (For a related discussion for spinful electrons, see Ref. [85].)

7.2.4 Finite-size scaling

Numerical results for the square lattices of various sizes up to 30 sites suggest that the energy difference is nonvanishing in the thermodynamic limit.

We plotted Fig. 7.5 and Fig. 7.6 to show the finite-size scalings. Figure 7.5 shows 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

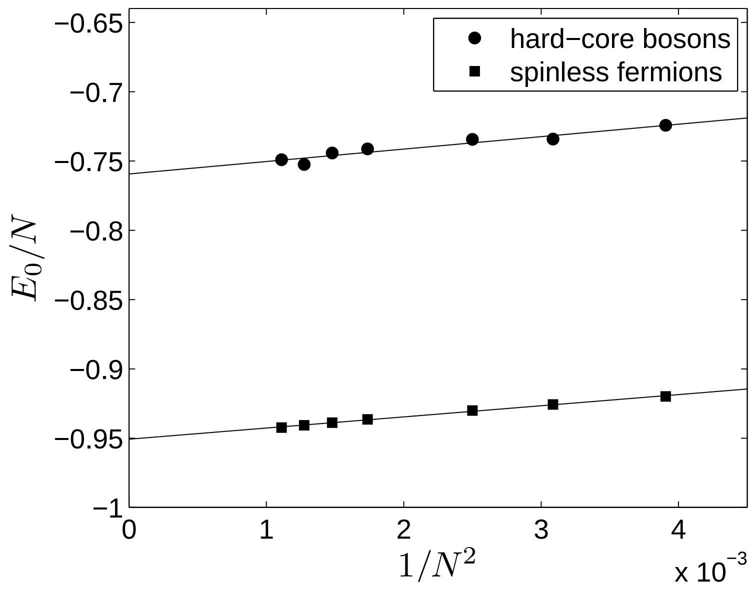


Figure 7.5: Finite size scaling of ground-state energies in two-dimensional square lattice with $(N/2-1)\Phi_0/N$ flux per plaquette at filling fraction $(N/2-1)/N$.

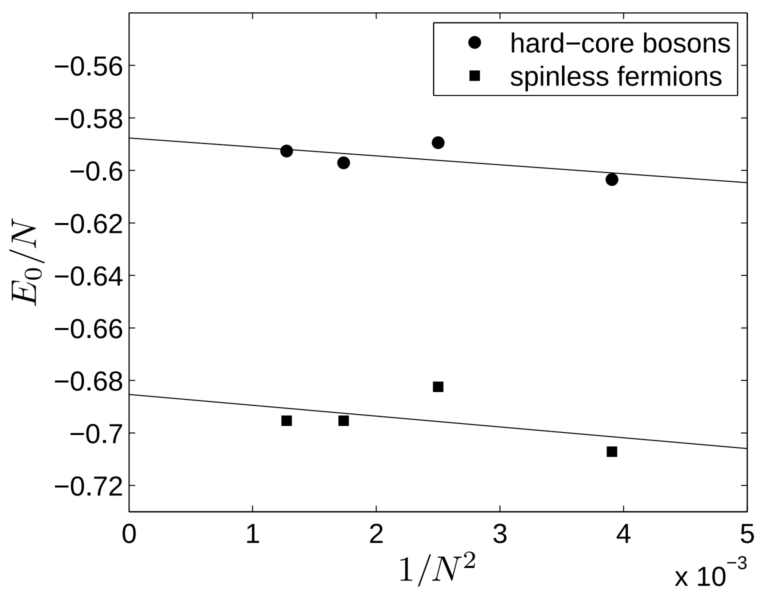


Figure 7.6: Finite size scaling of groundstate energies in two-dimensional square lattice with $\Phi_0/4$ flux per plaquette at quarter filling. While there is no proof at this present, the numerical extrapolation suggests that fermions have lower ground-state energy also in this case.

extrapolation suggests that the fermions have a lower ground-state energy in the thermodynamic limit, which is confirmed by rigorous proof in the π-flux model [57] and will be discussed in Sec. 7.3.1. The fitting functions are

$$E_0^{\mathrm{B}}/N = -0.7593 + 8.973/N^2 + O(N^{-4}),$$

for hard-core bosons and

$$E_0^{\mathrm{F}}/N = -0.9507 + 8.043/N^2 + O(N^{-4}),$$

for fermions respectively. The extrapolated groundstate energy density for fermions matches well with the exact result -0.958091 (see Ref. [57], and Sec. 7.3.1).

The finite size scaling with $\Phi_0/4$ flux per plaquette at quarter filling is shown in Fig 7.6, suggesting the ground-state energy of hard-core bosons is still higher than fermions at quarter filling in the thermodynamic limit. The fitting functions are

$$E_0^{\mathrm{B}}/N = -0.5877 - 3.405/N^2 + O(N^{-4}),$$

for hard-core bosons and

$$E_0^{\mathrm{F}}/N = -0.6853 - 4.125/N^2 + O(N^{-4}),$$

for fermions, respectively.

In fact, in the following, we will prove rigorously in the thermodynamic limit that the fermions have a lower energy at half filling with $\Phi = \pi$ flux per plaquette, as suggested by our numerical calculation and the statistical transmutation argument discussed in Sec. 7.2.3.

7.3 Cluster decomposition by Anderson's argument

Since exact diagonalization only works on small clusters, to overcome the fatal disadvantage of numerical method, from this section, we will make use of various methods to provide rigorous proof in the thermodynamic limit. In this section, we present the cluster decomposition technique by Anderson's argument.

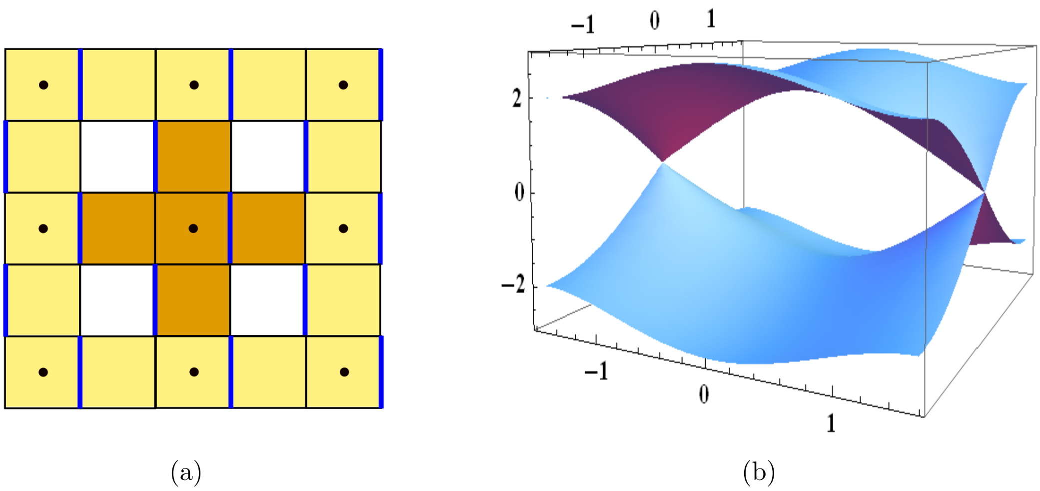


Figure 7.7: (a) The square lattice with π flux in each plaquette. The brown cross represents a cluster of 12 sites. The whole lattice is covered by clusters, whose centers are denoted by black dots. (b) The energy bands in the first Brillouin zone.

7.3.1 2D π-flux square lattice

We note that Lieb has shown that π flux minimizes the ground-state energy of fermions at half-filling on the square lattice [30]. On the other hand, an argument similar to the Proof of Theorem 1 can be used to prove a lattice version of Simon's theorem on diamagnetism of bosons [18]. Namely, for bosons, introduction of a flux always increases the ground-state energy. These, together with the statistical transmutation argument discussed earlier, suggest a possibility of violation of Eq. (4.1) with π flux per plaquette.

Let us discuss the square lattice with π flux per plaquette. The Hamiltonian reads

$$\mathcal{H} = -\sum_{<j,k>} (t_{jk} c_j^\dagger c_k + \text{H.c.}). \tag{7.16}$$

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. 7.7.

For technical convenience, we restrict ourselves to the case of the "grand canonical ensemble" ground state at $\mu = 0$. For π-flux square lattice, it turns out to be equivalent to finding the ground state at half filling (1/2 particle per site). We first discuss the dispersion relation of a single particle on the square lattice with a π flux through each plaquette. By taking a 2×2 unit cell (which is twice as large as the minimal magnetic unit cell), the dispersion relation is

$$E_{\pm} = \pm\sqrt{4 + 2\cos 2k_x - 2\cos 2k_y}, \tag{7.17}$$

where (k_x, k_y) is the wavenumber which belongs to the reduced Brillouin zone $-\pi/2 \leq k_{x,y} < \pi/2$. Each energy level is doubly degenerate. The ground-state energy of fermions at $\mu = 0$, which corresponds to the half-filling, is given as

$$E_0^{\mathrm{F}} = \sum_{k_x, k_y} 2E_{-}(k_x, k_y), \tag{7.18}$$

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 to integral multiples of $2\pi/L_{x,y}$. Thus, in the thermodynamic limit $L_{x,y} \to \infty$, the ground-state energy of the fermionic model at $\mu = 0$ is obtained exactly as

$$\frac{E_0^{\mathrm{F}}}{N} = -\frac{1}{2}\int_{-\pi}^{\pi} \frac{d\tilde{k}_x}{2\pi} \int_{-\pi}^{\pi} \frac{d\tilde{k}_y}{2\pi} \sqrt{4 + 2\cos\tilde{k}_x - 2\cos\tilde{k}_y} = -0.958091. \tag{7.19}$$

Now we turn to the "grand canonical" ground-state energy, of the corresponding boson model at the same chemical potential ($\mu = 0$). Here we use Anderson's argument [37, 86, 87] by writing the Hamiltonian as

$$\mathcal{H} = \sum_{\alpha} h_{\alpha}, \tag{7.20}$$

where

$$h_{\alpha} = -\frac{1}{2}\sum_{\langle j,k\rangle \in +_{\alpha}} (t_{jk} c_j^{\dagger} c_k + \mathrm{H.c.}). \tag{7.21}$$

Here $+_{\alpha}$ refers to a cross-shaped cluster of 12 sites as shown in Fig. 7.7 (a). We consider all the clusters with the same pattern of hopping amplitudes within the cluster, in the square lattice. As a consequence, each cluster as shown in Fig. 7.7 (a), overlaps with 4 other clusters and each link appears in two different clusters when periodic boundary conditions are imposed. The factor 1/2 in Eq. (7.21) compensates this double counting.

The ground-state energy E_0 of $\mathcal{H}$ satisfies

$$E_0 \geq \sum_{\alpha} \epsilon_0^{\alpha}, \tag{7.22}$$

where ϵ_0^{α} is the ground-state energy of h_{α}, which is shown in Table 7.3. The grand canonical ground-state energy of the cross-shaped cluster is obtained by

m	$\epsilon_0^{+}(m)$
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 7.3: The lowest energy of the π-flux model on a 12-site cross-cluster of square lattice, where m is the number of particles.

exact diagonalization as $\epsilon_0^\alpha = -3.609035$. Since there are $N/4$ such clusters in the square lattice of N sites, we obtain

$$E_0^{\mathrm{B}}/N \geq -3.609035/4 = -0.902259 > E_0^{\mathrm{F}}/N. \tag{7.23}$$

Thus the inversion of the ground-state energies for the π-flux square lattice model with $\mu = 0$, as expected from the statistical transmutation argument discussed earlier, is now proved rigorously.

7.3.2 Pyrochlore lattice

This argument is not restricted to two-dimensional systems. Let us consider the standard tight-binding model on the three-dimensional pyrochlore lattice:

$$\mathcal{H} = \sum_{\langle j,k \rangle} (c_j^\dagger c_k + \mathrm{H.c.}), \tag{7.24}$$

where $\langle j, k \rangle$ runs over all pairs of nearest-neighbor sites in the three-dimensional pyrochlore lattice. Again we set the chemical potential $\mu = 0$. We note that this model has frustrated hoppings with this choice of the sign in hopping amplitudes.

The model in the single-particle sector has two degenerate flat bands at the energy $\epsilon = -2$ and two dispersive bands touching the flat bands [88]. Thus for

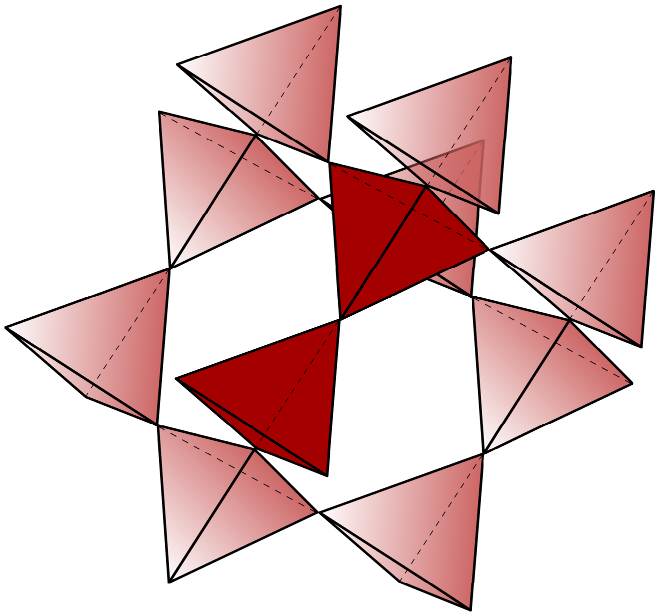


Figure 7.8: The lattice structure of pyrochlore. A dimer of two tetrahedra made up of 7 sites are shown in dark in pyrochlore lattice.

fermions, the ground-state energy at $\mu = 0$ satisfies

$$E_0^{\mathrm{F}} < -2(N/2) = -N, \tag{7.25}$$

where N is the number of sites of the lattice. We note that, because of the lack of the particle-hole symmetry, $\mu = 0$ does not imply half-filling for this model. The hard-core boson version of this model can be decomposed as Eq. (7.20) with

$$h_\alpha = (1/4) \sum_{\langle j,k \rangle \in \mathrm{TD}_\alpha} (c_j^\dagger c_k + \mathrm{H.c.}), \tag{7.26}$$

where TD_α refers to each dimer of elementary tetrahedra of the pyrochlore lattice sharing a vertex (site) (see Fig. 7.8). Here we count dimers in any direction; each tetrahedron (and thus each link) belongs to 4 dimers. The factor 1/4 in the definition of h_α is introduced to compensate the overcounting. The ground-state energies of the cluster in each sector with fixed number of particles m are shown in Table 7.4, The lowest ground-state energy of a tetrahedra dimer is obtained by exact diagonalization as $\epsilon_0^\alpha = -(2+\sqrt{2})/4 = -0.853554$. Since there are N dimers of tetrahedra, the GS energy of bosons at $\mu = 0$ satisfies

$$E_0^{\mathrm{B}}/N \geq -(2+\sqrt{2})/4 > E_0^{\mathrm{F}}/N. \tag{7.27}$$

Thus we have proved the violation of Eq. (4.1) for the simple tight-binding model on the three-dimensional pyrochlore lattice.

m	0	1	2	3	4	5	6	7
$\epsilon_0(m)$	0	-0.411438	-0.628534	-0.853554	-0.853554	-0.628534	-0.411438	0

Table 7.4: The lowest energy of the NN hopping model on a tetrahedron-dimer of pyrochlore lattice, in sectors of different numbers of particles.

7.4 Cluster decomposition by min-max principle

The example of the pyrochlore lattice in Sec. 7.3 exhibits a flat band as the lowest energy band. While the existence of a flat band is neither a necessary nor sufficient condition to violate Eq. (4.1), it does tend to help: as long as all the fermions occupy the lowest flat band, the Pauli exclusion principle plays no role in increasing the ground state energy. Thus, such flat band models would have a better chance to realize the inversion of the ground state energies.

In this section, we will present rigorous proof that the inequality (4.1) is indeed violated in the thermodynamic limit, in a few models with a lowest flat band in a range of filling fraction, using a cluster decomposition technique [89]. They include the delta-chain model, for which the violation of Eq. (4.1) was numerically found for small clusters [55, 56], and the kagome lattice model. Rigorous proof of the optimal lower bound of the filling fraction to reverse natural inequality on delta-chain is presented in Sec. 7.4.4.

7.4.1 Flat band models

In fermionic system, flat band models play an important role in the study of strongly correlated systems, for example in the context of ferromagnetism of the Hubbard model [90, 91, 92, 93, 94]. One way to a flat band is achieved by destructive interference of electron hoppings. The distinct characteristic of flat band model is that it provides huge degeneracy of localized states in the single-particle spectrum. The well known one flat band model, the Landau level, can be regards as one in continuum rather than lattice model.

To make use of this advantage of flat band models, think about a system with positive semi-definite Hamiltonian with lowest flat band, in which all the localized states of flat bands are occupied by fermions with zero energy, described by filling factor ν. If we can find that the ground-state energy of corresponding bosonic

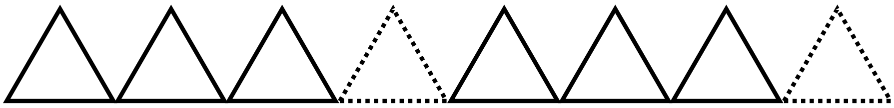


Figure 7.9: An example of decomposition of the delta-chain Hamiltonian to clusters, with $p = 4$ unit cells per cluster, including one decoupled site at the top of the dashed triangle.

model is strictly positive at the same filling, the reversal of natural inequality is realized.

7.4.2 Delta chain

First we discuss the delta-chain model, for which the violation of Eq. (4.1) was numerically found for small clusters [55, 56]. The Hamiltonian of the model can be written in the following form [93, 94]:

$$\mathcal{H} = \sum_{j=1}^{N} a_j^\dagger a_j, \tag{7.28}$$

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. (4.6)), 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 (7.28) is modified from that in Ref. [55] by a constant chemical potential, so that the flat band has exactly zero energy. Thus the ground-state energy of the fermionic version of the model (7.28) is zero as long as the filling fraction (particle number per site) ν satisfies $\nu \leq 1/2$. On the other hand, the ground-state energy E_0^{B} of bosons is zero as long as $\nu \leq 1/4$ since the localized zero-energy states do not overlap with each other in this range of filling [95].

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

$$\mathcal{H} = \sum_{n=0}^{N/p-1} \mathcal{H}_n^{(p)} + \sum_{n=1}^{N/p} a_{np}^\dagger a_{np}, \tag{7.29}$$

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 7.9. 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 $\tilde{E}_0^{\mathrm{B}}$ of the first term $\tilde{\mathcal{H}} = \sum_{n=0}^{N/p-1} \mathcal{H}_n^{(p)}$ satisfies $\tilde{E}_0^{\mathrm{B}} \leq E_0^{\mathrm{B}}$. $\tilde{\mathcal{H}}$ is a sum of mutually commuting cluster Hamiltonians $\mathcal{H}_n^{(p)}$. Thus $\tilde{E}_0^{\mathrm{B}}$ 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. 7.9. The cluster contains 8 sites. The ground-state energy in each sector with fixed particle number m is obtained by a numerical exact diagonalization of the 8-site cluster. The results are shown in Table 7.5. It is found that $\epsilon_0^{(4)}(m) = 0$ for $m \leq 3$ and $\epsilon_0^{(4)}(m) \geq \Delta_{\mathrm{DC}}^{(4)} = 0.372605$ for $4 \leq m \leq 8$.

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

Table 7.5: Ground-state energy ϵ_0 of the cluster Hamiltonian $\mathcal{H}_n^{(4)}$ for delta-chain, with m particles in the cluster. The cluster contains 8 sites, as shown in Fig. 7.9.

If we consider the filling fraction in the range $3/8 < \nu \leq 1/2$, it follows from Dirichlet's box principle that there is at least one cluster which contains 4 or more particles. Thus, in this range, $\tilde{E}_0^{\mathrm{B}} \geq \Delta_{\mathrm{DC}}^{(4)}$ for any system size N, while $E_0^{\mathrm{F}} = 0$. 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. (4.1) is not optimal. In an alternative approach generalizing the techniques used in the context of flat-band ferromagnetism [93, 94] and of frustrated antiferromagnets near the saturation field [95, 96], we can extend the region to $1/4 < \nu \leq 1/2$. The lower bound 1/4 is in fact optimal. The detail will be presented in the Sec. 7.4.4.

7.4.3 Kagome lattice

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

$$\mathcal{H} = \sum_{\alpha} a_{\Delta_\alpha}^\dagger a_{\Delta_\alpha} + \sum_{\alpha} a_{\nabla_\alpha}^\dagger a_{\nabla_\alpha}, \tag{7.30}$$

where Δ_α and ∇_α are elementary triangles pointing up and down respectively, of the kagome lattice, as shown in Fig. 7.10. We define $a_{\Delta_\alpha} \equiv c_{\alpha_1} + c_{\alpha_2} + c_{\alpha_3}$, where

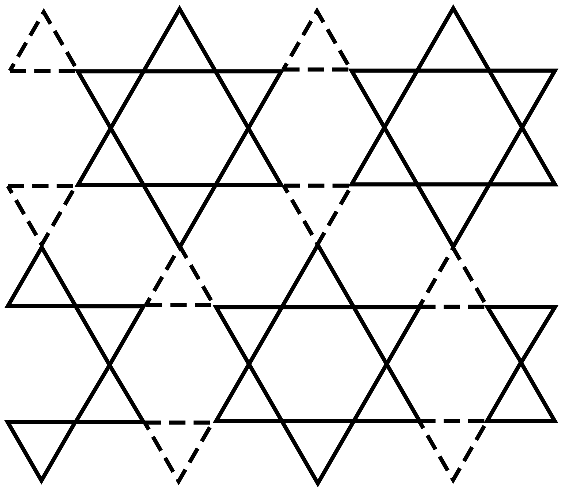


Figure 7.10: The 12-site clusters of "Star of David" shape are shown in solid lines on a kagome lattice.

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 7.6: The lowest energy of cluster Hamiltonian $\mathcal{H}^{\text{cluster}}$ on 12-site "Star of David" shape, in sectors with different numbers of particles m.

$\alpha_{1,2,3}$ 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 [88]. Thus $E_0^{\mathrm{F}} = 0$ when $\nu \leq 1/3$.

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. The ground-state energy of the cluster in each sector with m particles is shown in Table 7.6. The ground-state energy ϵ_0 of each cluster is zero with $m \leq 3$, but is positive with $m \geq 4$. Thus, invoking Dirichlet's box principle again, Eq. (4.1) is violated for filling fraction $1/4 < \nu \leq 1/3$. This conclusion also holds for infinite-size system, or in the thermodynamic limit.

7.4.4 Optimal lower bound of filling fraction for violation in delta-chain model

Let us improve the estimate of the range of the filling fraction, for which the violation of Eq. (4.1) occurs in the delta-chain. Our result is that the violation occurs, namely the reversed inequality $E_0^{\mathrm{B}} > E_0^{\mathrm{F}}$ holds, for $1/4 < \nu \leq 1/2$. 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 on-site $U > 0$ in the enlarged Hilbert space first,

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

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 $U \to \infty$, and this problem is reduced to Eq. (7.28) in this limit.

Obviously, the hopping term $\mathcal{H}_{\mathrm{hop}}$ is positive semi-definite. The on-site interaction, the U term, is also positive semi-definite because $U n_i (n_i - 1) = U c_i^\dagger c_i^\dagger c_i c_i$ for bosons. As a consequence, all the energy eigenvalues can not be negative.

Therefore, any state with $E^{\mathrm{B}} = 0$ is a ground state. If such a ground state $|\Phi_{\mathrm{GS}}\rangle$ exists, it satisfies

$$\mathcal{H}_{\mathrm{hop}}|\Phi_{\mathrm{GS}}\rangle = \mathcal{H}_{\mathrm{int}}|\Phi_{\mathrm{GS}}\rangle = 0, \tag{7.31}$$

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

Consider the zero-energy ground state of $\mathcal{H}_{\mathrm{hop}}$ first. Define 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 of but not orthogonal to each other. The zero energy state (valley state) $b_j^\dagger|0\rangle$ is shown in Fig. 7.11 by blue lines, which is the first excited state of spin-1/2 antiferromagnetic Heisenberg model near saturation field, with single magnon trapped in the valley of the delta-chain [95, 96]. 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 $\mathcal{H}_{\mathrm{hop}}$ can be constructed out of b-operators as,

$$|\Phi_0^{\mathrm{B}}\rangle = \sum_{\{n_1,\cdots,n_N\}} f(n_1,\cdots,n_N)(b_1^\dagger)^{n_1}(b_2^\dagger)^{n_2}\cdots(b_N^\dagger)^{n_N}|0\rangle, \tag{7.32}$$

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

Now we require those zero-energy ground states (7.32) of $\mathcal{H}_{\mathrm{hop}}$ to satisfy $\mathcal{H}_{\mathrm{int}}|\Phi_0^{\mathrm{B}}\rangle = 0$. This is equivalent to require $c_i c_i|\Phi_0^{\mathrm{B}}\rangle = 0$, which imposes restrictions on the coefficients $f(n_1,\cdots,n_N)$. We first note that

$$\begin{aligned} c_{2j+1}^2|\Phi_0^{\mathrm{B}}\rangle &= \sum_{\{n_1,\cdots,n_N\}} 2n_j(n_j-1)f(n_1,\cdots,n_N)\times \\ &\quad (b_1^\dagger)^{n_1}\cdots(b_j^\dagger)^{n_j-2}\cdots(b_N^\dagger)^{n_N}|0\rangle. \end{aligned} \tag{7.33}$$

Then the linear independence of b-operators, together with $c_{2j+1}^2|\Phi_0^{\mathrm{B}}\rangle = 0$, implies that $n_j = 0$ or 1 for nonzero $f(n_1,\cdots,n_N)$. If $n_j > 1$ for any j, the coefficient $f(n_1,\cdots,n_N)$ vanishes. We thus restrict out attention to the case where $n_j = 0$ or 1 for all j. We successively find

$$\begin{aligned} c_{2j}^2|\Phi_0^{B}\rangle &= \sum_{\{n_1,\cdots,n_N\}} 2n_{j-1}n_j f(n_1,\cdots,n_N)\times \\ &\quad (b_1^\dagger)^{n_1}\cdots(b_{j-1}^\dagger)^{n_{j-1}-1}(b_j^\dagger)^{n_j-1}\cdots(b_N^\dagger)^{n_N}|0\rangle, \end{aligned} \tag{7.34}$$

where $n_j = 0$ or 1 has been applied. From the linear independence of b-operators and $c_{2j}^2|\Phi_0^{\mathrm{B}}\rangle = 0$, we obtain the condition for the zero-energy ground state, which reads $n_{j-1}n_j = 0$. This implies that, for bosons, in the construction of the zero-energy ground state, no $b^\dagger$-operators on adjacent valleys can 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. 7.11. In the range $\nu \leq 1/4$, we can find a particle configuration that satisfies the exclusion rule. However, in the case $\nu > 1/4$ we cannot find such configuration, implying the absence of zero-energy state.

These zero-energy ground states remain as ground states for any $U > 0$, and hence in the limit $U \to \infty$. Since the on-site U term is positive semi-definite, no state joins the zero-energy sector with increasing U. Therefore, the ground-state energy of hard-core boson (corresponding to infinite U) is strictly positive in the range of filling $\nu > 1/4$.

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 $\nu \leq 1/2$ can also be constructed by b operators,

$$|\Phi_0^{\mathrm{F}}\rangle = \sum_{\{n_1,\cdots,n_N\}} f(n_1,\cdots,n_N)(b_1^\dagger)^{n_1}(b_2^\dagger)^{n_2}\cdots(b_N^\dagger)^{n_N}|0\rangle, \tag{7.35}$$

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

From the above analysis, it also follows that both bosonic and fermionic systems have exactly zero-energy groundstate for $\nu \leq 1/4$. Thus the lower bound of the range of the filling fraction for the reversed inequality to hold, 1/4, is in fact optimal.

7.5 In presence of interaction

Theorems 1, 2 and 3 are valid even in the presence of interaction term. In the remainder of the thesis, we dropped the interactions for technical simplicity: fermions are then free, while bosons are subject only to the hard-core interaction. Introduction of additional density-density interactions should not essentially modify

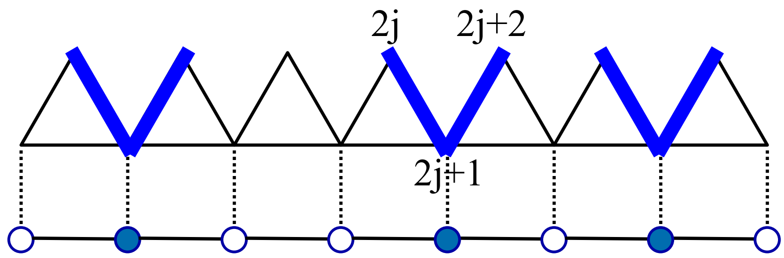


Figure 7.11: Schematic figure of mapping to particle configurations in one-dimensional chain with nearest neighbor exclusion. Localized zero-energy states (valley states) are shown in blue lines.

physics, 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 models without interactions other than the hard-core interaction.

That said, in fact, one can actually prove that the inequality (4.1) is violated even in the presence of an additional interaction, in the one-dimensional ring with π flux discussed in Chap. 6. This can be seen by noting that the Jordan-Wigner transformation applies regardless of the presence of interaction (the number of particles is assumed as even),

$$E_0^{\mathrm{F}}(\Phi = \pi) = E_0^{\mathrm{B}}(\Phi = 0), \tag{7.36}$$

$$E_0^{\mathrm{F}}(\Phi = 0) = E_0^{\mathrm{B}}(\Phi = \pi). \tag{7.37}$$

And a lattice version of Simon's theorem [18] also applies in the presence of the interaction:

$$E_0^{\mathrm{B}}(\Phi = \pi) \geq E_0^{\mathrm{B}}(\Phi = 0), \tag{7.38}$$

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

Chapter 8

Conclusion

The goal of this thesis is to investigate the effect of particle statistics and frustration on the ground-state energy. We compare the ground-state energy of hard-core bosons and fermions with the same Hamiltonian.

The comparison turns out to be nontrivial in the presence of interaction. With the hard-core interaction among bosons, the simple argument based on the perfect BEC breaks down. We rigorously proved sufficient conditions for the natural inequality and the strict natural inequality. Namely, when all the hopping amplitudes are nonnegative, the ground-state energy of hard-core bosons is still lower than that of fermions, for the spinless (Theorem 1) and spinful cases (Theorem 2 and Theorem 3) respectively.

The sufficient condition for the natural inequality can be understood as the absence of frustration among hoppings. We map the original many-body Hamiltonian to a single particle tight-binding problem on a fictitious lattice. When all the hopping amplitudes are nonnegative and the particles are bosons, the corresponding single-particle problem also has only nonnegative hopping amplitudes. In such a case, there is no frustration in the quantal phase of the wavefunction. On the other hand, the 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 wavefunction, induced by the Fermi statistics. We nominate it as "statistical frustration", because it is introduced by the Fermi statistics and results in destructive quantum interferences among different paths. In this sense, the non-strict version of the natural inequality is a corollary of the lattice version of the diamagnetic inequality. In fact, we proved the strict version of the diamagnetic inequality on a general lattice (Theorem 4), which is a byproduct of the strict natural inequality. To our knowledge, the strict diamagnetic inequality has not been discussed previously. We emphasize that this picture does not rely on the assumption of a perfect BEC and thus its applicability is not limited to noninteracting systems of particles.

The origins of the hopping frustration and the statistical frustration are rather different. The latter is introduced by the Fermi statistics and is unique for fermions. However, upon mapping to the single-particle problem on the fictitious lattice, both the hopping frustration and the statistical frustration are represented by a non-vanishing flux in the fictitious lattice. We provide a unified understanding of the hopping frustration and the statistical frustration. In this sense, the effect of particle statistics can be included in the scope of general frustration.

In terms of a fictitious lattice, for a frustration-free systems, introduction of any frustration into such system is expected not to decrease the ground-state energy. Simon's universal diamagnetism of bosons is best explained by this understanding. Another example, which is non-trivially explained by this understanding, is the natural inequality proved by us. On the other hand, when one type of frustration already exists, the effect of introducing another type of frustration is a non-trivial problem. For example, what happens in a system of fermions when the hopping frustration is introduced, where the statistical frustration already exists? There cannot be any general answer to this question. The ground-state energy of fermions may or may not decrease, depending on the model. The orbital magnetism of fermions can be either paramagnetic or diamagnetic, depending on the system.

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 the possibility that the natural inequality can be reversed in the presence of hopping frustration. For simplicity, we limit ourselves to the comparison between spinless fermions and hard-core bosons, with no interaction other than the hard-core constraint. Introduction of additional density-density interactions should not essentially modify physics, as it would affect bosonic and fermionic models in a similar manner. We proved that the natural inequality is indeed reversed in the presence of hopping frustration, in various examples (in Chap. 6 and Chap. 7), by rigorous proof assisted by exact diagonalization.

Finally we suggest some possible future work and open questions of our work.

- The comparison of the ground-state energies of soft-core bosons (without hard-core constraint) and fermions:
  In this thesis, 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 on-site interaction $\frac{\mathcal{U}}{2}n_i(n_i-1)$; the hard-core constraint can be then implemented by taking $\mathcal{U} \to +\infty$. The on-site interaction term is positive semi-definite 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 introduced 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. Numerically, without hard-core constraint, the dimension of the Hilbert space of bosons is much larger than that of fermions. Exact diagonalization is not suitable due to computation cost for memory. To simplify this problem, we can start with a "quasi hard-core bosons". Namely, the number of bosons allowed at the same site can be relaxed to be greater than 1 but still small. We can use DMRG to investigate this problem in one-dimensional or small two-dimensional systems, for example a coupled-ladder system. Other open problems include comparison in the presence of other degrees of freedom such as the orbital/flavor of particles.

- The investigation of the reversed natural inequality in a spinful system, in the presence of hopping frustration:
  In this thesis, 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 Zeeman term. Thus, 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 the present 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 are usually introduced as "synthetic gauge field" [97], 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.

- Extension to continuous systems:
  The theorems in this thesis are proved for finite lattices, which are discrete systems. The continuous limit of a lattice system can be obtained by discretization with extremely fine meshes. The first halves of our theorems (the non-strict natural/diamagnetic inequality) can be extended to the continuous limit of lattice systems. However, the latter halves (the strict natural/diamagnetic inequality) are not guaranteed by taking the continuous limit. The Perron-Frobenius theorem invoked in our theorems are applicable to a finite lattice. Extension of the discussion to an infinite lattice is mathematically nontrivial.

- Features of the ground state:
  In this thesis, we focus on the comparison of the ground-state energies between hard-core bosons and fermions. Our study could give some implications on the features of the ground state. For example, if statistical transmutation occurs, where the ground-state energy of bosons should be higher than fermions, the ground state of fermions is always ferromagnetic [85], because the ground state of spinful bosons (composite spinful bosons) is always polarized [98, 68, 99].

- Experimental realization:

A ultracold quantum gas provides an exciting setting for quantum simulation of interacting many-body systems, due to highly experimental tunability and novel detection possibilities. Given the great controllability of cold atoms in optical lattices, they would be a natural playground to examine related physics in this thesis. It would be worth noting that introduction and control of an artificial "magnetic flux" for cold atoms in optical lattices is an active area of current experimental research. For example, people use atom tunneling assisted by Raman transitions to create a strong effective magnetic field with a staggered flux alternating between $\pi/2$ and $-\pi/2$ per plaquette [100]. We hope the our theoretical conclusions can be verified in some experiments in future.

Appendix A

Proof of Simon's diamagnetism

In this appendix, I present the proof of the inequality (2.2) in Section 2.1

$$\int d\tau \; |\psi|^* \mathcal{H}(0) |\psi| \leq \int d\tau \; \psi^* \mathcal{H}(\vec{A}) \psi,$$

which holds for any ψ. This inequality is the foundation of Simon's diamagnetism. To prove this inequality, let me derive some useful relations first [18].

The first term in Hamiltonian (2.1) $\sum_{j=1}^{N} \frac{1}{2m_j}[\nabla_j - ie_j \vec{A}(\vec{r}_j)]$ can be written as an operator $\mathbf{\nabla} - i\mathbf{A}$, acting on a $3N$-dimensional space. The N-particle wave function $\psi(\vec{r}_1, \cdots, \vec{r}_N)$ is also $3N$ dimensional in coordinate space. Not to lose the generality, the wave function ψ is assumed as a complex one $\psi = Re^{i\Theta}$.

According to $|\psi|\big|\mathbf{\nabla}|\psi|\big| = \big|\psi \mathbf{\nabla}|\psi|\big| = |R\mathbf{\nabla}R|$, and $\psi^* \mathbf{\nabla} \psi = R\mathbf{\nabla}R + iR^2 \mathbf{\nabla}\Theta$, we have

$$|\psi|\big|\mathbf{\nabla}|\psi|\big| = \big|\mathrm{Re}(\psi^* \mathbf{\nabla} \psi)\big|. \tag{A.1}$$

Because $\mathbf{A}$ is a real function,

$$\big|\mathrm{Re}[\psi^*(\mathbf{\nabla} - \mathrm{i}\mathbf{A})\psi]\big| = \big|\mathrm{Re}(\psi^* \mathbf{\nabla} \psi)\big|. \tag{A.2}$$

For any a, $b \in \mathbb{C}$, it is easy to prove $\big|\mathrm{Re(ab)}\big| \leq |\mathrm{a}||\mathrm{b}|$. Therefore,

$$\big|\mathrm{Re}[\psi^*(\mathbf{\nabla} - \mathrm{i}\mathbf{A})\psi]\big| \leq \big|\psi\big|\big|(\mathbf{\nabla} - \mathrm{i}\mathbf{A})\psi\big|. \tag{A.3}$$

From equations (A.1) (A.2) (A.3), we have $|\psi|\big|\mathbf{\nabla}|\psi|\big| \leq |\psi|\big|(\mathbf{\nabla} - i\mathbf{A})\psi\big|$.

Furthermore we have $\big|\mathbf{\nabla}|\psi|\big|^2 \leq \big|(\mathbf{\nabla} - i\mathbf{A})\psi\big|^2$. Assume $d\tau$ is the $3N$-dimensional integral element. Integrating over τ in the whole space,

$$\int d\tau \; \big|\mathbf{\nabla}|\psi|\big|^2 \leq \int d\tau \; \big|(\mathbf{\nabla} - i\mathbf{A})\psi\big|^2. \tag{A.4}$$

Do integration by parts,

$$\int d\tau \ \left|\boldsymbol{\nabla}|\psi|\right|^2 = -\int d\tau \ |\psi|^* \boldsymbol{\nabla}^2 |\psi|, \tag{A.5}$$

$$\int d\tau \ \left|(\boldsymbol{\nabla} - i\mathbf{A})\psi\right|^2 = -\int d\tau \ \psi^* [\boldsymbol{\nabla} - i\mathbf{A}]^2 \psi. \tag{A.6}$$

Because $\boldsymbol{v}$ is a real function, we obtain $\int d\tau \ |\psi|^* \boldsymbol{v} |\psi| = \int d\tau \ \psi^* \boldsymbol{v} \psi$. Add $\int d\tau \ |\psi|^* \boldsymbol{v} |\psi|$ and $\int d\tau \ \psi^* \boldsymbol{v} \psi$ to both sides of equations (A.5) and (A.6), respectively, and consider the inequality (A.4), we have

$$\int d\tau \ |\psi|^* (-\boldsymbol{\nabla}^2 + \boldsymbol{v}) |\psi| \leq \int d\tau \ \psi^* (-[\boldsymbol{\nabla} - i\mathbf{A}]^2 + \boldsymbol{v}) \psi, \tag{A.7}$$

Therefor $\int d\tau \ |\psi|^* \mathcal{H}(0) |\psi| \leq \int d\tau \ \psi^* \mathcal{H}(\vec{A}) \psi$ is proved for any ψ. The rest of the proof for Simon's universal diamagnetism of bosons is presented in Sec. 2.4.

Bibliography

[1] P.W. Anderson. More is different. *Science*, 177:393–396, Aug 1972.

[2] Steven R. White. Density matrix formulation for quantum renormalization groups. *Phys. Rev. Lett.*, 69:2863–2866, Nov 1992.

[3] G. Vidal. Classical simulation of infinite-size quantum lattice systems in one spatial dimension. *Phys. Rev. Lett.*, 98:070201, Feb 2007.

[4] G. Vidal. Entanglement renormalization. *Phys. Rev. Lett.*, 99:220405, Nov 2007.

[5] Elliott H. Lieb and Werner Liniger. Exact analysis of an interacting bose gas. i. the general solution and the ground state. *Phys. Rev.*, 130:1605–1616, May 1963.

[6] H. Bethe. Zur theorie der metalle. i. eigenwerte und eigenfunktionen der hnearen atomkette. *Zeitschrift für Physik*, 71(3-4):205–226, 1931.

[7] V.E. Korepin, N.M. Bogoliubov, and A.G. Izergin. *Quantum Inverse S-cattering Method and Correlation Functions*. Cambridge University Press, 1997.

[8] T. Giamarchi. *Quantum physics in one dimension*, volume 121. Oxford University Press, 2004.

[9] Hal Tasaki. The hubbard model - an introduction and selected rigorous results. *Journal of Physics: Condensed Matter*, 10(20):4353, 1998.

[10] Yosuke Nagaoka. Ferromagnetism in a narrow, almost half-filled s band. *Phys. Rev.*, 147:392–405, Jul 1966.

[11] Elliott Lieb and Daniel Mattis. Theory of ferromagnetism and the ordering of electronic energy levels. *Phys. Rev.*, 125:164–172, Jan 1962.

[12] Elliott H. Lieb. Two theorems on the hubbard model. *Phys. Rev. Lett.*, 62:1201–1204, Mar 1989.

[13] Tohru Koma and Hal Tasaki. Decay of superconducting and magnetic correlations in one- and two-dimensional hubbard models. *Phys. Rev. Lett.*, 68:3248–3251, May 1992.

[14] Masanori Yamanaka, Masaki Oshikawa, and Ian Affleck. Nonperturbative approach to luttinger's theorem in one dimension. *Phys. Rev. Lett.*, 79:1110–1113, Aug 1997.

[15] M. Girardeau. Relationship between systems of impenetrable bosons and fermions in one dimension. *Journal of Mathematical Physics*, 1(6):516–523, 1960.

[16] M. D. Girardeau. Permutation symmetry of many-particle wave functions. *Phys. Rev.*, 139:B500–B508, Jul 1965.

[17] Belen Paredes, Artur Widera, Mandel Olaf Murg, Valentin, Simon Folling, Ignacio Cirac, Gora V. Shlyapnikov, Theodor W. Hansch, and Immanuel Bloch. Tonks-girardeau gas of ultracold atoms in an optical lattice. *Nature*, 429:277–281, May 2004.

[18] Barry Simon. Universal diamagnetism of spinless bose systems. *Phys. Rev. Lett.*, 36:1083–1084, May 1976.

[19] Elliott H. Lieb and Michael Loss. Fluxes, laplacians, and kasteleyn's theorem. *Duke Math. J.*, 71:337, 1993.

[20] Stephen Blundell. *Magnetism in Condensed Matter (Oxford Master Series in Physics)*. Oxford University Press, 2001.

[21] Tosis Kato. Schrödinger operators with singular potentials. *Israel Journal of Mathematics*, 13(1-2):135–148, 1972.

[22] R. P. Feynman. *Statistical Mechanics*. Westview Press, 1972.

[23] Conjun Wu. Unconventional bose-einstein condensation beyond the "no-node" theorem. *Mod. Phys. Lett. B*, 23:1–24, Jan 2009.

[24] Douglas R. Hofstadter. Energy levels and wave functions of bloch electrons in rational and irrational magnetic fields. *Phys. Rev. B*, 14(6):2239–2249, Sep 1976.

[25] Ian Affleck and J. Brad Marston. Large-n imit of the heisenberg-hubbard model: Implications for high-T_c superconductors. *Phys. Rev. B*, 37:3774–3777, Mar 1988.

[26] Y. Hasegawa, P. Lederer, T. M. Rice, and P. B. Wiegmann. Theory of electronic diamagnetism in two-dimensional lattices. *Phys. Rev. Lett.*, 63:907–910, Aug 1989.

[27] Daniel S. Rokhsar. Quadratic quantum antiferromagnets in the fermionic large-N limit. *Phys. Rev. B*, 42:2526–2531, Aug 1990.

[28] X. G. Wen, Frank Wilczek, and A. Zee. Chiral spin states and superconductivity. *Phys. Rev. B*, 39:11413–11423, Jun 1989.

[29] G. Kotliar. Resonating valence bonds and d-wave superconductivity. *Phys. Rev. B*, 37:3664–3666, Mar 1988.

[30] Elliott H. Lieb. Flux phase of the half-filled band. *Phys. Rev. Lett.*, 73:2158–2161, Oct 1994.

[31] F. Calogero. Solution of a three-body problem in one dimension. *Journal of Mathematical Physics*, 10(12):2191–2196, 1969.

[32] M. A. Cazalilla, R. Citro, T. Giamarchi, E. Orignac, and M. Rigol. One dimensional bosons: From condensed matter systems to ultracold gases. *Rev. Mod. Phys.*, 83:1405–1466, Dec 2011.

[33] Mikhail Zvonarev. In *Notes on Bethe Ansatz*. 2010.

[34] A. Lenard. *Momentum Distribution in the Ground State of the One-dimensional System of Impenetrable Bosons*. Princeton University Plasma Physics Laboratory, 1963.

[35] R.A. Horn and C.R. Johnson. *Matrix Analysis*. Cambridge University Press, 2012.

[36] Carl D Meyer. *Matrix Analysis and Applied Linear Algebra*. Society for Industrial and Applied Mathematics, 2001.

[37] P. W. Anderson. Limits on the energy of the antiferromagnetic ground state. *Phys. Rev.*, 83:1260–1260, Sep 1951.

[38] Daniel Shanks. *Soved and Unsolved Problems in Number Theory.* American Mathematical Society, 2000.

[39] Gary Chartrand. *Introductory Graph Theory.* Dover Publications, 1977.

[40] Tetsuro Yamamoto. *Fundament of Matrix Analysis (in Japnese).* Sainensusha Co. Ltd. Publishers, 2010.

[41] E Seneta. *Non-negative Matrices And Markov Chains.* Springer New York, 1980.

[42] Elliott H. Lieb. Residual entropy of square ice. *Phys. Rev.*, 162:162–172, Oct 1967.

[43] Elliott H. Lieb. Bound on the maximum negative ionization of atoms and molecules. *Phys. Rev. A*, 29:3018–3028, Jun 1984.

[44] Elliott H. Lieb. Two theorems on the hubbard model. *Phys. Rev. Lett.*, 62:1201–1204, Mar 1989.

[45] J. K. Freericks and Elliott H. Lieb. Ground state of a general electron-phonon hamiltonian is a spin singlet. *Phys. Rev. B*, 51:2812–2821, Feb 1995.

[46] W. Pauli. über den zusammenhang des abschlusses der elektronengruppen im atom mit der komplexstruktur der spektren. *Zeitschrift für Physik*, 31(1):765–783, 1925.

[47] von Bose. Plancks gesetz und lichtquantenhypothese. *Zeitschrift für Physik*, 26(1):178–181, 1924.

[48] A. Einstein. Quantentheorie des einatomigen idealen Gases. *Sitzungsberichte der Preußischen Akademie der Wissenschaften*, Physikalisch-mathematische Klasse:261–267, 1924.

[49] A. J. Leggett. *Quantum Liquids: Bose condensation and Cooper pairing in condensed-matter systems.* Oxford University Press, 2006.

[50] Tom Kennedy, Elliott H. Lieb, and B. Sriram Shastry. The XY model has long-range order for all spins and all dimensions greater than one. *Phys. Rev. Lett.*, 61:2582–2584, Nov 1988.

[51] P. C. Hohenberg. Existence of long-range order in one and two dimensions. *Phys. Rev.*, 158:383–386, Jun 1967.

[52] N. D. Mermin and H. Wagner. Absence of ferromagnetism or antiferromagnetism in one- or two-dimensional isotropic heisenberg models. *Phys. Rev. Lett.*, 17:1133–1136, Nov 1966.

[53] N. D. Mermin. Crystalline order in two dimensions. *Phys. Rev.*, 176:250–254, Dec 1968.

[54] John Cardy. *Scaling and Renormalization in Statistical Physcis.* Cambridge University Press, 1996.

[55] Sebastian D. Huber and Ehud Altman. Bose condensation in flat bands. *Phys. Rev. B*, 82:184502, Nov 2010.

[56] Ehud Altman. private communications, 2010.

[57] Wenxing Nie, Hosho Katsura, and Masaki Oshikawa. Ground-state energies of spinless free fermions and hard-core bosons. *Phys. Rev. Lett.*, 111:100402, Sep 2013.

[58] Takeo Matsubara and Hirotsugu Matsuda. A lattice model of liquid helium, i. *Progress of Theoretical Physics*, 16(6):569–582, 1956.

[59] T. Holstein and H. Primakoff. Field dependence of the intrinsic domain magnetization of a ferromagnet. *Phys. Rev.*, 58:1098–1113, Dec 1940.

[60] M E Fisher. The theory of equilibrium critical phenomena. *Reports on Progress in Physics*, 30(2):615, 1967.

[61] N. G. Zhang and C. L. Henley. Stripes and holes in a two-dimensional model of spinless fermions or hardcore bosons. *Phys. Rev. B*, 68:014506, Jul 2003.

[62] Siew-Ann Cheong and Christopher L. Henley. Exact ground states and correlation functions of chain and ladder models of interacting hardcore bosons or spinless fermions. *Phys. Rev. B*, 80:165124, Oct 2009.

[63] Hal Tasaki. From nagaoka's ferromagnetism to flat-band ferromagnetism and beyond: An introduction to ferromagnetism in the hubbard model. *Prog. Theo. Phys.*, 99(4):489, Apr. 1998.

[64] L. D. Landau and E. M. Lifshitz. *Statistical physics.* Butterworth-Heinemann, 1980.

[65] W. Vincent Liu and Congjun Wu. Atomic matter of nonzero-momentum bose-einstein condensation and orbital current order. *Phys. Rev. A*, 74:013607, Jul 2006.

[66] Vladimir M. Stojanović, Congjun Wu, W. Vincent Liu, and S. Das Sarma. Incommensurate superfluidity of bosons in a double-well optical lattice. *Phys. Rev. Lett.*, 101:125301, Sep 2008.

[67] Federico Becca, Luca Capriotti, Sandro Sorella, and Alberto Parola. Exact bounds on the ground-state energy of the infinite-u hubbard model. *Phys. Rev. B*, 62:15277–15278, Dec 2000.

[68] Eli Eisenberg and Elliott H. Lieb. Polarization of interacting bosons with spin. *Phys. Rev. Lett.*, 89:220403, Nov 2002.

[69] J. E. Hirsch. Two-dimensional hubbard model: Numerical simulation study. *Phys. Rev. B*, 31:4403–4419, Apr 1985.

[70] E. Fradkin. *Field Theories of Condensed Matter Physics (2 edition)*. Cambridge University Press, 2013.

[71] Roderich Moessner and Arthur P. Ramirez. Geometrical frustration. *Physics Today*, 59:24–29, Feb 2006.

[72] G. Möller and N. R. Cooper. Condensed ground states of frustrated bose-hubbard models. *Phys. Rev. A*, 82:063625, Dec 2010.

[73] H. T. Diep. *Frustrated Spin Systems*. World Scientific, 2004.

[74] Elliot H. Lieb, T. Schultz, and D. J. Mattis. *Ann. Phys. (N. Y.)*, 16:407, 1961.

[75] Shigetoshi Katsura. Statistical mechanics of the anisotropic linear heisenberg model. *Phys. Rev.*, 127:1508–1518, September 1962.

[76] Paul Ginsparg. Applied conformal field theory. In *Fields, Strings and Critical Phenomena*. North-Holland, 1989.

[77] F. C. Alcaraz and M. J. Martins. Conformal invariance and critical exponents of the takhtajan-babujian models. *Journal of Physics A: Mathematical and General*, 21(23):4397, 1988.

[78] Francisco C. Alcaraz, Michael N. Barber, and Murray T. Batchelor. Conformal invariance and the spectrum of the *XXZ* chain. *Phys. Rev. Lett.*, 58:771–774, Feb 1987.

[79] Claudio Chamon. private communications, 2013.

[80] Y. Hatsugai, K. Ishibashi, and Y. Morita. Sum rule of hall conductance in a random quantum phase transition. *Phys. Rev. Lett.*, 83(11):2246–2249, Sep 1999.

[81] Y. Natsume, T. Hamada, S. Nakagawa, J. Kane, and M. Katagiri. The accurate expression of the ground state for square lattice s=1/2 heisenberg antiferromagnet by rvb-strings spreading over any n-th n.n. *Physica B*, 165:175–176, August 1990.

[82] Gordon W. Semenoff. Canonical quantum field theory with exotic statistics. *Phys. Rev. Lett.*, 61:517–520, Aug 1988.

[83] Eduardo Fradkin. Jordan-wigner transformation for quantum-spin systems in two dimensions and fractional statistics. *Phys. Rev. Lett.*, 63:322–325, Jul 1989.

[84] G. Möller and N. R. Cooper. Condensed ground states of frustrated bose-hubbard models. *Phys. Rev. A*, 82:063625, Dec 2010.

[85] Yasuhiro Saiga and Masaki Oshikawa. Saturated ferromagnetism from statistical transmutation in two dimensions. *Phys. Rev. Lett.*, 96(3):036406, Jan 2006.

[86] Rolf Tarrach and Roser Valentí. Exact lower bounds to the ground-state energy of spin systems: The two-dimensional S =1/2 antiferromagnetic heisenberg model. *Phys. Rev. B*, 41:9611–9613, May 1990.

[87] R. Valentí, P. J. Hirschfeld, and J. C. Anglés d'Auriac. Rigorous lower bounds on the ground-state energy of correlated fermi systems. *Phys. Rev. B*, 44:3995–3998, Aug 1991.

[88] Doron L. Bergman, Congjun Wu, and Leon Balents. Band touching from real-space topology in frustrated hopping models. *Phys. Rev. B*, 78:125104, Sep 2008.

[89] Wenxing Nie, Hosho Katsura, and Masaki Oshikawa. Particle statistics, frustration, and ground-state energy. *arXiv:cond-mat/1401.2090*, 2014.

[90] A Mielke. Ferromagnetic ground states for the hubbard model on line graphs. *Journal of Physics A: Mathematical and General*, 24(2):L73, 1991.

[91] A Mielke. Ferromagnetism in the hubbard model on line graphs and further considerations. *Journal of Physics A: Mathematical and General*, 24(14):3311, 1991.

[92] A Mielke. Ferromagnetism in the hubbard model on line graphs and further considerations. *Journal of Physics A: Mathematical and General*, 24(14):3311, 1991.

[93] Hal Tasaki. Ferromagnetism in the hubbard models with degenerate single-electron ground states. *Phys. Rev. Lett.*, 69:1608–1611, Sep 1992.

[94] Andreas Mielke and Hal Tasaki. Ferromagnetism in the hubbard model. *Commun.Math.Phys.*, 158:341–371, Nov 1993.

[95] M. E. Zhitomirsky and Hirokazu Tsunetsugu. Exact low-temperature behavior of a kagomé antiferromagnet at high fields. *Phys. Rev. B*, 70:100403, Sep 2004.

[96] M. E. Zhitomirsky and Hirokazu Tsunetsugu. High field properties of geometrically frustrated magnets. *Prog. Theor. Phys. Supplement*, 160:361, 2005.

[97] Immanuel Bloch, Jean Dalibard, and Sylvain Nascimbene. Quantum simulations with ultracold quantum gases. *Nat. Phys.*, 8:267–276, April 2012.

[98] A Suto. Percolation transition in the bose gas. *Journal of Physics A: Mathematical and General*, 26(18):4689, 1993.

[99] A. Fledderjohann, A. Langari, E. Mller-Hartmann, and K.-H. Mtter. Ferromagnetism in a hard-core boson model. *The European Physical Journal B - Condensed Matter and Complex Systems*, 43(4):471–478, 2005.

[100] M. Aidelsburger, M. Atala, S. Nascimbène, S. Trotzky, Y.-A. Chen, and I. Bloch. Experimental realization of strong effective magnetic fields in an optical lattice. *Phys. Rev. Lett.*, 107:255301, Dec 2011.

Acknowledgement

I would like to express my sincere gratitude to all those who helped me in every aspect during my three years' study in Japan.

My deepest gratitude goes first and foremost to Professor Masaki Oshikawa, my supervisor, for his constant guidance, encouragement and patience. He led me into the world of strongly correlated quantum many-body systems. He suggested me the interesting subject of this thesis and supervised me through all the stages of my research and writing. I greatly appreciate the uncountable enlightening discussions with him. I benefit a lot from his advice and insight which are always stimulating and capture the essence of the problem. His insightful advice, constant encourage and great patience help me to overcome the difficulty confronted every time. I would like to thank him for his effort and support to provide as many opportunities as he could for my academical activities. I have learned a lot from him about physics and much more beyond physics. His serious attitudes in physics, gentle attitudes to people, working enthusiasm, immense knowledge and passion in science will influence me all my life.

I would like to sincerely thank our collaborator, Professor Hosho Katsura. I learned a lot from him in mathematical physics. I appreciate his generosity and sharing his vast knowledge with us. I appreciate his contributions in our work, without which this work would never reached this level. In numerical diagonalization, we partially used TITPACK ver. 2 developed by Professor Hidetoshi Nishimori. I would like to thank all the questions from the members of defense committee and discussions with them. I appreciate the serious reviewing of this thesis by Professor Naomichi Hatano.

I would like to gratefully acknowledge the cooperation and discussion with Yasuhiro Tada on the research of chiral superfluid issue. He widened my horizon and led me to the world of superconductivity.

I would like to thank Professor Shaojing Qin and Professor Tao Xiang for their acceptance and financial support for me as a visiting student in Institute of Theoretical Physics (ITP), Chinese Academy of Science, during my half-year leave of absence due to the East Japan Earthquake. I appreciate their timely help such that I can continue and concentrate on my study in an academic environment.

I would like to thank the following people for valuable discussion and support in the last three years: Professor Karo Penc, Wei-Feng Tsai, Thomas Eggel, Shunsuke Furukawa, Masahiro Sato, Shintaro Takayoshi, Shunsuke Furuya, Yuta Kumano, Hidetaka Nishihara, Yohei Fuji, Emika Takata, Soichiro Mohri, Yuya Nakagawa and Miklos Lajko. I appreciate the wonderful time spent with them together.

I would like to thank Ms. Tsuji, Ms. Matsushita and Ms. Habu for their patience and help for my academic activities. I especially appreciate the help from Ms. Tsuji and Yuta Kumano for my movings.

My thanks also go to my friends Yu Wang, Bing Bai, Lin Zhu, Weihang Zhou and Hui-hai Zhao for sharing the wonderful time in the University of Tokyo, their encouragement and help, so that I can overcome every obstacle in my daily life. I would like to thank my officemates Qiaoni Chen, Yanyan Bu, Zhenhua Zhang and Xunwang Yan, during my visit in ITP. I appreciate the stimulating discussions with them and as much convenience as they could provide, which made me feel at home. I would like to thank my old friends Xuejun Qiu, Fan Jin, Shijun Mao and Wenchao Zhang. Their encouragement makes me feel I am not lonely on the way.

I would like to acknowledge the financial support of Government Scholarship from Ministry of Education, Culture, Sports, Science and Technology of Japan. I would like to acknowledge University of Tokyo. It provides me a precious opportunity to study and do research in this well known university. And I appreciate the financial support from the Young Researcher Over Sea Program from my university for my visit to Kavli Institute for Theoretical Physics, UC Santa Barbara. Part of the work was started there. I would like to acknowledge the hospitality from Professor Xiwen Guan for my visit in Wuhan Institute of Physics and Mathematics, Chinese Academy of Science.

Finally, I would like to thank all the members in my family for their constant encouragement and support for my academic pursuit. They did anything they could such that I did not need to worry anything in my family. Their love and trust are stimulating me for a better me.

Publication List

- Wenxing Nie, Hosho Katsura and Masaki Oshikawa,
  "Ground-State Energies of Spinless Free Fermions and Hard-Core Bosons"
  Phys. Rev. Lett. **111**, 100402 (2013).

- Wenxing Nie, Hosho Katsura and Masaki Oshikawa,
  "Particle Statistics, Frustration, and Ground-State Energy"
  preprint: arXiv:1401.2090