STRONGLY-INTERACTING SPINLESS FERMIONS AND HARDCORE BOSONS ON THE SQUARE LATTICE

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STRONGLY-INTERACTING SPINLESS FERMIONS AND HARDCORE BOSONS ON THE SQUARE LATTICE

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This thesis deals with a two-dimensional model of strongly-interacting spinless fermions and hard-core bosons. This model is a simplified version of the Hubbard model and is the simplest model of correlated electrons. In this thesis we study in detail the phase diagram of this model, and our work contributes to the understanding of strongly-interacting fermions and bosons in two dimensions which is essential in elucidating the mysteries of high-temperature superconductivity.

Our work is divided into two parts, one on the dilute limit, with a few bosons and fermions, and one on stripes which are holes lining up across the lattice.

We explain the relevance of our model to models of high-temperature superconductors, and describe in detail our exact diagonalization program using the Lanczos method.

We study the two-particle problem using the lattice Green functions and obtain the ground state energy of a few particles in the large-lattice limit. The two-particle problem is then reformulated using the scattering t-matrix, which is the sum of
all two-body interactions to infinite order, and we show the qualitative difference between boson and fermion t-matrices.

We study the problem of a single stripe and show how it can be mapped to a spin-1/2 chain, the problem of one and two holes on the stripe and calculate stripe effective mass, and the interaction of two, three, and four stripes and find that stripes repel and the interaction energy decays as a power-law as a function of stripe separation. We investigate the stability of an array of stripes against phase separation into particle-rich and hole-rich regions, and find that the stripe-array is not stable for bosons, and is possibly stable for fermions.

Using a modified t-matrix, the interacting energy spectrum for a few particles is calculated. The boson and fermion energy curves at the low-density limit are fitted. Schick's result for bosons is checked, and we explain that p-wave scattering terms are needed for the fermion problem in our model.

This thesis is the first systematic study of the strongly-interacting spinless fermion model in two dimensions. Chapters 4 and 7 contain the first systematic investigation of the t-matrix on a lattice, and Chapters 5 and 6 are one of the first exact diagonalization studies of interacting quantum stripes. Chapter 2 can be used as a guide for coding exact diagonalization programs in two and higher dimensions.
Biographical Sketch

The author grew up in Beijing. His father is a biophysicist working for the Chinese Academy of Sciences and his mother a professor of physical chemistry at the Beijing University of Science and Technology, where his family has been living since before he was born. As a child, the author enjoyed reading picture books that told old Chinese stories and thought about becoming a historian. That career path was changed in high school when he, following the crowd, attended weekend preparatory schools for mathematics and physics Olympiads, where he learned a lot of geometry and found it fascinating.

In the fall of 1990, the author came to the United States on a scholarship to study at the Hackley School in Tarrytown, New York, which is a small and beautiful school by the Hudson River. He spent two very happy years there and got to know many very kind people.

It was a shock for him to go to Harvard University, where he was thrust into the big world for the first time in his life. He enjoyed the courses very much and was especially interested in writing long papers. He liked physics but at the beginning he took many different courses, including Chinese classical poetry, Salem witchcraft, and macro economics history. In the winter of his freshman year, he found in Lamont Library a copy of Richard Feynman’s autobiography, and was
greatly impressed by the person in the book. He decided to take more advanced courses in physics, and in the fall of his sophomore year, he enrolled in a classical mechanics course taught by a mathematical physicist. He was fascinated by the Lagrangian and Hamiltonian formulations of classical mechanics and continued to take physics courses. In his junior year, he took a group theory in physics course, in which he was introduced to various symmetries of the physical world that he has since found extremely aesthetically appealing.

He moved to Cornell for graduate school and spent a busy first year taking courses and teaching undergraduate physics. In the spring of his first year, he took a solid state physics course and was introduced to the world of magnetism and superconductivity, which he found to his liking. He decided to work for the instructor of the course the following summer and ended up writing this thesis five years later.

In his five-and-a-half years at Cornell, the author, not knowing what he would like to do and feeling restless about life, tried many things, including drawing class, writing class, wildflower class, and he sat in on courses ranging from Greek literature, to introductory philosophy, to social psychology, to poetical and literary theory. He went to eleven book sales offered by the public library and bought a room full of books very cheaply, including a set of Harvard Classics and a set of Encyclopedia Britannica. Browsing freely at home, he was introduced to Keats, Samuel Johnson, Proust, Bertrand Russell, Shakespeare, Flaubert, Kleist, and James Joyce, and he went to the Kroch Asian Library often and reread many Chinese classics that he enjoyed so much when he was young. It was among these books that he found lasting happiness, and his thesis topic has turned out to be fascinating too. He will leave Ithaca in a few weeks and move to Washington, DC, but he will not
forget the happy time he spent in the wildflower garden, looking at the trillium,
bloodroot, black-eyed Susan, wild sunflower; the walks he took at the arboretum,
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To my parents, Jizhen Zhang and Wen Ye
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Chapter 1

Introduction

In this thesis, we study a model of strongly interacting spinless fermions and hard-core bosons on a square lattice. Since the discovery of the high-temperature superconductors in 1986, there has been tremendous interest in strongly interacting electronic systems in two dimensions. From the theoretical aspect, a number of two-dimensional models have gained prominence, and one of the most extensively studied is the Hubbard model. Yet, after fifteen years of intense work, because of the lack of good analytical and numerical methods for two dimensional, strongly interacting, fermion systems, there are still many unanswered questions surrounding the phase diagram of the Hubbard model. The model that we will study in this thesis is closely related to this research activity; it is a simplified version of the Hubbard model, and it is what we believe the simplest microscopic model of correlated electrons in two dimensions.

Our model is motivated by a number of considerations that arose from the work on high-temperature superconductors and the Hubbard model but have not been satisfactorily answered. One is related to the validity of the Fermi liquid theory at the low-density limit in two dimensions, and another is the need for microscopic un-
derstanding of interacting stripes. In this introduction, we describe the physical and mathematical considerations that have led us to this model of strongly interacting spinless fermions and hardcore bosons, and we describe the larger context in which our results should be placed.

This chapter is organized as follows. First, we introduce the high-temperature superconductors, focusing on \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \), and the relevance of the Hubbard model. We then describe the phase diagram of the Hubbard model, and introduce our model of spinless fermions and hardcore bosons. After a brief note on electronic and spin models, we describe some of the motivations for studying our model. And we close by giving brief overviews of the thesis chapter by chapter.

1.1 High-Temperature Superconductors

Superconductivity has always held our fascination since the discovery by Kamerlingh Onnes in 1911. He was measuring the temperature dependence of mercury’s electrical resistance and recorded a sudden drop from a finite value to zero at 4.2 Kelvin. It was a totally unexpected observation and was only made possible by the availability of liquified helium from a few years before. In the years after that many superconducting materials were discovered, but their mysterious mechanism was not fully elucidated until the BCS theory appeared in 1957, which says that electrons form pairs of bosonic nature via a phonon-mediated mechanism and condense.

The search for materials with higher transition temperature progressed slowly, reaching 23.2 K for \( \text{Nb}_3\text{Ge} \) in the 1970s. Fifteen years ago, in January 1986, J. Georg Bednorz and K. Alex Muller discovered superconductivity in \( \text{La}_{2-x}\text{Ba}_x\text{CuO}_4 \), a ceramic material that can superconduct at about 30 K, surprising just about everybody. And in a year’s time, the transition temperature reached an amazing 100 K
in a related family of copper oxides, well beyond liquid nitrogen temperature. (In Fig. 1.1, we borrow the figure from Ref. [1] to show the remarkable period of discovery in historical context.) Now fifteen years later, superconducting power lines have been laid in some North American cities, but the microscopic mechanism of these high-temperature superconductors remains unsolved and is as challenging and fascinating as ever. This thesis is about a model that is closely related to the family of models that have been devised to understand the cuprate superconductors, and we now start to introduce its relevance.

This section follows closely discussions in Ref. [2] and Ref. [3]. We will discuss La$_{2-x}$Sr$_x$CuO$_4$ whose crystal unit cell is shown in Fig. 1.2. This compound has a layered structure: three Cu-O planes are shown in the figure and they are separated from each other by nonmagnetic La$_2$O$_2$ layers. The pure La$_2$CuO$_4$ (without Sr doping) is an antiferromagnetic insulator which we can understand from the following argument. An isolated Cu$^{2+}$ ion has nine electrons in the 3$d$ orbital, but because it is embedded in a crystal environment surrounded by oxygens, the degeneracy between the $d$ orbitals is split. The bonding between a Cu$^{2+}$ and two O$^{2-}$ ions are shown in Fig. 1.3. We cannot go into detail of this calculation, but it suffices to say that the orbitals separate and the resulting highest energy state is the $d_{x^2-y^2}$ state with one electron. That is also to say that this $d_{x^2-y^2}$ orbital carries a missing hole, which gives the ion spin 1/2. Thus the pure La$_2$CuO$_4$ is described by a square lattice of spin-1/2 states, and they couple antiferromagnetically via the well-known superexchange mediated by oxygens on the same plane.

The interesting physics happens when we dope with Sr, i.e., La$^{3+}$ is randomly replaced by Sr$^{2+}$. To maintain charge neutrality electrons must be taken out of the system, or equivalently holes must be added. It is interesting to ask where the holes
Figure 1.1: The remarkable discovery of the high-temperature superconductors in 1986 in historical context. Taken from Ref. [1].
Figure 1.2: Left, crystal structure of La$_{2-x}$Sr$_x$CuO$_4$ (LSCO). Taken from Ref. [3]. The body-centered-tetragonal structure is shown, with three Cu-O planes that are 6.6 Å apart. Sr substitution of La is also noted. Right, a single Cu-O plane. Taken from Ref. [2]. The $d_{x^2-y^2}$ orbital of a Cu$^{2+}$ ion is shown. When doping Sr, the holes will go to O$^{2-}$, making it O$^-$, and the outer electron is at the $p_x$ orbital (shown), which interacts with $d_{x^2-y^2}$ of Cu$^{2+}$. 
Figure 1.3: Bonding between a Cu$^{2+}$ and two O$^{2-}$ ions. Taken from Ref. [3]. The highest energy state $d_{x^2-y^2}$ has only one electron, making the ion a spin-1/2 hole. Will the $d_{x^2-y^2}$ electron from Cu$^{2+}$ be removed and give Cu$^{3+}$? Apparently this is not true [2]. The holes go to O$^{2-}$ ions in CuO$_2$ to give O$^-$ ($1s^2 2s^2 2p^5$). The outer electron is apparently in the so-called $p_\sigma$ orbital (see Fig. 1.2) which binds with the $d_{x^2-y^2}$ of Cu$^{2+}$. We will consider this binding in Sec. 1.2 on microscopic models; here, it suffices to say that with Sr concentration greater than 0.05, the oxygen holes can move from site to site, creating a metallic state.

The experimentally determined phase diagram [2] is shown in Fig. 1.4. At low temperatures and Sr doping concentration from 0.05 to 0.30, the famous high-temperature superconducting state is achieved, with optimal doping at 0.15, giving the highest transition temperature for this compound at around 40 K.\footnote{The first high-temperature superconducting state discovered by Bednorz and Muller in 1986 is a closely related compound La$_{2-x}$Ba$_x$CuO$_4$, with Ba$^{2+}$ instead of Sr$^{2+}$. The highest transition temperature there is about 30 K.} Note also in the phase diagram (Fig. 1.4), the undoped state and its vicinity is the Neel state (doping $x < 0.02$), i.e., the antiferromagnetic state with staggered magnetization that we considered above with spins coupled by superexchange.
Figure 1.4: Phase diagram of La$_{2-x}$Sr$_x$CuO$_4$ with Sr doping concentration $x$. Taken from Ref. [2]. Antiferromagnetic Neel state $x < 0.02$. Superconducting $0.05 < x < 0.30$ at low temperatures, with optimal doping at $x = 0.15$, giving the highest Tc at around 40 K.
1.2 The Hubbard Model

Fig. 1.3 is the starting point for constructing microscopic models for cuprate superconductors. From the beginning of the work on these superconductors, it is believed that the essential physics lies in the electronic properties of a single CuO$_2$ plane. We will first introduce the Hubbard model and then discuss its relevance to the physics of the CuO$_2$ plane. The Hubbard Hamiltonian is

$$H = -t \sum_{\langle i,j \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}. \quad (1.1)$$

Here $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ are the usual fermion creation and annihilation operators of spin $\sigma$ at site $i$ and $\hat{n}_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ the number operator. The first term is the hopping term (i.e., kinetic energy) with the sum over nearest neighbors and $t$ is the hopping amplitude. The second term is the on-site interaction term (potential energy) with amplitude $U$ and it only kicks in when there is an up-down spin pair at one site.

The Hubbard model is a four-state model: at each site there can be four choices of state $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, and $|\uparrow, \downarrow\rangle$. In Fig. 1.5 we show more graphically the content of Eq. 1.1 on the square lattice.

```
  o o o o o o o
  o o o o o o o
  o o o o o U o
  o o o o o o o
  o o o o o o o
  o o o o o o o
```

onsite interaction $U$

nearest neighbor

hopping $t$

Figure 1.5: Hubbard model on the square lattice with nearest-neighbor hopping $t$ and on-site interaction $U$, as in Eq. 1.1.

How is Hubbard model related to the physics of the CuO$_2$ plane in cuprates? In
Sec. 1.1 we mentioned that each Cu$^{2+}$ ion of the CuO$_2$ plane has one electron in the outer $d_{x^2-y^2}$ orbital, making the ion a spin-1/2 hole, and without doping these spins couple antiferromagnetically via superexchange. With doping, holes go into O$^{2-}$ ions, making them O$^-$, where the outer electrons are at the $p_\sigma$ orbital. A natural way to develop a microscopic Hamiltonian for electrons in the doped CuO$_2$ plane is to take into account of the two O$^-$ 2$p_\sigma$ orbitals and the Cu$^{2+}$ 3$d_{x^2-y^2}$ orbital. The resulting Hamiltonian is the so-called three-band Hubbard Hamiltonian (see Ref. [3] for detail) and is rather complicated, including creation and annihilation operators for different orbitals.

An important contribution was made by Zhang and Rice [4]. The O$^-$ hole from doping can combine with the Cu$^{2+}$ hole from the 3$d_{x^2-y^2}$ electron, forming singlet or triplet states, and Zhang and Rice showed that the singlet state (the so-called Zhang-Rice singlet) has the lowest energy. So instead of considering holes moving from oxygen to oxygen, one can consider singlets centered on the copper ions moving in a spin-1/2 background. In the Hubbard model, Eq. 1.1, if there is large repulsion (i.e., $U$ large and positive), at half-filling, we have one spin-1/2 electron per site. Then holes in the Hubbard model doped away from the half-filled limit describe effectively the Zhang-Rice singlets in the spin-1/2 copper background. Therefore, the large-$U$ Hubbard model, Eq. 1.1, near the half-filled limit has been intensely investigated.

The Hubbard model was invented in the 1960s in the context of transition metal magnetism, and has since become, thanks to high-Tc, one of the most studied (and perhaps still the least understood) models in physics. There have been many attempts to justify more quantitatively its relevance to high-Tc superconductivity, for example the validity of the on-site repulsion (see Ref. [3] for a small sample), but
here we will, as many workers in this field, take it as something that captures some of the essential physics that should be understood as a reasonable starting point.

1.3 Phase Diagram of the Hubbard Model

This section follows Ref. [5]. In this section, we introduce some of the known results about the Hubbard model. For those who are not familiar with research works in the fields of high-Tc, strongly correlated electrons, or magnetism, we want to use this section on the Hubbard model phase diagram to give a flavor of what people often do with theoretical models in these fields. This helps to place the present thesis work in a larger perspective. For those who would like to see specifically what our model is and what our work is about, please proceed to Sec. 1.6.

In Fig. 1.6 we plot the phase diagram of the Hubbard model for any dimensionality. The largest particle density or filling is 2, corresponding to two particles per site. Because of the particle-hole symmetry of the Hubbard Hamiltonian (1.1), the phase diagram should be symmetric about $n = 1$, so we only plot $0 \leq n \leq 1$. The half-filled case $n = 1$ plays a large role in the study of the Hubbard model; it is the case with one particle per site. The attractive Hubbard model $U < 0$ is not so interesting because it always favors two-electron pairs energetically. The repulsive case $U > 0$ is much more interesting and is the case we consider here.

1.3.1 $U = 0$, Noninteracting

This is the noninteracting case, and the Hubbard Hamiltonian Eq. 1.1 contains the hopping term only, which can be diagonalized by

$$|	ext{k}\rangle = \frac{1}{\sqrt{N}} \sum_i e^{-i\text{k} \cdot r_i} c_i^\dagger |0\rangle.$$  \hspace{1cm} (1.2)
Figure 1.6: Phase diagram of the Hubbard model (for any dimensions). The “undiscovered country” is for two and higher dimensions.
The eigenstate $|k\rangle$ is the Bloch electron, so this limit is also called the band limit. The one-particle energy is

$$\mathcal{E}(k) = -2t \sum_{i=1}^{d} \cos k_i a, \quad (1.3)$$

where $d$ is the dimensionality and $a$ the lattice constant. In Fig. 1.7 we show $\mathcal{E}(k)$ in one dimension for a chain of 20 sites, emphasizing the discrete nature of the dispersion curve. The Brillouin zone is $-\pi \leq k \leq \pi$. The ground state is obtained by filling the lowest energy levels up, with two (up and down spin) electrons at each level.

![Figure 1.7: $\mathcal{E}(k)$ for a one-dimensional chain of twenty sites with $t = 1$.](image)

### 1.3.2 $t = 0$, Atomic Limit

Without hopping there are two atomic (one-particle) energy levels: $\epsilon = 0$ or $\epsilon = U$. If $n \leq 1$, there is room for one particle at each site, so the ground state energy is zero (there is a large degeneracy). When $n > 1$, we must have two electrons at
one site, so adding each electron will raise the energy by $U$, which is the chemical potential. In Fig. 1.8 we show the chemical potential vs filling $n$.

![Diagram of chemical potential vs filling $n$ for $t = 0$ Hubbard model. The chemical potential jumps by $U$ after the half-filled case of one electron at each site ($n = 1$) because of the on-site repulsion.](image)

**Figure 1.8:** Chemical potential $\mu$ vs filling $n$ for $t = 0$ Hubbard model. The chemical potential jumps by $U$ after the half-filled case of one electron at each site ($n = 1$) because of the on-site repulsion.

### 1.3.3 $n = 1$, $U/t \to \infty$, Neel Antiferromagnet

For the exactly half-filled case, in the strong coupling limit $U/t \to \infty$, there is one particle at each site. The Hubbard Hamiltonian (1.1) can be written in terms of spin-1/2 operators at each site $s_i$. It can be shown [6] that the effective Hamiltonian obtained is the well-known antiferromagnetic Heisenberg’s Hamiltonian:

$$H = J \sum_{\langle i,j \rangle} s_i \cdot s_j,$$

where $J = 4t^2/U$ and the sum is over nearest-neighbor sites. The spin-1/2 Heisenberg is obviously a two-state model.

The Heisenberg exchange interaction $s_i \cdot s_j$ is of course the corner stone of magnetism, and it dates back to the very early days of quantum mechanics. For the
ferromagnetic problem, the ground state is trivial, and in the 1930s Hans Bethe solve exactly the wavefunctions of the one-dimensional antiferromagnetic Heisenberg model (see the book by Mattis [7]). Since the discovery of high-Tc superconductors, there has been a big industry studying the two-dimensional Heisenberg model (see Ref. [8]). There is no exact solution, but the consensus from many analytical and computational studies is that the ground state at zero temperature is the usual Neel antiferromagnet.

1.3.4 $U/t = \infty$, One Hole, Nagaoka State

We have seen that when we approach $U/t = \infty$ from the $n = 1$ line, the ground state is the Neel antiferromagnet. We get something very different when we have $U/t = \infty$ but a little bit away from half filling. When there is exactly one hole, we have one of the few nontrivial exact results of the Hubbard model, namely the surprising and celebrated Nagaoka theorem, that the ground state is ferromagnetic, i.e., all $N - 1$ spins are aligned ($N$ is the number of sites) (see Ref. [9]).

1.3.5 $U/t$ Large, Small Number of Holes, $t - J$ Model

When there are two or more holes, whether the ferromagnetic (Nagaoka) state is stable or not is a question still not settled (see for example Ref. [10] and Ref. [6]). However, when investigating hole motion in the large $U$ limit, using second-order perturbation theory, we get the following model [6]

$$H = -t \sum_{\langle i,j \rangle \sigma} \left( (1 - n_{i,-\sigma}) c_{i\sigma}^\dagger c_{j\sigma} (1 - n_{j,-\sigma}) + \text{h.c.} \right) + J \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j,$$  \hspace{1cm} (1.5)

where $J = 4t^2/U$. This is another famous model, the so-called $t - J$ model. The first term (hopping) is basically nearest-neighbor hopping (like that in the Hubbard
model, Eq. 1.1) except the factor $(1 - n_{i,-\sigma})$ in front of $c_{i\sigma}^\dagger c_{j\sigma}$ restricts hopping to the $i$-th site if there is already a particle. Therefore the $t - J$ model is a three-state model: at each site we can have $|0\rangle$, $|\uparrow\rangle$, and $|\downarrow\rangle$. No double occupation is allowed. There has also been an industry studying the $t - J$ model (see Ref. [3] and Ref. [11] for a small sample). Some of the questions addressed are hole binding and phase separation.

1.3.6 $n = 1$, $U = U_{MI}$, Metal-Insulator Transition

Following the $n = 1$ line down, starting from the large $U$ limit where we have a Neel antiferromagnetic insulator, to $U = 0$ where we have free electrons, there is a fascinating transition: the metal-insulator transition. We have already considered the $t = 0$ atomic limit, where we have two bands at $0$ and $U$ (see Fig. 1.8). And we know that when $U = 0$ we have an energy band that is depicted in Fig. 1.7, with a spread of $4t$ for a one-dimensional model. So when we have both nonzero $t$ and $U$, we have a combination of the two situation. The left figure in Fig. 1.9 shows the $U \ll t$ limit, with two bands of width $4dt$, for the $d$-dimensional model, separated by $U$. This is the insulator state. When $U$ decreases, the two bands are closer and we have a correlation-induced metal-insulator transition at a critical value $U_{MI}$, as illustrated in Fig. 1.9.

Metal-insulator transition is often associated with the physicist N. F. Mott, and it has had a long and distinguished history, since long before high-Tc superconductivity was known (see [12]). High-Tc has brought metal-insulator transition under the lime light, yet many aspects of this transition are still not well understood.
1.3.7 Two-Particle Problem, Exactly Solvable

The one-particle problem (i.e., one electron in the Hubbard model) is trivial because there cannot be interaction. The eigenstate is Eq. 1.2 and the eigenenergy is Eq. 1.3. The two-particle problem is a lot more complicated but tractable. The problem of two particles in the Hubbard model is closely related mathematically to a number of two-particle problems, in particular, the two-magnon problem in the Heisenberg model. The Heisenberg Hamiltonian, Eq. 1.4, can be written in the following form,

$$H = \frac{1}{2} J \sum_{\langle i,j \rangle} \left( s_i^+ s_j^- + s_j^+ s_i^- \right) + J \sum_{\langle i,j \rangle} s_i^z s_j^z. \quad (1.6)$$

The first term looks like a hopping term and the second an interaction term. The spin operators on different sites commute, $s_i^+ s_j^+ |0\rangle = s_j^+ s_i^+ |0\rangle$, so if we consider Eq. 1.6 as a particle Hamiltonian, we have boson particles. For the two-particle problem in the Hubbard model, it turns out that the mathematics is (almost) identical for bosons and fermions (except plus and minus signs that can be treated
simultaneously for the two cases). And it turns out that the two-magnon problem in the Heisenberg model has been solved a long time ago by researchers in the magnetism field when they studied magnon-magnon interaction.

The key idea in many two-body problems from different contexts is that the two-body problem can be reduced to a one-body problem using relative coordinate and momentum, and the resulting one-body problem can be further reduced by symmetry. The leftover problem can be solved analytically at certain limits using special integrals or special functions. For magnon problems see Ref. [7], and for two particles in the Hubbard model see Ref. [13].

1.3.8 \( n \ll 1 \), Dilute Limit, T-Matrix

At the dilute limit, with more than two particles, no exact solutions are available, but the result from the two-particle problem can be employed to study this case systematically. At the center of this calculation is the two-particle scattering matrix, the so-called t-matrix, which includes all two-body scattering terms and calculates the interaction correction to the noninteracting energy of the pair. If there are more than two particles, summing up the t-matrix corrections for all pairs gives an approximation to the exact interacting energy, with errors due to the neglect of three and more-body interaction terms. However, at the very dilute limit, in three dimensions this method gives good results. See Kanamori [14] and Mattis [7] for detail. In two dimensions, the case relevant for high-Tc, the dilute fermion problem is far from settled. There is a controversy regarding whether the system is a Fermi liquid state, and it will be discussed in more detail later in this chapter.

We should also mention that the few-body problem (on or off-lattice) is also a small field in itself, engaging many mathematically oriented researchers (see Ref. [15]
for a review).

1.3.9 The Great Interior

We have so far covered the borders and corners of the Hubbard model phase diagram (Fig. 1.6). The $U = 0$ (noninteracting), $t = 0$ (atomic), and $M = 1$ (one-particle, $M$ is the number of particles) lines are trivial. The $M = 2$ and the one-hole-with-$U = \infty$ (Nagaoka theorem) points are exactly understood. The $n = 1$, $U/t \rightarrow \infty$ segment is well-studied (Neel antiferromagnet) and the half-filled case can be studied using quantum Monte Carlo (see next section). Some immediate vicinities of these spots have been studied using analytical methods such as perturbation, mean-field, and self-consistent methods, but in a lot of the cases these methods are not well-controlled because of strong correlation. Therefore the rest of the phase diagram (that means everything in Fig. 1.6 except not much more than a measure zero set) has to be investigated using numerical methods.

1.4 Hubbard Model: Special Cases, Variations, and Results

Before we introduce the numerical methods, we describe some special cases and variations of the Hubbard model.

$d = 1$

The one-dimensional Hubbard model is exactly solved using the so-called Bethe ansatz technique that Hans Bethe originally used to solve the spin-$1/2$ Heisenberg antiferromagnetic chain (which we mentioned above) [16, 9]. A host of one-
dimensional quantum problems can be solved using this deep and beautiful method (see the book by Lieb and Mattis [17] for a sampling) which has since found application in areas such as pure mathematics (e.g., quantum group) and string theory (e.g., conformal field theory).

\[ d = \infty \]

The classical Ising model in infinite dimensions is exactly solvable. In search of controlled approximations for strongly correlated systems, the infinite dimension limit of the Hubbard model has been studied [18]. At far as we know, unlike the Ising case, the \( d = \infty \) Hubbard model is not exactly solvable, but it is found that a class of mean-field techniques can be applied with control [19].

**Extended Hubbard Models**

If in the Hubbard Hamiltonian Eq. 1.1, hopping is not constrained to nearest neighbors, or if on-site interaction is extended to neighboring sites, we have extended Hubbard models. If we have completely unconstrained (infinite-range) hopping, the Hubbard model at the thermodynamic (infinite-lattice) limit is exactly solvable [20].

**Bose-Hubbard Model**

The boson version of the Hubbard model exhibits a number of interesting phases as well, including superfluid, charge-density wave, insulator, and a so-called supersolid phase where superfluidity coexists with the crystalline order [21]. The Bose-Hubbard model has been used to study quantum phase transitions and Bose-Einstein condensation.
Symmetries

The exact symmetries of a model are often the basis for a reduction of the problem. It is easy to see that the Hubbard Hamiltonian, Eq. 1.1, commutes with the total particle number operator, lattice translations and point group operations (reflections and rotations), and the total spin operator. It takes more work to show the so-called pseudospin symmetry: \((SU(2) \times SU(2))/\mathbb{Z}_2 = SO(4)\) [22]. These symmetries have all been used in numerical diagonalization studies that we will explain next.

1.5 Numerical Methods

There are two widely used and one up-and-coming method for studying strongly interacting electronic systems numerically.

1.5.1 Exact Diagonalization

This is an exact method for every quantum mechanical problem with a finite number of basis states. All basis states are enumerated; the Hamiltonian matrix is computed within these basis states; it is then diagonalized, giving eigenenergies and eigenfunctions. Of course the problem is the exponential growth of the number of basis states which severely limits the size of the system that can be studied. For example, the Hubbard model is a four-state model, i.e., with \(N\) sites, there are \(4^N\) basis states. If \(N = 16\) (for \(4 \times 4\) lattice), \(4^{16} = 4,294,967,296\), well beyond the computational power of the day.

There are indeed ways to reduce the number of states (i.e., block-diagonalize the Hamiltonian matrix), using particle number conservation, space group symmetries, and special symmetries of special models, that we introduced above. The \(4 \times 4\)
Hubbard model with \( M = 16 \) electrons (8 up and 8 down), after reduction by particle conservation, translation, and the symmetries of the square, has 1,310,242 states in the largest matrix block [23]. To store a 1 million by 1 million matrix in memory requires to much space, so one diagonalization method, the Lanczos method, has been widely used because it requires the storage of only a few vectors, not the full matrix (see [23]). The Lanczos method can obtain the low-lying eigenvalues and eigenvectors with high accuracy. This thesis is heavily based on a Lanczos exact diagonalization program, which will be explained in great detail in Chapter 2.

We should mention that these methods of Hilbert space reduction are only delaying temporarily the exponential growth, which will very quickly make the biggest and fastest supercomputers feel helpless. (We will describe the renormalization group method later, which tries to beat the exponential growth with more drastic reductions than the symmetry considerations here, but that method is still in early development stage.) So it is absolutely crucial to think carefully and hard about whatever model we want to study and make educated reductions. That is what we will do with our model of spinless fermions and hardcore bosons.

### 1.5.2 Quantum Monte Carlo (QMC)

The Monte Carlo method does not enumerate all basis states; it moves around in state space using a random choice according to certain known statistical distributions. The half-filled case in the Hubbard model can be studied using lattice quantum Monte Carlo, but for \( n \neq 1 \), at low temperatures, the repulsive Hubbard model has a notorious fermion “sign problem.” See Dagotto [3] for a detailed description of the problem and the attempts to overcome or alleviate the problem. The sign problem severely restricts the fermion systems that can be studied using quantum
Monte Carlo and gives unacceptable statistical errors close to zero temperature for many interesting regimes that we want to study. On the other hand, there is no such problem with boson systems, and as we will see in Chapter 8 the boson version of the model that we will introduce has been studied (though very fleetingly) using quantum Monte Carlo.

1.5.3 Renormalization Group: DMRG

The problem with exact diagonalization is that the method keeps all basis states and the number of basis states often grows exponentially as the system grows, severely limiting the size of the system we can compute. One way to beat the exponential growth is to keep only the “important” states and throw away the rest. The question is which states should we keep. In 1992, S. R. White devised a procedure using the density matrix: the density matrix renormalization group (DMRG) [24, 25]. He considered a Heisenberg spin chain, and starting from two sites, he grew the chain at the two ends. The number of basis states of course grows exponentially as new sites are added, but White only kept a fix number of states which are the highest-weight states in the ground state density matrix determined from the previous iteration. The number of states kept is in the order of hundreds and the accuracy is almost unprecedented for numerical calculations in physics.

It is a great challenge to extend the DMRG to two dimensions. A straightforward way is to turn a two-dimensional system into a one-dimensional one by tracing the 2D lattice with a linear order (the scanline approach). A number of ingenious ways have been developed (see Ref [26] for a recent attempt), but it is fair to say that an accurate renormalization group method in two dimensions is still in its infancy. The idea of keeping the most important states is absolutely necessary, and the density
matrix method is very promising and is a method to watch in the days ahead.

1.6 Our Model

Before the 2D DMRG comes of age and the QMC solves the sign problem, the most reliable method in the study of strongly correlated fermion systems is exact diagonalization. After a great deal of symmetry considerations to reduce the size of the matrix, the Hubbard model has been exactly diagonalized on the $4 \times 4$ lattice [27] and for up to four particles on the $6 \times 6$ lattice [28] (that is where the exponential growth in basis states catches up with computer memory availability). We have asked the question:

Is there a model that contains the basic ingredients of short-range hopping and interaction but is simpler (in the exact diagonalization sense) than Hubbard model?

The answer is yes: we can neglect the spin. We obtain the following Hamiltonian for spinless fermions,

$$ H = -t \sum_{\langle i,j \rangle} \left( c_i^\dagger c_j + c_j^\dagger c_i \right) + V \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j, \quad (1.7) $$

where $c_i^\dagger$ and $c_i$ are spinless fermion creation and annihilation operators at site $i$, $\hat{n}_i = c_i^\dagger c_i$ the number operator, $t$ the nearest-neighbor hopping amplitude, and $V$ the nearest-neighbor interaction. Note that with spinless fermions, there can be at the most one particle per site; no on-site interaction (as that in the Hubbard model) is possible, and we have included in our Hamiltonian nearest-neighbor repulsion.

The spinless fermion model, Eq. 1.7, is a two-state model, and the number of basis states for a $N$-site system is $2^N$, which is a significant reduction from the $4^N$
of the Hubbard model. We can further reduce the number of basis states by taking the nearest-neighbor interaction $V = +\infty$, i.e., infinite repulsion, which excludes nearest neighbors, giving roughly $2^{N/2}$ states. In Fig. 1.10 we show the hopping and exclusion that are involved in our model (compare with Fig. 1.5 for the Hubbard model).

![Diagram of the spinless fermion and hardcore boson model with nearest-neighbor hopping amplitude $t$ and nearest-neighbor repulsion $V$. The crosses show the four excluded neighbors of a particle when $V = +\infty$.](image)

Figure 1.10: The spinless fermion and hardcore boson model with nearest-neighbor hopping amplitude $t$ and nearest-neighbor repulsion $V$. The crosses show the four excluded neighbors of a particle when $V = +\infty$.

The spinless fermion model with infinite repulsion Eq. 1.7 contains a significant reduction of the Hilbert space. We have mentioned above that after using particle conservation, translation symmetry, and the symmetries of the square, the Hubbard model on the $4 \times 4$ lattice has $1,310,242$ at half-filling. In our model with infinite $V$, after using particle conservation and translation symmetry (but not point group symmetry), the largest matrix for the $7 \times 7$ system has $1,906,532$ states (for 11 particles). We can therefore compute for all fillings the $7 \times 7$ system whereas for the Hubbard model $4 \times 4$ is basically the limit. This of course means that for
certain limits we can also go much further than the Hubbard model. For example, we can handle four particles on a $20 \times 20$ lattice where the number of basis states is 2,472,147, whereas for the Hubbard model, Ref. [28] studied four particles on a $6 \times 6$ lattice. This extended capability with our model enables us to obtain a number of new results (on stripe-stripe interaction for example) that are difficult to obtain with the Hubbard model.

An added feature of our model is that the basis set for the spinless fermion problem is identical to that for the hardcore boson problem, because with hardcore repulsion, there can be one boson at one site also. Therefore, without computational difficulty, we can study numerically both the spinless fermion and hardcore boson problem, killing two birds with one stone. The comparison of the fermion and boson cases in our model has helped us understand the fermion case better (in stripe-array stability problem especially, as we will see later).

**Previous Work**

Spinless fermions can also be realized in experiments, for example, the spin polarized $^3$He due to a strong magnetic field, or ferro or ferri-magnetic electronic systems where one spin-band is filled. The one-dimensional spinless fermion model with finite repulsion is solved exactly using Bethe ansatz [29]. The infinite-dimensional problem is studied in Ref. [30]. A very different approach using the renormalization group for fermions is done in Ref. [31]. A Monte Carlo study of the two-dimensional model at half-filling only and low temperatures is in Ref. [32], which, dating back to 1985, may be the earliest quantum Monte Carlo simulation for fermions. (It is no coincidence that they chose the model with the smallest Hilbert space.)

Considering the tremendous effort that has been devoted to the Hubbard model
and the close resemblance of our model to the Hubbard model, it is surprising that
works on this spinless model have been rather sparse, though it has been commented
that the spinless model offers considerable simplifications [33]. This thesis work
is the first systematic study of the two-dimensional strongly interacting spinless
fermion model. Some of the results included here have appeared in Ref. [34].

1.7 A Note on Models

Those who are new to the field of strongly correlated electrons or magnetism might
perhaps be somewhat puzzled by the plethora of models floating around in the
literature of this field. In this brief introduction, we have already mentioned plenty
of models (Hubbard, $t - J$, Heisenberg, for example) and we will be studying one
extensively in this thesis. It is useful to organize the models in a better way, and
we offer, from experience, a crude set of rules of thumb.

When encountering a model, ask these three questions.

1. Is this a quantum model or a classical model?

2. What is the dimensionality of the model?

3. Is the kinetic or interaction term infinite-range?

For example, the Hubbard model important to high-$T_c$ is a quantum model, two-
dimensional, and neither the hopping nor interaction is infinite-range (they are
nearest-neighbor). As another example, the Ising model that Onsager solved is
a classical model, two-dimensional, and not infinite-range. As yet another example,
the Heisenberg spin chain that Bethe solved is a quantum model, one-dimensional,
and not infinite-range.
The relevance of these three questions is answered by the following. There is an important result that has to be determined on a case-by-case basis, but in general: solving a \((d + 1)\)-dimensional classical statistical mechanical model is equivalent to solving a \(d\)-dimensional quantum model (see Cardy [35] for detail). For example, the two-dimensional classical Ising model (solved by Onsager) is equivalent to a quantum Ising chain in a transverse magnetic field [35]. We can now answer the question: how difficult are these models?

1. Zero-dimensional models have just one particle and are trivial to solve. Solving a quantum spin-1/2 particle for example involves diagonalizing a \(2 \times 2\) Hamiltonian matrix.

2. One-dimensional classical models are easy to solve, because they are equivalent to zero-dimensional quantum models. For example, a classical Ising chain (solved in elementary statistical mechanics textbooks using transfer matrix) is equivalent to just one quantum spin-1/2 (see Chandler [36] for the exact map).

3. One-dimensional quantum models and two-dimensional classical models are hard but there are nontrivial exact solutions (Bethe ansatz, and Onsager’s solution for example). Also the computational technique DMRG mentioned above can solve the 1D quantum problem accurately and relatively painlessly.

4. Infinite-dimensional models often have exact solutions and often mean-field theories work well.

5. If there is infinite-range hopping or interaction, then often there are exact solutions that are mean-field like.
6. Two-dimensional quantum models (e.g., 2D Hubbard, $t - J$, and Heisenberg) and three-dimensional classical models (e.g., 3D Ising model) with short-range correlations are very difficult to solve. Few exact results are known.

In Table 1.1 we organize some of the most familiar models in a table.

1.8 Two Motivations

In this thesis, we will study in detail the spinless fermion and hardcore boson model on a square lattice with infinite nearest-neighbor repulsion. The computational tool that we will rely on is exact diagonalization. And we are able to obtain a great deal of information about the phase diagram of this model, including the dilute, near-half-filled, and intermediate limits. We are especially motivated by the following two important considerations about strongly correlated fermions in two dimensions.

1.8.1 2D Fermi Liquid?

The Fermi liquid theory is one of the most important theories in condensed matter physics. Here we will quote P. W. Anderson’s explanation from Ref. [37].

The idea is to imagine oneself starting from a completely noninteracting Fermi gas and gradually turning on the interactions between the particles. Landau’s argument is that there will be a one-to-one correspondence between states before and after this adiabatic turning-on process, and that states of similar symmetry do not cross, so that he can label the new states with the quantum numbers of the old and they will be in roughly the same order. The noninteracting gas can be described as having a distribution function $n(k)$ (assumed to be very close
Table 1.1: Models organized by dimensionality and quantum/classical nature (all with short-range correlations). \((d + 1)\)-dim classical models are often equivalent of \(d\)-dimensional quantum models. The difficult ones that are within the class of our model are bold.

<table>
<thead>
<tr>
<th>Dim</th>
<th>$\infty$</th>
<th>$\infty$ D Ising (Exact)</th>
<th>$\infty$ D Hubbard (Meanfield)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\infty$</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>3</td>
<td>3D Ising Model</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>2</td>
<td>2D Ising (Onsager)</td>
<td>2D Hubbard Model</td>
<td>2D (t - J), Heisenberg \nOur Model</td>
</tr>
<tr>
<td>1</td>
<td>Ising Chain (Easy)</td>
<td>Spin-1/2 Chain (Bethe)</td>
<td>1D Hubbard (Lieb&amp;Wu)</td>
</tr>
<tr>
<td>0</td>
<td>...</td>
<td>Spin-1/2 Particle (Easy)</td>
<td>...</td>
</tr>
<tr>
<td>Dim</td>
<td>Classical</td>
<td>Quantum</td>
<td>...</td>
</tr>
</tbody>
</table>
to the $T = 0$ Fermi distribution of the ground state), so Landau labels the new states by $n(k)$ and asks how the energy can depend functionally on $n(k)$. The fictional particles that occupy the states $k$ are called “quasiparticles.”

The idea is fascinating that states from an interacting system can be in one-to-one correspondence with a noninteracting system and an interacting system can be approximated by a system of noninteracting quasiparticles. The Landau Fermi liquid theory is not an isolated result but one in a class of important and deep results in which the independent particle approximation works very well in an interacting system. (See Feynman Lectures Vol. III [38] for interesting examples from different fields.) It has worked well for us in three dimensions (so well that we take the independent electrons in metals for granted even though the electron-electron interaction is by no means negligible). But when it was known that the high-temperature superconductors are quasi-two-dimensional electron systems, it was not clear whether the Fermi liquid idea would apply.

Exact solutions in one dimension have given rise to the Luttinger liquid state, which behaves drastically different (with, for example, spin-charge separation) from the Fermi liquid state. But what about in two dimensions? Anderson advocated shortly after the discovery of the high-Tc materials that the physics in the two-dimensional Cu-O plane of the cuprates is not a Fermi liquid. He [39] specifically claimed that a calculation by Bloom [40] for dilute fermions in two dimensions which gives Fermi liquid behavior contained errors. In the early 1990s, a number of researchers [41, 42] studied the dilute limit of the Hubbard model and concluded that the Fermi liquid picture does not break down there. Now after ten years, this question of whether the dilute limit of the two-dimensional Hubbard model is a
Fermi liquid is still not convincingly settled (see Ref. [43]).

We are interested in this important question. It is a motivation to study the dilute limit of our model, which we will do in great detail in this thesis. Starting with an exact solution of the two-particle problem, we will construct the so-called t-matrix, which contains all two-body scattering terms, and we will use it to study scattering in the dilute limit.

1.8.2 Stripes

One of the more recent results from the high-Tc labs is the observation of stripes in a class of cuprates. Stripes are modulations of charge and spin densities, and they can be static or dynamic. In 1995, Tranquada and coworkers [44] observed the coexistence of superconducting and stripe domain order for the material La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$ at around doping $x = 0.125$. The stripes are one-dimensional objects on a two-dimensional plane (see Fig. 1.11 for a schematic drawing), and they have been called “self-organized one dimensionality” [45]. Search for stripes in the Hubbard and $t - J$ models has been intense and is still going strong [46].

In the infinite nearest-neighbor repulsion model that we will study, stripes are natural objects. They are aligned holes stretching across the system, and they fluctuate and interact with one another, following the movement of the underlying particles. In this thesis we will study such stripes. Starting with one single stripe, which is essentially a one-dimensional system, we study holes added to a stripe, stripe-stripe interaction, and finally the stability of an array of stripes.
Figure 1.11: Schematic drawing of stripes in the CuO$_2$ plane at $1/8$ doping. Stripes are domain walls separating antiferromagnetically ordered regions of spins. There is a $180^\circ$ spin order change across each stripe. Filled circles indicate holes; there is one for every eight copper ions ($1/8$ doping). Adapted from Ref. [44].

1.9 Outline of the Thesis

After this long introduction, starting from the experimental results of the high-temperature superconductors, to the Hubbard model, to the different parts of Hubbard model’s phase diagram, to a note on the world of models, to numerical techniques for strongly correlated systems, to finally the introduction of our model and our motivations, we hope that the reader now has a good sense of what our model is and why we want to study it.

Because we have infinite repulsion $V = +\infty$, the only parameter in our model is particle density $n$ (filling, particle per lattice site). In Fig. 1.12 we show, in the spirit of the Hubbard model phase diagram in Fig. 1.6, the phase diagram of our model. The horizontal axis is particle density $n$ which in our model with infinite nearest-neighbor repulsion can only go up to $1/2$. The vertical axis is energy per site, and the data curves are fermion ground state energies from a range of lattices. As is in the Hubbard model case, a walk in the parameter space from the boundaries to the
interior will go from the trivial part to not trivial but exact solvable to something very hard, requiring numerical assistance.

Chapter 2, Exact Diagonalization Program

In Chapter 2, we introduce the exact diagonalization computer program, which is the main numerical software for this thesis work. Most of the issues that we discuss here are important issues in any exact diagonalization program. These include representing the lattice, building the basis set with a fix number of particles, ordering and searching the basis set, and building the Hamiltonian matrix efficiently. One of the main issues in this chapter is using symmetry to reduce the number of basis states. Here we consider translation symmetry, which can reduce the basis set by a factor of N where N is the total number of sites. We show in detail how we can build the Hamiltonian matrix efficiently using the translation-reduced (Bloch) basis states.

Another important issue in this chapter is regarding the fermion sign. Because of the anticommutation relation, as two fermions change order, a minus sign is produced. In one dimension, this is not a significant problem, because fermions cannot hop over one another. But in two dimensions, with a lot more freedom to move around on the lattice, we need to consider the fermion sign with care. And we will show in detail where the sign appears in calculations.

Finally, an important implementation issue is matrix diagonalization, the most time-consuming part of our program. A commonly used and very accurate method is the Lanczos method, which is what we use for matrix dimension larger than several thousands. We will introduce this method at the end of Chapter 2.
Figure 1.12: Schematic phase diagram of the two-dimensional spinless fermion and hardcore boson model with infinite nearest-neighbor repulsion. This is a roadmap for the thesis.
Chapter 3, The Two-Particle Problem I: Lattice Green Function

The two-particle problem plays a large role in our study of the dilute limit of our model because two-body scatterings dominate the interactions of a few particles. In general, the two-particle problems in various contexts are also some of the few problems that can be analytically solved in physics. The two-particle problem in our model follows the tradition of the Kepler problem in classical mechanics, the hydrogen atom problem in quantum mechanics, the two-magnon problem in magnetism, the two-electron problem in the Hubbard model, problems that appear in (and perhaps dominate) standard textbooks.

In this chapter, the mathematical techniques that we use to solve the two-particle problem on a lattice are centered around the lattice Green functions. Lattice Green functions are not as well known as their counterparts in the continuum (for example the Green functions in electrostatics and quantum scattering theory), but in the lattice setting they are just as powerful. Often analytical results that are difficult to obtain from the Schrodinger equation formulation emerges from the Green function formulation. We will, in this chapter, formulate the two-particle problem using lattice Green function, employ some of its recursion relations to significantly reduce the complexity of the problem, and obtain the two-boson ground state energy on a large lattice. At the end of Chapter 3, the two-particle result is used to study the problem of a few particles on a large lattice, and the ground state energy is obtained by considering two-body interactions.

Chapter 4, The Two-Particle Problem II: T-Matrix

In Chapter 4, the two-particle problem is cast into a different form, emphasizing the scatterings between the two particles. The result is the scattering matrix, the so-
called t-matrix, that is exact for the two-particle problem and contains all two-body scattering terms (these are the ladder diagrams in the field-theoretical setting).

The t-matrix is useful when the interaction is strong, so the usual perturbation theory, using the Born approximations, does not apply. It is the centerpiece in dilute-limit calculations, and because it packages interaction effects and calculates corrections to noninteracting energies, it is crucial in understanding the effect of interaction. In explaining our interest in the 2D Fermi liquid in Sec. 1.8.1, we discussed the interesting independent-particle approximation for interacting systems. The t-matrix is, simply, the key here. It is basically the effective interaction that turns a strongly-interacting system to an noninteracting one. And we will study the two-particle t-matrix in great detail in this chapter.

Chapter 5, Stripes and Holes on a Stripe

Near half-filled limit. Before we go on to use the t-matrix for more than two particles in the dilute limit, we switch gears and study the near-half-filled limit, in part because the work on the dilute limit is still on-going and because near the half-filled limit, we have another exactly solvable problem that we understand well.

In Sec. 1.7 on various models, we have mentioned that two-dimensional short-range quantum models are in general very difficult to solve, except at certain limits. Here we have a case that a two-dimensional problem is, because of the specific form of the interaction, turned into a one-dimensional problem. The specific form of the interaction in our model is the infinite nearest-neighbor repulsion, which severely restricts the motion of a particle on the lattice when there are many particles around. At exactly the half-filled limit, no particle can move. As we put holes into the system, motion is possible when the holes align, stretching across the system, forming a
stripe. The stripe of holes can then fluctuate and interact, moving up and down the system.

It turns out that with a single stripe, particles can only move in one direction, effectively reducing the 2D problem to a 1D one. We will show that this one-stripe problem maps exactly to a 1D spin-1/2 chain, which can be solved exactly using Bethe ansatz (see Sec. 1.4).

We then study the problem of one-hole-with-a-stripe. For this situation, the bosons and fermions have the same energy spectrum. We will introduce a conjecture that explains why this is so. Basically, it says that the hole can only move in a few ways, and by inspecting its motion, we see that two particles cannot exchange with each other. There are complications with periodic boundaries, and we check this conjecture numerically for a number of cases. For the one-hole-with-a-stripe problem we also study the energy dependence on the two directions of the lattice.

We then study the two-hole-with-a-stripe problem. In this case, with more freedom to move, two particles can exchange, so boson and fermion energies are not the same. We study the binding of two holes, and as in the one-hole problem, the energy dependence on the two directions of the lattice.

For both the one-hole and two-hole problems with a stripe, we use a simple double-well potential to explain the exponential decay of energy on the lattice size perpendicular to the stripe. We use this one-dimensional model to calculate stripe effective mass, thus extracting a macroscopic parameter from exact diagonalization data of a microscopic model.

Chapter 6, Stripe-Stripe Interaction and the Stripe-Array

*Intermediate-filling limit*. In Sec. 1.8.2, we mentioned that one of the motivations
for studying our model is our interest in a simple model of interacting stripes. In this chapter, we study interacting stripes, building on the work with one stripe plus holes in Chapter 5.

We have exactly diagonalized systems with two, three, and four stripes, and we observe that stripes repel and the dependence of stripe-stripe interaction energy on stripe separation is a power-law decay. This power-law can be best explained when the stripes are short, e.g., stripes of length 4 in a $4 \times 40$ system, which is more or less a one dimensional system with a number of interacting particles (short stripes). This problem can be understood using a particle-in-a-box potential which shows a $1/L^2$ dependence for ground state energy. That is what we observe from diagonalization, and we use this result to obtain stripe effective mass.

This thesis work is one of the first using exact diagonalization to investigate the properties of interacting stripes with a microscopic Hamiltonian. We discuss the stability of an array of stripes by fitting the diagonalization results in the intermediate filling limit and using a Maxwell construction. Our interest is whether at the intermediate-filling limit we have the stripe-array case or a phase-separated case with hole-rich regions and particle rich-regions. The conclusion is, interestingly, that the boson stripe-array is not stable and the fermion stripe-array is very close to the stability limit and is possibly stable.

Chapter 7, A Few Fermions: Shell Effect and T-Matrix

*Dilute limit.* In Chapter 7, we study the problem of a few fermions. First, the fermion shell effect is discussed and demonstrated from diagonalization. Because of Pauli exclusion two identical fermions cannot occupy the same state, so as we add fermions to the system, they fill up the lowest energy states. If there is degeneracy in
one-particle energy, we fill degenerate shells progressively. That is what we observed with diagonalization results, which show drastic differences for bosons and fermions.

The problem of more than two fermions can be studied using the two-particle t-matrix (constructed in Chapter 4), because with only a few particles in the system, we can ignore three or more-body interaction terms. We show the modifications to the two-fermion t-matrix that enable us to calculate energies for three, four, and five particles. Using this t-matrix, we can compute the interaction corrections to the noninteracting energy, and we can trace the change in the energy spectrum from the noninteracting one to the interacting one.

Chapter 8, The Dilute Limit: Energy Curves

Dilute limit. Finally, in Chapter 8, we discuss the energy per particle curve for dilute bosons and fermions. This problem has a 50-year history, dating back to Bogoliubov’s study of weakly interacting boson gas in 1947, Yang and coworkers’ study of hard-sphere fermions and bosons in the 1950s, and Galitskii and Beliaev’s diagrammatic calculations in 1958. (See Introduction in Chapter 8 for references.) We have studied the two-dimensional results derived by Schick for bosons and Bloom for fermions by fitting the data from diagonalization for a number of lattices. Schick’s result for dilute bosons is checked nicely, and work is in progress for the fermion problem. We explain that for spinless fermions in our model we will need the p-wave scattering term, which is not included in Bloom’s calculation.

Chapter 9, Conclusion and Outlook

The thesis is concluded and a parting outlook is made.

Fig. 1.13 shows the relationships between the thesis chapters and appendices.
Figure 1.13: The relationships between the thesis chapters and appendices. (1)-(9) are chapter numbers, and (A)-(F) are appendix numbers.
Bibliography


Chapter 2

Exact Diagonalization Program

Exact diagonalization is an important computational tool to study properties of quantum systems. It is most natural when there is a discrete number of basis states. The simplest example is the diagonalization of a two-by-two Hamiltonian matrix in the problem of a single spin one-half particle in a magnetic field, a problem that most of us encounter in our first quantum mechanics course. Here the Hilbert space is two-dimensional, and the basis states are simply the spin up state and the spin down state. For more complicated physical systems, the Hilbert space of basis states is larger and more complicated. Exact diagonalization methods have been used extensively to study interacting quantum spin systems, for example, quantum spins on a chain or a plane with nearest-neighbor Heisenberg interactions, and interacting boson and fermion models, for example, the Hubbard model. The method can also be used for problems with apparently continuous degrees of freedom, with the introduction of a large box and the associated boundary conditions for example. The inherent limitation of this method is that the size of the Hilbert space and therefore the size of the Hamiltonian matrix to be diagonalized often grows exponentially with the size of the system, for example, the addition of spins or particles, so we are
limited by the capabilities of our computers. Still, exact diagonalization is a valuable
tool. For one-dimensional quantum problems there are good analytical methods
(e.g., Bethe ansatz) and numerical methods (e.g., the density matrix renormalization
group) (see Chapter 1), but for two or higher dimensional quantum problems, such as
our problem on the square lattice, where no exact solutions are known and the Monte
Carlo methods are plagued by the negative sign problem, exact diagonalization is a
good and reliable method to get a basic understanding of complex physical systems.

There are good introductory articles on the exact diagonalization method [1, 2].
Our program is especially close to the method described by Leung and Oppenheimer
[1]. However, both of these articles are working with a one-dimensional model, and
in two dimensions a number of new problems appear and are not covered in these
articles. Here we will describe in detail our exact diagonalization program for our
two-dimensional strongly interacting model. We will try to pay special attention to
the complications of the two-dimensional world, and will try to give implementation
details for a newcomer to replicate the program.

This chapter is divided into the following sections. First we introduce the repre-
sentation of the two-dimensional square lattice with periodic boundary conditions.
The boundary conditions can create a rectangular system or a skewed one, and we
will cover both cases. An important requirement for the two-dimensional fermion
problem is that we choose an order for the lattice sites to keep track of the sign
changes as fermions move on the lattice (this point will be explained in detail).
Second, we establish the basis set. We will use position space representation and
will first not use translation symmetry. We will show how the Hamiltonian matrix
can be computed one column at a time. Next, we employ translation symmetry and
this is computationally the most difficult part of our program. We will give some
detailed examples to make the calculation more explicit. A number of bookkeeping
details have to be kept as these new basis states are stored and used to compute the
Hamiltonian matrix. After this, we introduced the Lanczos algorithm, an important
numerical method to compute eigenvalues of a matrix without storing the full matrix
in memory. It uses matrix-vector multiplication only and is crucial in our push to
larger and larger systems. Overall, in this chapter we will address issues from both
mathematics (e.g., basis states construction using symmetry) and implementation
(e.g., storage and efficient search methods).

2.1 Model

Our objective is very clear. We have a square lattice with periodic boundary con-
ditions. On the lattice we have a number of particles, spinless fermions or hardcore
bosons, that interact. The Hamiltonian of this problem (as introduced in Sec. 1.6,
Eq. 1.7) is,

$$H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) + V \sum_{\langle ij \rangle} \hat{n}_i \hat{n}_j.$$  \hspace{1cm} (2.1)

Here $c_i^\dagger$ creates a particle at site $i$ and $c_j$ annihilates a particle at site $j$. The
commutation relation for spinless fermions is $\{c_i, c_j^\dagger\} = \delta_{ij}$ and hardcore bosons
$[c_i, c_j^\dagger] = \delta_{ij}$. $\hat{n}_i = c_i^\dagger c_i$ is the number operator. In this Hamiltonian only the ratio of
$V/t$ matters. In our study we take $t = 1$ and $V = +\infty$, i.e., the particles experience
infinite nearest-neighbor repulsion (as introduced in Sec. 1.6). For bosons we also
have an additional hardcore condition, $(c_i^\dagger)^2 |0\rangle = 0$ (which is of course satisfied by
fermions due to the Pauli exclusion principle). The preceding is all that we have
from mathematical definitions. Our problem is of course to study the properties of
this model, especially the ground state eigenenergy and eigenvector. In the following
we will put this problem on the computer and use exact diagonalization to solve it.

2.2 Lattice

Our underlying lattice is a square lattice, and we take the lattice constant to be unity. The periodic boundary conditions are specified by two lattice vectors $\mathbf{R}_1$ and $\mathbf{R}_2$, such that for any lattice vector $\mathbf{r}$ we have $\mathbf{r} + n_1 \mathbf{R}_1 + n_2 \mathbf{R}_2 \equiv \mathbf{r}$, where $n_1$ and $n_2$ are two integers. In Fig. 2.1, we show two systems. The first one has $\mathbf{R}_1 = (4, 0)$ and $\mathbf{R}_2 = (0, 5)$ so the number of lattice sites is $N = 20$. The second one has $\mathbf{R}_1 = (4, 1)$ and $\mathbf{R}_2 = (1, 5)$ so $N = |\mathbf{R}_1 \times \mathbf{R}_2| = 19$. From this example we see immediately the advantage of having skewed boundary conditions: we can have reasonably shaped systems with number of sites (here 19) not possible for an usual rectangular system.\footnote{When we say a rectangular system, we mean a square lattice with rectangular boundaries. In this thesis, our underlying lattice is always square, with rectangular or skewed boundaries.} As exact diagonalization is limited by the size of the system, it helps to have many different systems.

The computer representation of the lattice is straightforward. We have a list of sites labeled by site positions. The order of this list is our choice and it is convenient to choose an order that reflects in some sense the neighboring properties of the lattice (so that when we construct the Hamiltonian matrix, more entries will be close to diagonal, as we will see later). The convention we use is starting the zeroth site from the lower left corner and move progressive upward and rightward following the square lattice structure until we encounter boundaries of the lattice defined by the periodic boundary condition vectors $\mathbf{R}_1$ and $\mathbf{R}_2$. Fig. 2.1 should make this order clear.\footnote{So that for the $(4, 1) \times (1, 5)$ lattice our list of sites goes as $(0, 0)(1, 1)(1, 2)(1, 3)(1, 4)(2, 1)\ldots$} For the rectangular lattice, the chosen order is convenient in the sense that
Figure 2.1: Square lattices with periodic boundary conditions: \((4, 0) \times (0, 5)\) on the left and \((4, 1) \times (1, 5)\) on the right. Site numbers are shown, following the numbering convention, upward and rightward.

the conversion between the site number on the list and the coordinates is easy: for the \(n\)th site on the list \((0 \leq n < N)\) and for a \(L_x \times L_y\) lattice, the coordinates are \((x, y) = (n/L_y, n\%L_y)\), where \(/\) gives the quotient and \(\%\) the remainder, and conversely, given \((x, y)\) the site number on the list is \(n = xL_y + y\). These simple relations are used over and over again in later parts of the program where lattice translations are performed.

We here note that specifying an order for lattice sites is not just a computer implementation issue. It will be explained in Sec. 2.3 that for a fermionic system in more than one dimension, the order of sites is important in keeping track of the sign change as the fermions move around on the lattice. It will be seen that because a particular state is created by a number of creation operators in linear order, as the fermions move on the lattice the order of operators can change and minus signs are introduced. Therefore we must have a linear order of sites with which to keep track of the sign. In a one-dimensional world we have less of a sign
problem because fermions cannot hop over each other and the only sign change is introduced by fermions moving out of one side of the lattice and re-emerging from the opposite side, if there is periodic boundary condition, on the other hand, in our two-dimensional problem moving in the interior of the lattice can create sign changes.

Finally, in our lattice representation, during program initiation, we also store a list of four nearest neighbors for each lattice sites in the order of right, left, up, and down. For example, for the \((4,1) \times (1,5)\) lattice in Fig. 2.1, the \(n = 1\) site \((1,1)\) has a nearest-neighbor list of \((5,10,2,4)\) which gives conveniently the information that the right nearest-neighbor is the \(n = 5\) site on the list and so on. For our square lattice with periodic boundary conditions this neighbor information can be computed easily. We store it because it will be used extensively when we compute the Hamiltonian matrix using the nearest neighbor hopping term of the Hamiltonian. Also if we are given the nearest-neighbor list we can use our program for an arbitrarily connected lattice (not just square lattice but also triangular lattice for example\(^3\)). This list is the key ingredient of the lattice structure because our Hamiltonian in Eq. 2.1 involves nearest-neighbor terms only.

### 2.3 Basis States

The very first and obvious observation about our Hamiltonian (2.1) is that it conserves particle number\(^4\) which means that a state with \(M\) particles will always have

---

\(^3\)This capability of the program has not been utilized in this thesis. It may well be the basis for a future project, as work has been done for the boson version of our model on the triangular lattice [3].

\(^4\)The number of creation operators equals the number of annihilation operators in each term of the Hamiltonian.
zero matrix element with a state that does not have exactly $M$ particles, and we can therefore just limit our calculation to states with a definite number $M$ of particles. A convenient choice of basis states is the position space representation. In Fig. 2.2 we show a state with $M = 3$ particles that is represented by the three site numbers of the locations of the three particles, i.e., $[2, 6, 8] = c_2^\dagger c_6^\dagger c_8^\dagger |0\rangle$. Note that in this state, the four nearest-neighbor sites for each occupied site are unoccupied, in compliance with the infinite nearest-neighbor repulsion $V = +\infty$ restriction of our Hamiltonian. If a state has two n.n. sites both occupied, the Hamiltonian operator acting on it will give infinity. The energy is not finite, and we exclude these states from our basis set. Note that in the position space representation, the spinless fermions and hardcore bosons have the same basis states, which is convenient, as we can use the same basis set for both problems.

\[
\begin{array}{cccc}
4 & 9 & 14 & 19 \\
3 & 8 & 13 & 18 \\
2 & 7 & 12 & 17 \\
1 & 6 & 11 & 16 \\
0 & 5 & 10 & 15 \\
\end{array}
\]

Figure 2.2: A particular basis state for the $4 \times 5$ lattice, with three particles ($M = 3$). Using the lattice site numbering convention, we represent this state by the $M$ occupied sites, $[2, 6, 8] = c_2^\dagger c_6^\dagger c_8^\dagger |0\rangle$.

Before we go on to tell the construction of the basis state list, we should mention that we can also use the momentum space representation of basis states, i.e.,

\[ [6, 2, 8] = c_6^\dagger c_2^\dagger c_8^\dagger |0\rangle, \]

which is the same state with a possible minus sign for fermions.

\[ ^5 \text{A different order of the site numbers represents a different order of the creation operators, e.g.,} \]

\[ [6, 2, 8] = c_6^\dagger c_2^\dagger c_8^\dagger |0\rangle, \]
$|p_1, p_2, ..., p_M\rangle$. In fact, for the few-particle problem that we will calculate in later chapters, basis states in momentum space has more clear physical meaning in scattering calculations. The difficulty here is that in our problem infinite nearest-neighbor repulsion requirement is straightforward to implement in the position space representation, but not straightforward in the momentum space. Also in momentum space more than two bosons (even though they are hardcore) can occupy the same momentum state, so the basis states are not the same for fermions and bosons.\footnote{For only two particles, as we will see later, this is not a big problem, but for a many-particle system, the possibility of a boson condensate significantly changes the physics.} In our computer program we will use position representation.

To enumerate all basis states with $M$ particles and infinite n.n. repulsion, we use recursion. Starting from the first site on the lattice site list, either put it in our state (i.e., let a particle occupy it) and then exclude its neighbors, or skip it and put the next site on the list into our state. When the state reaches $M$ particles, it is added to the basis set list. And the process terminates when we get to the end of the site list. For $4 \times 5$ lattice with $M = 3$ we have 540 states. Some of them are listed in Table 2.1. The state [2,6,8] in Fig. 2.2 is number 182. The index numbers for the basis states are important in building the Hamiltonian matrix.

We add that to construct this basis set list, all we need is the list of nearest-neighbors to exclude the four n.n. sites for an occupied site. This procedure can be applied to a general lattice without modification. Also, discerning readers may raise the point that in this list of 540 states many are related by translation symmetry, for example the state [1,3,7] is [0,2,6] translated by vector (0,1). For our translation invariant Hamiltonian (2.1) using the 540 basis states is much more work than needed. Later we will employ translation symmetry. Here we discuss the general
case for a general lattice and for a Hamiltonian without translation symmetry (e.g., with disorder).

Table 2.1: Some position basis states for $4 \times 5$ lattice with three particles. The total number of states is 540. Note that this list of states follows the dictionary order of the particles. This is because when we construct the list we go down the list of lattice sites in increasing order. The 182nd state $[2,6,8]$ was shown in Fig. 2.2.

<table>
<thead>
<tr>
<th>index</th>
<th>state</th>
<th>index</th>
<th>state</th>
<th>index</th>
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<th>state</th>
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</thead>
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<td>8</td>
<td>[0,2,16]</td>
<td>178</td>
<td>[2,5,15]</td>
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<td>179</td>
<td>[2,5,16]</td>
<td>192</td>
<td>[2,8,10]</td>
</tr>
<tr>
<td>2</td>
<td>[0,2,9]</td>
<td>10</td>
<td>[0,2,19]</td>
<td>180</td>
<td>[2,5,18]</td>
<td>193</td>
<td>[2,8,11]</td>
</tr>
<tr>
<td>3</td>
<td>[0,2,10]</td>
<td>11</td>
<td>[0,3,6]</td>
<td>181</td>
<td>[2,5,19]</td>
<td>194</td>
<td>[2,8,12]</td>
</tr>
<tr>
<td>4</td>
<td>[0,2,11]</td>
<td>12</td>
<td>[0,3,7]</td>
<td>182</td>
<td>[2,6,8]</td>
<td>195</td>
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<td>13</td>
<td>[0,3,9]</td>
<td>183</td>
<td>[2,6,9]</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>6</td>
<td>[0,2,13]</td>
<td>14</td>
<td>[0,3,10]</td>
<td>184</td>
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</tr>
<tr>
<td>7</td>
<td>[0,2,14]</td>
<td>15</td>
<td>[0,3,11]</td>
<td>...</td>
<td>...</td>
<td>539</td>
<td>[14,16,18]</td>
</tr>
</tbody>
</table>

2.4 Hamiltonian Matrix

2.4.1 Rule for Computing Matrix Entries

Given the basis set obtained in the preceding section, the rules for computing Hamiltonian matrix elements are straightforward. With infinite-$V$, the only term in the Hamiltonian that we need to consider is the n.n. hopping term. Because it is summed over all n.n. pairs, if we have a state $|n\rangle$, and we applied the Hamiltonian operator to it, $H|n\rangle$, what we get is a linear combination of states each with one
particle of $|n\rangle$ hopped to a n.n. site (if it is allowed). This contributes to the following rule for calculating matrix elements. Take states $|m\rangle$ and $|n\rangle$, and superimpose them. The matrix element $\langle m|H|n\rangle$ is nonzero if and only if the superimposed state has one n.n. pair which comes from one hop. In Fig. 2.3, we have $|m\rangle = [2, 6, 8]$ and $|n\rangle = [2, 8, 11]$, and superimposed state $[2, 6, 8, 11]$ differs from each by one single n.n. hop, such that 11 in $|n\rangle$ goes to 6 in $|m\rangle$. The hop is highlighted in the superimposed state.

\[
\begin{array}{ccc}
4 & 9 & 14 & 19 \\
3 & 8 & 13 & 18 \\
2 & 7 & 12 & 17 \\
1 & 6 & 11 & 16 \\
0 & 5 & 10 & 15 \\
\end{array}
\quad
\begin{array}{ccc}
4 & 9 & 14 & 19 \\
3 & 8 & 13 & 18 \\
2 & 7 & 12 & 17 \\
1 & 6 & 11 & 16 \\
0 & 5 & 10 & 15 \\
\end{array}
\quad
\begin{array}{ccc}
4 & 9 & 14 & 19 \\
3 & 8 & 13 & 18 \\
2 & 7 & 12 & 17 \\
1 & 6 & 11 & 16 \\
0 & 5 & 10 & 15 \\
\end{array}
\]

Figure 2.3: The rule for computing Hamiltonian matrix elements. The state $|m\rangle = [2, 6, 8]$ is shown on the left, $|n\rangle = [2, 8, 11]$ in the middle, and the superimposed state $[2, 6, 8, 11]$ on the right. The rule is that the matrix element $\langle m|H|n\rangle$ is nonzero if and only if one and exactly one particle hopped from state $|n\rangle$ to $|m\rangle$, as indicated by the box in the right figure.

We now calculate the exact matrix element for these two sample states with attention to signs. First for the fermion case, we have,

\[
\langle m|H|n\rangle = \langle 0|c_s c_6 c_2| - \sum_{i<j} (c_i^\dagger c_j + c_j^\dagger c_i) |c_2^\dagger c_s^\dagger c_{11}^\dagger |0\rangle = -\langle 0|c_s c_6 c_2 |c_6^\dagger c_{11}^\dagger c_s^\dagger c_{11}^\dagger |0\rangle = -\langle 0|c_s c_6 c_2 |c_11|c_{11}^\dagger c_s^\dagger c_{11}^\dagger |0\rangle (-1)^2 = -\langle 0|c_{11} c_s c_6 c_2 |c_2^\dagger c_6^\dagger c_s^\dagger c_{11}^\dagger |0\rangle (-1)^2(-1)^3 = -(-1)^{2+3}. \quad (2.2)
\]

This simple calculation illustrates the fact that one and only one term in the Hamiltonian can contribute, and for fermions, the signs (from the anticommutation rela-
tion) have to be kept track of as we change the order of the creation and annihilation operators. They can be determined by comparing the two original states with the superimposed state. In our example in Eq. 2.2, it takes two operator order changes to place \( c_6^\dagger \) into \([2, 8, 11]\) and three changes to move \( c_{11} \) into \([2, 6, 8]\) so both become \([2, 6, 8, 11]\). Therefore the matrix element is \(-(-1)^{243}\). On the other hand, for bosons, switching the order of creation and annihilation operators does not introduce minus signs (because of the commutation relation), so if the matrix element is not zero, it must be \(-1\) always (it comes from the \(-t\) coefficient in the Hamiltonian (2.1) and we have taken \( t = 1\).

The preceding calculation says that the Hamiltonian matrix element between state \([2, 6, 8]\) and \([2, 8, 11]\) is \(1\) for the fermion case and \(-1\) for the boson case. Using the basis set list in Table 2.1, we see that the matrix element \(H_{182, 193} = 1\) for fermion and \(-1\) for boson. We can thus fill the \(540 \times 540\) matrix. Fig.2.4 shows the calculated Hamiltonian matrix, where the entries are \(1\) or \(-1\) for fermions and all \(-1\) for bosons. Out of the 291600 entries, only 3880, about one percent of the full matrix, are nonzero. This is indeed a sparse matrix.

2.4.2 Calculate Nonzero Entries Only

Given the sparse nature of the matrix, that for this example only one percent of the entries are nonzero, it is unwise to compute all the matrix elements. We now introduce the improvement that lets us compute only the nonzero entries. And we can fill the matrix one column at a time. Take our old state \(|n\rangle = [2, 6, 8]\), and when we apply the Hamiltonian operator to it, we get only a few states from nearest-neighbor hopping (see Fig. 2.2). Here we write for the fermion case.

\[
H[2, 6, 8] = -([6, 8, 17] - [2, 8, 11] + [2, 5, 8] + [2, 6, 13] + [2, 6, 9]),
\] (2.3)
Figure 2.4: The nonzero matrix elements of the Hamiltonian matrix (real symmetric) calculated using the basis set in Table 2.1, for a $4 \times 5$ lattice, with three particles. The entries are 1 or $-1$ for the fermion case and all $-1$ for the boson case (see Eq. 2.5). The matrix is $540 \times 540$ and the total number of nonzero elements is 3880, which is about 1 percent of the whole matrix.
where the first minus sign is the $-t$ factor in the Hamiltonian. The minus sign in front of $[2,8,11]$ comes from fermion operator exchange brought about by hopping: $[2,6,8] \rightarrow [2,11,8] = -[2,8,11]$. We need to sort the site order after hopping because in our basis set, the site numbers in each state have increasing order (see Table 2.1).

From Eq. 2.3, we see immediately that out of the 540 matrix elements corresponding to the state $[2,6,8]$, only five are nonzero, and we know the values right away. The state $[2,6,8]$ is number 182 on the basis set list, $[6,8,17]$ is 395, $[2,8,11]$ is 193, $[2,5,8]$ is 173, $[2,6,13]$ is 186, $[2,6,9]$ is 183. So $H_{595,182} = -1$, $H_{193,182} = 1$, $H_{173,182} = -1$, and so on. For the boson case, these five are still the only nonzero entries in this column, and the entries are all $-1$.

In general we have the following procedure. Take state $|n\rangle$, and for each of the $M$ particles in this state, hop it to nearest neighbor sites if it is not excluded by other particles, and this gives the set of states having nonzero matrix elements with $|n\rangle$. We can write this fact as

$$H|n\rangle = -\sum_{m \in \mathcal{M}} s_m |m\rangle,$$

(2.4)

where $\mathcal{M}$ is the set obtained by n.n. hopping and $s_m = \pm 1$ is the fermionic sign introduced, with $s_m = 1$ always for bosons.\footnote{$s_m$ is in fact a function of $m$ and $n$, but in our discussion in this chapter, we always consider a fixed column $n$, so we omitted the $n$ dependence in the notation $s_m$.} Then the matrix elements are

$$\langle m| H|n\rangle = \begin{cases} -s_m, & m \in \mathcal{M} \\ 0, & \text{otherwise} \end{cases}.$$

(2.5)

When computing the matrix, for the column corresponding to $|n\rangle$ we then only need to consider the set $\mathcal{M}$. Here we should mention that with this new procedure, we now need to search for a state in the basis set list. For example, in the example just
discussed, we must know the index number of the state \([6, 8, 17]\) is 395 to filled the entry at \((395, 182)\). In a later section, Sec. 2.6.4, we will discuss the implementation of a hash table to facilitate searching.

### 2.4.3 Diagonalization Methods

To diagonalize a matrix, there are basically two kinds of methods. One requires storing the entire matrix in memory and all eigenvalues can be obtained. For this we use a widely used linear algebra package, LAPACK [4]. Another method, the Lanczos method, does not require storing the full matrix and can therefore be used for much larger matrices. We will discuss this method in Sec. 2.7.

### 2.4.4 Summary

We summarize our diagonalization program described up to this point. This is for a general lattice and a general Hamiltonian.

1. given \(R_1\) and \(R_2\), represent the lattice:
   
   (a) form lattice site list
   
   (b) form nearest neighbor list

2. given \(M\), the number of particles, construct position space basis set

3. compute Hamiltonian matrix one column at a time:
   
   (a) take a particular state \(|n\rangle\) (say \(q\)-th on basis set list), apply the Hamiltonian operator to it (i.e., hop each particle to allowed n.n. sites) \(H|n\rangle = -\sum_{m \in M} s_m |m\rangle\)
   
   (b) for \(m \in M\) search the basis set list for the index of \(|m\rangle\) (say \(p\)-th)
(c) fill matrix element \( H_{p,q} = -s_m \)

4. diagonalize the matrix

2.5 Translation Symmetry

Now we come to the most complicated part of our diagonalization program: using lattice translation symmetry to block diagonalize the Hamiltonian matrix. Up to this point, the implementation is fairly straightforward, but with symmetry, a number of complications arise in constructing the basis set, storing basis set information, and calculating matrix elements.

2.5.1 Symmetry in Quantum Physics

First let us briefly consider the use of symmetry in quantum mechanics in general. If the Hamiltonian is invariant under certain symmetry operations, how can we simplify the problem? Let us consider the simplest example: a two-state system with reflection symmetry such that reflection takes state \(|1\rangle\) to \(|2\rangle\). We know that instead of using the basis states \(|1\rangle\) and \(|2\rangle\) to form the \(2 \times 2\) Hamiltonian matrix, if the Hamiltonian is invariant under reflection, we can use a new set of states, \((|1\rangle + |2\rangle)/\sqrt{2}\) (the symmetric state) and \((|1\rangle - |2\rangle)/\sqrt{2}\) (antisymmetric). The matrix is then block diagonalized, with two independent \(1 \times 1\) matrices.

For a more complicated symmetry, we use group theory to construct the new basis states. Here we explain very briefly the reflection symmetry case. The reflection group has two elements: identity (do nothing) and reflection. This group has two so-called irreducible representations, both one-dimensional. One is the trivial representation, with 1 and 1 representing the two group elements, and the other
is 1 and −1. The coefficients of the new basis states come from these irreducible representations, with normalization factors, here $\sqrt{2}$. For more complicated groups a mathematical procedure exists for constructing irreducible representations (and thus the new basis set with which the Hamiltonian matrix is block diagonal). An introductory reference with many examples is Harter’s book [5]. Short notes are provided in Ref. [6, 7] for the symmetry considerations needed to exact diagonalize the two-dimensional Hubbard model.

### 2.5.2 Translation Symmetry Basis States

For our problem we have lattice translation symmetry for all lattices, and reflection and rotation symmetries for some lattices. Constructing basis states simultaneously for non-commuting symmetries, e.g., translation and rotation, is mathematically involved (see [7]). In our program, we only implement translation symmetry, in part because it works for all lattices, with rectangular as well as skewed boundary conditions. The new basis states we will use is [1],

$$ |n\mathbf{k}\rangle = \frac{1}{N_{n\mathbf{k}}} \sum_{i=0}^{N-1} e^{-i\mathbf{k} \cdot \mathbf{R}_i} |T_i|n\rangle. $$ (2.6)

In this expression $\mathbf{k}$ is a reciprocal lattice vector (one of $N$, where $N$ is the number of sites), $\mathbf{R}_i$ is a lattice vector (one of $N$). The order of $\{\mathbf{R}_i\}$ in the sum should not matter as long as we use a consistent one; we have used the same order as the lattice sites (see Fig. 2.1). $T_i$ is a short hand notation for translation by $\mathbf{R}_i$. For a state with $M$ particles, $|n\rangle = |r_1, r_2, ..., r_M\rangle$, we have $T_i|n\rangle = |r_1 + \mathbf{R}_i, r_2 + \mathbf{R}_i, ..., r_M + \mathbf{R}_i\rangle$. $N_{n\mathbf{k}}$ is a normalization factor.

To connect with the general symmetry statement discussed in Sec. 2.5.1, the translation group has one-dimensional irreducible representations which are simply
complex numbers, $e^{-i k \cdot R_i}$ for the element $T_i$, and these numbers are used as coefficients in the new basis states just as 1, 1 and 1,−1 are used for the reflection case. Our basis states (2.6) are obviously related to the Bloch states in solid state physics, and we will call these states (2.6) Bloch states.

How exactly does this set of basis states simplify our problem? First if $|n\rangle$ and $|n'\rangle$ are connected by some translation, say $T_j|n'\rangle = \sigma_j|n\rangle$, where $\sigma$ is the fermion sign, we show that the translation basis states $|nk\rangle$ and $|n'k\rangle$ are multiples of each other.

$$|nk\rangle = \frac{1}{N_{nk}} \sum_{l=0}^{N-1} e^{-i k \cdot R_i} T_i|n\rangle = \frac{1}{N_{nk}} \sum_{l=0}^{N-1} e^{-i k \cdot R_i} T_i \sigma_j T_j|n'\rangle$$

$$= \sigma_j e^{i k \cdot R_j} \frac{1}{N_{nk}} \sum_{l=0}^{N-1} e^{-i k (R_i + R_j)} T_{i+l}|n'\rangle = \sigma_j e^{i k \cdot R_j} |n'k\rangle,$$  

(2.7)

where we have used the fact that $N_{nk} = N_{nk}$. What this calculation implies is that if we have two states connected by translation symmetry, the corresponding Bloch states cannot be both used in computation (because they are the same state except a phase factor). This says that we need to take our basis states constructed in earlier sections (see Table 2.1) and group them into classes connected by translation symmetry. Each class will contribute a Bloch state (for a particular wave vector $k$) which is used to build the Hamiltonian matrix. Group theory says that two states with different $k$ have zero matrix element. That means that the Bloch states (2.6) block diagonalize the Hamiltonian matrix, i.e., if the original matrix is $N_s \times N_s$, then with the Bloch states, we have $N$ matrices and each is $N_s/N \times N_s/N$. Because matrix diagonalization is a matrix dimension cube operation. This will significantly reduce computation time, not mentioning storage space. Furthermore, as will be

\footnote{In some cases, $|nk\rangle$ is zero, so the matrix can be smaller than $N_s/N$. In practice, it is easier to leave these zero states in the basis set as the resulting zero eigenvalues do not make a difference in our study.}
explained in later sections, in many cases we know by symmetry which $k$ vectors to study, thus further reducing computational needs.

### 2.5.3 Representative States

As mentioned above, the original basis states are divided by translation into classes, and any two states in the same class give the same Bloch state with an overall phase factor. What we need to do is to choose a representative from each class, and use this state consistently to build Bloch states. For a state $|n\rangle$ we denote its representative $|\bar{n}\rangle$. For each translation class, it does not matter mathematically which state we choose as the representative. Computationally, we choose the state $[\bar{i}_1, \bar{i}_2, \ldots, \bar{i}_M]$ with the lowest dictionary order, i.e., the lowest $\bar{i}_1$, if a tie, lowest $\bar{i}_2$, etc. In Table 2.2, our old state $[2, 6, 8]$ is translated with the 20 lattice vectors of the $4 \times 5$ lattice. The representative state for this class is $[0, 2, 16]$.

### 2.5.4 Implementation

In this section we discuss some implementation issues related to the Bloch state basis set. To construct the basis set, we use the same recursion calculation used to construct the old basis set (see Sec. 2.3). The difference is that we only keep the representative states. How do we know if a state is a representative? First, to be a representative, because of the dictionary order we use to define representatives, the first particle must be at the first site (with site number zero) (because otherwise we can translate the state to obtain lower order). Then, as we build the basis set, we translate each state to test if it is the representative. If yes, we keep it, if no, we discard it.

It turns out that after running optimization programs with the compiler, basis
Table 2.2: The state $[2,6,8]$ translated with the 20 lattice vectors $(R_x, R_y)$ on a $4 \times 5$ lattice. The representative of this translation class is $[0,2,16]$ which has the lowest dictionary order.

<table>
<thead>
<tr>
<th>index</th>
<th>$R_x$</th>
<th>$R_y$</th>
<th>new state</th>
<th>sign</th>
<th>index</th>
<th>$R_x$</th>
<th>$R_y$</th>
<th>new state</th>
<th>sign</th>
</tr>
</thead>
<tbody>
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<td>0</td>
<td>0</td>
<td>[2,6,8]</td>
<td>1</td>
<td>10</td>
<td>2</td>
<td>0</td>
<td>[12,16,18]</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>1</td>
<td>[3,7,9]</td>
<td>1</td>
<td>11</td>
<td>2</td>
<td>1</td>
<td>[13,17,19]</td>
<td>1</td>
</tr>
<tr>
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<td>0</td>
<td>2</td>
<td>[4,5,8]</td>
<td>-1</td>
<td>12</td>
<td>2</td>
<td>2</td>
<td>[14,15,18]</td>
<td>-1</td>
</tr>
<tr>
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<td>3</td>
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<td>3</td>
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<td>-1</td>
</tr>
<tr>
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<td>4</td>
<td>[1,5,7]</td>
<td>1</td>
<td>14</td>
<td>2</td>
<td>4</td>
<td>[11,15,17]</td>
<td>1</td>
</tr>
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</tr>
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<td>1</td>
<td>[8,12,14]</td>
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<td>16</td>
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<td>1</td>
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</tr>
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<td>-1</td>
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<td>2</td>
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<td>-1</td>
</tr>
<tr>
<td>8</td>
<td>1</td>
<td>3</td>
<td>[5,11,14]</td>
<td>-1</td>
<td>18</td>
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<td>3</td>
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<td>-1</td>
</tr>
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<td>9</td>
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<td>4</td>
<td>[6,10,12]</td>
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<td>19</td>
<td>3</td>
<td>4</td>
<td>[0,2,16]</td>
<td>1</td>
</tr>
</tbody>
</table>

State translation is one of the most often called subroutines of the program. Because subroutine calls are time-consuming, it pays to have the most efficient translation subroutine. For rectangular-shaped lattices this can be done efficiently. Given a particular site number $i$, to translate it by vector $(R_x, R_y)$, we first obtain the coordinates $(x = i/L_y, y = i\%L_y)$, where $/$ is quotient operator and $\%$ remainder, then add the vector to it to get $(x_1 = x + R_x, y_1 = y + R_y)$. The addition may move the site out of the lattice, we convert it back by $(x_2 = x_1\%L_x, y_2 = y_1\%L_y)$, and finally we get the translated index $i' = x_2L_y + y_2$. This procedure is used for each particle in the basis state, so $[i_1, ..., i_M]$ goes to $[i'_1, ..., i'_M]$. The resulting state might not be in the dictionary order. We reorder it and obtain a fermion sign, $\sigma_i$ corresponding to translation $T_i$ (by $\mathbf{R}_i$). $N$ such signs are stored for each basis state
because they are used repeatedly in matrix element computation.

At this point, as we carry out the translations, it is convenient to compute and store the normalization factors $N_{nk}$ in Eq. 2.6 (because again these are used repeatedly in calculating matrix elements). We have $N$ terms in the sum of Eq. 2.6, but $T_i|n\rangle$ are not necessarily all different. Generally speaking, for states with some symmetry, the number of different terms in the sum is less than $N$. An extreme case is the half-filled case depicted in Fig. 2.5 on a $4 \times 4$ lattice. Out of the 16 translations in the sum in (2.6), there are only two different states. This shows that the computation of the normalization factor $N_{nk}$ is not simply adding the modulus square of the exponential coefficients. It involves identifying identical states after translation and adding the coefficients before computing the modulus.

![Figure 2.5: A half-filled state on a $4 \times 4$ lattice. This highly symmetric state shows some complication for calculating new basis states using translation symmetry. The normalization factor $N_{nk}$ in Eq. 2.6 has to be calculated with care, by combining identical states after translations.](image)

In summary, to build the Bloch basis set, we first build recursively states with first particle at site zero. For each of these states we translate it by the $N$ lattice vectors. If the state has the lowest order, it is the representative of a translation class, and we keep it in our basis set. Otherwise we do nothing and continue to the next state. As we carry out the $N$ translations, we compute fermionic signs
and normalization factor for all k vectors needed. So in the end, we have a list of representative states |\tilde{\eta}\rangle, for each state we have N fermionic signs \sigma_i and a number of normalization factors N_{nk} (depending on the number of k vectors wanted). For our old problem of 4 \times 5 lattice with M = 3, now our Bloch basis set of translation representatives has only 27 states, instead of 540 (see Table 2.3).

Table 2.3: Bloch basis set for 4 \times 5 lattice with M = 3. These are representatives of the translation classes. Dictionary order is used and the first particle must be at site zero.

<table>
<thead>
<tr>
<th>index</th>
<th>state</th>
<th>index</th>
<th>state</th>
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<td>[0,7,10]</td>
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<td>[0,2,19]</td>
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<tr>
<td>2</td>
<td>[0,2,9]</td>
<td>11</td>
<td>[0,6,10]</td>
<td>20</td>
<td>[0,7,14]</td>
</tr>
<tr>
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<td>[0,2,10]</td>
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<td>[0,6,12]</td>
<td>21</td>
<td>[0,7,16]</td>
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<tr>
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<td>[0,2,11]</td>
<td>13</td>
<td>[0,6,13]</td>
<td>22</td>
<td>[0,7,17]</td>
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<tr>
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<td>[0,2,13]</td>
<td>15</td>
<td>[0,6,16]</td>
<td>24</td>
<td>[0,8,12]</td>
</tr>
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<td>[0,2,14]</td>
<td>16</td>
<td>[0,6,17]</td>
<td>25</td>
<td>[0,8,16]</td>
</tr>
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<td>[0,2,16]</td>
<td>17</td>
<td>[0,6,18]</td>
<td>26</td>
<td>[0,9,13]</td>
</tr>
</tbody>
</table>

2.6 Hamiltonian Matrix with Translation

With the Bloch states (2.6) matrix element computation is more involved. A straightforward formula is

\begin{equation}
\langle \tilde{\eta}k|H|\tilde{\eta}k\rangle = \frac{1}{N_{nk}} \sum_{p=0}^{N-1} \sum_{l=0}^{N-1} e^{i\mathbf{k} \cdot (\mathbf{R}_p - \mathbf{R}_l)} \langle T_p \tilde{\eta}|H|T_l \tilde{\eta}\rangle.
\end{equation}
Note we are using \( \tilde{n} \) to denote the representative of a translation class that includes the state \( n \). The problem with this formula is that there are \( N^2 \) terms involved. So for a very small lattice of \( 4 \times 5 \), we need to do 400 calculations to obtain one entry of the matrix. We should be able to do better.

### 2.6.1 Matrix Element Formula

Let us start from a representative state \( |\tilde{n}\rangle \). We have, as in Eq. 2.4, \( H|\tilde{n}\rangle = -\sum_{m \in \mathcal{M}} s_m |m\rangle \), where \( \mathcal{M} \) denotes the set of states created by hopping one particle in \( |\tilde{n}\rangle \) to an allowed n.n. site and the overall minus sign comes from the \( -t \) term in the Hamiltonian. Then \( H|T_i|\tilde{n}\rangle = T_i H|\tilde{n}\rangle = -\sum_m s_m T_i |m\rangle \), where we have used the fact that \( T_i \) commutes with the Hamiltonian. We have,

\[
H|\tilde{n}\rangle = \frac{1}{N_{nk}} \sum_{l=0}^{N-1} e^{-i k \cdot R_i H T_i |\tilde{n}\rangle}
\]

\[
= -\frac{1}{N_{nk}} \sum_{m \in \mathcal{M}} s_m \sum_{l=0}^{N-1} e^{-i k \cdot R_i T_i |m\rangle} = -\frac{1}{N_{nk}} \sum_{m \in \mathcal{M}} N_{mk} s_m |m_k\rangle. \tag{2.9}
\]

Next because we are interested in matrix elements between representative states, we want to connect \( |m_k\rangle \) in the preceding equation to \( |\tilde{n}\rangle \). We have done this earlier in Eq. 2.7. To recapitulate, if \( T_{j(m)} |\tilde{n}\rangle = \sigma_{j(m)} |m\rangle \), then \( |m_k\rangle = \sigma_{j(m)} e^{i k \cdot R_{j(m)}} |\tilde{n}\rangle \).

So we have

\[
H|\tilde{n}\rangle = -\frac{1}{N_{nk}} \sum_{m \in \mathcal{M}} N_{mk} s_m \sigma_{j(m)} e^{i k \cdot R_{j(m)}} |\tilde{n}\rangle. \tag{2.10}
\]

We should note that for all \( m \in \mathcal{M} \) there can be more than one element having the same representative \( |\tilde{n}\rangle \). That is to say in the sum in Eq. 2.10, there can be more than one term with \( |\tilde{n}\rangle \). (We will show an example of this situation in Sec. 2.6.3.)

We write a new set \( \mathcal{M}' = \{m | m \in \mathcal{M} \text{ and } m \text{ has rep } \tilde{n} \} \). Then we can write our matrix element equation as follows,

\[
\langle \tilde{n}k | H | \tilde{n}k \rangle = -\frac{N_{nk}}{N_{nk}} \sum_{m \in \mathcal{M}'} \sigma_{j(m)} e^{i k \cdot R_{j(m)} s_m}. \tag{2.11}
\]
Eq. 2.11 is the centerpiece of the Bloch state calculation. It includes many of the complications that come with the Bloch basis set.

2.6.2 Summary of the Procedure

Let us summarize what this important formula Eq. 2.11 says. We have representative states $|\tilde{n}\rangle$ in our basis state list (say it is number $q$ on the list) (see Table 2.3). For each state on the list apply the Hamiltonian operator to it, $H|\tilde{n}\rangle = -\sum_{m \in \mathcal{M}} s_m |m\rangle$. For each $m \in \mathcal{M}$ find the representative $|\tilde{m}\rangle$ and record $j(m)$ such that $T_{j(m)}|\tilde{m}\rangle = \sigma_{j(m)} |m\rangle$. For all $m \in \mathcal{M}$ find the subset $\mathcal{M}' = \{m | m \in \mathcal{M}$ and $m$ has rep $\tilde{m}\}$ and use Eq. 2.11 to compute matrix elements. We then search the basis state list for the position of $|\tilde{n}\rangle$ (say it is number $p$). Finally, we fill in the matrix element at $H_{p,q}$.

We can also summarize this procedure in the following.

1. input: $q$-th state in basis state list $|\tilde{n}\rangle$

2. $H|\tilde{n}\rangle = -\sum_{m \in \mathcal{M}} s_m |m\rangle$, find $\mathcal{M}$

3. for each $m \in \mathcal{M}$

   (a) find the representative $|\tilde{m}\rangle$

   (b) record $j(m)$ such that $T_{j(m)}|\tilde{m}\rangle = \sigma_{j(m)} |m\rangle$

   (c) find the subset $\mathcal{M}' = \{m | m \in \mathcal{M}$ and $m$ has rep $\tilde{m}\}$

   (d) use Eq. 2.11 to compute matrix elements $\langle \tilde{m}k | H | \tilde{n}\rangle$

   (e) search basis state list for the position of $|\tilde{n}\rangle$ (say $p$-th)

   (f) fill in the matrix element at $H_{p,q}$

4. go back to 1. for the next $|\tilde{n}\rangle$
2.6.3 An Explicit Calculation

Because the procedure in Sec. 2.6.2 is the most important part of our diagonalization program, it pays to make it more clear by doing an explicit calculation. We will show for this example exactly what $\mathcal{M}$, $s_m$, $j(m)$, $\sigma_{j(m)}$, and $\mathcal{M}'$ are.

The example that we will compute is again the $4 \times 5$ lattice with $M = 3$ particles. The representatives of the Bloch basis set is shown earlier in Table 2.3. We will explicitly build the Hamiltonian matrix for reciprocal lattice vector $k = (0,1)$. The notation $k = (n_1, n_2)$ stands for $k = n_1 k_1 + n_2 k_2$ where $k_1$ and $k_2$ are Bravais unit vectors in the reciprocal lattice space. For a rectangular lattice $k = (2\pi n_1/L_x, 2\pi n_2/L_y)$. From the list of representatives, we simply pick one, $q = 17$, $[0, 6, 18]$, and compute matrix elements for the 17th column.

The first step is to apply the Hamiltonian to it. We have

$$H[0, 6, 18] = -(-[6, 15, 18] + [4, 6, 18] + [0, 11, 18] + [0, 7, 18]$$

$$- [0, 3, 6] + [0, 6, 13] + [0, 6, 19] + [0, 6, 17]).$$

(2.12)

Here $\mathcal{M} = \{[6, 15, 18], [4, 6, 8], ..., [0, 6, 17]\}$. The signs $s_m$ are simply the signs in front of the terms in the sum. Next we find representatives $|\tilde{m}\rangle$ for each state in $\mathcal{M}$ and record the translation that takes $|\tilde{m}\rangle$ to $|m\rangle$. Here we collect the necessary information in Table 2.4.

For $k = (0, 1)$, the normalization factors $N_{n_k}$ are all equal to 4.4721 for all states. From Eq. 2.11, we see that the normalization factors cancel out. Now with Table 2.4 in hand, we can calculate all nonzero matrix entries in the 17-th column. The nonzero entries are $(1, 17)$, $(6, 17)$, $(12, 17)$, $(13, 17)$, and $(20, 17)$. What is $\mathcal{M}'$? For the case $p = 6$ we have only one term contributing to the sum. So $H_{6,17} = -\sigma_{j(m)} e^{ik R_{j(m)}} s_m = -(-1) \exp(i(0, 2\pi/5) \cdot (3, 3)(-1) = -\exp(i(6\pi/5)).$ For $p = 20$
Table 2.4: Information used to calculate matrix element using Eq. 2.11. $|\tilde{\mu}\rangle$ is the representative of $|m\rangle$. $p$ is index number of $|\tilde{\mu}\rangle$ on the basis set list. $T_{j(m)}|\tilde{\mu}\rangle = \sigma_{j(m)}|m\rangle$. $\mathbf{R}_{j(m)}$ is the translation vector.

| $|m\rangle$ | $s_m$ | $|\tilde{\mu}\rangle$ | $p$ | $j(m)$ | $\sigma_{j(m)}$ | $\mathbf{R}_{j(m)}$ |
|-------|-------|-------|-----|-------|----------|----------------|
| $[6, 15, 18]$ | -1 | $[0,2,13]$ | 6 | 18 | -1 | (3,3) |
| $[4, 6, 18]$ | 1 | $[0,6,13]$ | 13 | 18 | 1 | (3,3) |
| $[0, 11, 18]$ | 1 | $[0,7,14]$ | 20 | 11 | 1 | (2,1) |
| $[0, 7, 18]$ | 1 | $[0,7,14]$ | 20 | 18 | 1 | (3,3) |
| $[0, 3, 6]$ | -1 | $[0,2,8]$ | 1 | 3 | -1 | (0,3) |
| $[0, 6, 13]$ | 1 | $[0,6,13]$ | 13 | 0 | 1 | (0,0) |
| $[0, 6, 19]$ | 1 | $[0,6,12]$ | 12 | 19 | 1 | (3,4) |
| $[0, 6, 17]$ | 1 | $[0,6,17]$ | 16 | 0 | 1 | (0,0) |

There are two terms contributing to the sum, i.e., $\mathcal{M}' = \{[0,11,18],[0,7,8]\}$. We have $H_{20,17} = -(\exp(i(0,2\pi/5) \cdot (2,1)) + \exp(i(0,2\pi/5) \cdot (3,3))) = -\exp(i(2\pi/5)) - \exp(i(6\pi/5))$.

This fact that $\mathcal{M}'$ can have more than one states is apparently true for two or high dimensional systems only. In Ref. 1 for a one dimensional system, a formula (4.4) similar to our (2.11) is given, with one term only. The example calculated in this section shows clearly that in our two-dimensional system we must be careful about combining states. The block diagonalized matrix is given in Fig. 2.6 (compare this with the original sparse matrix in Fig. 2.4).
Figure 2.6: The nonzero matrix elements of the Hamiltonian matrix (complex Hermitian) calculated using the Bloch basis set in Table 2.3, for a $4 \times 5$ lattice, with three particles. Here we are plotting block diagonal Hamiltonian matrices with 20 $k$ vectors.
2.6.4 Comments

Here we make a few comments on this calculation procedure in Sec. 2.6.2. First, we see why when we build the basis set, we should store the signs $\sigma$ and normalization factor $N_{nk}$. They are used repeatedly in matrix element calculation. Second, it is clear that this process is calculating one column of the matrix at a time. Starting from a state $|\bar{n}\rangle$ ($q$-th state), we find all states linked to it by hopping, i.e., we are computing the $q$-th column of the matrix. Third, in the procedure we will be searching for the index number of the state $|\tilde{n}\rangle$ in the representative state list. When the list is long, for example in the order of millions, it is good to have a good search method. Here we have implemented a hash table.

The hash table is a simple idea. Instead of searching the whole list, let us remember the position of some states, so we can jump right to a point close to the position we want. Take a look at Table 2.3. Let’s say that we want to search the index number of the state $[0, 6, 16]$. If we know where the second number first becomes 6, that is index number 11, we can start searching from number 11. If in addition we know the place where the second number first becomes 7, that is number 18, we can limit our search from 11 to 17. This is the thumb index for a dictionary. Of course, we cannot store positions of all states (that is like having a thumb index for for every word). We are fine with indexing the first few particles, say three or four (the first one is zero always, so we do not need that). As far as implementation is concerned, when we construct the list of representatives, as in Table 2.3, because we are going in the increasing dictionary order, it is easy to record the index number first appearance of the first few particles. We have a two-dimensional array $hashTable[[]]$ such that $hashTable[i][j]$ stores the index number of the first appearance of state $[0, i, j, ...]$.
One other point need to be made is that this whole process outlined here works without modification for skewed lattices. The main implementation problem is translation. The optimized way that worked well for rectangular lattices using quotient (/) and remainder (%) operators that we outlined above does not apply now. But this does not pose a significant performance problem.

2.7 Matrix Diagonalization: Lanczos Algorithm

We come to the last part of our diagonalization program: namely finding the actual eigenvalues of the Hamiltonian matrix, that is constructed either using the regular basis set or the Bloch basis set. There are two options. First, if we want to find all the eigenvalues, i.e., if we are interested in many of the excited states, we need to have the full matrix stored in memory. Then we can use the commercially available software package, (we have used LAPACK) to find all eigenvalues and eigenvectors. Our program is written in Java, using extensively the object-oriented features of the language, and because the diagonalization packages are in Fortran, we have written Java to Fortran interfaces to call these subroutines. The problem here is that we quickly run out of memory space with a full matrix in storage, so we can only compute matrices with dimension in the several thousand range. To go beyond this we must seek a new method.

The Lanczos algorithm [8] is a method that does not need the storage of the full matrix. If one has a $n \times n$ matrix $H$, and if one only wants to find the lowest eigenvalue (not excited state eigenvalues, not eigenvectors), the Lanczos method requires the storage of only two vectors of $n \times 1$ only. It is an iterative method, and at the $m$-th iteration a $m \times m$ tridiagonal symmetry matrix $T_m$ is built. The smallest eigenvalue of this matrix, $\epsilon_m$, approximates the ground state eigenvalue of
the full matrix $H$. We iterate until $\epsilon_m$ converges to satisfy some tolerance value. In many of our calculations, $H$’s dimensionality is several hundred thousands, and to achieve $10^{-15}$ convergence of $\epsilon_m$ requires often not more than $m = 100$ iterations. That is to say a $T_m$ matrix with about $100 \times 100$ contains information (about the ground state) of the original matrix $H$ that is more than $100,000 \times 100,000$.

The procedure is described in Ref. [1]. Here we record what it says.

1. start with a random vector $w$ and apply the matrix to it, $Hw = v$

2. find $\alpha_1$ and $\beta_1$ by doing, $\alpha_1 = w^*v$, $v = v - \alpha_1 w$, and $\beta_1 = |v|$

3. for $j=2,3,\ldots$, find $\alpha_j$ and $\beta_j$ from $\alpha_{j-1}$ and $\beta_{j-1}$, build $T_j$, and find $e_j$ and $u_j$

   (a) $t = w$, $w = v/\beta_{j-1}$, $v = -\beta_{j-1} t$

   (b) $v = v + Hw$

   (c) $\alpha_j = w^*v$, $v = v - \alpha_j w$, $\beta_j = |v|$

   (d) form $T_j$ matrix (using information from previous steps and the new $\alpha_j$)

$$
T_j = \begin{pmatrix}
\alpha_1 & \beta_1 \\
\beta_1 & \alpha_2 & \beta_2 \\
& \ddots & \ddots & \ddots \\
& & \beta_{j-2} & \alpha_{j-1} & \beta_{j-1} \\
& & & \beta_{j-1} & \alpha_j
\end{pmatrix}
$$

(2.13)

(e) diagonalize $T_j$ and find lowest eigenvalue $e_j$ and the corresponding eigenvector $u_j$

(f) if $|e_j - e_{j-1}| < $ Tolerance, done, and $e_j$ is an approximation for the lowest eigenvalue, and an approximation for the lowest eigenvector is

$$
U_j = \sum_{i=1}^{j} u_j^i w_i,
$$

(2.14)
where $\mathbf{w}_i$ are the vectors $\mathbf{w}$ from the iterations. (Because $\mathbf{w}$ is not stored during iteration, if we want to find the eigenvector $\mathbf{U}_j$, we need to redo the iterations again, and we would then need three vectors, $\mathbf{w}$, $\mathbf{v}$, and $\mathbf{U}_j$.) Otherwise, go back to (a), find $\alpha_{j+1}$, $\beta_{j+1}$, $T_{j+1}$, $e_{j+1}$ and $\mathbf{u}_{j+1}$, etc.

Note first that the tridiagonal matrix $T_j$ is not built from scratch at each $j$; it uses the information from previous steps. The computationally intensive part of the calculation does not lie in the diagonalization of $T_j$, because this is a small matrix. It is when we set up the matrix $T_j$ during iteration. There we are required to do matrix vector multiplication $H\mathbf{w}$ where $H$ is $100,000 \times 100,000$ and we do not have the matrix in storage. This is where the table of information (Table 2.4) is important. The most important knowledge is which entries of a given column (or row, because our matrix is Hermitian) are nonzero (the $p$ column in Table 2.4). Once we have this information, it is easy to do matrix-vector multiplication.

One small note is that earlier we mentioned that to obtain ground state energy we only need two vectors of $n \times 1$. It seems that from the procedure outlined, we will need three, $\mathbf{v}$, $\mathbf{w}$, and $\mathbf{t}$. In fact if we look more closely, we see that $\mathbf{t}$ is simply a temporary storage space during essentially a swap process. We only need a complex number to store the entry of the vector being calculated.

Finally, there are commercial packages that implements Lanczos diagonalization. We have implemented the Lanczos ourselves using the procedures outlined in this section. We have also installed ARPACK [9], a popular package that uses the closely related so-called Arnoldi methods and can obtain excited state eigenvalues and eigenvectors as well. If we only need information about the ground state, our program is considerably faster than ARPACK.
2.8 Summary

In this section we collect together all the details from the previous sections and list the main steps for our diagonalization program. We will only describe the Bloch basis set case, because the regular basis set method has been summarized earlier.

1. given $\mathbf{R}_1$ and $\mathbf{R}_2$ represent the lattice
   
   (a) form lattice site list (using upward then rightward convention)
   
   (b) form nearest neighbor list for each site (using right, left, up, down convention)

2. given $M$, the number of particles, and $k$ vectors, construct Bloch basis set
   
   (a) using dictionary order, store $hashTable[i][j]$
   
   (b) keep only representative state of each translation class only $|\vec{n}\rangle$
   
   (c) store signs $\sigma_i$ and normalization constants $N_{nk}$

3. store Hamiltonian matrix information one column at a time
   
   (a) input: $q$-th state in basis state list--$|\vec{n}\rangle$
   
   (b) $H|\vec{n}\rangle = - \sum_{m \in \mathcal{M}} s_m |m\rangle$, find $\mathcal{M}$
   
   (c) for each $m \in \mathcal{M}$
      
      i. find the representative $|\vec{m}\rangle$
      
      ii. search basis state list (using $hashTable$) and record the position of $|\vec{m}\rangle$: $p$
      
      iii. record $j(m)$ such that $T_{j(m)}|\vec{m}\rangle = \sigma_{j(m)} |m\rangle$
      
      iv. record $s_m$
(d) for each $q$, store a set of $(p, j(m), s_m)$ triplets

4. Lanczos iterations

(a) compute $Hw = v$

i. $q$-th column: combine those triplets $(p, j(m), s_m)$ with the same $p$

ii. use $s_m, j(m)$ (these are from the stored matrix information), $\sigma_j$, $N_{nk}$

(these are from the stored Bloch state information) and plug into

Eq. 2.11 to compute matrix elements $H_{p,q}$

iii. use $H_{p,q}$ to do matrix-vector multiplication

(b) compute $T_m$ matrix

(c) diagonalize $T_m$ to get $\epsilon_m$: $\epsilon_m$ is ground state energy after it satisfies our
tolerance requirement

2.9 Discussions and Conclusion

Let us use $N$ to denote the number of Bloch basis states, i.e., the dimensionality of
the Hamiltonian matrix for one $k$ vector.

In Fig. 2.7, we show for the $7 \times 7$ lattice, $N$ vs the number of particles $M$, with
$M = 2, 3, ..., 20$. The largest matrix is the $M = 11$ case, with $N = 1,906,532$, i.e.,
close to 2 million Bloch basis states. In Fig. 2.8, we show the case of four particles
$M = 4$ on the $L \times L$ lattice, with increasing $L$ ($L = 5, 6, ..., 20)$. For $L = 20$,$N = 2,472,147$, and $N$ increases rapidly as $L$ increases.

Detailed instructions for running the diagonalization program are in Append-
dices A which also includes a discussion of the time and memory issues in Sec. A.4.
Here we will be brief.
Figure 2.7: Matrix (translation-reduced) dimensionality $\mathcal{N}$ for one k vector for the $7 \times 7$ lattice with $M = 2, 3, \ldots, 20$ particles. The largest matrix is for $M = 11$, with $\mathcal{N} = 1,906,532$.

The following times are obtained using an Intel Pentium III 700 processor.$^9$

Using LAPACK, full diagonalization of a $3156 \times 3156$ matrix ($7 \times 7$ with $M = 18$) takes about 27 minutes. Full diagonalization is limited by memory availability to $\mathcal{N}$ up to a few thousands.

Using the Lanczos algorithm, we have two options. First, we store information about the matrix (i.e., for each column, a set of $(p, j(m), \sigma_{j(m)})$ described in Sec. 2.6.2 that contains information about the nonzero entries of the Hamiltonian matrix in this column). The $M = 9$ case on $7 \times 7$ lattice with $\mathcal{N} = 1,120,744$ and tolerance $10^{-15}$ takes about 45 minutes (32 Lanczos iterations) and uses about 1.5

$^9$The machine charming at the CCMR.
Figure 2.8: Matrix (translation-reduced) dimensionality $\mathcal{N}$ for one $k$ vector for four particles $M = 4$ on the $L \times L$ lattice with $L = 5, 6, ..., 20$. For $L = 20$, $\mathcal{N} = 2,472,147$. Numerical data for this graph is in Table D.4.

GB of memory. This basically reaches our memory limit.

On the other hand, we can also do Lanczos without storing matrix information. The same $M = 9$ case on $7 \times 7$ uses only 200 MB of memory but takes more than four hours (263 minutes), for a larger tolerance $10^{-7}$ (therefore fewer Lanczos iterations, 14). Without storing matrix information, we can calculate for larger matrices: the $M = 11$ case on $7 \times 7$, with $\mathcal{N} = 1,906,532$ (the largest for the $7 \times 7$ system) and tolerance $10^{-7}$, is done in 10 hours, using less than 400 MB of memory. The largest matrix we computed for this thesis work is $\mathcal{N} = 2,472,147$, i.e., about 2.5 million Bloch states, for $M = 4$ on $20 \times 20$. This takes 10 hours and uses about 550 MB of memory, for a tolerance of $10^{-7}$. Tables A.2, A.3, A.4, and A.5 at the end of
Appendix A contains detailed time and memory information.

The $7 \times 7$ lattice, with maximum $\mathcal{N}$ around 2 million, is basically the largest lattice for which we can calculate eigenenergies at all fillings. The exponential growth is very rapid after this. The $8 \times 8$ lattice with 8 particles has $9,151,226$ Bloch states, and with one more particle, $M = 9$, there are $30,658,325$, i.e., more than 30 million states.

To conclude, in this chapter, we introduced the exact diagonalization method applied to our two-dimensional quantum model. We first introduced the method for a general lattice with a general Hamiltonian, showing the rules for computing matrix elements and the important idea of computing one column of the matrix at a time. We then turned to the case with translation symmetry using the Bloch states (2.6). The idea is to choose a representative state from each translation class, and we showed in detail the complications related to computing the matrix elements. Eq. 2.11 is the key result in this calculation. We then considered an important computational technique for diagonalizing very large matrices: the Lanczos method.

The Lanczos exact diagonalization program described in this chapter, using Bloch states for matrices up to 2 million by 2 million, is the computational hardware for this thesis.

The preceding sections in this chapter have focused on the implementation issues of the program. With a computer program in hand, how to use it, what to use it for, and what the program’s results are telling us are more challenging questions that will be explored in the chapters that follow. As an example, the program says nothing about which of the $N$ reciprocal lattice vectors $\mathbf{k}$ we should use in diagonalization. Questions like this requires actual understanding of the physics of the problem. And that is what we will turn to now.
Bibliography

Chapter 3

The Two-Particle Problem I:
Lattice Green Function

In this chapter, we study analytically the problem of two particles (spinless fermions or hardcore bosons) on an otherwise empty lattice. As introduced in Sec. 1.9 of the Introduction, we are interested in studying dilute fermions and bosons, and the two-particle problem plays a large role in this investigation, because at the low-density limit, two-body interaction is the dominant interaction. The two-particle problem is also a natural starting point, after the trivial one-particle problem, and it is a good entry point to lattice physics. In this chapter we will acquaint ourselves with lattice sums, reciprocal lattice vectors, lattice Fourier transforms, lattice Green functions—objects and tools that are important in the lattice setting but are perhaps a bit less familiar, due to the emphasis on continuous problems in introductory physics courses. One good thing about the two-particle problem is that the equations can be reduced analytically to a simple form and all the eigenenergies and eigenstates can be determined without much computational effort.
3.1 Previous Work and Introduction

The two-particle problem has appeared in many different contexts. The most familiar one is the hydrogen atom problem in introductory quantum mechanics textbooks. That is a continuum problem, but as we will see in what follows, the main mathematical steps are the same as those in our problem: the two-body problem is reduced, using relative coordinates, to a one-body problem, which is further reduced using symmetries (rotational symmetries in the hydrogen case, giving spherical harmonics, and reflection symmetries in our case).

As already mentioned in Sec. 1.3.7 on the two-particle problem in the Hubbard model, the Heisenberg spin Hamiltonian can be considered as a boson model, with nearest-neighbor hopping. The two-magnon problem is closely related mathematically to our two-particle problem, and it has been solved in arbitrary dimensions for ferromagnets. Some of the original research articles are Refs. [2, 3, 4], and Mattis's book on magnetism contains a very clear explanation [5].

Another important two-particle problem is the Cooper problem, with two electrons in the presence of a Fermi sea. What is of interest here is whether a bound state exists and therefore whether a Cooper pair can form. To solve for energy, the Schrödinger equation for the pair of electrons is rewritten, using a Green function, as an implicit equation for energy, which is in turn solved graphically (see Baym [1] for details).

Motivated by the possibility of Cooper pair formation in high-temperature superconductors, there have also been a number of studies on bound states on a two-dimensional lattice (see Refs. [6, 7, 8, 9, 10, 11]). The question is whether two electrons can bind in a model with repulsive interactions. Various terms, in different forms but all attractive, have been added to the standard Hubbard Hamiltonian
to make binding possible. The two-electron problem in the plain two-dimensional repulsive Hubbard model is studied in Ref. [13], and ground state energy in the large-lattice limit is obtained analytically. The key in these calculations is the lattice Green function. The Schrodinger equation is written in the Green function language, and a self-consistent equation for energy is obtained. The infinite lattice limit of some of the lattice Green functions is known analytically, and is the basis for many of the calculations.

On the other hand, the two-boson problem has not attracted as much attention as its fermion counterpart. The difference between the boson problem and the fermion problem is that the boson total wave function has to be symmetric while the fermion total wave function is antisymmetric. In the Hubbard model, if two electrons form a spin singlet (so the spin wave function is antisymmetric with respect to particle permutation) then their spatial wave function need to be symmetric, which is like our boson problem (except we have hardcore and nearest-neighbor interactions).

In this chapter, we present a rather complete calculation for the two-particle problem in our model, treating both bosons and fermions. With infinite repulsive interaction in our model, we are not interested in finding bound states. We are first of all interested in calculating energies (for all states) for a finite-size lattice. Our formulation uses the lattice Green function, and our calculation is more complicated than the Hubbard model case because of nearest-neighbor interaction (while the Hubbard model contains only on-site interaction). As we will show in this chapter, our Green function is a $4 \times 4$ matrix, corresponding to interaction with four nearest neighbors. We formulate for arbitrary interaction (any range, any strength), and then show the simplification from short-range interaction and infinite repulsion.

Another of our interests is to obtain analytically the two-particle energies in the
infinite-lattice limit. To achieve this end, we must simplify the $4 \times 4$ lattice Green function. For a rectangular-boundary lattice and zero total momentum, we show how this can be done, using lattice reflection symmetries, and for a square-boundary lattice,\footnote{The name “square-boundary” lattice denotes a lattice with square periodic boundaries. We try to differentiate the term from that referring to the underlying square lattice.} we obtain the two-boson energy in the large-lattice limit, which we check with exact diagonalization results. The two-fermion problem is more difficult, as we will explain, and is work in progress.

Using the two-particle, large-lattice result, we can obtain the energy of a few particles on a large lattice, because here two-body interaction is the dominant interaction. We show that the total energy of a few particles (bosons and fermions) can be obtained by adding the energy of each pair of particles.

This chapter is organized as follows. First, we formulate the Schrodinger equation for two particles using lattice Green function. The resulting implicit equation for energy is solved and eigenstates are plotted. We then restrict our attention to the rectangular-boundary lattice and zero total momentum and further reduce the problem using lattice symmetries. Finally, we will show that we can obtain an analytical form for the two-boson energy for a large square-boundary lattice, and we study the energy of a few particles (three, four, and five) on a large lattice.

\section{3.2 Preliminary}

\subsection{3.2.1 Fourier Transform and Commutation Relations}

For future convenience, we collect in this section some results that will be used repeatedly in our calculation. First, the commutation relations for creation and
annihilation operators are
\[
[c_r, c_{r'}^\dagger]_{bf} = \delta_{rr'}, \quad [c_r, c_{r'}]_{bf} = [c_{r'}^\dagger, c_r^\dagger]_{bf} = 0,
\]
(3.1)
where we have used the subscript \(bf\) (short for boson and fermion) to denote both the commutator and the anticommutator. That is to say, for operators \(A\) and \(B\),
\[
[A, B]_{bf} = AB - s_{bf}BA,
\]
(3.2)
where
\[
s_{bf} = \begin{cases} 
+1, & \text{boson}, \\
-1, & \text{fermion}.
\end{cases}
\]
(3.3)
Next we write down the lattice Fourier transform convention that we use in our calculation,
\[
c_r = \frac{1}{\sqrt{N}} \sum_q e^{i q r} c_q, \quad c_q = \frac{1}{\sqrt{N}} \sum_q e^{-i q r} c_r.
\]
(3.4)
Taking complex conjugate, we get the expressions for the creation operators,
\[
c_r^\dagger = \frac{1}{\sqrt{N}} \sum_q e^{-i q r} c_q^\dagger, \quad c_q^\dagger = \frac{1}{\sqrt{N}} \sum_q e^{i q r} c_r^\dagger.
\]
(3.5)
An important property of the lattice sum is
\[
\sum_r e^{i q r} = N \delta_{q,0},
\]
(3.6)
where \(N\) is the number of lattice sites. Then in momentum space, we have
\[
[c_q, c_{q'}^\dagger]_{bf} = \delta_{qq'}, \quad [c_q, c_{q'}]_{bf} = [c_{q'}^\dagger, c_q^\dagger]_{bf} = 0.
\]
(3.7)
We can rewrite these relations to get a formula that will be used repeatedly in the calculation,
\[
c_q c_{q'}^\dagger = \delta_{qq'} + s_{bf} c_{q'}^\dagger c_q, \quad c_q c_{q'} = s_{bf} c_q^\dagger c_{q'};
\]
(3.8)
and an especially useful identity,
\[
\langle 0| c_{q'} c_{q}^\dagger c_{k}^\dagger c_{k'}^\dagger |0\rangle = \delta_{qk} \delta_{q'k'} + s_{bf} \delta_{qk} \delta_{q'k'}.
\]
(3.9)
3.2.2 Hamiltonian in Momentum Space

In this two-particle calculation, we will work in momentum space, and we will start with a Hamiltonian more general than that introduced in Sec. 1.6, Eq. 1.7,

\[ H = T + U, \]
\[ T = \sum_{\mathbf{r}_1 \mathbf{r}_2} t(\mathbf{r}_2 - \mathbf{r}_1) c_{\mathbf{r}_1}^\dagger c_{\mathbf{r}_2}, \quad U = \sum_{\mathbf{r}_1 \mathbf{r}_2} V(\mathbf{r}_2 - \mathbf{r}_1) c_{\mathbf{r}_1}^\dagger c_{\mathbf{r}_2}^\dagger c_{\mathbf{r}_2} c_{\mathbf{r}_1}. \quad (3.10) \]

Here we have allowed hopping and interaction between any two lattice sites, but we require that both depend only on the separation between the two vectors and both have inversion symmetry. That is \( t(\mathbf{r}_1, \mathbf{r}_2) = t(\mathbf{r}_2 - \mathbf{r}_1), t(-\mathbf{r}) = t(\mathbf{r}), V(\mathbf{r}_1, \mathbf{r}_2) = V(\mathbf{r}_2 - \mathbf{r}_1), \) and \( V(-\mathbf{r}) = V(\mathbf{r}). \) In momentum space, this more general Hamiltonian (3.10) becomes,

\[ T = \sum_{\mathbf{p}} \mathcal{E}(\mathbf{p}) c_{\mathbf{p}}^\dagger c_{\mathbf{p}}, \quad U = \frac{1}{2N} \sum_{\mathbf{pp}'\mathbf{k}} V(\mathbf{k}) c_{\mathbf{p}}^\dagger c_{\mathbf{p}}^\dagger c_{\mathbf{p}'+\mathbf{k}} c_{\mathbf{p}'}, \quad (3.11) \]

where

\[ \mathcal{E}(\mathbf{p}) = \sum_{\mathbf{r}} t(\mathbf{r}) e^{i\mathbf{p}\mathbf{r}}, \quad V(\mathbf{k}) = \sum_{\mathbf{r}} V(\mathbf{r}) e^{i\mathbf{k}\mathbf{r}}. \quad (3.12) \]

It is easy to check that \( \mathcal{E}(-\mathbf{p}) = \mathcal{E}(\mathbf{p}) \) and \( V(-\mathbf{k}) = V(\mathbf{k}) \). An important property of this Hamiltonian (3.11) is that it conserves total momentum, a fact that will be used when we write down the wave function.

We note that the Hamiltonian (3.10) reduces to our nearest-neighbor Hamiltonian (1.7) if we take,

\[ t(\mathbf{r}) = \begin{cases} -t, & \mathbf{r} = (\pm 1, 0)(0, \pm 1), \\ 0, & \text{otherwise}, \end{cases} \]

\[ V(\mathbf{r}) = \begin{cases} V, & \mathbf{r} = (\pm 1, 0)(0, \pm 1), \\ 0, & \text{otherwise}, \end{cases} \quad (3.13) \]
where we have taken the lattice constant to be unity. Then we have,

\[ \mathcal{E}(\mathbf{p}) = -2t(\cos p_x + \cos p_y), \quad V(\mathbf{k}) = 2V(\cos k_x + \cos k_y). \]  (3.14)

The energy dispersion expression in Eq. 3.14, for nearest-neighbor hopping, is of crucial importance in our calculation. We plot it in Fig. 3.1 for a 10 \times 10 lattice. The energy is minimum at \( \mathbf{k} = (0, 0) \), around which a quadratic approximating function can be used. In Fig. 3.1 we also include a density plot of \( \mathcal{E}(\mathbf{p}) \), demonstrating more explicitly the discrete reciprocal lattice vectors (here 100 in the first Brillouin zone for 10 \times 10 lattice). It emphasizes the fact that in the calculations to follow for finite lattices, we have a finite sum of terms.

\[ \begin{align*}
\text{Figure 3.1: Energy dispersion function } &\mathcal{E}(\mathbf{k}) \text{ (3.13) for a 10 } \times \text{ 10 lattice. Four} \\
&\text{Brillouin zones are plotted. The density plot of } \mathcal{E}(\mathbf{k}) \text{ on the right emphasizes the} \\
&\text{discrete quality of our problem, that there are a finite number of (here 100) reciprocal} \\
&\text{lattice vectors in one Brillouin zone.}
\end{align*} \]

\(^{2}\text{We are slightly abusing the notation } V. \text{ } V(\mathbf{r}) \text{ is the potential function for all space. } V \text{ is} \]
\[ \text{the value of the potential at four points } (V = V(\mathbf{r} = (1, 0))) \text{ for example). And } V(\mathbf{k}) \text{ the Fourier} \]
\[ \text{transform of } V(\mathbf{r}). \text{ We will differentiate these meanings by including explicitly the argument, } \mathbf{r} \text{ or} \]
\[ \mathbf{k}. \text{ Without argument, we then mean } V = V(\mathbf{r} = (1, 0)). \]
3.2.3 The Two-Particle State

In this section we discuss the two-particle state $|\psi\rangle$ that will be used in our Schrodinger equation. The wavefunction that we will use is,

$$|\psi\rangle = \sum_{\mathbf{q}_1} f(\mathbf{q}_1)|\mathbf{q}_1, \mathbf{P} - \mathbf{q}_1\rangle,$$

where $\mathbf{P}$ is the total momentum of the two particles (because we know that our Hamiltonian conserves total momentum). We make a few comments about this wave function.

First, we can also write our wavefunction in a more symmetric form,

$$|\psi\rangle = \sum_{\mathbf{q}_1} f(\mathbf{q}_1)|\mathbf{q}_1 + \mathbf{P}/2, -\mathbf{q}_1 + \mathbf{P}/2\rangle,$$

which is the form used in some theoretical calculations (see for example [9]). We use the form in Eq. 3.15 with computer implementation in mind. For example, the reciprocal lattice vectors for a rectangular-boundary $L_x \times L_y$ lattice are $\mathbf{k} = 2\pi(n_x/L_x, n_y/L_y)$, where $n_x$ and $n_y$ are integers. (In this chapter, we only deal with rectangular-boundary lattices, and we will write, in short, $\mathbf{k} = (n_x, n_y)$.) If we choose the form $|\mathbf{q}_1 + \mathbf{P}/2, -\mathbf{q}_1 + \mathbf{P}/2\rangle$, and if the total momentum $\mathbf{P} = (1, 0)$ and $\mathbf{q}_1 = (m_x, m_y)$, then for $\mathbf{q}_1 + \mathbf{P}/2 = (m_x + 1/2, m_y)$ to be a reciprocal lattice vector, $m_x$ cannot be an integer. Of course, in $|\mathbf{q}_1 + \mathbf{P}/2, -\mathbf{q}_1 + \mathbf{P}/2\rangle$, $\mathbf{q}_1$ need not be a reciprocal lattice vector; $\pm \mathbf{q}_1 + \mathbf{P}/2$ should be. This means that if $\mathbf{P} = (0, 0)$, we should use $\mathbf{q}_1 = (l_x, l_y)$ where $l_x$ and $l_y$ are integers; and if $\mathbf{P} = (1, 0)$, we should use $\mathbf{q}_1 = (-1/2 + l_x, l_y)$ where $l_x$ and $l_y$ are integers. The sum in Eq. 3.16 then depends on the choice of $\mathbf{P}$. With our choice Eq. 3.15 on the other hand, the sum can be chosen as $\mathbf{q}_1 = (l_x, l_y)$ with $l_x = 0, 1, \ldots, L_x - 1$ and $l_y = 0, 1, \ldots, L_y - 1$ for all $\mathbf{P}$. Also with our form of the wave function (3.15), we can generalize to $M$ particles easily by writing $|\mathbf{q}_1, ..., \mathbf{q}_{M-1}, (\mathbf{P} - \mathbf{q}_1 - ... - \mathbf{q}_{M-1})\rangle$. 
Another point about this wave function is that if we sum over all reciprocal lattice vectors, we can have two states that differ only by a sign, namely, \( |q_1, P - q_1\rangle = s_{bf}|P - q_1, q_1\rangle \). One way to deal with this is to restrict the sum so that only one of these two states remains. But this is cumbersome in part because of the existence of a special case, that when \( P = 2q_1 \), \( q_1 = P - q_1 \), i.e., permutation gives the same state. Instead, note the following relation,

\[
|\psi\rangle = \frac{1}{2} \left( \sum_{q_1} f(q_1)|q_1, P - q_1\rangle + \sum_{q_1} f(P - q_1)|P - q_1, q_1\rangle \right)
\]

\[
= \frac{1}{2} \left( \sum_{q_1} (f(q_1) + s_{bf}f(P - q_1))|q_1, P - q_1\rangle \right)
\]

\[
= \frac{1}{2} \sum_{q_1} g(q_1)|q_1, P - q_1\rangle, \tag{3.17}
\]

where in the last step we have defined a new quantity, \( g(q_1) = f(q_1) + s_{bf}f(P - q_1) \), which satisfies

\[
g(P - q_1) = s_{bf}g(q_1). \tag{3.18}
\]

In (3.17), instead of restricting the basis state, we still sum over all vectors, but require the coefficients to obey certain relations (3.18). This is also convenient because once we get an eigenstate of the Hamiltonian, we can use this relation (3.18) on the coefficients to test whether it is a boson or fermion state. We will also see later that when plugging the state (3.15) into the Schrodinger equation, we can only get an equation for \( g(q) \), not \( f(q) \). That is to say that we cannot determine \( f(q) \) individually. We can only obtain the symmetric or antisymmetric combinations of \( f(q) \), which are \( g(q) \) with plus and minus signs respectively.\(^3\)

\[^3\]We could have started this section with Eq. 3.17, requiring the coefficients \( g(q) \) to have the symmetry property Eq. 3.18. That is what we will do in a research paper. We have chosen to start with \( f(q) \) in Eq. 3.15 and Eq. 3.16 to show (or remind) the reader some of the considerations that go into choosing the form of the wavefunction.
3.3 Schrödinger Equation

3.3.1 The First Schrödinger Equation

Now we derive the Schrödinger equation for the two-particle coefficients \(g(\mathbf{q})\) in \(|\psi\rangle\) (3.17). Applying the more general form of the Hamiltonian operator (3.11) to the state (3.15), we get,

\[
T|\psi \rangle = \sum_{\mathbf{q_1}} f(\mathbf{q}_1)(\mathcal{E}(\mathbf{q}_1) + \mathcal{E}(\mathbf{P} - \mathbf{q}_1))|\mathbf{q}_1, \mathbf{P} - \mathbf{q}_1\rangle, \tag{3.19}
\]

\[
U|\psi \rangle = \frac{1}{N} \sum_{\mathbf{q_1}} f(\mathbf{q}_1) \sum_{\mathbf{k}} V(\mathbf{k})|\mathbf{q}_1 + \mathbf{k}, \mathbf{P} - \mathbf{q}_1 - \mathbf{k}\rangle. \tag{3.20}
\]

The Schrödinger equation \((E - T)|\psi \rangle = U|\psi \rangle\) then becomes

\[
\sum_{\mathbf{q_1}} f(\mathbf{q}_1)(E - \mathcal{E}(\mathbf{q}_1) - \mathcal{E}(\mathbf{P} - \mathbf{q}_1))|\mathbf{q}_1, \mathbf{P} - \mathbf{q}_1\rangle = \frac{1}{N} \sum_{\mathbf{q_1}} f(\mathbf{q}_1) \sum_{\mathbf{k}} V(\mathbf{k})|\mathbf{q}_1 + \mathbf{k}, \mathbf{P} - \mathbf{q}_1 - \mathbf{k}\rangle. \tag{3.21}
\]

Take the inner product of Eq. 3.21 with a generic state \(|\mathbf{q}, \mathbf{P} - \mathbf{q}\rangle\), we get,

\[
(E - \mathcal{E}(\mathbf{q}) - \mathcal{E}(\mathbf{P} - \mathbf{q}))g(\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{k}} V(\mathbf{q} - \mathbf{k})g(\mathbf{k}). \tag{3.22}
\]

First, note that Eq. 3.22 is for \(g(\mathbf{q})\) not \(f(\mathbf{q})\), because as mentioned earlier only the symmetric and antisymmetric coefficients of the initial state (3.15) can be determined. Second, Eq. 3.22 is a matrix equation \(\mathcal{A}g = Eg\) where \(\mathcal{A}_{\mathbf{qk}} = (\mathcal{E}(\mathbf{q}) + \mathcal{E}(\mathbf{P} - \mathbf{q}))\delta_{\mathbf{qk}} + V(\mathbf{q} - \mathbf{k})/N\). If \(V\) is not infinity, this \(N \times N\) matrix \(\mathcal{A}\) can be diagonalized, and \(E\) and \(g(\mathbf{q})\) are respectively the eigenvalue and eigenvector. To deal with \(V = +\infty\), we need some further manipulations.

3.3.2 Green Function Equation

We consider the case when \(E \neq \mathcal{E}(\mathbf{q}) + \mathcal{E}(\mathbf{P} - \mathbf{q})\), for any \(\mathbf{q}\), which is to say, the energy \(E\) is not the energy of a noninteracting pair. Using the definition (3.12),
\[ V(q - k) = \sum_{r'} V(r') e^{i(q-k) \cdot r'}, \text{ the equation (3.22) becomes,} \]

\[
g(q) = \frac{1}{N} \sum_{k} \frac{V(q - k)}{E - \varepsilon(q) - \varepsilon(P - q)} g(k) \]
\[
= \sum_{r'} \frac{1}{N} \frac{e^{-iq \cdot r'}}{E - \varepsilon(q) - \varepsilon(P - q)} V(r') \sum_{k} e^{-ik \cdot r'} g(k). \quad (3.23)\]

Multiply this equation by \( e^{-iq \cdot r} \) and sum over \( q \), we get

\[
\sum_{q} e^{-iq \cdot r} g(q) = \sum_{r'} \left[ \frac{1}{N} \sum_{q} \frac{e^{iq \cdot (r' - r)}}{E - \varepsilon(q) - \varepsilon(P - q)} \right] V(r') \sum_{k} e^{-ik \cdot r'} g(k). \quad (3.24)\]

Now define the lattice Fourier transform of the coefficients \( g(q) \),

\[
\tilde{g}(r) = \sum_{q} e^{-iq \cdot r} g(q), \quad (3.25)\]

and the lattice Green function,

\[
G(E, P; r, r') = \frac{1}{N} \sum_{q} \frac{e^{iq \cdot (r' - r)}}{E - \varepsilon(q) - \varepsilon(P - q)}, \quad (3.26)\]

then our Schrodinger equation (3.22) becomes,

\[
\tilde{g}(r) = \sum_{r'} G(E, P; r, r') V(r') \tilde{g}(r'). \quad (3.27)\]

This equation is equivalent to the Schrodinger equation for the general Hamiltonian (3.10). The meaning of the Green function is clear: \( G(E, P; r, r') \) takes the (Fourier transformed) coefficient of the eigenstate and potential at \( r' \) and gives via (3.27) the coefficient at \( r \). Also from Eq. 3.26, we see that \( G(E, P; r, r') \) is always a function of \( r - r' \). This is a consequence of our assuming \( t(r_1, r_2) \) and \( V(r_1, r_2) \) to be translation invariant in deriving the Hamiltonian, Eq. 3.11.

Because our general form of the Hamiltonian (3.10) allows interactions between particles at any two lattice sites, the sum in Eq. 3.27 is over all lattice vectors. But if the potential \( V(r) \) is finite-range, we get simplifications. Next we show how nearest-neighbor interaction gives rise to a \( 4 \times 4 \) matrix equation for \( E \).
3.3.3 Matrix Equation

This section is indebted to Ref. [10] which solved a similar problem. In the following we return to the nearest-neighbor potential \( V(\mathbf{r}) \) in Eq. 3.13. The Green function sum in Eq. 3.27 then has only four terms,

\[
\tilde{g}(\mathbf{r}) = \sum_j G(E, \mathbf{P}; \mathbf{r}, \mathbf{R}_j)(V\tilde{g}(\mathbf{R}_j)),
\]

where we have used \( \mathbf{R}_j \in \{(\pm 1, 0), (0, \pm 1)\} \). If we also restrict \( \mathbf{r} \) to the four nearest-neighbor vectors, then Eq. 3.28 becomes,

\[
\tilde{g}(\mathbf{R}_i) = \sum_j G(E, \mathbf{P}; \mathbf{R}_i, \mathbf{R}_j)(V\tilde{g}(\mathbf{R}_j)).
\]

If we define the \( 4 \times 4 \) matrix,

\[
\mathcal{G}_{ij}(E, \mathbf{P}) = G(E, \mathbf{P}; \mathbf{R}_i, \mathbf{R}_j),
\]

and a \( 4 \times 1 \) vector \( \phi_j = \tilde{g}(\mathbf{R}_j) \), then we obtain a simple matrix equation,

\[
(I - \mathcal{G}(E, \mathbf{P})V)\phi = 0.
\]

Here \( E \) is the unknown energy, \( \mathbf{P} \) is the total momentum that we can specify, and this equation says that \( E \) is the special number that makes the \( 4 \times 4 \) matrix \( I - \mathcal{G}(E, \mathbf{P})V \) singular, and the \( 4 \times 1 \) vector \( \phi \) is the null vector of \( I - \mathcal{G}(E, \mathbf{P})V \).

We can also rewrite this equation as an equation for energy using the determinant,

\[
\det(I - \mathcal{G}(E, \mathbf{P})V) = 0.
\]

With \( V = +\infty \), we have an even simpler equation

\[
\mathcal{G}(E, \mathbf{P})(V\phi) = 0,
\]

which says that \( V\phi \) is the null vector of \( \mathcal{G}(E, \mathbf{P}) \). And we have an equation for energy,

\[
\det \mathcal{G}(E, \mathbf{P}) = 0.
\]
These equations (3.28, 3.33, 3.34) and the Green function (3.26) are all we need for our two-particle problem. The original problem of two particles can be considered as a $N^2 \times N^2$ problem, because each particle can be at $N$ site so the number of basis states is roughly $N^2$. Using total momentum conservation in our starting wave function (3.15) we immediately reduce the two-particle problem to a one-particle problem, with $N$ basis states and a $N \times N$ matrix in (3.22). Here we have gone further, using the fact that there is only nearest-neighbor interaction, we obtain, via Fourier transform (3.25), a $4 \times 4$ matrix equation (3.33).

For the Hubbard model, there is only on-site interaction, so $V(r)$ is nonzero only when $r = 0$, and the sum in Eq. 3.27 has only one term. Eq. 3.29 is simply a scalar equation, which, after $\tilde{g}$ cancels from both sides of the equation and using Eq. 3.26, gives,

$$1 = \frac{V}{N} \sum_{\mathbf{q}} \frac{1}{E - \varepsilon(\mathbf{q}) - \varepsilon(\mathbf{P} - \mathbf{q})},$$

which is exactly the result in Ref. [13]. Eq. 3.35 is an implicit equation for $E$ and is much simpler than our determinant equation (3.34). We will show in Sec. 3.7 that for rectangular-boundary lattices, our equation (3.34) also simplifies. And for square-boundary lattices, our two-boson equation looks very much like Eq. 3.35.

Next, from the matrix equation (3.33) we will retrace our steps back to the coefficients of the original wavefunction $g(\mathbf{q})$ in Eq. 3.17.

### 3.3.4 Solution of the Two-Particle Problem Summarized

We solve the two-particle problem for the nearest-neighbor infinite-repulsion Hamiltonian (1.7) using the following steps.

1. Given a total momentum $\mathbf{P}$, solve for $E$ in $\det \mathcal{G}(E, \mathbf{P}) = 0$, with Green function (3.26).
2. Obtain the corresponding null vector \( V\phi_j = V\tilde{g}(R_j) \).

3. Obtain \( \tilde{g}(\mathbf{r}) \) for all \( \mathbf{r} \) by using \( \tilde{g}(\mathbf{r}) = \sum_j G(E, \mathbf{P}; \mathbf{r}, R_j)(V\phi_j) \).

4. Using inverse Fourier transform to get \( g(\mathbf{q}) \)

\[
g(\mathbf{q}) = \frac{1}{\mathcal{N}} \sum_{\mathbf{r}} e^{i\mathbf{q}\mathbf{r}} \tilde{g}(\mathbf{r}).
\]

(3.36)

\( g(\mathbf{q}) \) is the coefficient in our wave function, \( |\psi\rangle = (1/2) \sum_{\mathbf{q}} g(\mathbf{q}) |\mathbf{q}, \mathbf{P} - \mathbf{q}\rangle \). \( g(\mathbf{P} - \mathbf{q}) = g(\mathbf{q}) \) is the boson solution, and \( g(\mathbf{P} - \mathbf{q}) = -g(\mathbf{q}) \) the fermion solution.

3.4 Solving for Energy

The section 3.3.4 summarizes the steps for solving the two-particle problem. In this section, we will show some example solutions for specific lattices and total momentum vectors.

We will begin with a small rectangular-boundary lattice \( L_x = 4 \) and \( L_y = 5 \), with total momentum \( \mathbf{P} = (0, 0) \). Fig. 3.2 shows the function \( \det \mathcal{G}(E, (0, 0)) \) as a function of \( E \). The Green function (3.26) diverges when \( E \) equals one of the noninteracting energies. And the intersections of \( \det \mathcal{G}(E, (0, 0)) \) with the horizontal axis are the exact two-particle energies we want to find. In Table 3.1 we show all noninteracting and exact energies of this problem.

Finding roots of \( \det \mathcal{G}(E) \) (we have dropped \( \mathbf{P} \) from \( \mathcal{G}(E, \mathbf{P}) \) because \( \mathbf{P} \) is fixed for each calculation) in one-dimension is straightforward. We can use the bisection method if we can bracket the roots. This is where the noninteracting energies are useful. From the plot in Fig. 3.2, we can see that one root is bracketed by the two noninteracting energies \(-8.0\) and \(-5.236\). Using the bisection algorithm on \( \det \mathcal{G}(E) \)
Figure 3.2: $\det \mathcal{G}(E, \mathbf{P})$ vs $E$ for the $4 \times 5$ lattice with $\mathbf{P} = (0,0)$. The Green function diverges as $E$ equals one of the noninteracting energies. The intersections with the horizontal axis are the exact two-particle energies.

For this range gives the lowest boson energy $6.89226$ quickly. Similarly, we see that $-5.236$ and $-4.0$ bracket a root, which is the lowest fermion energy $-4.27745$. For other intervals, the noninteracting energies may bracket more than one root and the shape of $\det \mathcal{G}(E)$ becomes more complicated. The good thing is that evaluating $\mathcal{G}_{ij}(E)$ using Eq. 3.26 is relatively easy (a lattice sum), and no matter how big the lattice size, we only need to evaluate the determinant of a $4 \times 4$ matrix. This is to say that we can graph $\det \mathcal{G}(E)$ in great detail to obtain bisection brackets, without the difficulties associated with for example large matrix diagonalization. In a later section, after we simplify the equation $\det \mathcal{G}(E) = 0$, root finding is easier still.
Table 3.1: All noninteracting and exact two-particle energies of the 4 × 5 lattice with total momentum $\mathbf{P} = (0,0)$. $\mathbf{q}_1$ and $\mathbf{q}_2 = \mathbf{P} - \mathbf{q}_1$ are the momentum vectors.

The energy $\mathcal{E}(\mathbf{q})$ is given in Eq. 3.14.

<table>
<thead>
<tr>
<th>$\mathbf{q}_1$</th>
<th>$\mathbf{q}_2$</th>
<th>$\mathcal{E}(\mathbf{q}_1) + \mathcal{E}(\mathbf{q}_2)$</th>
<th>boson</th>
<th>fermion</th>
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<td></td>
</tr>
</tbody>
</table>

3.5 $\tilde{g}(\mathbf{r})$ Explained

Our Green function equation (3.33) is for $\tilde{g}$, but what is $\tilde{g}$ physically? In this section we will see that it is basically the wave function (3.15) in the relative coordinate representation. First we have, using (3.25),

$$
\tilde{g}(-\mathbf{r}) = \sum_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{r}} g(\mathbf{q}) = \sum_{\mathbf{q}} e^{i(\mathbf{P}-\mathbf{q}) \cdot \mathbf{r}} g(\mathbf{P} - \mathbf{q}) \\
= s_{bf} e^{i\mathbf{P} \cdot \mathbf{r}} \sum_{\mathbf{q}} e^{-i\mathbf{q} \cdot \mathbf{r}} g(\mathbf{q}) = s_{bf} e^{i\mathbf{P} \cdot \mathbf{r}} \tilde{g}(\mathbf{r}),
$$

where we have used the symmetry property of $g(\mathbf{q})$ in Eq. 3.18. For a wave function $\psi$ in the relative coordinate $\mathbf{r}$ we should have $\psi(-\mathbf{r}) = s_{bf} \psi(\mathbf{r})$, where the sign comes from boson and fermion exchange. Here Eq. 3.37 has an extra phase factor. We
show where this factor comes from.

We start with a two-particle state with definite relative position,

\[ |r\rangle = \sum_{r'} e^{iP\cdot R} |r', r' + r\rangle = e^{-iP\cdot r/2} \sum_q e^{iq\cdot r} |q, P - q\rangle, \tag{3.38} \]

where \( P \) is the total momentum and \( R = (r' + r' + r)/2 \) is the center-of-mass position and the second expression is the momentum space expression. It is easy to check that this state satisfies the desired relation, \( | - r\rangle s_{bf}|r\rangle \). And its inner product with our wave function (3.17) is

\[ \psi(r) \equiv \langle r|\psi\rangle = e^{iP\cdot r/2}\tilde{g}(r), \tag{3.39} \]

where \( \psi(r) \) is used to denote the representation of our wave function \( |\psi\rangle \) in the relative position \( r \) space. Using the reflection property of \( \tilde{g}(r) \) (3.37), we get \( \psi(-r) = s_{bf}\psi(r) \), as desired. The extra phase factor in Eq. 3.39 is the consequence of not choosing the wave function \( |\psi\rangle \) in a symmetrical form in Eq. 3.15. We chose implementation simplicity instead, but fortunately, this is not causing a big problem.

In summary, our \( \tilde{g}(r) \) is the Fourier transform (3.25) of the coefficients \( g(q) \) in our wave function \( |\psi\rangle \). It is also \( |\psi\rangle \) in the relative coordinate representation (3.39), except an overall phase factor. We have \( |\tilde{g}(r)|^2 = |\psi(r)|^2 \) which is the probability of finding two particles at a relative distance \( r \). This explanation of the physical meaning of \( \tilde{g}(r) \) also gives us an understanding of the Green function equations (3.27, 3.28). These equations are Schrodinger’s equations in the relative coordinate space. That is to say for our two-particle problem we fix one particle at the origin, so the other particle is at \( r \), and we have a one-particle problem described by the wavefunction \( \tilde{g}(r) \) and the equations (3.27, 3.28).
3.6 Eigenstates

In Sec. 3.4 we outlined the procedures for computing energy. In this section we follow the steps summarized in Sec. 3.3.4 to compute energy eigenstates in the relative position representation \( \tilde{g}(r) \) and momentum representation \( g(q) \).

The sample system that we choose here to present is the \( 10 \times 11 \) lattice. For the two-particle problem, as long as the energy and the corresponding null vector \( V\phi \) are known, the computation of eigenstate is straightforward and easy. It involves Green function computation and lattice Fourier transform only. We can compute eigenstates for very large systems without difficulty, and here we simply choose a system that is large enough to capture the essential physics. We will focus on the low-lying states. In Table 3.2, the lowest few noninteracting and exact energies are collected. The lowest three boson eigenstates are plotted in Fig 3.3 and the fermion states in Fig 3.4.

The reason that we choose a \( L_x \neq L_y \) lattice here is that our exact eigenstates are not degenerate (see Table 3.2), so the eigenvectors are uniquely determined. If we choose the \( 10 \times 10 \) lattice, the fermion energies will come in degenerate pairs, corresponding to reflection symmetry about \( y = x \). As can be seen in Table 3.2, the low-lying fermion energies are closely placed pairs but not degenerate.

From the Re(\( \tilde{g}(r) \)) plots, we see that boson wave functions are symmetric and fermion wave functions are antisymmetric. The momentum probability function \( |g(q)|^2 \) is very instructive in this calculation. The boson ground state has a sharp peak at \( q = 0 \) which means that in this state the two particles are most likely found with zero momentum. The first excited boson state has most probable momenta at \( (\pm 1, 0) \) and \( (0, \pm 1) \). The next one is more complicated, with \( (\pm 1, \pm 1) \) joining the group.
Figure 3.3: Lowest three boson eigenstates for the $10 \times 11$ lattice with $P = (0, 0)$ ($E_0 = -7.906815$ (top), $E_1 = -7.299892$ (middle), $E_2 = -6.971337$ (bottom)). Four copies of the lattice are plotted. The left column is $\text{Re}(\tilde{g}(r))$ (real part of the wavefunction in relative position space) and the right column is $|g(q)|^2$ (probability of finding one particle with momentum $q$).
Figure 3.4: Lowest three fermion eigenstates for the $10 \times 11$ lattice with $\mathbf{P} = (0, 0)$ ($E_0 = -7.311780$ (top), $E_1 = -7.177059$ (middle), $E_2 = -6.499407$ (bottom)). Four copies of the lattice are plotted. The left column is $\text{Re}(\tilde{\psi}(\mathbf{r}))$ (real part of the wavefunction in relative position space) and the right column is $|g(\mathbf{q})|^2$ (probability of finding one particle with momentum $\mathbf{q}$).
Table 3.2: The 12 low-lying noninteracting and exact two-particle energies of the 10×11 lattice with total momentum P = (0, 0). q₁ and q₂ = P − q₁ are the momentum vectors. (Note we do not imply correspondence when we list the noninteracting exact energies side by side.)

<table>
<thead>
<tr>
<th>q₁</th>
<th>q₂</th>
<th>E(q₁) + E(q₂)</th>
<th>boson</th>
<th>fermion</th>
</tr>
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<td>-2.82420928838594</td>
</tr>
</tbody>
</table>

For the fermion states, it is not possible, due to Pauli exclusion, to have two particles both with momentum zero. From diagonalization, the ground state is seen to be concentrated at momenta (0, ±1), the first excited state at (±1, 0), and the second excited state is concentrated at (±1, ±1). It is interesting to observe that these three states correspond to the momentum vectors of the three low-lying noninteracting states (excluding q₁ = q₂ = (0, 0) which cannot be a fermion state).
fermion states. We will return to this important concept in later chapters as the
t-matrix makes this correspondence explicit.

3.7 Equations for Rectangular-Boundary Lattices

Our equation for energy \( \det G(E) = 0 \) (3.34) is good for arbitrary boundaries. But
because it is a determinant equation, it involves all 16 matrix elements. In order to
extract some analytical content from this equation we would much prefer equations
that involve only a small number of matrix elements. In this section we look more
closely at the structure of the matrix \( G_{ij}(E) \) for rectangular lattices and use lattice
symmetries to obtain simpler versions of the determinant equation (3.34).

We specialize to the case \( P = 0 \) and rectangular-boundary lattices. We have
from Eq. 3.30,

\[
G_{ij}(E) = \frac{1}{N} \sum_{q} \frac{\epsilon_{i} q (R_{j} - R_{i})}{E - 2 \epsilon(q)} = \frac{1}{N} \sum_{q} \frac{\cos(q_{x}(R_{jx} - R_{ix})) \cos(q_{y}(R_{jy} - R_{iy}))}{E - 2 \epsilon(q)},
\]

(3.40)

where \( R_{i} = \{ (\pm 1, 0), (0, \pm 1) \} \) corresponding to the relative positions where the poten-
tial is nonzero (see Eq. 3.13) and in the last step we have used the symmetry
properties of the energy function \( \epsilon(q_{x}, q_{y}) = \epsilon(q_{x}, -q_{y}) = \epsilon(-q_{x}, q_{y}) \). It is conve-
nient for this and later sections to define a new notation for the Green function \( G_{ij} \),
emphasizing its dependence on \( R_{j} - R_{i} \),

\[
\Gamma(E, m, n) = \frac{1}{N} \sum_{q} \frac{\cos(m q_{x}) \cos(n q_{y})}{E + 4 \cos q_{x} + 4 \cos q_{y}},
\]

(3.41)

where the sum is over the \( N \) reciprocal lattice vectors \( q = (2\pi l_{x}/L_{x}, 2\pi l_{y}/L_{y}) \) with
\( 0 \leq l_{x} < L_{x} \) and \( 0 \leq l_{y} < L_{y} \) (for one Brillouin zone), and we have used the
expression for \( \epsilon(q) \) from Eq. 3.14 (and taken \( t = 1 \)).
This Green function for rectangular-boundary lattices satisfies the following reflection properties,

\[
\Gamma(E, m, n) = \Gamma(E, -m, n) = \Gamma(E, m, -n) = \Gamma(E, -m, -n). \tag{3.42}
\]

And if we have a square lattice \((L_x = L_y)\) we also have

\[
\Gamma(E, m, n) = \Gamma(E, n, m), \tag{3.43}
\]

a relation that will be used in a later section. With this new notation for Green function \((3.41)\) our matrix elements are

\[
G_{ij}(E) = \Gamma(E, R_{jx} - R_{ix}, R_{jy} - R_{iy}). \tag{3.44}
\]

Table 3.3 shows the vectors \(R_j - R_i\).

Table 3.3: The matrix \(R_j - R_i\) for nearest-neighbor vectors \((\pm 1, 0)\) and \((0, \pm 1)\).

<table>
<thead>
<tr>
<th>(R_j - R_i)</th>
<th>(1,0)</th>
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<td>(-1,-1)</td>
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<td>(-1,1)</td>
<td>(0,2)</td>
<td>(0,0)</td>
</tr>
</tbody>
</table>

Using the reflection properties of \(\Gamma(E, m, n)\), Eq. 3.42, and the definition Eq. 3.44, our matrix becomes,

\[
G_{ij}(E) = \begin{pmatrix}
  a & c & b & b \\
  c & a & b & b \\
  b & b & a & d \\
  b & b & d & a
\end{pmatrix}, \tag{3.45}
\]
where \(a = \Gamma(E, 0, 0), b = \Gamma(E, 1, 1), c = \Gamma(E, 2, 0), \) and \(d = \Gamma(E, 0, 2).\) The eigenvalues and eigenvectors of this matrix are,

\[
\lambda_{f1} = a - c, \quad (1, -1, 0, 0) \\
\lambda_{f2} = a - d, \quad (0, 0, 1, -1) \\
\lambda_{b1,b2} = a + \frac{c + d}{2} \pm \frac{\sqrt{16b^2 + (c - d)^2}}{2}, \quad (v_{1,2}, v_{1,2}, 1, 1) \quad (3.46)
\]

where \(v_1\) and \(v_2\) are complicated functions of \(a, b, c,\) and \(d.\)

The exact energy \(E\) makes the matrix \(G_{ij}(E)\) singular, which means that one of the eigenvalues has to be zero. Setting \(\lambda_{f1} = 0,\) we get \(a = c\) and setting \(\lambda_{f2} = 0,\) \(a = d,\) which are

\[
\Gamma(E, 0, 0) - \Gamma(E, 2, 0) = 0, \quad \Gamma(E, 0, 0) - \Gamma(E, 0, 2) = 0. \quad (3.47)
\]

From Eq. 3.33, the null eigenvector of \(G\) is \(V\phi = V(\tilde{g}(R_1), \tilde{g}(R_2), \tilde{g}(R_3), \tilde{g}(R_4)),\)
where \(R_i = \{(1, 0)(-1, 0)(0, 1)(0, -1)\}, \) \(i = 1, 2, 3, 4.\) From symmetry (Eq. 3.37, with \(P = 0),\) for fermions we should have \(V\phi_1 = -V\phi_2\) and \(V\phi_3 = -V\phi_4,\) and for bosons \(V\phi_1 = V\phi_2\) and \(V\phi_3 = V\phi_4.\) Inspecting the eigenvectors we obtained in Eq. 3.46, we see that the two eigenvalues \(\lambda_{f1,f2}\) are fermion eigenvalues and \(\lambda_{b1,b2}\) are boson eigenvalues, and the two equations in Eq. 3.47 are equations for fermions.

In Fig. 3.5 we have plotted these two relations (3.47) versus \(E\) for the 4×5 lattice. The intersections with the horizontal axis are the exact energies. Comparing these plots with the plot for the determinant equation, Fig. 3.2, we see that we have made some good progress. We have separated the the determinant equation into equations for bosons and fermions. This will not only assist us in extracting analytical results but also facilitate us in doing numerical root finding (now bracketing is much easier, see Sec. 3.4). The eigenstates are easy to find also. For the fermions we know that
\( V \tilde{g}_j = (1, -1, 0, 0) \) or \((0, 0, 1, -1)\), and from Eq. 3.28, we have

\[
\tilde{g}(r) = G(E, P; r, (1, 0)) - G(E, P; r, (-1, 0)), \quad (3.48)
\]

\[
\tilde{g}(r) = G(E, P; r, (0, 1)) - G(E, P; r, (0, -1)), \quad (3.49)
\]

where the \( G \) function here is the original Green function in Eq. 3.26, the first equation corresponds to the eigenvalue \( a - c \) and the second to \( a - d \).

### 3.8 Equations for Square-Boundary Lattices

For bosons, the eigenvalues, Eq. 3.46, are rather complicated for general rectangular-boundary lattices, and we do not have simple equations as those for fermions, Eq. 3.47. We have noted in Sec. 3.7 that for a square-boundary lattice, \( \Gamma(E, m, n) = \Gamma(E, n, m) \), that is to say \( c = d \) in the matrix (3.45). And the boson eigenvalues in (3.46) simplify greatly to \( \lambda_{b1} = a + 2b + c \) and \( \lambda_{b2} = a - 2b + c \), which means that the boson energy equations are,

\[
\Gamma(E, 0, 0) + 2 \Gamma(E, 1, 1) + \Gamma(E, 2, 0) = 0, \quad (3.50)
\]

\[
\Gamma(E, 0, 0) - 2 \Gamma(E, 1, 1) + \Gamma(E, 2, 0) = 0. \quad (3.51)
\]

The corresponding eigenvectors simplify too, to \((1, 1, 1)\) and \((1, 1, -1, -1)\) respectively. These functions of energy on the left-hand side of Eq. 3.50 and Eq. 3.51 can be plotted in the same fashion as the fermion relations in Fig. 3.5 and they facilitate root finding. In the next section, they will also be used for analytical calculations at the large-lattice limit.
Figure 3.5: Plots of two-fermion energy equations, Eq. 3.47, for a $4 \times 5$ lattice. The top graph is $\Gamma(E, 0, 0) - \Gamma(E, 2, 0)$ vs $E$ and the bottom $\Gamma(E, 0, 0) - \Gamma(E, 0, 2)$. The intersections with the horizontal axis are the interacting fermion energies. Compare these with the full plot of the determinant equation (3.34); we have used lattice symmetry to reduce the determinant equation.
3.9 The Large-$L$ Limit For Bosons

The equations (3.47), (3.50) and (3.51) are much better starting points for analytical calculations than the original determinant equation (3.34). In the center of the problem is the lattice Green function $\Gamma(E,m,n)$ defined in Eq. 3.41. Many of the lattice calculations come down to evaluating these lattice Green functions [7, 8, 9, 10, 11]. Incidentally the interesting problem of computing the resistance between two points on a lattice resistor network turns out to be an application of the lattice Green functions [16]. In this section, we derive the large-lattice two-boson energy using the recursion and symmetry relations of the Green function $\Gamma(E,m,n)$.

3.9.1 Recursion Relations

The Green function $\Gamma(E,m,n)$ for general $m$ and $n$ are difficult to evaluate. Ref. [15] gives $\Gamma(E,0,0)$ and $\Gamma(E,1,1)$ for the infinite lattice using the complete elliptic integrals of the first and second kind. The good thing is that there are a number of recursion relations connecting the Green functions at different $m$ and $n$ [14, 15]. In two dimensions, it turns out that if we know $\Gamma(E,0,0)$ and $\Gamma(E,1,1)$, we can use the recursion relations to obtain any $\Gamma(E,m,n)$. For our calculation, some of the recursion relations are of particular convenience and can help us obtain an equation for bosons even simpler than Eq. 3.51.

The two recursion relations that we will use are

\[ E \Gamma(E,0,0) + 4 \Gamma(E,1,0) + 4 \Gamma(E,0,1) = 1, \]  \hfill (3.52)

\[ \Gamma(E,0,0) + 2 \Gamma(E,1,1) + \Gamma(E,2,0) + \frac{1}{2} E \Gamma(E,1,0) = 0. \]  \hfill (3.53)

These relations are easy to check. Note that in the expression for $\Gamma(E,m,n)$ in Eq. 3.41 the denominator is $E + 4\cos q_x + 4\cos q_y$. In Eq. 3.52 the sum of the
numerators is also $E + 4 \cos q_x + 4 \cos q_y$, so the sum of the three Green functions is simply $(1/N) \sum_q 1 = 1$. Eq. 3.53 is proved in the same fashion.

### 3.9.2 Boson, $L \times L$ Lattice

Now we go to the square-boundary lattice case and start with Eq. 3.50 for boson energy. Using the recursion relation (3.53) we get that $\Gamma(E, 1, 0) = 0$. And then using recursion relation (3.52), and the fact that for square-boundary lattices $\Gamma(E, 1, 0) = \Gamma(E, 0, 1)$, we get a simplified equation of Eq. 3.50,

$$\Gamma(E, 0, 0) = \frac{1}{E}, \quad (3.54)$$

with eigenvector $(1, 1, 1, 1)$. This is where we can start doing analytical calculation, because $\Gamma(E, 0, 0)$ is the easiest among all $\Gamma(E, m, n)$ to evaluate. In the following, we will work on the boson problem on the square-boundary lattice.

### 3.9.3 $\Gamma(E, 0, 0)$

In this section we compute the leading form of $\Gamma(E, 0, 0)$ for large $L$ of a square-boundary lattice. The calculation is close to that in Ref. [13] for the Hubbard model. We have, from Eq. 3.41,

$$\Gamma(E, 0, 0) = \frac{1}{N} \sum_q \frac{1}{E + 4 \cos q_x + 4 \cos q_y} = \frac{1}{4N} \sum_q \frac{1}{2 - \cos q_x - \cos q_y - \Delta E/4}, \quad (3.55)$$

where we have defined $E = -8 + \Delta E$. Because the lowest energy of an independent particle is $\mathcal{E}(0) = -4$, $\Delta E$ is the energy correction to two independent particle energy at zero momentum. In Eq. 3.55, the largest contribution from the sum is from the $q = 0$ term, we take that out of the sum and get,

$$\Gamma(E, 0, 0) = \frac{1}{L^2 \Delta E} - \frac{1}{4N} \sum_{q \neq 0} \frac{1}{2 - \cos q_x - \cos q_y - \Delta E/4}$$
\[
\frac{1}{L^2 \Delta E} - \frac{1}{4} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{d^2 q}{(2\pi)^2} \frac{1}{2 - \cos q_x - \cos q_y}
\approx \frac{1}{L^2 \Delta E} - \frac{1}{4\pi} \int_{2\pi/L}^{\pi} dq
\approx \frac{1}{L^2 \Delta E} - \frac{\ln L}{4\pi} + \text{const.}
\]

(3.56)

We should discuss the number of approximations we have made to extract this leading dependence in \(L\). First except in the \(q = 0\) term we have ignored the \(\Delta E\) term, assuming it is small as compared to \(q^2\) (with \(q \neq 0\)). This is justified as we only want the leading term in the large-\(L\) limit. Using an integral for a lattice sum is another approximation. We choose the lower limit of integration to be \(2\pi/L\) corresponding to the first reciprocal lattice vectors after \((0,0)\) is taken out of the sum. We also used the harmonic approximation for the energy function. (See Fig. 3.1 for a plot of the energy.)

### 3.9.4 The Large-\(L\) Limit of Two Bosons

Using the boson energy equation (3.54) and the large-\(L\) limit of the Green function (3.56), we get,

\[
\frac{1}{-8 + \Delta E} \approx \frac{1}{L^2 \Delta E} - \frac{\ln L}{4\pi} + \text{const.}
\]

(3.57)

In the large-\(L\) limit, \(\Delta E \to 0\) (as it is the interaction correction to the noninteracting energy), so we get, to the leading order of \(L\),

\[
\Delta E = \frac{4\pi}{L^2 \ln L},
\]

(3.58)

and the two-boson energy is,

\[
E \approx -8 + \Delta E,
\]

(3.59)

where \(-8\) is the energy for two noninteracting bosons with zero momentum. In Fig. 3.6 we plot the two-particle energies from exact diagonalization for \(L \times L\) lattices,
including bosons with total momentum $\mathbf{P} = (0, 0)$ and fermions with $\mathbf{P} = (0, 0)$ and $(0, 1)$. (See Table D.2 for numerical values.) Not surprisingly, the energies approach the noninteracting energy, $-8$, in the large-$L$ limit ($\Delta E \rightarrow 0$). Also included in the figure is $-8 + \Delta E = -8 + 4\pi/(L^2 \ln L)$ (bold line), which approaches the boson curve at the large-$L$ limit.

Note that in our calculation for $\Gamma(E, 0, 0)$ (3.56), we have neglected the contribution of $\Delta E$ in the denominator except for the first term ($\mathbf{q} = 0$). Now with the leading form of $\Delta E$ we can obviously plug (3.59) into (3.56) to get the form of the next term. We use the following fitting form (which is also used in Ref. [13] for three electrons in the two-dimensional Hubbard model),

$$\Delta E = \frac{4\pi}{L^2 \ln L} \left( A + \frac{B}{\ln L} + \frac{C}{(\ln L)^2} \right). \quad (3.60)$$

In Fig. 3.7, we plot $(E - (-8))L^2 \ln L/(4\pi)$ vs $1/\ln L$. According to our functional form (3.60), we should have $(E - (-8))L^2 \ln L/(4\pi) = A + B/\ln L + C/(\ln L)^2$, i.e., the leading order coefficient $A$ can be determined from quadratic fitting. Fig. 3.7 shows that $A \approx 1$, agreeing with the analytical calculation (3.58).

### 3.9.5 Comments on Fermion Large-$L$

How about two fermions on a large lattice? We expect that we can also write $E = E_0 + \Delta E$. Can we obtain $\Delta E$ for large $L$? For $\mathbf{P} = (0, 0)$, our formalism in Sec. 3.7 applies, and the equation that we need to use is Eq. 3.47. However, as can be seen in Fig. 3.6, the $\mathbf{P} = (0, 0)$ ground state is not the absolute ground state for two fermions on a $L \times L$ lattice; the energy from the $\mathbf{P} = (0, 1)$ sector is lower. Therefore, if we wish to obtain the two-fermion ground state energy in the large-$L$ limit, we cannot use the formalism in Sec. 3.7, and we should go back to the determinant equation Eq. 3.34. We have not worked out this problem.
Figure 3.6: Two-particle groundstate energies for $L \times L$ lattice. Bosons with $\mathbf{P} = (0,0)$ and fermions with $\mathbf{P} = (0,0)$ and $(0,1)$. In the large-$L$ limit the energies approach the energy for two independent particles (-8). The bold line is $-8 + 4\pi/(L^2 \ln L)$. 
Figure 3.7: Groundstate energy of two bosons on a $L \times L$ lattice with $\mathbf{P} = (0, 0)$.

$(E - (-8))L^2 \ln L / (4\pi)$ vs $1/\ln L$. Quadratic fitting gives $(E - (-8))L^2 \ln L / (4\pi) = A + B / \ln L + C / (\ln L)^2$. We get $A \approx 1$. 
3.10 A Few Particles on a Large $L \times L$ Lattice

The procedure used in Sec. 3.9.4 for two bosons can also be applied to problems with a few particles. For a few particles on a large lattice with short-range (here nearest-neighbor) interaction, two-particle interaction is the main contribution to energy. We write for two particles,

$$E(2, L) = E_0(2, L) + \Delta E(L). \quad (3.61)$$

Here in this section we use the notation $E(M, L)$ and $E_0(M, L)$ to denote the $M$-particle exact and noninteracting ground state energies respectively and emphasize the dependence of $\Delta E$ on $L$ by using $\Delta E(L)$. It is reasonable to expect that the energy for $M$ particles is the noninteracting energy plus interaction corrections from the $M(M - 1)/2$ pairs of particles. We then have,

$$E(M, L) \approx E_0(M, L) + \frac{M(M - 1)}{2} \Delta E(L). \quad (3.62)$$

For bosons, $E_0(M, L) = -4M$, because in the ground state, all bosons occupy the zero-momentum state. On the other hand, for fermions, because of Pauli exclusion, no two fermions can occupy the same state, the noninteracting ground state is obtained from filling the $M$ fermions from the lowest state ($k = 0$) up (see Sec. B.6 for a simple program we wrote to calculate the noninteracting ground state energy of a few spinless fermions).

Eq. 3.62 implies that plotting $2(E(M, L) - E_0(M, L))/(M(M - 1))$ vs $L$ for different $M$ should all asymptotically at large $L$ approach $\Delta E(L)$. In Fig. 3.8, we do such plots, for bosons and fermions with $M = 2, 3, 4, 5$. (See Tables D.2, D.3, D.4, and D.5 for numerical values.) The fermion results, from p-wave scattering (as our spinless fermion wave function has to be antisymmetric), are much smaller than the boson results (bold curves) from s-wave scattering. We will return to
this observation in Chapter 8 when we fit the energy vs particle density curve for fermions.

For bosons, \( \Delta E(L) = 4\pi/(L^2 \ln L) \) (Eq. 3.58), and to check the coefficient \( 4\pi \) for \( M > 2 \) in Eq. 3.62, we include higher order terms, as we did for the two-boson calculation in Eq. 3.60. Using Eq. 3.62 and Eq. 3.60, we get, for a few bosons \( (E_0(M, L) = -4M) \),

\[
\frac{(E(M, L) + 4M)L^2 \ln L}{2\pi M(M - 1)} = A + B \frac{1}{\ln L} + C \left( \frac{1}{\ln L} \right)^2. \tag{3.63}
\]

In Fig. 3.9, we plot \( (E(M, L) + 4M)L^2 \ln L/(2\pi M(M - 1)) \) vs \( 1/\ln L \) for \( M = 2, 3, 4, 5 \), using the boson data in Fig. 3.8. (The \( M = 2 \) case has been plotted and fitted in Fig. 3.7.) Quadratic polynomial fitting is done for \( M = 2, 3 \), where we have more data than \( M = 4, 5 \). The coefficient \( A \approx 1 \) for both fits, implying, from Eq. 3.60, the leading-order term in \( \Delta E(L) \) is indeed \( 4\pi/(L^2 \ln L) \). \( B \) and \( C \) from two fits are also comparable.

To summarize, from Eq. 3.62 and Eq. 3.60 and fitting in Fig. 3.9, we find that in our model the energy of a small number \( M \) of bosons on a large \( L \times L \) lattice is to the leading order of \( L \),

\[
E(M, L) \approx -4M + \frac{M(M - 1)}{2} \frac{4\pi}{L^2 \ln L}. \tag{3.64}
\]

For fermions, \( \Delta E(L) \) requires, as we explained in Sec. 3.9.5, studying the Green function with \( \mathbf{P} = (0, 1) \). We hope to treat this problem in a future work.

### 3.11 Summary and Outlook

This chapter contains lots of equations, but the idea is clear. We want to study the problem of two particles in our system. We start with the Schrödinger equation and
Figure 3.8: Boson and fermion $2(E(M, L) - E_0(M, L))/(M(M - 1))$ vs $L$ for $M = 2, 3, 4, 5$. All curves appear to converge at large $L$. The fermion (p-wave) result is much less than the boson result (s-wave). The $M = 4$ plot goes to $L = 20$ and the $M = 5$ plot to $L = 10$. The boson $M = 5$ curve is too high to be included in this plot. See Tables D.2, D.3, D.4, and D.5 for numerical values.
Figure 3.9: Boson \((E(M, L) + 4M)L^2 \ln L/(2\pi M(M - 1))\) vs \(1/\ln L\) for \(M = 2, 3, 4, 5\). Quadratic polynomial fitting is done for \(M = 2\) and \(M = 3\). The fitted constant coefficients are approximately one, and the other coefficients from \(M = 2\) and \(M = 3\) are comparable.
derive a lattice Green function formulation. We numerically solve the resulting determinant equation for eigenenergies and eigenstates. But this determinant equation is too hard to study analytically. We specialize to rectangular-boundary lattice and $P = 0$ and obtain simplified equations. For the boson case, on the square-boundary lattice, we get an especially simple equation, which we use to obtain the two-boson energy in the large-lattice limit. And using the two-body result, we show that we can obtain the energy of a few particles on a large lattice.

The key in this calculation is lattice Green function. Schrodinger equation is written in terms of the Green function and the manipulations afterwards rely on symmetry properties of the Green function. Finally, the large-lattice limit is obtain by evaluating $\Gamma(E, 0, 0)$, the simplest of all two-dimensional lattice Green functions.

The following is a more detailed summary, collecting together the important equations.

**Hamiltonian and Wavefunction**

We start by transforming the Hamiltonian to momentum space (3.11)

\[
T = \sum_p \mathcal{E}(p) c_p^+ c_p, \quad U = \frac{1}{2N} \sum_{pp'k} V(k) c_p^+ c_{p'}^+ c_{p+k} c_{p-k}.
\]

We then introduce the two-particle wave function in momentum space $|\psi\rangle$ and the coefficient function $g(q)$ (3.17)

\[
|\psi\rangle = \frac{1}{2} \sum_{q_1} g(q_1) |q_1, P - q_1\rangle.
\]

**Schrodinger Equation and Green Function**

We apply the Hamiltonian operator to $|\psi\rangle$ and obtain a Schrodinger equation on $g(q)$ (3.22). Then we transform $g$ to the relative coordinate space and using the
lattice Green function (3.26)

\[ G(E, \mathbf{P}; \mathbf{r}, \mathbf{r}') = \frac{1}{N} \sum_{\mathbf{q}} \frac{e^{i\mathbf{q} \cdot (\mathbf{r}' - \mathbf{r})}}{E - \mathcal{E}(\mathbf{q}) - \mathcal{E}(\mathbf{P} - \mathbf{q})}, \]

we obtain a new form of the Schrodinger equation (3.27). This equation is then simplified for the case of nearest-neighbor interaction, and we obtain a closed set of 4 × 4 equations in a matrix form (3.29)

\[ \tilde{\mathcal{g}}(\mathbf{R}_i) = \sum_j G(E, \mathbf{P}, \mathbf{R}_i, \mathbf{R}_j) (V \tilde{\mathcal{g}}(\mathbf{R}_j)). \]

This has also been written as a determinant equation (3.34)

\[ \det \mathcal{G}(E, \mathbf{P}) = 0. \]

**Eigenenergies and Eigenstates**

We then plotted this determinant function and find roots numerically using the bisection method. With energy computed numerically, the eigenstates are obtained and plotted. We see that \( g(\mathbf{q}) \) for the low-lying states suggests close relation to the noninteracting problem.

**Rectangular-Boundary Lattice, New Fermion Equations**

Then by employing the reflection properties of the Green function we simplify the determinant equation and after defining \( \Gamma(E, m, n) \) (3.41)

\[ \Gamma(E, m, n) = \frac{1}{N} \sum_{\mathbf{q}} \frac{\cos(mq_x) \cos(nq_y)}{E + 4 \cos q_x + 4 \cos q_y}, \]

we obtain Eq. 3.47

\[ \Gamma(E, 0, 0) - \Gamma(E, 2, 0) = 0, \quad \Gamma(E, 0, 0) - \Gamma(E, 0, 2) = 0. \]

for fermions on a general rectangular-boundary lattice and Eq. 3.50.
Square-Boundary Lattice, New Boson Equations

We also obtain Eq. 3.51 for bosons on a square lattice

\[ \Gamma(E, 0, 0) + 2 \Gamma(E, 1, 1) + \Gamma(E, 2, 0) = 0, \]
\[ \Gamma(E, 0, 0) - 2 \Gamma(E, 1, 1) + \Gamma(E, 2, 0) = 0. \]

One of the equations for bosons (3.51) can be simplified using the recursion relations for Green functions. We obtain a particularly simple equation in Eq. 3.54

\[ \Gamma(E, 0, 0) = \frac{1}{E} \]

which can be analytically studied in the large-lattice limit.

Two-Boson in Large-Lattice Limit

Using the Green function \( \Gamma(E, 0, 0) \) we extract the leading order term of the two-boson groundstate energy (3.59)

\[ E = -8 + \frac{4\pi}{L^2 \ln L} \]

and it compares well with numerical fitting of the exact diagonalization data.

A Few Particles

The two-particle (boson and fermion) large-lattice result can be used to obtain the energy for a few particles on a large lattice,

\[ E(M, L) \approx E_0(M, L) + \frac{M(M - 1)}{2} \Delta E(L). \]

For bosons, we know \( \Delta E(L) = 4\pi/(L^2 \ln L) \), so we have

\[ E(M, L) \approx -4M + \frac{M(M - 1)}{2} \frac{4\pi}{L^2 \ln L}. \]

We do not yet know \( \Delta E(L) \) for fermions and we hope it can be calculated in a future work.
Outlook

Why do we need this Green function formalism while we can numerically diagonalize the two-particle problem relatively easily.\(^4\) The Green function formalism enables us to study the problem analytically, and we are able, as we showed in this chapter, to obtain the large-$L$ dependence of energy. Also the Green function formalism works for arbitrary interaction range and strength. For example, with next-nearest-neighbor interaction, our Green function matrix $G_{ij}$ (Eq. 3.30) becomes $8 \times 8$ with $R_i \in \{[\pm1,0],(0,\pm1),(\pm1,\pm1)\}$, but the solution procedure summarized in Sec. 3.3.4 applies without modification. On the other hand, changing the interaction range or using finite interaction will require significant changes in our diagonalization code.

Furthermore, we know that quantum mechanics can be formulated in a number of different ways: the most familiar one is the Schrödinger equation formulation, but there are also Green function and path integral formulations that are more useful in certain situations. Different approaches often bring added understanding, and the lattice Green function formalism presented in this chapter certainly adds to our understanding of interacting particles on a lattice.

In Chapter 4, we will continue our discussion of the two-particle problem. We will introduce a new formulation, the t-matrix formulation, that captures the essence of two-particle interaction, even for an infinite potential. We will get back to the important problem that was touched upon in this chapter, namely, the correspondence of interacting states with the noninteracting ones. We will see that the t-matrix formulation is particularly useful in addressing this problem and will be crucial in a

\(^4\) The Hamiltonian matrix is at most $N \times N$, where $N$ is the number of lattice sites, because for each total momentum vector $P$, there can be no more than $N$ two-particle basis states.
more precise understanding of the problem with more than two particles than the large-lattice results presented in Sec. 3.10.
Bibliography


Chapter 4

The Two-Particle Problem II: T-Matrix

In Chapter 3, we studied the two-particle problem using lattice Green function and obtained implicit equations for energy. In this chapter, we reformulate the equations for two particles and derive a scattering matrix, the t-matrix, that is the sum of two-body scattering terms to all orders. The t-matrix is essential in studying the dilute (i.e., low particle density) limit. In this chapter we derive the t-matrix for two particles (fermions and bosons) only, where the t-matrix formulation is exact. In Chapter 7, we will use this two-particle t-matrix to study fermion problems with more than two particles; there, the t-matrix is an approximation because it only includes two-body interactions and ignores three or more-body terms.
4.1 Introduction

4.1.1 From Noninteracting to Interacting

One of the interesting observations we made in Chapter 3 (the two-particle problem with lattice Green function) is that in the $10 \times 11$ system we studied, the momentum space distribution of the low-lying two-fermion exact states roughly correspond to the noninteracting states each labeled by a particular set of momentum vectors $\mathbf{q}_1$ and $\mathbf{q}_2$ (see Fig. 3.4 and discussions after that in Sec. 3.6). The equations for energy that we obtained, either the determinant equation (3.34) or the simplified equations (3.47, 3.50, 3.51, 3.54), involve the lattice Green functions $G(E, \mathbf{P}, \mathbf{r}, \mathbf{r}')$ (3.26) or $\Gamma(E, m, n)$ (3.41), which are sums over all reciprocal lattice vectors $\mathbf{q}$ and does not distinguish any subset. For example, Eq. 3.54 says,

$$\Gamma(E, 0, 0) = \frac{1}{N} \sum_{\mathbf{q}} \frac{1}{E + 4 \cos q_x + 4 \cos q_y} = \frac{1}{E}. \quad (4.1)$$

On the other hand, we expect that, at least when the potential $V$ is small, we should be able to write a perturbative equation for energy,

$$E = \mathcal{E}(\mathbf{q}_1) + \mathcal{E}(\mathbf{q}_2) + \Delta E(\mathbf{q}_1, \mathbf{q}_2), \quad (4.2)$$

which is to say that the exact interacting energy of two particles is the noninteracting energy $\mathcal{E}(\mathbf{q}_1) + \mathcal{E}(\mathbf{q}_2)$, for a pair of momenta $\mathbf{q}_1$ and $\mathbf{q}_2$, plus a correction term $\Delta E$ due to the interaction $V$. And with more than two particles, at least when the particle density is low, we expect to have

$$E = \sum_{\mathbf{q}} \mathcal{E}(\mathbf{q}) + \frac{1}{2} \sum_{\mathbf{q}, \mathbf{q}'} \Delta E(\mathbf{q}, \mathbf{q}'). \quad (4.3)$$

In Eq. 4.3, we have used the interaction correction to the two-particle energy $\Delta E$ from Eq. 4.2 to compute two-body interactions, and we used the assumption that
in the low-density limit two-body interactions dominate over three or more-body interactions.

In Sec. 3.9.4 and Sec. 3.10, we studied the ground state energy of a few particles on a large lattice, and we showed that the energy of $M$ particles can be approximated by summing the energy of the $M(M-1)/2$ pairs. Eqs. 4.2 and 4.3 are more precise statements of the ideas presented in Sec. 3.9.4 and Sec. 3.10. They apply to small lattices and to excited states.

Eq. 4.2 and Eq. 4.3 correspond to the so-call “adiabatic continuation” idea, which says that interacting fermion states correspond one-to-one to noninteracting ones as we slowly switch on a potential (see our discussion on Fermi liquid theory in Sec. 1.8.1). In the boson case, because many bosons can occupy one quantum mechanical state and form a condensate, Eq. 4.3 should be modified, but on the other hand, with only two bosons, we expect Eq. 4.2 should be valid.

Eq. 4.2 and Eq. 4.3 highlight the effect of interaction, which is packaged in the energy-shift term $\Delta E$. These formulas enable us to look at a list of noninteracting energies and draw correspondences with the interacting energies. We illustrate this idea in Fig. 4.1 using the two-fermion data in Table. 3.2, for the $10 \times 11$ system with total momentum $\mathbf{P} = (0,0)$. (We will return to this figure at the end of this chapter (Fig. 4.8), after we developed the t-matrix formalism.)

The objective of this chapter is to make Eq. 4.2 explicit for our lattice model, and the objective of Chapter 7 is to make Eq. 4.3 explicit.

### 4.1.2 Infinite (Singular) Potential

One possible objection to our formulas (4.2 and 4.3) is that in our problem, the interaction is infinitely strong. Can the idea of perturbation be applied to a singular
Figure 4.1: From noninteracting energies to interacting energies using t-matrix, for two fermions on the $10 \times 11$ lattice with total momentum $\mathbf{P} = (0, 0)$. Numerical values are in Table 3.2.

potential? This is a problem in the familiar two-particle scattering calculation. The first-order correction to the scattering amplitude, i.e., the first Born approximation, is proportional to the potential, which is infinite. However, this singular potential scattering problem (e.g., hard-sphere interaction in 3D) has been solved (see [1]) by replacing the potential with the so-called scattering length, which is finite even when the potential is infinite. We will show in this chapter (Sec. 4.6) that first of all a perturbation series (Born series) can be written down (that corresponds to a series of the so-called ladder diagrams) and even though each term is proportional to the potential, the sum of all terms (the t-matrix) is finite.
4.1.3 Previous Work

Because the t-matrix captures two-body interaction effects, it is the centerpiece of dilute fermion and boson calculations. Field-theoretical calculations in both three and two dimensions are based on the ladder diagrams and the t-matrix. See Fetter [2] for the 3D problem, Schick [3] for the 2D boson problem and Bloom [4] the 2D fermion problem. (More detailed references are in Chapter 8, where we study the dilute fermion and boson problem in our model.) For lattice fermion problems, Kanamori [5] derived the t-matrix for a tight-binding model that is essentially a Hubbard model (this work is also described in Yosida [6]). And in Mattis’s book [7], §6.11, the t-matrix is worked out explicitly for the Hubbard model, and Kanamori’s result is obtained. The t-matrix formula that Kanamori and Mattis derived is for any dimensions, and Ref. [7] also evaluated the t-matrix for the dilute limit in three dimensions and obtained a functional dependence on particle density.

Rudin and Mattis [8] used the t-matrix expression derived in Refs. [5, 7] and found upper and lower bounds of the fermion t-matrix in two dimensions in terms of particle density. Rudin and Mattis mentioned in Ref. [8] that their bounds, at the time of writing (1985), had not been checked by “M.C. or other means” (Monte Carlo, we presume). In fact, as far as we know, even now, the two-dimensional t-matrix results by Rudin and Mattis have not been checked by numerical calculations.

Rudin and Mattis’s result for energy for the low-density limit of the two-dimensional Hubbard model is of the same functional form as Bloom’s calculation for the two-dimensional fermion hard disks [4]. Since the discovery of high-temperature superconductors, and after it became clear that these materials are quasi-two-dimensional systems, Bloom’s calculation has received a lot of attention because of its relevance to the 2D Fermi liquid controversy (see Sec. 1.8.1). There have been a number of
works on the 2D dilute Fermi gas [9] and on the dilute limit of 2D Hubbard model [10], all using the t-matrix, but these results, as Rudin and Mattis’s result [8], have not been checked by numerical simulations.

In fact, we are not aware of a systematic study of the t-matrix for a lattice model. (The work by Kanamori, Mattis, and Rudin and Mattis are for fermions, and we are not aware of t-matrix studies of lattice boson problems.) We believe that our study here, for the two-particle problem in this chapter (for bosons and fermions) and the few-fermion problem in Chapter 8, is a first such study.

4.1.4 Chapter Organization

This chapter is organized as follows. First we derive the t-matrix in momentum space for both fermions and bosons. We will use symmetry to reduce the problem and as we will see, the fermion and boson equations separate. We then use the symmetry-reduced t-matrix to study the two-particle problem on the $10 \times 11$ lattice. We show how the t-matrix can connect the noninteracting energies to the interacting energies, and we comment on the difference between the boson case and the fermion case. Finally, we write down the Born series for our problem, show that each term corresponds to a ladder diagram, and that the sum is precisely our t-matrix. The Born series makes explicit the physical meaning of the t-matrix: it is the sum total of all two-body scattering terms.

4.2 Setup and Symmetry

To have an equation in the form of Eq. 4.2, we start with any pair of momentum vectors $\mathbf{q}_1$ and $\mathbf{q}_2$ and write noninteracting energy of the pair $E_0 = \mathcal{E}(\mathbf{q}_1) + \mathcal{E}(\mathbf{q}_2)$
and total momentum $\mathbf{P} = \mathbf{q}_1 + \mathbf{q}_2$. Because our Hamiltonian (3.11) conserves total momentum, we can restrict our basis states to $|\mathbf{q}, \mathbf{P} - \mathbf{q}\rangle$. It is tempting to take $|\mathbf{q}_1, \mathbf{P} - \mathbf{q}_1\rangle$ and $|\mathbf{q}_2, \mathbf{P} - \mathbf{q}_2\rangle$ as our nonperturbed states, but there can be other two-particle states with the same total momentum $\mathbf{P}$ and energy $E_0$.

In fact, our energy dispersion function is (3.14),

$$\mathcal{E} (\mathbf{q}) = -2t (\cos q_x + \cos q_y), \quad (4.4)$$

So if we write $\mathbf{q}_1 = (q_{1x}, q_{1y})$ and $\mathbf{q}_2 = (q_{2x}, q_{2y})$, and define $\mathbf{q}_3 = (q_{1x}, q_{2y})$ and $\mathbf{q}_4 = (q_{2x}, q_{1y})$ then we have, $\mathbf{q}_1 + \mathbf{q}_2 = \mathbf{q}_3 + \mathbf{q}_4$ and $\mathcal{E}(\mathbf{q}_1) + \mathcal{E}(\mathbf{q}_2) = \mathcal{E}(\mathbf{q}_3) + \mathcal{E}(\mathbf{q}_4)$. We call this fact, that component exchanges in the pair $\mathbf{q}_1$ and $\mathbf{q}_2$ gives a pair $\mathbf{q}_3$ and $\mathbf{q}_4$ that have the same total momentum and energy, the *pair component exchange symmetry* of our energy dispersion function $\mathcal{E}(\mathbf{q})$. This symmetry is illustrated in Fig. 4.2 and is due to the fact that our $\mathcal{E}(\mathbf{q})$ is separable into an $x$ part and a $y$ part (i.e., $\mathcal{E}(\mathbf{q}) = \mathcal{E}_x(q_x) + \mathcal{E}_y(q_y)$ where $\mathcal{E}_x(q) = -2t \cos q = \mathcal{E}_y(p)$ in our model\(^1\).

\[ \begin{align*}
\mathbf{q}_1 &= (q_{1x}, q_{1y}) & \bullet & \mathbf{q}_2 &= (q_{2x}, q_{2y}) \\
\mathbf{q}_3 &= (q_{1x}, q_{2y}) & \bullet & \mathbf{q}_4 &= (q_{2x}, q_{1y})
\end{align*} \]

\[ \text{Figure 4.2: Pair component exchange symmetry of our energy dispersion function} \]

\[ \mathcal{E}(\mathbf{k}) \text{ in Eq. 4.4. We have } \mathbf{q}_1 + \mathbf{q}_2 = \mathbf{q}_3 + \mathbf{q}_4 \text{ and } \mathcal{E}(\mathbf{q}_1) + \mathcal{E}(\mathbf{q}_2) = \mathcal{E}(\mathbf{q}_3) + \mathcal{E}(\mathbf{q}_4). \]

\(^1\)Note that, anisotropic hopping dispersion $\mathcal{E}(\mathbf{q}) = -2t_x \cos q_x - 2t_y \cos q_y$, where $\mathcal{E}_x(q) = -2t_x \cos q$ and $\mathcal{E}_y(q) = -2t_y \cos q$, also has this pair component exchange symmetry.
The pair component exchange symmetry says that if \( q_{1x} \neq q_{2x} \) and \( q_{1y} \neq q_{2y} \), then the state \(|\mathbf{q}_3, \mathbf{q}_4\rangle\), with \( \mathbf{q}_3 \) and \( \mathbf{q}_4 \) defined above using component exchange, has the same total momentum and energy as \(|\mathbf{q}_1, \mathbf{q}_2\rangle\). The degenerate perturbation theory requires \(|\mathbf{q}_3, \mathbf{q}_4\rangle\) should be included in the set of nonperturbed states with \(|\mathbf{q}_1, \mathbf{q}_2\rangle\).

With a noninteracting two-particle energy \( E_0 \) and total momentum \( \mathbf{P} \), we divide the \( N \) reciprocal lattice vectors into two disjoint sets,

\[
Q_I = \{ \mathbf{q} | \mathcal{E}(\mathbf{q}) + \mathcal{E}(\mathbf{P} - \mathbf{q}) = E_0 \}, \quad Q_{II} = \{ \mathbf{q} | \mathbf{q} \notin Q_I \}. \tag{4.5}
\]

Note that if \( \mathbf{q} \in Q_I \) then \( \mathbf{P} - \mathbf{q} \in Q_I \). Denote \( N_1 \) the number of elements in \( Q_I \) and \( N_2 = N - N_1 \) the number of elements in \( Q_{II} \).

With this separation of \( \mathbf{q} \), our eigenstate (3.17) becomes

\[
|\psi\rangle = \sum_{\mathbf{q} \in Q_I} g(\mathbf{q})|\mathbf{q}, \mathbf{P} - \mathbf{q}\rangle + \sum_{\mathbf{q} \in Q_{II}} g(\mathbf{q})|\mathbf{q}, \mathbf{P} - \mathbf{q}\rangle, \tag{4.6}
\]

where the first sum contains all states whose noninteracting energy is degenerate.\(^2\)

Using the idea of degenerate perturbation theory, we expect to be able to find a secular matrix \( \mathbf{T} \), \( N_1 \times N_1 \), for the degenerate states in \( Q_I \) only, and \( \mathbf{T} \) will eventually be our momentum space t-matrix, which we will derive now.

Note that \(|\mathbf{q}, \mathbf{P} - \mathbf{q}\rangle = s_{bf}|\mathbf{P} - \mathbf{q}, \mathbf{q}\rangle\), where \( s_{bf} \) is the sign defined in Eq. 3.3, \( s_{bf} = 1 \) for bosons, and \( s_{bf} = -1 \) for fermions. This is to say that the number of independent states in the first sum of Eq. 4.6 is less than \( N_1 \). We include both \(|\mathbf{q}, \mathbf{P} - \mathbf{q}\rangle \) and \(|\mathbf{P} - \mathbf{q}, \mathbf{q}\rangle \) in our calculation because we are considering boson and fermion problems at the same time: the symmetric solution \( g(\mathbf{q}) = g(\mathbf{P} - \mathbf{q}) \) is a boson solution and the antisymmetric solution \( g(\mathbf{q}) = -g(\mathbf{P} - \mathbf{q}) \) is a fermion solution (see Eq. 3.18).

\(^2\)In Eq. 4.6, we left out an overall \( 1/2 \) factor in 3.17.
4.3 Derivation of the T-Matrix

Our purpose is to derive a set of closed equations for \( g(\mathbf{q}) \), the coefficient in our two-particle state Eq. 4.6, with \( \mathbf{q} \in Q_I \).

4.3.1 Schrodinger Equation and Fourier Transform

We start with the Schrodinger equation for the two-particle state \(|\psi\rangle\), Eq. 3.22,

\[
(E - \mathcal{E}(\mathbf{q}) - \mathcal{E}(\mathbf{P} - \mathbf{q}))g(\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{k}} V(\mathbf{q} - \mathbf{k})g(\mathbf{k}).
\]

(4.7)

which we derived in Sec. 3.3.1. Expressing \( V(\mathbf{q} - \mathbf{k}) \) in terms of the Fourier transform, we get from Eq. 4.7,

\[
(E - \mathcal{E}(\mathbf{q}) - \mathcal{E}(\mathbf{P} - \mathbf{q}))g(\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{r'}} e^{i\mathbf{q}\cdot\mathbf{r'}} V(\mathbf{r'}) \tilde{g}(\mathbf{r'}),
\]

(4.8)

where \( \tilde{g}(\mathbf{r}) \) is the Fourier transform of \( g(\mathbf{q}) \) as defined in Eq. 3.25

\[
\tilde{g}(\mathbf{r}) = \sum_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{r}} g(\mathbf{q}).
\]

(4.9)

Eq. 4.8 is for a general potential \( V(\mathbf{r}) \), as in the general Hamiltonian Eq. 3.10, where \( \mathbf{r} \) is the separation between two particles.

4.3.2 \( G^{II} \) and \( \tilde{g} \)

For \( \mathbf{q} \in Q_{II} \), if we assume that \( E \neq \mathcal{E}(\mathbf{q}) + \mathcal{E}(\mathbf{P} - \mathbf{q}) \), i.e., the exact energy is not one of the noninteracting energies for the set \( Q_{II} \), then, after dividing the energy difference factor in Eq. 4.8 and summing over \( \mathbf{q} \in Q_{II} \), we have,

\[
\sum_{\mathbf{q} \in Q_{II}} e^{-i\mathbf{q}\cdot\mathbf{r}} g(\mathbf{q}) = \sum_{\mathbf{r'}} \left[ \frac{1}{N} \sum_{\mathbf{q} \in Q_{II}} e^{i\mathbf{q}\cdot(\mathbf{r'} - \mathbf{r})} \frac{1}{E - \mathcal{E}(\mathbf{q}) - \mathcal{E}(\mathbf{P} - \mathbf{q})} V(\mathbf{r'}) \tilde{g}(\mathbf{r'}) \right].
\]

(4.10)

We next define a Green function for the set \( Q_{II} \),

\[
G^{II}(E, \mathbf{P}; \mathbf{r}, \mathbf{r'}) = \frac{1}{N} \sum_{\mathbf{q} \in Q_{II}} \frac{e^{i\mathbf{q}\cdot(\mathbf{r'} - \mathbf{r})}}{E - \mathcal{E}(\mathbf{q}) - \mathcal{E}(\mathbf{P} - \mathbf{q})}.
\]

(4.11)
and a Fourier transform with vectors in $Q_I$,

$$\tilde{g}^I(r) = \sum_{q \in Q_I} e^{-iqr} g(q). \quad (4.12)$$

Then Eq. 4.10 becomes,

$$\tilde{g}^I(r) = \tilde{g}(r) - \sum_{r'} G^{II}(E, P; r, r') V(r') \tilde{g}(r'). \quad (4.13)$$

### 4.3.3 $\phi$ in terms of $\phi^I$

We proceed by restricting to the nearest-neighbor repulsion potential (3.13),

$$V(r) = \begin{cases} V, & r = (\pm 1, 0)(0, \pm 1), \\ 0, & \text{otherwise} \end{cases} \quad (4.14)$$

Then Eq. 4.13 becomes,

$$\tilde{g}^I(r) = \tilde{g}(r) - \sum_{j} G^{II}(E, P; r, R_j)V(R_j), \quad (4.15)$$

where $R_{1,2} = (\pm 1, 0)$ and $R_{3,4} = (0, \pm 1)$. Now restricting $r = R_i$ in Eq. 4.15, we get a set of four equations,

$$\phi_i^I = \phi_i - \sum_j G^{II}_{ij}(E, P)(V\phi_j), \quad (4.16)$$

where we have written

$$G^{II}_{ij}(E, P) = G^{II}(E, P; R_i, R_j) \quad (4.17)$$

and $\phi_i = \tilde{g}(R_i)$ and $\phi_i^I = \tilde{g}^I(R_i)$. Eq. 4.16 is a matrix equation,

$$\phi^I = (I - G^{II}(E, P)V)\phi, \quad (4.18)$$

where $G^{II}$ is $4 \times 4$, $\phi$ and $\phi^I$ are $4 \times 1$, and $V$ is a scalar (strength of potential). And we can invert the matrix to get,

$$\phi = (I - G^{II}(E, P)V)^{-1} \phi^I. \quad (4.19)$$
Eq 4.19 is of crucial importance in this t-matrix calculation. It expresses the Fourier transform \( \tilde{g} \) of \( g(q) \) with all \( q \) in terms of the Fourier transform \( \tilde{g}' \) with only \( q \in Q_t \). The information about other \( q \in Q_t \) has been packaged into the Green function \( G_t(E,P) \). The main part of the t-matrix calculation has been completed with the derivation of Eq. 4.19.

### 4.3.4 T-Matrix \( T(E,P;q,q') \) and \( T_{q,q'} \)

At this point, there are two ways to proceed: one in real space and one in momentum space. Here we follow the momentum space formulation because we find that the momentum space t-matrix can be easily simplified by symmetry. The real space formulation, leading to a real space t-matrix, is presented in Appendix E.

Now we go back to Eq. 4.8, restrict the summation to \( R_i \), and substitute in \( V \tilde{g}_i \) from Eq. 4.19, and we get,

\[
(E - \varepsilon(q) - \varepsilon(P - q))g(q)
\]

\[
= \frac{1}{N} \sum_i e^{iq_{R_i}} V \tilde{g}_i
\]

\[
= \frac{1}{N} \sum_{ij} e^{iq_{R_i}} \left( V(I - G_t(E)V)^{-1}\right)_{ij} \tilde{g}'_{j}
\]

\[
= \sum_{q' \in Q_t} \left[ \frac{1}{N} \sum_{ij} e^{iq_{R_i}} e^{-iq'_{R_j}} \left( V(I - G_t(E)V)^{-1}\right)_{ij} \right] g(q'), \tag{4.20}
\]

where in the last step we have used the Fourier transform of \( \tilde{g}'(R_j) \) (4.12). Now let us define

\[
T(E,P;q,q') = \frac{1}{N} \sum_{ij} e^{iq_{R_i}} e^{-iq'_{R_j}} \left( V(I - G_t(E)V)^{-1}\right)_{ij}, \tag{4.21}
\]

then we have,

\[
(E - \varepsilon(q) - \varepsilon(P - q))g(q) = \sum_{q' \in Q_t} T(E,P;q,q')g(q'). \tag{4.22}
\]
If we restrict \( q \in Q_I \), then we have,

\[
(E - E_0)g(q) = \sum_{q' \in Q_I} T(E; \mathbf{P}; q, q')g(q'),
\]

which means,

\[
E = E_0 + \text{Eigenvalue}(\mathcal{T}(E)),
\]

where we have written

\[
\mathcal{T}_{q,q'}(E) = T(E; \mathbf{P}; q, q')
\]

and left out the dependence on \( \mathbf{P} \). Here \( \mathcal{T} (4.25) \) is the t-matrix in momentum space. Both \( q \) and \( q' \) in Eq.4.23 are in \( Q_I \), which means that if there are \( N_1 \) elements in \( Q_I \) then the matrix \( \mathcal{T}(E) \) is \( N_1 \times N_1 \).

Eq. 4.24 is our desired equation that shows explicitly the interaction correction to the noninteracting energy \( E_0 \). This t-matrix formalism for the two-particle problem is exact, and it is exactly equivalent to the Schrodinger equation and the Green function formalism in Chapter 3. The resulting equation is an implicit equation on \( E \). It is of the form \( E = E_0 + \Delta E(E) \) (Eq. 4.2), and we will show in a later section that for fermions the approximation \( E \approx E_0 + \Delta E(E_0) \) is often very good.

### 4.3.5 Connection to the Hubbard Model T-Matrix

The definition of \( T(E, \mathbf{P}; q, q') \) in Eq. 4.21 is a Fourier transform of the real space quantity \( V(I - \mathcal{G}^{II}(E)V)^{-1} \), where the superscript \( II \) denotes the summation over the set \( Q_{II} \) in the Green function (4.11). Here \( \mathcal{G}^{II} \) is \( 4 \times 4 \) because we have nearest-neighbor interaction. When there is only on-site interaction, as is in the usual Hubbard model case, \( \mathcal{G}^{II}(E) = \mathcal{G}^{II}(E, \mathbf{P}, (0, 0), (0, 0)) \), Eq. 4.11, is a scalar, we can simply use the scalar quantity \( V/(I - \mathcal{G}^{II}V) \), which is the t-matrix that has appeared in Kanamori [5], Mattis [7], Rudin and Mattis [8], and Yosida [6]. Our
expression, Eq. 4.21, is more complicated because we have nearest-neighbor interaction (and thus the relevance of \( R_j \)). Next we will see how symmetry considerations can diagonalize the matrix \( \mathcal{T}_{\mathbf{q}, \mathbf{q}'}(E) \).

### 4.3.6 Symmetry Considerations

In Sec. 3.7, after deriving the general Green function equation using \( \mathcal{G}(E) \), we specialized to rectangular-boundary lattices and used lattice reflection symmetries to diagonalize the \( 4 \times 4 \) matrix \( \mathcal{G}(E) \) and obtained scalar equations. Here our t-matrix equation Eq. 4.24 requires us to find the eigenvalues of the t-matrix \( \mathcal{T} \). In this section, we use particle permutation symmetry and pair component exchange symmetry to diagonalize the \( N_1 \times N_1 \) t-matrix \( \mathcal{T}(E) \) for a few special cases.

\( N_1 = 1 \)

There is only one momentum vector in \( Q_I \). Let us write \( Q_I = \{ \mathbf{q}_1 \} \) (this implies that \( \mathbf{p} - \mathbf{q}_1 = \mathbf{q}_1 \)). Then there is only one unperturbed two-particle basis state \( |\mathbf{q}_1, \mathbf{q}_1\rangle \) (see Eq. 4.6). This must be a boson state, and \( \mathcal{T}(E) \) is a number. We write the resulting scalar equation as,

\[
E = E_0 + T_1(E). \tag{4.26}
\]

\( N_1 = 2 \)

Here \( Q_I = \{ \mathbf{q}_1, \mathbf{q}_2 \} \) with \( \mathbf{q}_1 + \mathbf{q}_2 = \mathbf{p} \). The basis states are \( |\mathbf{q}_1, \mathbf{q}_2\rangle \) and \( |\mathbf{q}_2, \mathbf{q}_1\rangle \). The symmetric (boson) combination is \( (|\mathbf{q}_1, \mathbf{q}_2\rangle + |\mathbf{q}_2, \mathbf{q}_1\rangle) / \sqrt{2} \), and the antisymmetric (fermion) combination is \( (|\mathbf{q}_1, \mathbf{q}_2\rangle - |\mathbf{q}_2, \mathbf{q}_1\rangle) / \sqrt{2} \). These have to be the eigenvectors
of $T(E)$. And that is to say that if we define

$$S_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix},$$

then we have $S_2 = S_2^1, S_2^2 = I$, and

$$S_2 T(E) S_2 = \begin{pmatrix} T_{1,1}(E) & 0 \\ 0 & T_{1,-1}(E) \end{pmatrix}.$$

Here $T_{1,1}(E)$ and $T_{1,-1}(E)$ are scalars that correspond to boson and fermion symmetries respectively. And our $t$-matrix equation (4.24) is reduced to two scalar equations,

$$E = E_0 + T_{1,1}(E), \quad E = E_0 + T_{1,-1}(E),$$

for bosons and fermions respectively.

$N_1 = 4$

Here $Q_I = \{q_1, q_2, q_3, q_4\}$ with $q_1 + q_2 = q_3 + q_4 = P$. The basis states are $|q_1, q_2\rangle, |q_2, q_1\rangle, |q_3, q_2\rangle$, and $|q_2, q_1\rangle$. Using particle permutation symmetry, we get two boson states

$$a(|q_1, q_2\rangle + |q_2, q_1\rangle) + b(|q_3, q_4\rangle + |q_4, q_3\rangle),$$

$$a(|q_1, q_2\rangle + |q_2, q_1\rangle) - b(|q_3, q_4\rangle + |q_4, q_3\rangle),$$

and two fermion states,

$$a(|q_1, q_2\rangle - |q_2, q_1\rangle) + b(|q_3, q_4\rangle - |q_4, q_3\rangle),$$

$$a(|q_1, q_2\rangle - |q_2, q_1\rangle) - b(|q_3, q_4\rangle - |q_4, q_3\rangle)$$

where $a$ and $b$ are arbitrary coefficients to be determined.
If we have \( q_3 = (q_{1x}, q_{2y}) \) and \( q_4 = (q_{2x}, q_{1y}) \), i.e., the pair \( q_1 \) and \( q_2 \) and the pair \( q_3 \) and \( q_4 \) have same total momentum and energy due to the pair component exchange symmetry discussed in Sec. 4.2 (see Fig. 4.2), then we find from numerical calculations that \( a = b \). That is to say that if we define

\[
S_4 = \frac{1}{2} \begin{pmatrix}
1 & 1 & 1 & 1 \\
1 & 1 & -1 & -1 \\
1 & -1 & 1 & -1 \\
1 & -1 & -1 & 1
\end{pmatrix},
\]

(4.34)

with \( a \) and \( b \) both equal to 1/2 to get the normalization right, then we have \( S_4 = S_4' \), \( S_4^2 = I \), and

\[
S_4\mathcal{T}(E)S_4 = \begin{pmatrix}
T_{1,1,1,1}(E) & 0 & 0 & 0 \\
0 & T_{1,1,-1,-1}(E) & 0 & 0 \\
0 & 0 & T_{1,-1,1,-1}(E) & 0 \\
0 & 0 & 0 & T_{1,-1,-1,1}(E)
\end{pmatrix}.
\]

(4.35)

Here the four \( T' \)'s are scalars; they are the eigenvalues of \( \mathcal{T}(E) \). And our t-matrix equation (4.24) is reduced to

\[
E = E_0 + T_{1,1,1,1}(E), \quad E = E_0 + T_{1,1,-1,-1}(E),
\]

(4.36)

for bosons and

\[
E = E_0 + T_{1,-1,1,-1}(E), \quad E = E_0 + T_{1,-1,-1,1}(E),
\]

(4.37)

for fermions.

The three cases \( N_1 = 1, 2, \) and \( N_1 = 4 \) with pair component exchange symmetry are three special cases in which we know the eigenvectors of \( \mathcal{T} \) and can therefore diagonalize \( \mathcal{T} \) from symmetry considerations easily. For arbitrary cases, we return
to Eq. 4.24 and diagonalize $\mathcal{T}$ numerically. For example, on a $L \times L$ lattice, the pairs $(0,1)(0,-1)$ and $(1,0)(-1,0)$ have the same total energy and momentum, but this is not due to the pair component exchange symmetry. In this case, we numerically diagonalize the $4 \times 4$ matrix $\mathcal{T}(E)$, and we find that in the fermion eigenvectors, Eqs. 4.32 and 4.33, $a \neq b$.

### 4.3.7 T-Matrix Summarized

Here we summarize the steps of the t-matrix approach to the two-particle problem for a general potential strength $V$, and for both bosons and fermions.

1. Given $\mathbf{q}_1$ and $\mathbf{q}_2$, with the total noninteracting energy $E_0 = \mathcal{E}(\mathbf{q}_1) + \mathcal{E}(\mathbf{q}_2)$ and total momentum $\mathbf{P} = \mathbf{q}_1 + \mathbf{q}_2$, form $Q_I$ and $Q_{II}$ (with $N_1$ and $N_2$ elements).

2. Solve for $E$ in $E = E_0 + \text{Eigenvalue}(\mathcal{T}(E))$, where $\mathcal{T}(E)$ is given by

   (a) Form the $4 \times 4$ matrix $\mathcal{G}^{II}_{ij}(E) = G^{II}(E; \mathbf{P}; \mathbf{R}_i, \mathbf{R}_j)$ using Eq. 4.11,
   
   $$G^{II}(E; \mathbf{P}; \mathbf{r}, \mathbf{r}') = \frac{1}{N} \sum_{\mathbf{q} \in Q_{II}} \frac{e^{i \mathbf{q}(\mathbf{r}' - \mathbf{r})}}{E - \mathcal{E}(\mathbf{q}) - \mathcal{E}(\mathbf{P} - \mathbf{q})},$$

   (b) Invert $I - \mathcal{G}^{II}(E)V$.

   (c) Form the t-matrix $\mathcal{T}_{\mathbf{q},\mathbf{q}'} = T(E; \mathbf{P}; \mathbf{q}, \mathbf{q}')$ for $\mathbf{q}, \mathbf{q}' \in Q_I$, using Eq. 4.21,
   
   $$T(E; \mathbf{P}; \mathbf{q}, \mathbf{q}') = \frac{1}{N} \sum_{ij} e^{i \mathbf{q} \mathbf{R}_i} e^{-i \mathbf{q}' \mathbf{R}_j} \left(V(I - \mathcal{G}^{II}(E)V^{-1})\right)_{ij}.$$

   (d) If we have $N_1 = 2$ or $N_1 = 4$ with pair component exchange symmetry, we can find the eigenvalues of $\mathcal{T}(E)$ easily, by forming the symmetry reduced t-matrices, e.g., for $N_1 = 2$, $T_{1,1}(E)$ and $T_{1,-1}(E)$, and for $N_4$, $T_{1,1,1,1}(E)$, $T_{1,1,-1,-1}(E)$, $T_{1,-1,1,-1}(E)$, and $T_{1,-1,-1,1}(E)$. Then we just need to solve a scalar equation $E = E_0 + T(E)$, where $T(E)$ stands the
symmetry reduced functions, $T_{1,-1}(E)$ for example. (For a general case, we diagonalize $\mathcal{T}(E)$, and $T(E)$ is one of the eigenvalues.)

3. The corresponding eigenvector is $g(q)$ with $q \in Q_f$. $g(q) = g(P - q)$ is the boson solution, and $g(q) = -g(P - q)$ the fermion solution.

4. For $q \in Q_{II}$, using Eq. 4.22,

$$g(q) = \frac{1}{E - \mathcal{E}(q) - \mathcal{E}(P - q)} \sum_{q' \in Q_f} T(E; P; q, q') g(q').$$  \hfill (4.38)

Note that both the equation $E = E_0 + \text{Eigenvalue} (\mathcal{T}(E))$ and the symmetry reduced equation $E = E_0 + T(E)$ are implicit equations on $E$. The solution of such equations will be discussed below.

Note also that for our case $V = +\infty$, the t-matrix expression Eq. 4.21 becomes

$$T(E; P; q, q') = \frac{1}{N} \sum_{ij} e^{iqR_i} e^{-iq'R_j} \left(-G^{II}(E)^{-1}\right)_{ij},$$  \hfill (4.39)

where the potential $V$ cancels out, giving a finite value. This is one of the advantages of the t-matrix formalism, that it can deal with infinite (singular) potential.

### 4.4 Solving For Energy

The example system that we will study here is $10 \times 11$ with $P = (0,0)$, which was studied using lattice Green function in Sec. 3.6. To facilitate the reader in this section, as we will often refer to the noninteracting and interacting energies of the system, we reproduce Table 3.2 here as Table 4.1. It can be seen that all of the energies listed in Table 4.1 are of the three cases discussed in Sec. 4.3.6: $N_1 = 1$, $N_1 = 2$, and $N_1 = 4$ due to pair component exchange symmetry.
Table 4.1: The 12 low-lying noninteracting and exact two-particle energies of the $10 \times 11$ lattice with total momentum $\mathbf{P} = (0,0)$. $\mathbf{q}_1$ and $\mathbf{q}_2 = \mathbf{P} - \mathbf{q}_1$ are the momentum vectors. Reproduction of Table 3.2.

<table>
<thead>
<tr>
<th>$\mathbf{q}_1$</th>
<th>$\mathbf{q}_2$</th>
<th>$\mathcal{E}(\mathbf{q}_1) + \mathcal{E}(\mathbf{q}_2)$</th>
<th>boson</th>
<th>fermion</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0)</td>
<td>(0,0)</td>
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We solve for energy $E$ in the implicit equation, $E = E_0 + T(E)$, where $T(E)$ represents the eigenvalues of $\mathcal{T}(E)$, e.g., $T_{1, -1}(E)$. We plot $f(E) = E_0 + T(E)$ along with a line $y = E$. Their intersections are the desired energies $E$.

4.4.1 $N_1 = 1$ Case

In Fig. 4.3, we plot $f(E)$ vs $E$ for the $10 \times 11$ lattice with $\mathbf{P} = (0,0)$ and the noninteracting energy $E_0 = -8.0 = \mathcal{E}(0) + \mathcal{E}(0)$. Here $Q_I = \{(0,0)\}$, and the
nonperturbed state is \(|q_1 = (0, 0), P - q_1 = (0, 0)\) which can only be a boson state (because two particles occupy the same zero momentum state). The energy intersections from Fig. 4.3 are \(-7.906, -7.299, -6.971, -6.022,\) and so on. Looking into Table 4.1, we see that these are all boson energies.

![Graph showing the energy levels](image)

Figure 4.3: \(f(E) = E_0 + t_1(E)\) vs \(E\) for 10 \(\times\) 11 lattice with \(P = (0, 0)\) and \(E_0 = -8.0\) (i.e., \(E_0 = \mathcal{E}(0) + \mathcal{E}(0)\).) The intersections with the line \(y = E\) are the exact two-particle energies.

In Fig. 4.3, note also that the energy \(-6.601\), which is an exact eigenenergy from exact diagonalization, does not appear as an intersection in Fig. 4.3. This is a special energy, being also a noninteracting energy. Earlier, as mentioned at the
beginning of Sec. 4.3.2, we assumed that our $E \neq \mathcal{E}(q) + \mathcal{E}(P - q)$ for any $q \in Q_{II}$, so this energy is excluded from our t-matrix formulation. We will address later this kind of exact solutions that are also noninteracting energies.

Note that our equation $E = E_0 + T(E)$ is a reformulation of the Schrödinger equation with certain symmetry considerations ($T_{1,-1,1,-1}$ etc), and it should be satisfied by all energies $E$ with the same symmetry. Building $T(E)$ from $E_0$ and $P$ does not automatically give us a unique interacting energy $E$ that corresponds to the noninteracting energy $E_0$. However, we can see clearly from Fig. 4.3, if we perturb the exact solutions by a small amount $E \to E + \delta$, then $f(E)$ changes drastically except for the lowest energy $E = -7.906$. That is to say that these other energies, for example $E = -6.971$, are exact solutions of the equation $f(E) = E$, but they are not stable solutions. From the plot, only $E = -7.906$ comes close to being stable.

We can be more precise about this notion of stability. If we have an iteration $x_{n+1} = f(x_n)$, and $x^*$ is a fix point (i.e., $f(x^*) = x^*$), then the iteration is linear stable at $x^*$ if and only if $|f'(x^*)| < 1$. In our plots, we have included a line $y = E$ with slope one, which can be used as a stability guide. An intersection (fix point) is linearly stable when the function $f(E)$ at the intersection is not as steep as the straight line.

### 4.4.2 $N_1 = 2$ Case

In Fig. 4.4 we plot for $E_0 = -7.365$ and $P = (0,0)$ with $Q_1 = \{(0,1),(0,-1)\}$. The boson function $f(E) = E_0 + T_{1,1}(E)$ is the dotted line in the top graph, and the fermion function $f(E) = E_0 + T_{1,-1}(E)$ is the solid line in the bottom graph.

The intersections closest to $E_0 = -7.365$ are $-7.299$, the first excited boson
Figure 4.4: $f(E)$ vs $E$ for $10 \times 11$ lattice with $\mathbf{P} = (0, 0)$ and $E_0 = -7.365$ (i.e., $E_0 = \mathcal{E}(0, 1) + \mathcal{E}(0, -1)$.) The top graph (dotted line) is for boson $f(E) = E_0 + T_{1,1}(E)$, and the top graph (solid line) for fermion $f(E) = E_0 + T_{1,-1}(E)$. The fermion curve is essentially flat near $E = E_0$. 
energy (see Table 4.1), and \(-7.311\), the lowest fermion energy. Note that the curve on which the fermion intersection \((-7.311)\) lies is very flat. In other words for this fermion energy \(E \approx E_0 + T(E_0)\), i.e., the first iteration using the noninteracting energy gives an energy very close to the exact value. More precisely, we find with \(E_0 = -7.365014\), \(f(E_0) = E_0 + T(E_0) = -7.310584\), which is very close to \(E = -7.31178\). Many t-matrix calculations \([5, 7, 8, 6]\), use the first iteration \(E \approx E_0 + T(E_0)\) as an approximation to the exact energy, and we see in this case this approximation is very good. (We will come back to this point later in Sec. 4.5.)

### 4.4.3 \(N_1 = 4\) Case

In Fig. 4.5 and Fig. 4.6, we plot \(f(E)\) for \(E_0 = \mathcal{E}(1,-1) + \mathcal{E}(-1,1) = \mathcal{E}(1,1) + \mathcal{E}(-1,-1) = -6.601\) and \(P = (0,0)\). For this \(N_1 = 4\) case we have two boson functions, plotted in Fig. 4.5, \(f(E) = E_0 + T_{1,1,1,1}(E)\) (dotted line) and \(f(E) = E_0 + T_{1,1,-1,-1}(E)\) (dot-dashed line), and we have two fermion functions, plotted in Fig. 4.6, \(f(E) = E_0 + T_{1,-1,1,-1}(E)\) (solid line) and \(f(E) = E_0 + T_{1,-1,-1,1}(E)\) (dashed line). The fermion intersections closest to \(E_0\) are \(-6.499\) and \(-6.470\). Here again the \(f(E)\) curves for these two fermion branches are very flat. The two boson intersections closest to \(E_0\) are \(-6.022\) and \(-6.601\). Note that the latter is also a noninteracting energy, and it is the intersection of the horizontal line \(E = E_0\) with \(y = E\).

One interesting observation of the fermion plot in Fig. 4.6 is that the two closely spaced pair of energies (for example \(-7.311\) and \(-7.177\)) lie on different symmetry curves. We know that if we have a square lattice (for example \(10 \times 10\)) then the noninteracting fermion energies come in pairs. Here, we have chosen a \(10 \times 11\) lattice that is close to a square but does not have exact degeneracies. We see that
Figure 4.5: Boson $f(E)$ vs $E$ for $10 \times 11$ lattice with $P = (0, 0)$ and $E_0 = -6.601$. The dotted line is for $T_{1,1,1,1}$ and the horizontal dot-dashed line for $T_{1,1,-1,-1}$ (which corresponds to a noninteracting state, see text at the end of this section).
Figure 4.6: Fermion $f(E)$ vs $E$ for $10 \times 11$ lattice with $\mathbf{P} = (0, 0)$ and $E_0 = -6.601$. The solid line is for $T_{1,-1,1,-1}$ and the long-dashed line for $T_{1,1,-1,1}$. Note that closely spaced fermion energy pairs are separated by symmetry.
the resulting closely spaced pairs are separated by symmetry considerations.

**Exact Boson Eigenstate**

Another interesting observation from Fig. 4.5 for bosons is that we have a horizontal line that corresponds to \( T_{1,1,-1,-1}(E) = 0 \). For this case the noninteracting energy is an exact energy. That is to say, \((1, 1, -1, -1)\) is a null vector of \( T(E) \) (see Sec. 4.3.6), or the eigenstate,

\[
|\mathbf{q}_1, \mathbf{q}_2\rangle + |\mathbf{q}_2, \mathbf{q}_1\rangle - |\mathbf{q}_3, \mathbf{q}_4\rangle - |\mathbf{q}_4, \mathbf{q}_3\rangle,
\]

(4.40)

with \( \mathbf{q}_3 = (q_{1x}, q_{2y}) \) and \( \mathbf{q}_4 = (q_{2x}, q_{1y}) \) is an exact eigenstate of the Hamiltonian. This can be shown easily using the Schrodinger equation Eq. 4.7. We have \( g(\mathbf{q}_1) = g(\mathbf{q}_2) = 1, \) \( g(\mathbf{q}_3) = g(\mathbf{q}_4) = -1, \) and \( g(\mathbf{q}) = 0 \) for all other \( \mathbf{q} \), and what we want to show is \( V(\mathbf{q} - \mathbf{q}_1) + V(\mathbf{q} - \mathbf{q}_2) - V(\mathbf{q} - \mathbf{q}_3) - V(\mathbf{q} - \mathbf{q}_4) = 0 \). This is quite obvious using the formula for \( V(k) \) in Eq. 3.14 (because \( V(k) \) can be separated into a sum of two terms that involve the \( x \) and \( y \) components separately).

Transforming to the real space, without worrying about normalization, we can show easily,

\[
\tilde{g}(\mathbf{r}) = \sum_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{r}} g(\mathbf{q}) \sim \left( e^{-i q_{1x} x} - e^{-i q_{2x} x} \right) \left( e^{-i q_{1y} y} - e^{-i q_{2y} y} \right),
\]

(4.41)

where we have used the fact mentioned above that \( g(\mathbf{q}) \) is not zero for only four \( \mathbf{q} \)'s which are related by pair component exchange symmetry. It is clear from Eq. 4.41 that \( \tilde{g}(0, y) = 0 = \tilde{g}(x, 0) \), which means that the wave function in relative position space has nodes along \( x \) and \( y \) axes.

Fig. 4.7 is the relative position space plot of the boson exact eigenstate for the \( 10 \times 11 \) lattice with \( E = -6.60108 \) and \( \mathbf{P} = (0, 0) \). In momentum space, this state is \(|(1, 1), (-1, -1)\rangle - |(1, -1), (-1, 1)\rangle \), where both \(|(1, 1), (-1, -1)\rangle \) and
|(1, -1), (-1, 1)| have noninteracting energy $E_0 = -6.60108$. The nodes along $x$ and $y$ axes are clear.

Figure 4.7: Relative position space plot of the boson eigenstate with $E = -6.60108$, $\mathbf{P} = (0,0)$ on the $10 \times 11$ lattice: 3D plot (left) and density plot (right). There are nodes along $x$ and $y$ axes.

In relative position space, the requirement from hardcore and infinite nearest-neighbor repulsion is that $\tilde{g}(\mathbf{r})$ must vanish at $\mathbf{r} = (0,0)(\pm 1,0)(0,\pm 1)$. What we have shown in this section is that for bosons, the wavefunction can be arranged so that $\tilde{g}(\mathbf{r})$ vanish along the entire $x$ and $y$ axes, and trivially satisfies the requirement from the potential energy term in our model.

4.5 Fermion: Noninteracting to Interacting

In this section we use the t-matrix techniques developed in the preceding sections of this chapter to study the relationship between the noninteracting energies and the interacting energies. We start with the table of energies in Table 4.1 for the $10 \times 11$ lattice with $\mathbf{P} = (0, 0)$. We have asked in the introduction to this chapter whether
we can go from the noninteracting to the interacting energies (see Fig. 4.1) and now we know that we have an equation \( E = E_0 + T(E) \) where \( T(E) \) is the symmetry reduced scalar t-matrix function (see Sec. 4.3.7). From our graphs (Fig. 4.4 and Fig. 4.6) we have commented that for fermions the curve of \( T(E) \) around \( E_0 \) is quite flat (which is not the case for bosons). And we mentioned that this implies that the approximation \( E \approx E_0 + T(E_0) \) is close to the exact energy. Now in this section, we study the t-matrix approach for a specific system. We will denote \( E_1 = E_0 + T(E_0) \), the first iteration result, and \( E_{n+1} = E_0 + T(E_n) \), the \( n \)th iteration result.

In Table 4.2 we show the t-matrix calculation for the \( 10 \times 11 \) lattice. We show for the lowest few states the noninteracting energy \( E_0 \), the first t-matrix iteration \( E_1 \), the fifth t-matrix iteration \( E_5 \), and the exact energy \( E_{\text{exact}} \). In Fig. 4.8 these energy levels are plotted graphically. From the table, it is clear that the first t-matrix iteration result \( E_1 \) is quite close to the exact energy, and the fifth iteration result \( E_5 \) gives a value that is practically indistinguishable from the exact value. The t-matrix computations (for nondegenerate levels) are done using the program \texttt{tmat} described in Appendix F.

### 4.6 Physical Meaning of \( \mathcal{T}(E) \)

Our main work on the t-matrix has been completed. We have a set of explicit computational procedures that come from the Schrodinger equation and with which we can proceed to do calculations for pair interaction (see Sec. 4.3.7 for a summary). In this section we give yet another derivation of the t-matrix which makes more explicit the physical meaning of \( \mathcal{T}(E, \mathbf{p}; \mathbf{q}, \mathbf{q}') \) (4.21).
Figure 4.8: Two-fermion energy levels for the $10 \times 11$ lattice with $P = (0, 0)$. From left to right, the lowest few noninteracting energies $E_0$, first t-matrix iteration $E_1$, fifth t-matrix iteration $E_5$, and the exact energy $E_{exact}$ are plotted. Note that the third noninteracting energy from the bottom is doubly degenerate (see Table 4.2).
Table 4.2: Fermion energies for $10 \times 11$ lattice with $\mathbf{P} = (0, 0)$. $E_0 = \mathcal{E}(\mathbf{q}_1) + \mathcal{E}(\mathbf{q}_2)$ is the noninteracting energy. $E_n = E_0 + T(E_{n-1})$ where $T(E)$ is the symmetry reduced t-matrix. Here only fermion energies (from $T_{1,-1}$ or $T_{1,-1,1,-1}$ and $T_{1,-1,-1,1}$) are included. The t-matrix computations (for nondegenerate levels) are done using the program tmat described in Appendix F.

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<th>$E_0$</th>
<th>$E_1$</th>
<th>$E_5$</th>
<th>$E_{\text{exact}}$</th>
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4.6.1 Ladder Diagrams

Before we get into a lot of algebra, let us describe the physical idea. In scattering theory we know that the Born series is a perturbation series of the scattering amplitude in terms of the potential. In Fig. 4.9 we show the first three terms graphically, where the first term, the first Born approximation, is particularly simple—it is the Fourier transform of the potential. We also know that when the potential is weak the first few terms are a good approximation to the scattering amplitude, but when the potential is strong, we need all terms. In this section, we will show that our t-matrix $T(E, \mathbf{P}, \mathbf{q}, \mathbf{q}')$ is the sum of all such two-body scattering terms.
Figure 4.9: The three figures represent perturbative terms involving $V(q - q')$, $T_2(E, P; q, q')$ and $T_3(E, P; q, q')$. The t-matrix, $T(E, P; q, q')$, is the sum of all these terms, i.e., it is the sum of the ladder diagrams to infinite order.

4.6.2 Born Series

We start with Eq. 3.22 which we copy here for convenience,

$$ (E - \varepsilon(q) - \varepsilon(P - q))g(q) = \frac{1}{N} \sum_{q'} V(q - q')g(q'). \quad (4.42) $$

For $q \in Q_I$ we break up the sum over $q'$ into two terms and get,

$$ (E - E_0)g(q) = \frac{1}{N} \sum_{q' \in Q_I} V(q - q')g(q) + \frac{1}{N} \sum_{q' \in Q_{II}} V(q - q')g(q'). \quad (4.43) $$

For $q \in Q_{II}$ we can rewrite Eq. 4.42 to get,

$$ g(q') = \frac{1}{N} \sum_{q''} \frac{V(q' - q'')}{E - \varepsilon(q') - \varepsilon(P - q')}g(q''). \quad (4.44) $$

Plug Eq. 4.44 into the second sum in Eq. 4.43 and rearrange terms, we get,

$$ (E - E_0)g(q) = \frac{1}{N} \sum_{q' \in Q_I} V(q - q')g(q') + \frac{1}{N} \sum_{q'} T_2(E, P; q, q')g(q''), \quad (4.45) $$

where we have defined,

$$ T_2(E, P; q, q'') = \frac{1}{N} \sum_{q' \in Q_{II}} \frac{V(q - q')V(q' - q'')}{E - \varepsilon(q') - \varepsilon(P - q')} \quad (4.46) $$
Now break the sum over $\mathbf{q}''$ in Eq. 4.45 into two parts, and we get

\[
(E - E_0)g(\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{q}' \in Q_I} V(\mathbf{q} - \mathbf{q}') g(\mathbf{q}') \\
+ \frac{1}{N} \sum_{\mathbf{q}' \in Q_J} T_2(E; \mathbf{P}; \mathbf{q}, \mathbf{q}') g(\mathbf{q}') \\
+ \frac{1}{N} \sum_{\mathbf{q}' \in Q_{IJ}} T_3(E; \mathbf{P}; \mathbf{q}, \mathbf{q}') g(\mathbf{q}'). \tag{4.47}
\]

Plug Eq. 4.44 into the last term of Eq. 4.47 and we get

\[
(E - E_0)g(\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{q}' \in Q_J} V(\mathbf{q} - \mathbf{q}') g(\mathbf{q}') \\
+ \frac{1}{N} \sum_{\mathbf{q}' \in Q_J} T_2(E; \mathbf{P}; \mathbf{q}, \mathbf{q}') g(\mathbf{q}') \\
+ \frac{1}{N} \sum_{\mathbf{q}'} T_3(E; \mathbf{P}; \mathbf{q}, \mathbf{q}') g(\mathbf{q}'), \tag{4.48}
\]

where we have defined

\[
T_3(E; \mathbf{P}; \mathbf{q}, \mathbf{q}') = \frac{1}{N} \sum_{\mathbf{q}'' \in Q_{IJ}} \frac{T_2(\mathbf{q} - \mathbf{q}'') V(\mathbf{q}'' - \mathbf{q}')}{E - \mathcal{E}(\mathbf{q}'') - \mathcal{E}(\mathbf{P} - \mathbf{q}'')} \tag{4.49}
\]

\[
= \frac{1}{N^2} \sum_{\mathbf{q}'' \in Q_{IJ}} \sum_{\mathbf{q}''' \in Q_{IJ}} \frac{V(\mathbf{q} - \mathbf{q}'') V(\mathbf{q}'' - \mathbf{q}''') V(\mathbf{q}''' - \mathbf{q}')}{(E - \mathcal{E}(\mathbf{q}'')) - \mathcal{E}(\mathbf{P} - \mathbf{q}'')(E - \mathcal{E}(\mathbf{q}'') - \mathcal{E}(\mathbf{P} - \mathbf{q}''))(E - \mathcal{E}(\mathbf{q}''') - \mathcal{E}(\mathbf{P} - \mathbf{q}'''))}
\]

Continue this process, we obtain

\[
(E - E_0)g(\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{q}' \in Q_J} (V(\mathbf{q} - \mathbf{q}') + T_2(E; \mathbf{P}; \mathbf{q}, \mathbf{q}') + T_3(E; \mathbf{P}; \mathbf{q}, \mathbf{q}') + ...) g(\mathbf{q}'). \tag{4.50}
\]

What we have done here is the traditional perturbation theory using iteration. Eq. 4.50 is the Born series for scattering amplitude. The first term $V(\mathbf{q} - \mathbf{q}')$, the Fourier transform of the potential $V(\mathbf{r})$, is the first Born approximation. The content of higher order terms $T_2$, $T_3$, ... can be obtained from their definition. Eq. 4.46 says that $T_2$ involves two scatterings under $V$, and Eq. 4.49 says that $T_3$ involves three scatterings. Thus the Born series Eq. 4.50 can be graphically depicted at the ladders in Fig. 4.9, and it involves multiple scatterings to all orders. Note that each term in
the Born series is infinite for infinite potential \( V \). Next we will show that summing all the terms in the series gives the t-matrix and the potential \( V \) cancels out, giving a finite value.

### 4.6.3 T-Matrix

It is easy to check that

\[
T_2(E, P; q, q') = V^2 \sum_{ij} e^{iq_i^{R_j}} e^{-iq_j^{R_j}} G_{ij}^{II}(E, P),
\]

(4.51)

where \( G_{ij}^{II}(E, P) \) is our good old Green function (4.11),

\[
T_3(E, P; q, q') = V^3 \sum_{ij} e^{iq_i^{R_j}} e^{-iq_j^{R_j}} (G_{ij}^{II}(E, P))^2,
\]

(4.52)

and

\[
T_n(E, P; q, q') = V^n \sum_{ij} e^{iq_i^{R_j}} e^{-iq_j^{R_j}} (G_{ij}^{II}(E, P))^{n-1}.
\]

(4.53)

Now plug these results into Eq. 4.50, we get

\[
(E - E_0)g(q) = \sum_{q' \in Q} \left[ \frac{1}{N} \sum_{ij} e^{iq_i^{R_j}} e^{-iq_j^{R_j}} V \left( \delta_{ij} + V G_{ij}^{II} + V^2 (G_{ij}^{II})^2 + ... \right) \right] g(q')
\]

(4.54)

Now we come to the leap of faith,

\[
V \left( I + VG^{II} + V^2(G^{II})^2 + ... \right) = V(I - VG^{II}(E))^{-1}.
\]

(4.55)

This step is formal, and the interesting result is that the infinite potential \( V \) cancels out, giving a finite value \(-G^{II}(E)^{-1}\).

If we can do this formal sum, then we get from Eq 4.54,

\[
(E - E_0)g(q) = \sum_{q' \in Q} \left[ \frac{1}{N} \sum_{ij} e^{iq_i^{R_j}} e^{-iq_j^{R_j}} \left( V(I - VG^{II}(E))^{-1} \right)_{ij} \right] g(q')
\]

\[
= \sum_{q' \in Q} T(E, P; q, q') g(q'),
\]

(4.56)

which is exactly our momentum space T-matrix equation (4.22) and \( T(E, P; q, q') \) is exactly our t-matrix (4.21).
4.7 Summary and Outlook

Goal

This chapter starts with an observation that if the idea of one-to-one correspondence from noninteracting states to interacting states is correct, we should be able to write a perturbation equation for the interacting energy

\[ E = \mathcal{E}(q_1) + \mathcal{E}(q_2) + \Delta E(q_1, q_2). \]

Setup

We set up our calculation by dividing the basis set into an unperturbed one, with momentum vectors coming from \( Q_I \), and the complement, with momentum vectors from \( Q_{II} \),

\[ |\psi\rangle = \sum_{q \in Q_I} g(q) |q, P - q\rangle + \sum_{q \in Q_{II}} g(q) |q, P - q\rangle. \]

The pair component exchange symmetry due to the specific form of our energy dispersion \( \mathcal{E}(q) \) is also discussed.

T-Matrix

An important Green function quantity for momentum vectors in \( Q_{II} \) is essential in our calculation,

\[ G^{II}(E, P; r, r') = \frac{1}{N} \sum_{q \in Q_{II}} \frac{e^{i q (r' - r)}}{E - \mathcal{E}(q) - \mathcal{E}(P - q)}. \]

And using the matrix \( G^{II} \) defined from \( G^{II} \), the Schrodinger equation for two particles can be rewritten, exactly, as

\[ E = E_0 + \text{Eigenvalue}(T(E)), \]
where

\[ \mathcal{T}_{q,q'}(E) = T(E; P; q, q') \]

with \( q, q' \in Q_J \) and

\[ T(E; P; q, q') = \frac{1}{N} \sum_{ij} e^{i q R_i} e^{-i q' R_j} \left( V(I - G^{II}(E)V)^{-1} \right)_{ij} \]

The matrix \( \mathcal{T}(E) \) can be diagonalized in certain situations using symmetry, and we have shown three cases, where we can have a scalar equation,

\[ E = E_0 + T(E) \]

where \( T(E) \) is

1. \( N_1 = 1, T_1(E) \)
2. \( N_1 = 2, T_{1,1}(E) \) and \( T_{1,-1}(E) \)
3. \( N_1 = 4, T_{1,1,1,1}(E), T_{1,1,-1,-1}(E), T_{1,-1,1,-1}(E), \) and \( T_{1,-1,-1,1}(E) \) (pair component permutation symmetry case)

**Fermion**

The equation \( E = E_0 + T(E) \) is studied and it is found that \( E \approx E_0 + T(E_0) \) is a good approximation for fermions. The goal advertised at the beginning of the chapter \( E = E_0 + \Delta E \) is therefore answered for fermions and it has been shown that t-matrix does enable us to go from a spectrum of noninteracting energies to the exact, interacting energies.

**Boson Special State**

A special case for the bosons, where the noninteracting energy is the exact energy, is also discussed, where the eigenfunctions in relative position space are shown to have nodes along \( x \) and \( y \) axes.
Ladder Diagrams

The physical content of our t-matrix $T(E,P; q, q')$ is explained. It is the sum of all two-body scattering terms (described by the ladder diagrams) and is finite even for an infinite repulsive potential. The t-matrix contains the essential information about two-body interaction, is exact for the problem with two-particles, and will be used as a central ingredient for studying the low-density limit of our model.

Real Space T-Matrix

A real space t-matrix, running in parallel to the momentum space version in this chapter is in Appendix E.

Outlook

The t-matrix is an interesting physical quantity. It is not widely known because normally we are interested in problems with weak interactions where the usual perturbation theory from quantum mechanics textbooks, namely the Born approximation, works well. The t-matrix is an essential ingredient in strong interaction physics. It has been used extensively in scattering theories in the continuum, but has not been extensively studied on the lattice. One of the most interesting observations made from our study on the two-particle problem is the qualitative difference between the boson and fermion t-matrices, as shown in Fig. 4.4 and Figs. 4.5 and 4.6. Iterations $E_{n+1} = E_0 + T(E_n)$ starting with the noninteracting energy reach the exact energy quickly for fermions but not for bosons, i.e., the fermion solutions are linearly stable while the boson ones are not. Therefore, the t-matrix procedures described in this chapter (see Sec. 4.3.7) also provide a fast and easy way to obtain two-fermion energy: we only need a few iterations.
In Sec. 3.10, we used the large-lattice two-particle results to study the problem of a few particles on a large lattice. In Chapter 7, we will use the two-particle t-matrix results developed in this chapter to study the problem of a few fermions with more precision than that in Sec. 3.10, as we gradually map out the low-density limit of our model.
Bibliography


Chapter 5

Stripe and Holes on a Stripe

In this chapter we study the behavior of our model near the half-filled limit. Because of the infinite nearest-neighbor repulsion, the maximum filling fraction in our model is one half, and at this filling, the particles form a checkerboard configuration that cannot move.\footnote{That is to say that the Hamiltonian operator acting on this state gives zero, as no hopping is possible, and therefore the energy is zero.} Adding a single hole to it cannot produce motion either because the hole is confined by neighboring particles. A natural way to add holes to this system is to align them in a row going across the system, as indicated in Fig. 5.1. We call this row of holes a stripe and it is the subject of study in this chapter.

Stripes are natural objects in our model. For many systems with certain aspect ratios (e.g., the 6 \times 7 lattice depicted in Fig. 5.1), the stripe state is the one with the smallest number of holes and nonzero energy. Up to this point in the thesis, we have studied the dilute limit, which is dominated by pairwise scattering events of the few particles in the system. Here we have a new kind of physics of extended, fluctuating, quantum mechanical objects, that are results of collective motions of many particles.
Figure 5.1: An isolated hole (shown in the box) in a half-filled region cannot move. A row of holes (a stripe) can slide along in the vertical direction, with the arrows showing the possible moves.

Stripes have also been an area of active study in the high-temperature superconductivity research. Stripes that are modulations of spin and charge densities have been observed by neutron scattering in cuprates (see Ref. [1] and the schematic drawing in Fig. 1.11). And this observation has inspired further theoretical studies on stripe formation in a number of models believed to be important for cuprate superconductivity, e.g., the Hubbard and $t-J$ models (see e.g., Ref. [2]). Although the stripes in our model differ from those in the Hubbard and $t-J$ models in the obvious way that our underlying particles are spinless and we have infinite nearest-neighbor repulsion, we believe that our study of stripes in this simple model can shed light on the properties of stripes in spinfull models and those with on-site and finite nearest-neighbor repulsion. With the simplification of spinless particles and infinite repulsion, we have been able to obtain exact diagonalization results for a variety of situations including a single stripe, a hole on a stripe, hole-hole interactions on a stripe, and an interacting stripe-array for a large number of systems. In this
chapter we study the one-stripe problem and holes on a stripe, and in Chapter 6 we study interacting stripes and the stripe-array.

This chapter is organized as follows. We first study the single stripe and demonstrate how it can be mapped exactly to a one-dimensional spin-1/2 chain. Briefly, with infinite nearest-neighbor repulsion and a single stripe, particle motion is restricted to the direction perpendicular to the stripe only. An up step of the stripe can then be mapped to a spin up and a down step to a spin down. We then describe an extension to our exact diagonalization program that is suitable for the dense limit. Instead of enumerating all states, we build basis states from all possible hoppings from a starting state. Third, we study the problem of one hole added to a stripe. We demonstrate the two kinds of motions in this situation, that the hole can move along the stripe or the stripe can fluctuate away from the hole. We introduce a periodic-well model to understand the energy dependence (exponential decay) on the system size perpendicular to the stripe direction, and obtain effective mass of the stripe. We also consider the energy dependence on the length of the stripe. Finally, we present our data on two holes with a stripe, and calculate again the stripe effective mass. Note that in our analysis of stripes in this chapter and Chapter 6, we study both the spinless fermion and the hardcore boson cases. One of the important questions in many of the situations is the stability comparison of the two cases.

A number of the results in this chapter have appeared in condensed form in Ref. [3].
5.1 Single Stripe and Spin Chain

5.1.1 Stripe Examples

In this section we study the problem of a single stripe in the system. In Fig. 5.2 we show a \( L_x = 4 \) and \( L_y = 7 \) system with 12 particles. A stripe of length four is formed along the \( x \) direction. In each \( y \) column are three particles. The only four possible nearest-neighbor hops of the leftmost state are indicated with arrows and the resulting four states are shown on the right. Note that with a single stripe, the particles can only slide along in the \( y \) direction. It is not possible for them to move in any fashion in the \( x \) direction.

\[ \begin{array}{cccccccccccc}
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
\circ & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ \\
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\circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ \\
\circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ & \circ \\
\end{array} \]

Figure 5.2: A single stripe in a \( 4 \times 7 \) system. For the leftmost state, the four possible hops are labeled and the corresponding configurations are shown on the right. The corresponding spin chain configurations are shown below (see Sec. 5.1.3). The key fact illustrated here is that with a single stripe the particles can only slide in the direction perpendicular to the stripe.

\(^2\)The periodic boundaries at \( x = 0 \) and \( x = L_x \) force a stripe with even length only. The \( L_x \) even and \( L_y \) odd condition forces a stripe parallel to the \( x \) direction.

\(^3\)Of course, this does not mean that the stripe cannot move in the \( x \) direction. We know that transverse waves can travel in the longitudinal direction.
We also consider tilted boundaries with \((L_x, b) \times (0, L_y)\), which force a tilt of \(b\) steps to the stripe because the site \((0, y)\) is identified with \((L_x, y+b)\). In Fig. 5.3, we show the \((5,1) \times (0, 7)\) and the \((6,2) \times (0, 7)\) systems. Note because each stripe step is at 45 degree angle, an even (odd) horizontal length of the stripe \(L_x\) must produce an even (odd) number of total vertical steps \(b\). Thus \(L_x + b\) is always even. Note also that for the tilted stripes, vertical motion is again the only allowed motion of the system.

Figure 5.3: A single stripe in the \((5,1) \times (0, 7)\) and the \((6,2) \times (0, 7)\) systems. The boundary conditions force a tilt of the stripe. The corresponding spin-chains have total \(S_z\) equal to 1/2 and 1 respectively (see Sec 5.1.3).

### 5.1.2 Bose and Fermi Statistics

First, we show a sufficient condition that a stripe with fermions can have identical Hamiltonian matrix elements as a stripe of bosons.\(^4\) We know that when the

\(^4\)This simplifies the analytical calculation significantly because boson particles do not produce minus signs as their orders are switched. As we will see after we map the system to a spin chain we can simplify the problem further by using translation symmetries in the horizontal direction.
Hamiltonian operator acts on a state, we get $H|n\rangle = (-t) \sum_m s(n, m)|m\rangle$ (which is Eq. 2.4), where $s(n, m)$ is the sign introduced by hopping that is always 1 for bosons and ±1 for fermions depending on a chosen order to represent the states and the number of exchanges created by hopping. In Chapter 2 on exact diagonalization we introduced a convenient choice to number lattice sites that goes from the lower-left corner upward and then rightward (see Fig. 2.1), and this order is convenient for this discussion on stripes.

Commenting on Fig. 5.2 and Fig. 5.3, we have already mentioned that particles in the single stripe state are confined to move in the $y$ direction only. With our chosen site order, if a hop does not take a particle across the periodic boundaries, there is no change of order and therefore no fermion sign is introduced. If a hop does take a particle across the boundary, as it emerges from the opposite side, it has exchanged order with all other particles in its column. For the system in Fig. 5.2, there are three particles in one column, which means that a particle hopping across the boundary has always exchanged order in our state representation with exactly two particles. For fermions the cumulative sign from exchange is then 1. That is to say in the sum $H|n\rangle = (-t) \sum_m s(n, m)|m\rangle$, $s(n, m) = 1$ always. All the Hamiltonian matrix elements (without translation symmetry) are identical for boson and fermion cases (the nonzero ones are always $-t$).

It is not difficult to generalize this finding. For $L_y = 4p + 3$ where $p$ is an integer (there are $(L_y - 1)/2 = 2p + 1$ particles in one column), the fermion and boson systems with a single stripe have identical matrix elements. This argument works without modification for systems with tilted boundaries of the type $(L_x, b) \times (0, L_y)$ as there again motion is confined to the vertical direction.

---

for the spins, but this works for bosons only.
Note that having identical matrix elements is a much stronger condition than having identical eigenenergy spectra. We find from diagonalization that for one-stripe systems with rectangular boundaries, the boson and fermion spectra are identical. We also find the spectrum to be symmetric about zero. For a stripe in systems with tilted boundaries, there are complications. For the \((2m + 1, 1) \times (0, 2l + 1)\) system, the spectrum is not symmetric about zero. In this case, with \(l\) odd, the fermion spectrum is still identical to the boson spectrum, but for \(l\) even, the fermion energies are the boson ones with a minus sign (and because the spectrum is no longer symmetric about zero, the fermion energies are not the same as the boson energies). For the \((2m, 2) \times (0, 2l + 1)\) system, the boson and fermion spectra are symmetric about zero and identical. These complications are result of periodic boundary conditions. They do not introduce new physics and are one reason we stick to the simple case \(L_y = 4p + 3\) in many of our studies. And that is why the \(L_y = 7\) systems are so popular in this chapter.

### 5.1.3 Mapping to Spin Chain

**Stripe State to Spin-Chain State**

In Fig. 5.2 we have indicated a natural map to a spin chain state for a stripe configuration. The up step of the stripe is mapped to an up spin and the down step to a down spin. Here it is obvious the spins should be one-half because at each step the stripe can only move in two different ways.\(^5\) We write this map mathematically as

\[
S|n\rangle = |n_s\rangle, \tag{5.1}
\]

\(^5\)A generalization to higher spins is straightforward if the stripe can take more than two moves.

See Ref. [4] for a mapping of a strongly anisotropic \(t - J\) model to a spin-1 chain.
where the map \( \mathcal{S} \) takes a stripe state \( |n\rangle \) to a spin state \( |n_s\rangle \). For the leftmost state in Fig. 5.2, we have \( \mathcal{S}|n\rangle = |\downarrow\uparrow\downarrow\rangle \).

**Spin Hamiltonian and the Desired Map**

It is clear that each allowed particle hop takes the stripe either from up-step/down-step to down-step/up-step or from down-step/up-step to up-step/down-step. They correspond to the nearest-neighbor spin flips \( \uparrow\downarrow \) to \( \downarrow\uparrow \) and \( \downarrow\uparrow \) to \( \uparrow\downarrow \) respectively. Therefore the form of the equivalent spin Hamiltonian is

\[
H_{\text{spin}} = A \sum_i \left( S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ \right),
\]

where \( A \) is a constant to be determined. The map that we would have to have is

\[
\langle m|H|n\rangle \sim \langle Sm|H_{\text{spin}}|Sn\rangle,
\]

where \( H \) is our spinless fermion and hardcore boson Hamiltonian, Eq. 1.7, \( n \) and \( m \) are single-stripe states, and \( \mathcal{S}|n\rangle \) and \( \mathcal{S}|m\rangle \) are spin-chain states.

**Translation-Related Stripe States**

However there is a problem with this stripe-to-spin-chain map. If \( T_{R_y} \) translates a state in the \( y \) direction by \( R_y \), then \( \mathcal{S}T_{R_y}|n\rangle = \mathcal{S}|n\rangle \). This tells the obvious fact that for any stripe state in a \( L_x \times L_y \) system, all \( L_y \) translations give the same spin-chain state. This is a problem of mapping from a two-dimensional system to a one-dimensional one with a straightforward projection. When we say we map a system exactly to another we would like to have a one-to-one correspondence of the basis states, so something must be done to the stripe states.

We consider translation in the \( y \) direction and form the Fourier states as follows,

\[
|n, k_y\rangle = \frac{1}{\sqrt{L_y}} \sum_{R_y} e^{-ik_y R_y} T_{R_y}|n\rangle.
\]

(5.4)
When discussing translation symmetry in our exact diagonalization program in Sec. 2.5.2, we used translation states $|n, k\rangle$, including both $x$ and $y$ translations. Here we want the $y$ translation only because we want to project the stripe states to the $x$ direction. The normalization factor here is always $1/\sqrt{L_y}$ because the $L_y$ translations in the sum cannot produce two identical states. From group theory we know $\langle m, k'_y|H|n, k_y\rangle = 0$ if $k_y \neq k'_y$, so we only focus on states with the same $k_y$.

**Extra Sign and Phase**

When we apply the Hamiltonian to the state $|n\rangle$, we get $H|n\rangle = (-t) \sum_{m \in \mathcal{M}} s(n, m)|m\rangle$ (Eq. 2.4), where $\mathcal{M}$ is the collection of states that can be reached from $|n\rangle$ by a single hop, and $s(n, m)$ is the fermion sign (always $+1$ for boson). Because $H$ commutes with translation $T_{R_y}$, it is easy to show that

$$H|n, k_y\rangle = (-t) \sum_{m \in \mathcal{M}} s(n, m)|m, k_y\rangle. \quad (5.5)$$

For $q \in \mathcal{M}$, we then have

$$\langle q, k_y|H|n, k_y\rangle = (-t)s(n, q). \quad (5.6)$$

But if we translate $q$ by $R_y$ so we have $T_{R_y}|q\rangle = \sigma|q'\rangle$, where $\sigma$ is the fermion sign from translating the state $q$ by $R_y$, then the translation state $|q', k_y\rangle = \sigma e^{ik_y R_y}|q, k_y\rangle$ (we have shown this in the chapter on diagonalization that translation states built from two states in the same translation class differ by a phase factor and a sign, see Eq. 2.7). Then we have

$$\langle q', k_y|H|n, k_y\rangle = (-t)s(n, q)\sigma e^{-ik_y R_y}. \quad (5.7)$$
Map Defined

The states $|n, k_y\rangle$ are our candidates for the basis states to be mapped to the spin-chain states. The equation that we would like to have for the stripe to spin-chain map is, after modifying Eq. 5.3,

$$\langle q, k_y|H|n, k_y\rangle \sim \langle Sq|H_{\text{spin}}|Sn\rangle. \quad (5.8)$$

We know that $q$ belongs to a translation class (by $T_{R_y}$) with $L_y$ elements and $k_y$ can have $L_y$ values, so which $q$ and $k_y$ should we choose? Eq. 5.7 and Eq. 5.6 tell us that choosing $q'$ rather than $q$, the matrix element $\langle q', k_y|H|n, k_y\rangle$ has an extra sign $\sigma$ and an extra phase factor $e^{-ik_yR_y}$. However, in the spin-chain language, we have,

$$\langle Sq|H_{\text{spin}}|Sn\rangle = \langle Sq'|H_{\text{spin}}|Sn\rangle; \quad (5.9)$$

because $S|q\rangle = S|q'\rangle$. This means that we should have $\sigma e^{-ik_yR_y} = 1$ for all $R_y$. Choose $L_y = 4p + 3$, then, as we have shown in Sec. 5.1.2, all fermion hops for the one-stripe case produces +1 sign. Thus we have $s(n,q) = 1$ and $\sigma = 1$. In addition, if we choose $k_y = 0$, then we have,

$$\langle q, 0|H|n, 0\rangle = -t; \quad (5.10)$$

for any $|q\rangle$ and $|n\rangle$ in their respective translation classes. What we have done is choose $k_y = 0$ to get rid of the phase factor introduced by translation and choose $L_y = 4p + 3$ to get rid of the fermion minus sign introduced during translation and hopping.

Constant Determined

With the matrix element Eq. 5.10 for the stripe states organized by translation, the constant factor in the effective spin Hamiltonian, Eq. 5.2, can be easily determined...
using the following equation

$$\langle q, 0 | H | n, 0 \rangle = -t = \langle S q | H_{\text{spin}} | S n \rangle = A \langle S q | \sum_i (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) | S n \rangle,$$  
(5.11)

and a particular case, 

$$-t = A (\uparrow \downarrow | S_i^+ S_{i+1}^- | \downarrow \uparrow) = A,$$

which gives 

$$A = -t.$$ 

So finally, the spin Hamiltonian is,

$$H_{\text{spin}} = (-t) \sum_i \left( S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ \right) = (-2t) \sum_i \left( S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right).$$  
(5.12)

This is the so-called spin-1/2 XX chain (where the notation XX refers to the fact that the x and y terms have the same coefficient). It is well-studied and exactly solvable (see Ref. [5] for the solution of this problem and Ref. [6] for a range of related one-dimensional quantum problems).

### 5.1.4 Summary of Map

Let us summarize the exact conditions of this map from the stripe problem to the spin chain problem. For a $L_x \times L_y$ system with $L_x$ even and $L_y$ odd, with 

$$M = L_x (L_y - 1)/2$$

particles, a stripe forms along the $x$ direction. For each stripe state, pick one from each translation class, $|n\rangle$, and form state $|n, 0\rangle$ as in Eq. 5.4,

$$|n, 0\rangle = \frac{1}{\sqrt{L_y}} \sum_{R_y} T_{R_y} |n\rangle.$$ 

Then the stripe problem with hopping Hamiltonian $H$ and basis states $|n, 0\rangle$ is mapped to the spin-chain problem with Hamiltonian $H_{\text{spin}}$ (5.12) with basis states $S |n\rangle$, for bosons with any $L_y$ and fermions with $L_y = 4p + 3$. This map gives identical matrix elements,

$$\langle q, 0 | H | n, 0 \rangle = -t = \langle S q | H_{\text{spin}} | S n \rangle.$$
And note that because of periodic boundary conditions, the stripe returns to the same \( y \) coordinate after length \( L_x \). The corresponding spin chain states have length \( L_x \) with total \( z \) component of the spin zero.

For tilted boundaries, the map to the spin-chain works exactly as before: (i) the up-step/down-step maps to up-spin/down-spin; (ii) use \( k_y = 0 \) to get rid of fermion sign due to \( y \) translation; and (iii) use \( L_y = 4p + 3 \) to get rid of the fermion sign due to particles moving across the periodic boundaries. The only difference here is that the resulting spin problem have total \( S_z \) equal to \( b/2 \).

For bosons, we can further employ translation symmetry in the \( x \) direction to map the \((k_x, k_y = 0)\) problem to the spin-chain problem with wave vector \( k_x \).\(^6\) We also note that we have a spin diagonalization program written for an earlier project that can diagonalize arbitrary spin systems for both the full Hamiltonian matrix and the cyclic permutation symmetry-reduced problem. It is described briefly in [7] and was used for the work described in this section.

The map in this section has appeared in Ref. [3], but the exact state correspondence is not included there.

\[ \text{5.1.5 Stripe Effective Mass} \]

In Sec. 5.1.3, we showed how a single-stripe state with \( k_y = 0 \) can be mapped to a spin chain problem. The case with \( k_y \neq 0 \) is more complicated but tractable (we wish to describe this problem in a future publication), and here we use the diagonalization data for excited single-stripe states with \( k = (0, k_y) \) to obtain the stripe effective mass.

On a \( L_x \times L_y \) lattice, with the stripe stretching in the \( x \) direction, we can model\(^6\) For fermions we cannot do this because horizontal translations may introduce a fermion sign.
the motion of the stripe in the \( y \) direction by a free particle in one dimension. We then expect the energy dispersion to be,

\[
E_{\text{stripe}}(0, k_y) = E_{\text{stripe}}(0, 0) + \frac{\hbar^2 k_y^2}{2m^*},
\]

(5.13)

where \( m^* \) is the effective mass. In Fig. 5.4, we plot this dispersion \( E_{\text{stripe}}(0, k_y) - E_{\text{stripe}}(0, 0) \) vs \( k_y \) and also show the log-log plot for the 20 data points with the smallest \( k_y \). The \( k_y^2 \) dependence is checked for small \( k_y \).

To obtain the effective mass \( m^* \) we can use the slopes in the log-log plot of Fig. 5.4. Here we simply use the data point with the smallest \( k_y = 2\pi/L_y \) with a large \( L_y = 101 \). Eq. 5.13 gives the following expression for \( m^* \),

\[
m^* = \frac{(2\pi/L_y)^2}{2(E_{\text{stripe}}(0, 1) - E_{\text{stripe}}(0, 0))},
\]

(5.14)

where the notation \((l_x, l_y)\) stands for \( \mathbf{k} = (2\pi l_x/L_y, 2\pi l_y/L_y) \). The results are shown in Table 5.1.

Table 5.1: Stripe effective mass \( m^* \) calculated from Eq. 5.14 using single-stripe excited state energies with \( \mathbf{k} = (0, k_y) \). \((0, 1)\) denotes \( \mathbf{k} = (0, 2\pi/L_y) \) with \( L_y = 101 \).

<table>
<thead>
<tr>
<th>( L_x )</th>
<th>( E_{\text{stripe}}(0, 0) )</th>
<th>( E_{\text{stripe}}(0, 1) )</th>
<th>( m^* )</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>-2.828427125</td>
<td>-2.827058964</td>
<td>1.41432759</td>
</tr>
<tr>
<td>6</td>
<td>-4</td>
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<td>2.250080628</td>
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<td>-8.987563481</td>
<td>5.451798764</td>
</tr>
</tbody>
</table>
Figure 5.4: Single-stripe energy dispersion relation $E_{\text{stripe}}(0,k_y) - E_{\text{stripe}}(0,0)$ vs $k_y$ (top graph) for $0 < k_y = 2\pi l/L_y < \pi$, $L_y = 101$, $l = 1, 2, ..., 50$, and $L_x = 4, 6, 8$. And the log-log plot (bottom graph) for $l = 1, 2, ..., 20$. 
5.2 Diagonalization Program Revised

5.2.1 Introduction

In Chapter 2 we described the exact diagonalization program. It enumerates all basis states using recursion. Particles are placed into the system until the total number of particles in a state reaches the specified number $M$. This enumeration is good for the system at all fillings but is not efficient near the half-filled limit. Here a large part of each basis state has the checkerboard configuration, and computer time is wasted using exhaustive recursion to rediscover that in building the basis set. We should take into account of that knowledge and a natural idea is to start with the checkerboard configuration and take particles out of that state. This is also not efficient because many of states we obtain are states in which all holes are isolated, and they give zero matrix elements so we do not need to include them in our basis set.\footnote{In other words, if we say that two states are equivalent when by hopping one state can be changed to another, then for the dense limit the set of all possible states with total number of particles $M$ is divided into a number of subsets using this equivalence relation and many of these subsets have just one element that gives zero matrix elements.} For situations where we know the states involved, for example the single stripe case, we build the basis set starting from a particular state and find all states that can be reached by hopping. Below we outline the procedures for building the basis states and the Hamiltonian matrix.

5.2.2 Building Basis States without Translation Symmetry

First we numerate the procedures for basis states without translation symmetry.

1. Starting from a state $n$, apply hoppings to it and obtain states $n_1, n_2, n_3,...$
Figure 5.5: Building basis states from a given state \( n \). Applying all allowed hoppings to \( n \) (the level 0 state) gives the states \( n_1, n_2, n_3, \ldots \). Applying hoppings to \( n_1 \) (a level 1 state) gives level 2 states \( n_{11}, n_{12}, n_{13}, \ldots \). The basis state list is then \( n, n_1, n_2, n_3, \ldots ; n_{11}, n_{12}, n_{13}, \ldots ; n_{21}, n_{22}, \ldots ; n_{111}, n_{112}, \ldots \). Note that when applying hoppings to a state, only add states not already on the list.

See Fig 5.5.

2. Form the basis state list \( n, n_1, n_2, n_3, \ldots \) that are numbered 0, 1, 2, 3, \ldots.

3. Record the Hamiltonian matrix elements \( H_{0,1}, H_{0,2}, H_{0,3}, \ldots \).

4. Apply hoppings to the next state on the basis state list that has not been applied hopping to. Here from \( n_1 \) we get \( n_{11}, n_{12}, n_{13}, \ldots \). Add these to the basis state list to form \( n, n_1, n_2, n_3, \ldots ; n_{11}, n_{12}, n_{13}, \ldots \) (Note we should not add states that are already on the list. For example, applying hoppings to \( n_1 \) will certainly give \( n \) back again. Do not include this state in level 2 states. When computing Hermitian matrix elements we only need \( H_{p,q} \) for \( p < q \).

5. If \( n_{11} \) is the \( m \)-th element on the list, record the matrix elements \( H_{1,m}, H_{1,m+1}, \ldots \).
\[ H_{1,m+2}, \ldots \]

6. Repeat the previous two steps until all the states on the list have been applied hopping to and no new states are created.

7. We finish with a basis state list \( n, n_1, n_2, \ldots, n_{11}, n_{12}, n_{13}, \ldots, n_{21}, n_{22}, \ldots, n_{111}, n_{112}; \ldots \) And we have stored the Hamiltonian matrix elements.

5.2.3 Building Basis States with Translation Symmetry

Next we record the procedures for basis states with translation symmetry. The difference here from the case without translation is that we should store the representative of each class of translation related states.

1. Starting from a state \( n \), find the representative in its translation class, say \( \tilde{n} \). Initialized the basis state list to be \( \tilde{n} \) only.

2. Apply hoppings to the first element on the basis state list that has not been applied hopping to (say \( p \)-th) and for all states in its translation class apply hopping to get states \( m_1, m_2, m_3, \ldots \)

3. Find representatives for these new states, \( \tilde{m}_1, \tilde{m}_2, \tilde{m}_3, \ldots \). For the states not already on the list append them to the end (say they are the \( q_1, q_2, q_3, \ldots \) states).\(^8\)

4. Store matrix information, \( H_{p,q_1}, H_{p,q_2}, H_{p,q_3}, \ldots \).\(^9\)

\(^8\)Note that here and as in the case without translation above, we do not form a sorted basis state list; we store matrix information as we build the basis set, following the leads of the hopping Hamiltonian rather than using exhaustive enumeration.

\(^9\)With translation symmetry, we normally want to calculate the Hamiltonian matrix for a number of \( k \) vectors. So here we do not actually store the matrix element (because it depends on \( k \)), we
5. Repeat the previous three steps until all states on the list are treated with no new states generated.

6. We finish with a list of representative states $\tilde{n}_i, \tilde{n}_{i1}, \tilde{n}_{i2}, \tilde{n}_{i3}, \ldots, \tilde{n}_{i11}, \tilde{n}_{i12}, \tilde{n}_{i13}, \ldots$, $\tilde{n}_{i21}, \tilde{n}_{i22}, \ldots$. And we have a set of locations where the Hamiltonian matrix elements are nonzero.

### 5.3 One Hole on a Stripe

#### 5.3.1 Introduction

For a system with a single stripe, we have seen that the motion is strictly limited to sliding in the direction perpendicular to the stripe; and this enables us to map our two-dimensional system to a one-dimensional spin chain and solve it exactly. With holes added to the stripe state, a number of new motions are allowed. In Fig. 5.6 we show a $6 \times 7$ system with a single stripe and a hole. We see that the hole can now move along the stripe and the stripe can fluctuate and leave the hole stranded (i.e., immobile). In this section we study the one-hole-with-a-stripe problem. We first compare the fermion and boson statistics of this problem (like what we have done for the single stripe case but more complicated here). We then study the dependence of energy on $L_y$, the side of the lattice perpendicular to the stripe, which shows exponential decay as $L_y$ increases. We introduce a one-dimensional periodic well model to account for it and compute stripe effective mass. Finally we study the dependence of energy on $L_x$, the length of the stripe, and show a good $1/L$ fit which enables us to obtain the energy lowered by the hole on an infinitely long stripe. This is one of the stability conditions that we will use for the stripe-array state in store, among other things, the location of the nonzero matrix elements.
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Figure 5.6: A $6 \times 7$ system with a stripe and a hole. The hole is indicated in the box. It is initially lying on the stripe (leftmost state). The arrows indicate the particles hops that result in the hole moving along the stripe to the right (middle state). It is also possible for the stripe to fluctuate and leave the hole immobile (rightmost state).

5.3.2 Boson and Fermion Statistics

From diagonalization, we observe that for systems with rectangular boundaries, the boson and fermion one-hole-with-a-stripe spectra are identical. Here we cannot use the argument developed for the single stripe case earlier because, first the hole can move horizontally, and second the number of particles in each vertical column is not the same in different columns. Henley [8] has devised an interesting conjecture to explain why the two spectra are identical for the one-hole-with-a-stripe problem which we will explain in this section.

Say $|\alpha\rangle$ is a one-hole-with-a-stripe state. For the boson case we have $H|\alpha\rangle = (-t) \sum_{m \in \mathcal{M}} |m\rangle$. For the fermion case we have $H|\alpha\rangle = (-t) \sum_{m \in \mathcal{M}} s(\alpha, m)|m\rangle$, where we have written the fermion sign as $s(\alpha, m)$ to emphasize its dependence on
both the states $\alpha$ and $m$. Then if $|\beta\rangle$ is another one-hole-with-a-stripe state and $\beta \in \mathcal{M}$, we have

\[ \langle \beta | H | \alpha \rangle_f = s(\beta, \alpha) \langle \beta | H | \alpha \rangle_b, \tag{5.15} \]

where the subscripts $f$ and $b$ denote the fermion and boson matrix elements respectively. If we can write

\[ s(\beta, \alpha) = \sigma(\beta)\sigma(\alpha), \tag{5.16} \]

i.e., as a product of a function $\sigma$ that depends on one state only, then Eq. 5.15 can be written as a matrix equation,

\[ H_f = \Sigma H_b \Sigma, \tag{5.17} \]

where $\Sigma_{\alpha,\beta} = \delta_{\alpha,\beta}\sigma(\alpha)$. Because $\Sigma = \Sigma^{-1}$, it is a similarity transformation, and then the eigenvalues of $H_f$ are identical to that of $H_b$.

We can understand Eq. 5.16 with the help of Fig. 5.7. The point here is that $s(\beta, \alpha)$ is defined by hopping the state $|\alpha\rangle$ to $|\beta\rangle$. It is defined on the arrow pointing from $\alpha$ to $\beta$. The function $\sigma(\alpha)$ on the other hand is defined on the node $\alpha$ of the graph.

Fig. 5.7 suggests a natural way to define $\sigma(\alpha)$. First we choose a reference point. This should not matter and the one we choose is the starting state of the exact diagonalization program, say $0$. We set $\sigma(0) = 1$. Then if one hop takes $\alpha$ to $\beta$, define $\sigma(\beta) = s(\beta, \alpha)\sigma(\alpha)$. This definition will certainly give Eq. 5.16, but is it well defined? That is to say, for two paths leading to the same state $\beta$ from $0$ will they produce the same sign? Henley [8] conjectures that this is true.

We have checked this conjecture computationally for a number of systems with rectangular boundary conditions. Fig. 5.5 has described the procedure for building the basis set. We store a sign for each state, starting with $+1$ for $n$. As we expand
Figure 5.7: Obtaining \( \sigma(\alpha) \), that is defined for each state, from a reference state 0 and the step wise hopping sign function \( S(\beta, \alpha) \), that is defined on the arrow pointing from \( \alpha \) to \( \beta \). Define \( \sigma(\beta) = S(\beta, \alpha)\sigma(\alpha) \). Is this well defined? Will there be another path leading from 0 to \( \beta \) giving a different \( \sigma(\beta) \). See text for a conjecture.

The tree, we compute the sign for the next level of states. Whenever we come to a state that is already on the list we check to see that the sign we produce following the current path equals that already stored for that state. For the systems we checked, for example, \( 4 \times 9 \) with \( M = 15 \), \( 4 \times 11 \) with \( M = 19 \), and \( 6 \times 7 \) with \( M = 17 \), there has not been a violation.

### 5.3.3 Energy Dependence on \( L_y \)

In this section we study the energy dependence of the one-hole-with-a-stripe problem on the size of the lattice perpendicular to the stripe.

When a hole is added to a stripe, more hops are allowed and the state gains kinetic energy, so its energy is lower than that of the single stripe of the same length. We define the energy difference,

\[
\Delta(L_x, L_y) \equiv E_{\text{hole}}(L_x, L_y) - E_{\text{stripe}}(L_x),
\]

(5.18)

where \( E_{\text{hole}}(L_x, L_y) \) is the ground state energy of one hole with a stripe on a \( L_x \times L_y \)
lattice and \( E_{\text{stripe}}(L_x) \) the ground state energy of a single stripe with length \( L_x \). Here \( E_{\text{hole}}(L_x, L_y) \) is the same for bosons and fermions, as we discussed in Sec. 5.3.2. \( E_{\text{stripe}}(L_x) \) does not depend on \( L_y \) because, as we showed in Sec. 5.1.3, the single stripe problem with \( k = (0, 0) \) is mapped to a one-dimensional spin chain with \( k_x = 0 \). The ground state energy of the boson system is always in the \( k = (0, 0) \) sector, therefore \( E_{\text{stripe}} \) for the \( L_x \times L_y \) lattice is identical to the ground state energy of the length-\( L_x \) spin chain with \( k_x = 0 \), independent of \( L_y \).

In Fig. 5.8, we plot \( \Delta(L_x, L_y) \) vs \( L_y \) with \( L_x = 8 \). We only plot up to \( L_y = 15 \) because, as can be seen from the graph, the energy difference is essentially flat after that. The plots for \( L_x = 4, 6, 10, 12, 14 \) are qualitatively the same. (See Tables D.6 and D.7 for numerical data.)

Fig. 5.8 shows a fast decay of \( \Delta(L_x, L_y) \) in \( L_y \) so we try the following exponential fitting function,

\[
\Delta(L_x, L_y) = \tilde{\Delta}(L_x) - A(L_x)e^{-L_y/l(L_x)}, \quad (5.19)
\]

where \( \tilde{\Delta}(L_x) = \Delta(L_x, \infty), A(L_x), \) and \( l(L_x) \) are fitting parameters that depend on the length of the stripe \( L_x \).\(^{10}\) We choose a minus sign in front of \( A(L_x) \) because, as can be seen in Fig. 5.8, \( \Delta(L_x, L_y) < \tilde{\Delta}(L_x) \); in Eq. 5.19, \( A(L_x) \) is positive.

This fitting form Eq. 5.19, suggests the following linear regression check,

\[
\ln(\Delta(L_x, L_y + 2) - \Delta(L_x, L_y)) = C - \frac{L_y}{l(L_x)}, \quad (5.20)
\]

where \( C \) is a constant that depends on \( A, l, \) and \( L_x \), but not on \( L_y \). In Fig. 5.9 we plot \( \ln(\Delta(L_x, L_y + 2) - \Delta(L_x, L_y)) \) vs \( L_y \) for \( L_x = 4, 6, 8, 10, 12, 14 \) and \( L_y = 5, 7, 9, ... \). The linear fit is excellent for all data sets.

\(^{10}\) We will investigate the dependence on \( L_x \) of \( \tilde{\Delta}(L_x) \) later in Sec. 5.3.5.
Figure 5.8: Energy difference $\Delta(L_x, L_y) = E_{\text{hole}} - E_{\text{stripe}}$, Eq. 5.18, vs $L_y$ for $8 \times L_y$ lattices. The numerical data are in Table D.6.

### 5.3.4 Double-Well and Stripe Effective Mass

How can we account for the good exponential fitting form, Eq. 5.19, as shown in Fig. 5.9? Let us consider the hole fixed at some position and the stripe meandering in $y$ direction. In Fig. 5.6, we have shown that the hole can be in contact with the stripe or the stripe can fluctuate away, leaving the hole behind and immobile. When the stripe is in contact with the hole, the energy is lower than the energy of a single stripe $E_{\text{stripe}}$, which is also the energy when the stripe is separated from the hole. Because we have periodic boundary conditions in the $y$ direction, we can use
Figure 5.9: \( \ln(\Delta(L_x, L_y + 2) - \Delta(L_x, L_y)) \) vs \( L_y \) for \( L_x = 4, 6, 8, 10, 12, 14 \), where \( \Delta(L_x, L_y) = E_{\text{hole}} - E_{\text{stripe}} \), Eq. 5.18, is the energy difference between that of a hole with a stripe and that of a single stripe. The slope for each \( L_x \) curve is \(-1/l(L_x)\) in Eq. 5.20. The numerical data are in Tables D.6 and D.7.
a periodic-well potential to model the $y$ motion of the stripe.

\[
\begin{array}{c}
\hline
V_0 \\
\hline
E_0 \\
\hline
E_2
\end{array}
\]

$\hline$

$\hline$

Figure 5.10: Double-well potential used to understand the exponential decay of one-hole energy in $L_y$ in Eq. 5.19. Here $V_0$ is the depth of the well, $E_0$ the ground state energy of one single well, $E_2 < E_0$ the ground state energy of the double-well system (symmetric state), and $d$ the separation between two wells. $E_2 - E_0$ decays exponentially in $d$ as in Eq. 5.21.

For simplicity we consider a double-well system. In Fig. 5.10 we show two wells separated by $d$. $E_0$ is the ground state energy of an isolated well, and $E_2$ the ground state energy of the double-well system, which corresponds to a symmetric state and is lower than $E_0$. From standard quantum mechanics textbooks (see e.g., Ref. [9]), we know the energy difference decays exponentially with well separation,

\[ E_2 - E_0 = -A e^{-d/l}, \quad \text{where}, \quad \frac{1}{l} = \frac{\sqrt{2m(V_0 - E_0)}}{\hbar}, \quad (5.21) \]

where $A$ is a positive constant and $m$ the mass of the particle in the well.

The exponential decay in well separation in the double-well energy equation Eq. 5.21 is the result of tunneling between two wells. As far as our hole-with-a-stripe problem is concerned, the well separation $d$ is $L_y$, the well depth $V_0$ is $E_{\text{stripe}}$, the ground state energy of one isolated well $E_0$ is $E_{\text{hole}}(L_x, L_y = \infty)$, and the ground
state of the double-well system \( E_2 \) is \( E_{\text{hole}}(L_x, L_y) \). Therefore, Eq. 5.21 for the double-well problem translates into the following equation for our hole-with-a-stripe problem,

\[
E_{\text{hole}}(L_x, L_y) - E_{\text{hole}}(L_x, \infty) = -A(L_x)e^{-L_y/l(L_x)}. \tag{5.22}
\]

Using the definition for \( \Delta(L_x, L_y) \), Eq. 5.18, we see that Eq. 5.22 is exactly the fitting form we used before, Eq. 5.19. In addition, the double-well equation Eq. 5.21 gives us a way to calculate the effective mass \( m^*(L_x) \) of the stripe of length \( L_x \),

\[
\frac{1}{l(L_x)} = \sqrt{2m^*(L_x)(E_{\text{stripe}}(L_x) - E_{\text{hole}}(L_x, \infty))}, \tag{5.23}
\]

where we have set \( \hbar = 1 \). We get

\[
m^*(L_x) = \frac{1/l^2(L_x)}{2(E_{\text{stripe}}(L_x) - E_{\text{hole}}(L_x, \infty))}. \tag{5.24}
\]

Using the linear fitting slopes in Fig. 5.9 (that are \(-1/l(L_x)\)), we can compute \( m^*(L_x) \) using Eq. 5.24, and our results are shown in Table 5.2. We have used \( E(L_x, L_y) \) evaluated at large \( L_y \) to approximate \( E(L_x, \infty) \), because the exponential decay of \( E_{\text{hole}}(L_x, L_y) \) in \( L_y \) is fast (see Fig. 5.8 and the diagonalization data in Tables D.6 and D.7). The effective mass results are consistent with that obtained from the single-stripe energy dispersion relation in Table 5.1.

### 5.3.5 Energy Dependence on \( L_x \)

In this section we fix \( L_y \) and study the dependence of \( E_{\text{hole}} - E_{\text{stripe}} \) on the length of the stripe \( L_x \). In Fig. 5.11 we plot the energy difference \( \Delta(L_x, L_y) = E_{\text{hole}} - E_{\text{stripe}} \) as a function of \( 1/L_x \). The three curves correspond to \((L_x, b) \times (0, 7)\) systems with \( b = 0, 1, 2 \) respectively (those included in Table D.8).\(^{11}\) Eq. 5.19 gives a dependence

\(^{11}\)For \((L_x, 0) \times (0, 7)\) and \((L_x, 2) \times (0, 7)\) systems the boson and fermion energies are the same. For \((L_x, 1) \times (0, 7)\) this is not true, and here we plot the boson energies. Note that this does not
Table 5.2: Stripe effective mass \( m^* \) calculated from Eq. 5.24 using the double-well potential model for the one-hole-with-a-stripe problem. \( E_{\text{stripe}}(L_x) \) is the energy of a single stripe of length \( L_x \); \( l(L_x) \) is the decay length in Eq. 5.19 obtained from linear fitting in Fig. 5.9; \( E_{\text{hole}}(L_x, L_y) \) is used to approximate \( E_{\text{hole}}(L_x, \infty) \) using the large \( L_y \) listed in the table; and \( m^*(L_x) \) is the effective mass of the length-\( L_x \) stripe calculated using Eq. 5.24.

<table>
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<th>( L_x )</th>
<th>( L_y )</th>
<th>( E_{\text{hole}}(L_x, L_y) )</th>
<th>( E_{\text{stripe}}(L_x) )</th>
<th>( l(L_x) )</th>
<th>( m^*(L_x) )</th>
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</tr>
</tbody>
</table>

of \( \Delta(L_x, L_y) \) on \( L_y \). Here we fix \( L_y \) and study the \( L_x \) dependence.\(^{12}\)

We see from Fig. 5.11 the following fitting function works very well for both rectangular and tilted lattices,

\[
\tilde{\Delta}(L_x) = \Delta + \frac{B}{L_x}.
\]  

(5.25)

This fitting form enables us to extrapolate the energy gap formed by adding one hole to an infinitely long \( (L_x) \) stripe. The intercepts of the three curves for the three different classes of lattices all approach \( \Delta = -0.66 \). Later, in Sec. 6.5, we will study the stability of an array of stripes and we will use the value for \( \Delta \) because the \( \tilde{\Delta}(L_x, L_y) \) decays exponentially in \( L_y \), \( \Delta(L_x, 7) \) is numerically close to \( \Delta(L_x, \infty) \). See Fig. 5.8 and data in Tables D.6 and D.7.

\(^{12}\)Because \( \Delta(L_x, L_y) \) decays exponentially in \( L_y \), \( \Delta(L_x, 7) \) is numerically close to \( \Delta(L_x, \infty) \). See Fig. 5.8 and data in Tables D.6 and D.7.
Figure 5.11: $\Delta(L_x, L_y) = E_{\text{hole}} - E_{\text{stripe}}$ as a function of $1/L_x$ for three classes of lattices $(L_x, b) \times (0, 7)$ with $b = 0, 1, 2$. The numerical data are in Table D.8. The question there will be: will the holes added to a stripe stick to the stripe to form a wide one or will they form a new stripe? $\Delta$ is energy lowered by adding a hole to a stripe and will be relevant there. It is a binding energy in the sense that one hole off the stripe (immobile) has zero energy.
5.4 Two Holes with a Stripe

With two holes on a stripe, the particles have enough room to exchange with each other, so the boson and fermion energies are no longer the same. As in the one-hole case, we study the energy of the two-holes-with-a-stripe problem as a function of the two directions of the lattice.

5.4.1 Energy Dependence on \( L_y \)

As in Eq. 5.18 for the one-hole case, we define for the \( L_x \times L_y \) lattice the energy difference between the case of two holes with a stripe and that of a single stripe,

\[
\Delta_2(L_x, L_y) = E_{2\text{holes}}(L_x, L_y) - E_{\text{stripe}}(L_x),
\]

(5.26)

where the subscript 2 denotes the two-hole case. (Strictly speaking, we should write \( \Delta_2^{b,f}(L_x, L_y) \) and \( E_{2\text{holes}}^{b,f}(L_x, L_y) \) because these quantities are not the same for boson and fermion cases. Here, without the superscripts, they stand for both cases.)

In Fig. 5.12 we plot \( \Delta_2(L_x, L_y) \) vs \( L_y \) for bosons and fermions with stripe length \( L_x = 6 \). The fast decay behavior similar to that in the one-hole problem in Fig. 5.8 is observed, except here the boson and fermion curves approach different values at large \( L_y \).

As in Eq. 5.19 for the one-hole problem, we write the exponential decay suggested in Fig. 5.12 as,

\[
\Delta_2(L_x, L_y) = \tilde{\Delta}_2(L_x) - A_2(L_x)e^{-L_y/L_x},
\]

(5.27)

In Fig. 5.13 we plot, similar to what we have done in Fig. 5.9 for the one-hole case, \( \ln(\Delta_2(L_x, L_y + 2) - \Delta_2(L_x, L_y)) \) vs \( L_y \) for bosons and fermions, with \( L_x = 4, 6, 8, 10 \). Again the exponential dependence is checked nicely.
Figure 5.12: $\Delta_2(L_x, L_y)$ vs $L_y$ for bosons and fermions with stripe length $L_x = 6$. The decay is very fast after $L_y = 7$. See Table D.9 for numerical data.

### 5.4.2 Double-Well and Stripe Effective Mass

The resemblance of our treatment of the two-holes-with-a-stripe problem in Sec. 5.4.1 with that of the one-hole problem in Sec. 5.3.3 prompts us to ask whether the two-hole problem can be studied using a one-dimensional effective potential like the double-well potential used in Sec. 5.3.4. Here with two holes, we have a more complicated problem because the relative positions of the two holes and the stripe can have three cases: two holes on the stripe (with energy $E_{2\text{holes}}(L_x, \infty)$), one hole on the stripe with one isolated hole (with energy $E_{1\text{hole}}(L_x, \infty)$), or one stripe with two isolated holes (with energy $E_{\text{stripe}}(L_x)$).

As an approximation, we consider the deepest well ($E_{2\text{holes}}(L_x, \infty)$) only because
Figure 5.13: \( \ln(\Delta_2(L_x, L_y + 2) - \Delta_2(L_x, L_y)) \) vs \( L_y \) for \( L_x = 4, 6, 8, 10 \) (the top graph is for bosons and the bottom for fermions), where \( \Delta_2(L_x, L_y) = E_{\text{holes}} - E_{\text{stripe}} \), Eq. 5.26. The slopes are \(-1/\ell_2(L_x)\) in Eq. 5.27. Numerical data are in Tables D.9 and D.10.
that is the most probable position to find the particle. Then the effective mass equation Eq. 5.24 is modified to become,

\[ m^*_2(L_x) = \frac{1/l_2^2(L_x)}{2(E_{\text{stripe}}(L_x) - E_{2\text{holes}}(L_x, \infty))}, \]  

(5.28)

where \( l_2(L_x) \) comes from the linear fitting slopes in Fig. 5.13. The results for \( m^*_2 \) from this two-hole-with-a-stripe calculation are in Table 5.3. They are comparable to the one-hole results in Table 5.2.

Table 5.3: Stripe effective mass \( m^*_2 \) calculated from Eq. 5.28 using the double-well potential model for the two-holes-with-a-stripe problem. \( E_{\text{stripe}}(L_x) \) is the energy of a single stripe of length \( L_x \); \( l_2(L_x) \) is the decay length in Eq. 5.27 obtained from linear fitting in Fig. 5.13; \( E_{2\text{holes}}(L_x, L_y) \) is used to approximate \( E_{2\text{holes}}(L_x, \infty) \) using the large \( L_y \) listed in the table; and \( m^*_2(L_x) \) is the effective mass of the length-\( L_x \) stripe calculated using Eq. 5.28. The superscripts \( b \) and \( f \) denote bosons and fermions respectively.

<table>
<thead>
<tr>
<th>( L_x )</th>
<th>( L_y )</th>
<th>( E^b_{2\text{holes}} )</th>
<th>( E^b_{2\text{holes}} )</th>
<th>( E_{\text{stripe}} )</th>
<th>( l_2^b )</th>
<th>( l_2^f )</th>
<th>( m^*_2 )</th>
<th>( m^*_2 )</th>
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<td>-3.818556696</td>
<td>-2.828427125</td>
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<td>0.6135</td>
<td>1.3358</td>
<td>1.3417</td>
</tr>
<tr>
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<td>-5.204899112</td>
<td>-4</td>
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<td>0.4386</td>
<td>2.1664</td>
<td>2.1574</td>
</tr>
<tr>
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<td>19</td>
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<td>-6.510024144</td>
<td>-5.22625186</td>
<td>0.3621</td>
<td>0.3643</td>
<td>2.9375</td>
<td>2.9349</td>
</tr>
<tr>
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<td>-7.790359332</td>
<td>-6.472135955</td>
<td>0.3167</td>
<td>0.3274</td>
<td>3.7605</td>
<td>3.5377</td>
</tr>
</tbody>
</table>

5.4.3 Energy Dependence on \( L_x \)

To compare with Fig. 5.11 for one hole and a stripe, in Fig. 5.14 we plot \( \Delta_2(L_x, L_y) \), for three classes of lattices \((L_x, b) \times (0, L_y = 7)\) with \( b = 0, 1, 2 \), vs \( 1/L_x \). Here the \( 1/L_x \) fit, as in Eq. 5.25 for the one-hole problem, is no longer good. But we can still extrapolate the energy gap of the two-hole state and the stripe state for an
infinitely long stripe. For the \((L_x, 0) \times (0, 7)\) lattices, the gap is extrapolated to be 
\(-1.4\) approximately, for bosons and fermions.\(^{13}\) Comparing to the single hole gap 
of \(-0.65\), we see that binding between holes are not strong. This information will 
be useful when we consider stripe-array formation in Chapter 6.

![Graph](image)

**Figure 5.14:** \(\Delta_2(L_x, L_y) = E_{2\text{holes}} - E_{\text{stripe}}\) as a function of \(1/L_x\) for three classes of 
lattices \((L_x, b) \times (0, 7)\) with \(b = 0, 1, 2\). The numerical data are in Table D.11.

\(^{13}\)The \((L_x, 2) \times (0, 7)\) systems seem to produce a different gap, around \(-1.7\), and the \((13, 1) \times (0, 7)\) 
lattice appears to start a trend different from other lattices in the \((L_x, 1) \times (0, 7)\) series. This may 
be an effect of kink formation (holes congregate and the stripe forms a 90 degree turn) for these 
boundaries. The work on kinks along a stripe is on-going.
5.5 Summary

In this chapter we considered an extended, quantum-fluctuating object which is natural in our model—the stripe. We showed that for a single stripe the problem can be mapped exactly to the spin-1/2 XX chain which is exactly solvable. The key of this map is that with one stripe the particles can only move in the direction perpendicular to the stripe. For the single stripe case we show that for $L_y = 4p + 3$, where $p$ is an integer, the boson and fermion Hamiltonian matrices are identical.

We also explained the revisions done to the computer diagonalization program for the dense limit. Instead of exhaustively enumerating all basis states with a given number of particles, we start with one state and find all states connected to it by hopping (and record matrix elements during the process).

We then studied the one-hole-with-a-stripe problem. We checked numerically that for rectangular systems the boson and fermion spectra are identical. We explained a graph-based way to construct a similarity matrix that takes the boson problem to the fermion problem and vice versa. We also studied in detail the energy gap $\Delta(L_x, L_y)$ between the hole-with-a-stripe and the stripe cases. We showed that the dependence on $L_y$ is exponential and the dependence on $L_x$ is $1/L_x$.

We then studied the two-hole-with-a-stripe problem and found the same exponential decay in $L_y$ of the two-hole energy gap $\Delta_2(L_x, L_y)$ and extrapolated to the large-$L_x$ limit.

The exponential decay of one-hole and two-hole energies in $L_y$ was studied using a one-dimensional double-well potential and the stripe effective mass was calculated.

In Chapter 6, we will build on this knowledge on the single stripe and holes and study the interesting object that is the stripe-array.
Bibliography


Chapter 6

Stripe-Stripe Interaction and the Stripe-Array

6.1 Introduction

In Chapter 5 we studied the problem of one stripe in the system and that of one and two holes on a stripe. In this chapter we study the interaction among stripes and a very interesting object—the stripe array, that is an array of stripes lying parallel to each other, fluctuating and interacting (see Fig. 6.1 for a system with three stripes).

Experimental observations of stripes in a number of cuprates (La$_1.6-x$Nd$_x$Sr$_2$CuO$_4$ with $x = 0.125$ in Ref. [1]) has given more impetus to investigations of stripes. (See Fig. 1.11 for a schematic drawing of stripes in the CuO$_2$ plane adapted from Ref. [1], and see Ref. [2] for a review of some experimental results and theoretical considerations.) From the theory side, there are basically two roads. One approach is using microscopic models such as the Hubbard and $t-J$ models to study numerically stripe formation and phase separation. DMRG appears to be the best tool in such studies and has been applied to $t-J$ model in Refs. [3, 4]. Another ap-
Figure 6.1: An array of three stripes on a $10 \times 21$ lattice. Each column has $(21 - 3)/2 = 9$ particles, giving a total of 90 particles in this system.
proach to stripes is to use effective field theories, treating stripes as macroscopic objects (macroscopic in the sense of many-particle collective motion). For example in Ref. [5], Zaanen considered stripes as “a gas of elastic quantum strings in 2 + 1 dimensions.” The microscopic, numerical approach can be used to understand the mechanism for stripe formation, and it can be used to derive macroscopic parameters such as stripe-stripe interaction energy and stripe stiffness, but it is limited by computational power. The macroscopic approach on the other hand takes these macroscopic parameters as an input and can obtain results relevant to experiments, but it can explain less about mechanism.

We will follow the microscopic route which enables us to obtain macroscopic parameters from diagonalization data. We will obtain the stripe effective mass from stripe-stripe interaction. With our model, with spinless particles and infinite nearest-neighbor interaction, we can diagonalize systems much bigger (in terms of lattice size) than that can be done with the Hubbard or \( t-J \) models (for example, in Sec. 6.2.3, we study the interaction of two length-six stripes on the 6 x 112 lattice). We have also seen that stripes are natural in our model, and we believe that we have one of the simplest microscopic models based on underlying particle dynamics. Using this model the interaction of stripes and the formation of the stripe-array can be investigated.

In fact, one of the main reasons that we undertook this research on the spinless fermion and the hardcore boson model is our interest in the formation of the stripe-array. As we follow Chapter 5 and add more holes to the system, as we approach the intermediate-filling range (roughly quarter-filled), what happens to our system? Will the stripe-array be stable? or do we see phase separation? that is the separation of the system into a particle-rich region and a hole-rich region. In Fig. 6.2 we show
the two cases schematically.

\[
\begin{array}{cccccccc}
\bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc \\
\bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc \\
\bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc \\
\bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc \\
\bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc \\
\bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc \\
\bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc \\
\bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc & \bigcirc \\
\end{array}
\]

Figure 6.2: System at intermediate-filling (roughly quarter-filled). Phase separation (left), the separation of the system into particle-rich and hole-rich regions, vs stripe-array (right, schematic).

This chapter is organized around the three stability conditions that we study for the stripe-array: Do stripes repel or attract? Does adding holes to the system form new stripes or just a wider stripe? Are the stripe-array stable against phase separation? We will first consider the interaction among stripes and study systems with two, three, and (very briefly) four stripes. We demonstrate from exact diagonalization that states with evenly distributed stripes are the highest weighted states in the ground state. We show that stripes repel and when the stripe separation is large, the interaction among stripes decays as a power law with exponent 2 as a function of the distance between adjacent stripes. We use a one-dimensional model to study this behavior and calculate the stripe effective mass.

We then derive the chemical potential of the stripe-array in the infinite system limit (that is the energy per added hole to make additional stripes) and use it for the next two stability conditions. We compare this chemical potential with the energy of adding a hole to a stripe (calculated in Chapter 5). And we use a Maxwell
construction to see whether the stripe-array or the phase-separated state is stable. The interesting conclusion is that the boson stripe-array is not stable and the fermion stripe-array is very close to the stability limit. Some of the analytical and numerical work in this chapter has appeared in Henley and Zhang [6].

6.2 Two Stripes

6.2.1 Diagonalization

To study systems with two stripes, we use the same diagonalization program for the problem of one stripe and one stripe with holes that was introduced in Sec. 5.2. Again we do not exhaustively enumerate all possible states with a given number of particles \( M \). Instead, we build basis states starting from a given state. The starting state that we use for this two-stripe calculation is that with two stripes merged together. The left figure in Fig. 6.3 shows the starting state for a \( 8 \times 20 \) system. Here with two stripes in a rectangular system, the periodic boundary conditions require that \( L_x \) and \( L_y \) are both even. The number of particles in each column is \((L_y - 2)/2\) giving a total number of particles \( M = L_x(L_y - 2)/2 \) (with \( M = 72 \) for the \( 8 \times 20 \) system).

It may be somewhat surprising to know that we can exactly diagonalize a system as large as \( 8 \times 20 \) with 72 particles, considering the exponential growth in the number of basis states. Tables D.12 and D.13 include the number of basis states for two stripes, that are constructed from a starting state of two merged stripes We observe that the number of basis states grows extremely fast as a function of the length of the stripe \( L_x \) but only linearly in \( L_y \). If we consider a stripe as a spin-1/2 chain, as in Sec. 5.1.3, then increasing the length of the stripe by one step roughly doubles the
Figure 6.3: $8 \times 20$ lattice with two stripes. Each column has $(20 - 2)/2 = 9$ particles giving a total of $M = 8 \times 9 = 72$ particles. On the left is the starting state used for the diagonalization program, and on the right, one of the highest-weighted states in the boson ground state. The total number of basis states here is 73180.
number of basis states. With more than one stripe, this increase is more drastic. On the other hand, the linear increase in the direction perpendicular to the stripe is due to having a family of states which differ only by a shift in the relative y coordinate of the two stripes.

6.2.2 Boson and Fermion Statistics

We observe from exact diagonalization that for rectangular lattices with two stripes, the boson and fermion spectra are identical.\footnote{This is not true for systems with $L_x$ close to $L_y$. For example, for $6 \times 6$ with $M = 12$, the lowest boson energy is $-7.98357$ and the fermion energy is $-7.92667$. There we do not necessarily have two parallel stripes.} In Fig. 6.4, we show two configurations of two merged stripes. For a particle on the stripe we see that the horizontal hops are limited by nearest-neighbor repulsion to adjacent columns only. That means that with two stripes particles cannot move freely along the stripe and the motion in the system is still primarily in the vertical direction. From Fig. 6.4, we can also see, after trying some moves, that we cannot move one particle far away enough so as to exchange the position of two particles. This is a necessary condition in showing that the boson and fermion spectra are identical [7].

We also need to show that periodic boundary conditions do not affect the spectra, and we use again the idea outlined in Sec. 5.3.2 for the one-hole-with-a-striped problem. If we can get the state $\beta$ from $\alpha$ by hopping, define a sign for $\beta$, $\sigma(\beta)$, using the fermion sign from hopping $s(\beta, \alpha)$ and the sign of the state $\alpha$, by $\sigma(\beta) = s(\beta, \alpha)\sigma(\alpha)$. We have shown that if this function $\sigma$ is well-defined (i.e., all hopping paths leading to the same state give the same sign $\sigma$) then it defines a similarity transformation from the fermion to boson states and the spectra are identical. We have, as we did
Figure 6.4: Two configurations of two merged stripes. The arrows indicate the possible hops of one particle along the stripe. The horizontal movement is limited to the adjacent columns only.

for the one-stripe-with-a-hole problem, numerically checked a number of systems with two stripes, for example 4 × 10, 6 × 8, and 8 × 10, and we find that for the cases we checked the function \( \sigma(\alpha) \) is well defined.

### 6.2.3 Stripe-Stripe Interaction

In this section we use diagonalization results to study the interaction of two stripes. In Fig. 6.3, we have shown on the left the starting two-stripe state for the diagonalization program and on the right one of the highest weighted states of the boson ground state. It is clear that the stripes are well separated in this highest weight state of the ground state, \(^2\) and this suggests that two stripes may repel.

\(^2\)We plan, as a future project, to study the statistical average of the stripe separation from all basis states (not just the highest-weight state) of the ground state eigenvector.
To study the interaction between two stripes, we define the following function,
\[ \phi^{L_x}(d) = \frac{E_{2\text{ stripes}}(L_x, L_y) - 2E_{\text{stripe}}(L_x)}{2L_x}, \]  
where \( d \) is the distance between adjacent stripes (here \( d = L_y/2 \) for two evenly spaced stripes), \( E_{2\text{ stripes}} \) the energy of the two-stripe system, and \( E_{\text{stripe}} \) the energy of one single stripe. \( \phi \) is the energy cost per unit length per stripe due to stripe interaction,\(^3\) and it is positive for repelling stripes and negative for attracting stripes. In Fig. 6.5 we show \( \phi(d) \) for stripe length 4, 6, and 8. For all cases, \( \phi(d) \) is positive (the stripes repel) and decays as the stripe separation \( d \) increases.\(^4\)

It is clear that as \( d \to \infty \), \( \phi(d) \to 0 \) and from the graphs it does not decay exponentially. We try the following power-law fitting function,
\[ \phi(d) = \frac{A}{d^\alpha}. \]
In Fig. 6.6 we plot \( \ln(\phi(d)) \) vs \( \ln(d) \) for \( L_x = 4, 6 \) with \( d = 6, 8, \ldots, 56 \), i.e., the largest lattice for \( L_x = 4 \) is \( 4 \times 112 \) and for \( L_x = 6 \) is \( 6 \times 112 \). We see that the power-law assumption is good for \( L_x = 4 \) with the decay exponent \( \alpha \) (slope in Fig. 6.6) close to 2. For \( L_x = 6 \) we observe that the slope approaches 2 as the stripe separation \( d \) is large.

6.2.4 Power-Law Decay and Stripe Effective Mass

In Chapter 5 we explained the exponential decay of the one-hole-with-a-stripe energy in \( L_y \) by mapping the stripe motion to a one-dimensional problem with a double-well potential. Here with two stripes in the system, we have shown again that motion along the stripe is limited, and we expect a one-dimensional potential can be sufficient in capturing the essential physics.

\(^3\)When we are not considering the dependence of \( \phi^{L_x}(d) \) on \( L_x \), we will simply use \( \phi(d) \).

\(^4\)It is interesting to observe that \( \phi(d) \) for \( L_x = 8 \) is significantly smaller than that for \( L_x = 4, 6 \).
Figure 6.5: Stripe-stripe interaction energy cost $\phi(d)$ (Eq. 6.1) for stripe length 4, 6, and 8. $d$ is the distance between adjacent stripes ($d = L_y/2$). The numerical data are in Tables D.12 and D.13.
Figure 6.6: log-log plot of energy cost function $\phi(d)$ (Eq. 6.1) for stripe length $L_x = 4, 6$, with $d = 6, 8, ..., 56$. The slope (decay exponent $\alpha$ in Eq. 6.2) is close to 2 for $L_x = 4$, and for $L_x = 6$ the slope approaches 2 as stripe separation $d$ increases. Linear regression is used for all $L_x = 4$ data, and for the $L_x = 6$ data, only the ten points with the largest $d$ are used.
Here we consider two particles of mass $m^*$ moving in the $y$ direction only. In relative coordinates (center-of-mass frame), we have one particle with reduced mass $m_r = m^*/2$ moving freely but is confined by periodic boundary condition to a range of $L_y$. This is the particle-in-a-box problem and the energy is

$$E = \frac{\hbar^2}{2m_r} \left( \frac{\pi}{L_y} \right)^2 = \frac{\pi^2/m^*}{L_y^2}. \quad (6.3)$$

For the two-stripe problem, from curve fitting in Fig. 6.6, the decay exponent $\alpha$ is close to 2 for $L_x = 4$. Using Eq. 6.2 for $\phi(d)$, the definition for $\phi(d)$ in Eq. 6.1, and $d = L_y/2$ for two evenly spaced stripes, we have the following formula for the two-stripe interaction energy

$$E_{\text{2stripes}} - 2E_{\text{stripe}} = \frac{8L_x A}{L_y^2}, \quad (6.4)$$

where $A$ is the factor in Eq. 6.2.

Eq. 6.3 and Eq. 6.4 give an expression for the effective mass of a stripe from two-stripe interaction,

$$m^* = \frac{\pi^2}{8L_x A}. \quad (6.5)$$

From the linear fitting intercept in Fig. 6.6, we get, for $L_x = 4$, $A = \exp(-1.596418)$, and Eq. 6.5 then gives us the effective mass $m^* = 1.5222$. In Table 5.2, the $L_x = 4$ stripe effective mass calculated in the one-hole-with-a-stripe problem is 1.3561, and in Table 5.3 that from the two-hole problem is 1.3417 for fermions and 1.3358 for bosons. All these results for the effective mass of a short, length-four stripe are comparable.

It is clear that the shorter the stripes the better the one-dimensional approximating model is. For $L_x = 6$, it can be seen in Fig. 6.6 that the exponent approaches 2 in the large-$d$ limit, but for $d$ close to 56 (the largest system that we calculated),
linear regression still gives 1.91. The intercept for \( L_x = 6 \) in Fig. 6.6 is not yet sufficient for us to use Eq. 6.5 to calculate the stripe effective mass.

### 6.3 Three and Four Stripes

#### 6.3.1 Three-Stripe Results

We have also studied the interaction of three and four stripes with stripe length \( L_x = 4 \). In Fig. 6.7, on the left is the starting state in the diagonalization calculation for the \( 4 \times 19 \) lattice, and on the right, the highest weighted state in the fermion ground state. From diagonalization, we find that for 2, 3, and 4-stripe fermion systems we computed, the ground state energy always appears in the \( k = (0, 0) \) sector. The highest weight state in the ground state is identical for fermion and boson cases. Fig. 6.7 shows that, as in the two-stripe case in Fig. 6.3, the stripes tend to be far apart from each other.

To analyze the energy dependence more precisely, we define, in the same fashion as Eq. 6.1, the energy cost per unit length per stripe,

\[
\phi_3(d) = \frac{E_{3\text{stripes}}(L_x, L_y) - 3E_{\text{stripe}}(L_x)}{3L_x}, \tag{6.6}
\]

where \( d = L_y/3 \) here. In Fig. 6.8 we plot \( \phi_3(d) \) vs \( d \) and \( \ln(\phi_3(d)) \) vs \( \ln(d) \). First of all, with three or more stripes, unlike the two-stripe case, particles have enough room to exchange with each other when the stripes merge, and the fermion and boson energies are no longer the same.\(^5\) (However, we see from the graph that the boson and fermion energies are only slightly different.) It is clear that the stripes repel

\(^5\)So strictly speaking, we should write something like \( \phi_3^{L_x} \) to emphasize \( \phi_3 \)'s dependence on \( L_x \) and the boson and fermion statistics, but when we do not explicitly study these dependencies, we neglect them in \( \phi_3 \).
Figure 6.7: $4 \times 19$ lattice with three stripes. Each column has $(19 - 3)/2 = 8$ particles for a total of $M = 4 \times 8 = 32$ particles. On the left is the starting state used for the diagonalization program, and on the right, the highest-weighted state in the fermion ground state (boson state identical). The total number of basis states here is 77907.
and the exponent of $\phi_3(d)$ for $L_x = 4$ is 2.004 for the boson case (and practically the same for the fermion case, not shown in the graph), close to 1.983, the exponent for the two-stripe $L_x = 4$ case (see Fig. 6.6).

### 6.3.2 Stripe Effective Mass

As in the two-stripe case, we believe that this three-stripe problem can be mapped to a one-dimensional problem of three particles. Let us consider the ground state of three fermions of mass $m^*$ in a length-$L_y$ box. The energy is

$$E = \frac{\hbar^2}{2m^*} \left( 0 + 2 \left( \frac{2\pi}{L_y} \right)^2 \right) = \frac{4\pi^2/m^*}{L_y^2}. \quad (6.7)$$

For the three-stripe problem, we use the same $1/d^2$ relation for $\phi_3(d)$, as in Eq. 6.2 for the two-stripe problem,

$$\phi_3(d) = \frac{A_3}{d^2}, \quad (6.8)$$

where $A_3$ is a constant. Then Eqs. 6.7 and 6.8 give us a formula for stripe effective mass $m^*$, similar to the two-stripe formula in Eq. 6.5,

$$m^* = \frac{4\pi^2}{27L_x A_3}. \quad (6.9)$$

Using the linear fitting intercept in Fig. 6.8, we get for $L_x = 4$, $A_3 = \exp(-1.394246)$, and then from Eq. 6.9, we get $m^* = 1.4738$, which is consistent with the two-stripe result 1.5222 calculated in Sec. 6.2.4.

### 6.3.3 Four Stripe Results

We have also calculated the energy for the smallest system with four stripes: the $4 \times 12$ system with 16 particles. In Fig. 6.9 we show the starting state and one of the highest weighted states in the fermion ground state (the boson state is identical).
Figure 6.8: Stripe-stripe interaction energy cost $\phi_3(d)$ (Eq. 6.6) for three stripes with length 4 ($L_x = 4$). $d$ is the distance between adjacent stripes ($d = L_y/3$). The boson and fermion energies are slightly different. The log-log plot is shown below, showing for bosons an exponent 2.004. The numerical data are in Table D.14.
Here the boson energy is $-10.8525$ and the fermion energy $-10.8418$, both higher than the energy of four independent stripes with length 4, $-11.3137$.

Figure 6.9: $4 \times 12$ lattice with four stripes. Each column has $(12-4)/2 = 4$ particles for a total of $M = 4 \times 4 = 16$ particles. On the left is the starting state used for the diagonalization program, and on the right, one of the highest-weighted states in the fermion ground state (boson state identical). The total number of basis states here is 93290.

### 6.3.4 Stripe-Stripe Interaction Summary

We summarize the results for two, three, and four stripes. The boson and fermion energies are identical in the two-stripe case and are slightly different with more stripes. The stripes repel in all cases and the interaction as a function of stripe separation decays as a power law with exponent 2 when the stripe separation is large. We can understand the power-law behavior and the exponent using a one-dimensional
model of particles in a box, and the stripe effective mass is then calculated. With
intuition built from diagonalizing systems with a small number of stripes, we turn
to the stripe-array in the next section.

6.4 The Stripe-Array Chemical Potential

In this section we consider an array of stripes and calculate the chemical potential
of the stripe-array, i.e., the energy per hole in creating a new stripe. We will need
this information for stability analysis later. The calculation here has appeared in
Henley and Zhang [6].

Say we have a $L_x \times L_y$ system with $p$ stripes stretching in the $x$ direction. The
number of particles per column is $(L_y - p)/2$ and the total number of particles is

$$M = \frac{L_y - p}{2} L_x.$$  \hspace{1cm} (6.10)

Denote the total number of lattice sites $N = L_x L_y$, then the particle density is

$$n = \frac{M}{N} = \frac{1}{2} - \frac{p}{2L_y} = \frac{1}{2} - \frac{1}{2d},$$ \hspace{1cm} (6.11)

where $d$ is the separation between adjacent stripes and for even distributed stripe
we have $d = L_y/p$. We then have

$$d = \frac{1}{1 - 2n}. \hspace{1cm} (6.12)$$

The energy of the stripe-array has two contributions: the energy from independent
stripes and the energy due to stripe-stripe interaction. The energy per length $\sigma_0$ of
an infinitely long stripe is

$$\sigma_0 = -\frac{2}{\pi} t. \hspace{1cm} (6.13)$$
which can be obtained from mapping the stripe to the spin-1/2 chain (see Mila [8]).

Therefore the energy of \( p \) independent stripes is

\[
E_{\text{indep}} = p \sigma_0 L_x = \frac{\sigma_0}{d} L_x L_y,
\]

where we have used \( p = L_y/d \). On the other hand, the energy due to stripe-stripe interaction is

\[
E_{\text{interaction}} = p\phi(d) L_x = \frac{\phi(d)}{d} L_x L_y,
\]

where we have used the two-stripe interaction energy per length per stripe \( \phi(d) \) defined in Eq. 6.1. (Note that we have seen in Sec. 6.2.3 that \( \phi \) also depends on the length of the stripe \( L_x \). Fortunately, in the following, we will only work in the \( d \to \infty \) limit of \( \phi(d) \), which is independent of \( L_x \).) Combining Eq. 6.14 and Eq. 6.15, we obtain the energy density (per lattice site) of the stripe array as a function of particle density \( n \),

\[
\mathcal{E}_{sa}(n) = \frac{E_{\text{indep}} + E_{\text{interaction}}}{N} = \left( \sigma_0 + \frac{\phi(d)}{d} \right) \frac{1}{d} = \left( \sigma_0 + \phi(d) \right) (1 - 2n).
\]

Furthermore, we have seen, when we studied stripe-stripe interaction, \( \phi(d) \) is positive and \( \phi(d) \to 0 \) as \( d \to \infty \). So in the infinite-lattice limit we have

\[
\mathcal{E}_{sa}(n) = \sigma_0 (1 - 2n).
\]

That is to say that the chemical potential of the stripe-array is

\[
\mu^* = \frac{d\mathcal{E}_{sa}(n)}{dn} = -2\sigma_0 = \frac{4t}{\pi} = 1.273t,
\]

where the result for \( \sigma_0 \) from Eq. 6.13 is used. Eq. 6.18 says that the slope of the stripe energy density curve is \( 1.273t \), and if we have an array of stripes in the system then adding a particle to the system will raise the energy by \( 1.273t \), or equivalently, adding a hole to the stripe-array will lower the energy by \( 1.273t \). This is an important quantity in the stability analysis that is to follow.
6.5 Stripe-Array Stability

At the beginning of this chapter, we briefly introduced the stability considerations for the stripe-array. In Fig. 6.2 we showed two states at intermediate fillings: the separation of the system into particle-rich and hole-rich regions and the stripe-array. How do we know which state is the ground state for our model? How do we know whether the stripe-array state is stable?

**Stability Condition 1: Stripes Repel**

We have already studied stripe-stripe interaction, and we know that stripes repel. This is our first stability condition. In fact, we have seen in Figs. 6.3, 6.7, and 6.9 that starting with a phase separated state, exact diagonalization shows that states with highest weights in the exact ground state have stripes far apart.

**Stability Condition 2: Two Stripes Beat One Fat Stripe**

Our second stability condition comes from the work on the one-hole-with-a-stripe problem in Chapter 5. Here we want to know whether with more holes new stripes will form or the existing stripes just get wider (thus leading to phase separation). We showed in Sec. 5.3.5 that adding a hole to an infinitely long stripe lowers the energy by 0.66. Here we have shown that adding a hole to a stripe-array lowers the energy by 1.273 (with \( t = 1 \)). The stripe-array state is therefore preferred.

**Stability Condition 3: Stripe-Array Beats Phase Separation**

The third stability condition comes from free energy analysis in statistical mechanics. Here because we are considering zero temperature physics and \( F = E - TS \), energy is free energy. In Fig. 6.10 we show the two cases. The dashed tie-line is the Maxwell
construction. It is tangent to the liquid curve (small fillings) and is connected to the half-filled state at $n = 1/2$. It represents the coexistence of the liquid state and the half-filled state, i.e., the phase separated state. According to Sec. 6.4, the stripe-array line should have slope 1.273, and it is drawn from the half-filled limit. The stripe-array case is stable when the stripe-array line is below the dashed line, otherwise the phase separated state is stable. Therefore, to determine the stability of the stripe-array against phase separation, we need to determine the slope of the dashed line $\mu^{LC}$. Here we are following the notation in Ref. [6] and the superscript LC denotes the two states: liquid and CDW (charge-density-wave, i.e., half-filled state) that are connected by the dashed line.

To obtain $\mu^{LC}$, we need a fitting function for the energy density $E/N$ at intermediate fillings (the liquid part). We use a polynomial form, up to the third order in particle density $n = M/N$,

$$\mathcal{E}(n) = \frac{E(n)}{N} = A_1 n + A_2 n^2 + A_3 n^3,$$  \hspace{1cm} (6.19)

where $E(n)$ is the energy of the $M$ particle system. This fitting form can also be written as

$$\frac{E}{M} = A_1 + A_2 n + A_3 n^2,$$  \hspace{1cm} (6.20)

where $E/M$ is the energy per particle. We will use Eq. 6.20 to fit diagonalization results. The slope $\mu^{LC}$ can be determined by first solving for $n^*$, the $n$ coordinate of the intersection of the dashed tie-line with the liquid curve, using

$$\mu^{LC} = \frac{\mathcal{E}(n^*) - 0}{n^* - 1/2} = \frac{d\mathcal{E}(n)}{dn} \bigg|_{n^*}. \hspace{1cm} (6.21)$$

In Fig. 6.11, we plot, for fermions and bosons, $E/M$ vs $n$ at the intermediate fillings ($0.19 \leq n \leq 0.31$) for a number of lattices with lattice size ranging from
Figure 6.10: Stability of the stripe-array vs phase separation. Energy density $E/N$ vs particle density $n = M/N$. The stripe-array curve has slope $\mu^* = 1.273$. The dashed line is tangent to the liquid curve and is connected to the half-filled state. It represents the coexistence of the two phases: liquid and half-filled states, i.e., a phase separated state. On the left is the case where the stripe-array line is below the dashed line, and therefore the stripe-array is stable. On the right is the case where the dashed line is below the stripe-array line, i.e., the phase separated state is stable. $n^*$ is the intersection of the tie-line with the liquid curve, and the key quantity is the slope of the dashed line $\mu^{LC}$. 
Figure 6.11: Fermion (top) and boson (bottom) $E/M$ vs $n = M/N$ fit for intermediate fillings ($0.19 \leq n \leq 0.31$). The fermion data have larger spread than the boson data because of the fermion shell effect (that will be discussed in Sec. 7.1). The numerical data are in Tables D.15 to D.24.
25 to 42.\textsuperscript{6} In Table 6.1 we list the quadratic fitting parameters obtained from diagonalization data. For the ten lattices in Fig. 6.11, using Eq. 6.21, we obtain $\mu^{LC} = 1.254$ for fermions and $\mu^{LC} = 1.304$ for bosons.

Table 6.1: Fermion and boson fitting parameters (in Eq. 6.19) and the calculated $n^*$ and $\mu^{LC}$ (using Eq. 6.21), for all ten lattices in Fig. 6.11 and for the smallest and largest five lattices separately. Compared with the stripe-array slope $\mu^* = 1.273$, the fermion stripe-array is stable against phase separation ($\mu^{LC} < \mu^*$), and the boson stripe-array is unstable ($\mu^{LC} > \mu^*$).

<table>
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<th>Particle</th>
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<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$n^*$</th>
<th>$\mu^{LC}$</th>
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<td></td>
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<tr>
<td></td>
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<td>1.264</td>
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<tr>
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<td>all 10</td>
<td>-6.138</td>
<td>27.839</td>
<td>-33.950</td>
<td>0.233</td>
<td>1.304</td>
<td>Unstable</td>
</tr>
<tr>
<td></td>
<td>small 5</td>
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<td>-38.420</td>
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<td>1.301</td>
<td></td>
</tr>
<tr>
<td></td>
<td>large 5</td>
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<td>26.580</td>
<td>-31.251</td>
<td>0.233</td>
<td>1.307</td>
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</tbody>
</table>

In Table 6.1, we have also included calculations for the five smallest and five largest lattices in Fig. 6.11 separately. We find that $\mu^{LC}$ for both boson and fermion increases with increasing lattice size. For the boson case, this means that for large lattices, the stripe-array is not stable against phase separation ($\mu^{LC} > \mu^* = 1.273$). For the fermion case, the result is stable ($\mu^{LC} < \mu^*$) for the lattices that we have studied, but $\mu^{LC}$ is very close to the stability limit 1.273. The fermion stripe-array is possibly stable.

In our earlier publication, Ref. [6], we used the same polynomial fitting function,

\textsuperscript{6}These are square lattices $(a, -b)(b, a)$ with $a = 5, 6$ and $b = 0, 1, 2$, and rectangular lattices $5 \times 6, 5 \times 7, \text{and } 6 \times 7$. 
Eq. 6.19, but we fixed $A_1 = -4$, corresponding to the energy of an noninteracting particle, and our systems there went from 20 sites ($4 \times 5$) to 36 sites ($6 \times 6$). The analysis in this section and the results in Table 6.1 are obtained using the three-parameter ($A_1, A_2, A_3$) fit for bigger lattices, from 25 sites ($5 \times 5$) to 42 sites ($6 \times 7$). The conclusion in Ref. [6] was $\mu^{LC}_{\text{fermion}} = 1.25(2)$ and $\mu^{LC}_{\text{boson}} = 1.33(2)$.

6.6 Summary, Conclusion, and Future Work

Summary

In this chapter we studied an important object—the stripe-array. We began with an analysis of stripe-stripe interaction, for two, three, and four stripes. We saw that stripes repel and the interaction energy decreases to zero as power laws as the separation between adjacent stripes increases. We used a particle-in-a-box potential to study the interaction of short stripes and obtained stripe effective mass that is comparable to the one-hole and two-hole-with-a-stripe calculation in Chapter 5. We then computed the chemical potential of the stripe-array near the half-filled limit, and we considered in detail the stability conditions of the stripe-array. In addition to repulsion among stripes, we also showed that it is more favorable to form a stripe-array than adding holes to existing stripes. And using a Maxwell construction, we showed the interesting result that the boson stripe-array is not stable against phase separation into particle-rich and hole rich regions, while the fermion stripe-array is very close to the stability limit and is possibly stable.
Conclusion

This chapter and Chapter 5 taken as a whole are an attempt to understand stripes as macroscopic objects arising from microscopic components (the spinless fermion and hardcore boson particles in our model). The underlying physics is the quantum mechanics of the component particles that is described by a many-particle Schrödinger equation (which we solve by exact diagonalization). Stripes can perhaps be called an emergent phenomenon and are results of collective motions of many microscopic particles (the original particles or holes). They can perhaps be considered in the same fashion as phonons arising from collective lattice vibrations. And like phonons, the stripes in our problem have a life of their own, and we have tried, in these two chapters, to understand the new physics they bring.

Future Work

There are a number of investigations on stripes that we plan to do next. First, it is straightforward to study stripes in systems with tilted boundaries. Second, we would like to study stripes that go along the diagonal of systems such as $5 \times 5$. In this chapter and Chapter 5, we have confined ourselves to stripes parallel to an axis of the lattice, for example, in the horizontal direction, and then holes move along the stripe, also in the horizontal direction. With diagonal stripes, as holes move along the stripe, they can move in the horizontal and vertical directions, perhaps gaining more kinetic energy. Diagonal stripes are observed in La$_2$NiO$_4$ [1], and they are an interesting topic in the $t - J$ model [9]. Third, in this chapter and Chapter 5 we have not made use of excited state information. We would like to see whether we can understand the low-lying excitations using simple models. Fourth, we showed in Figs. 6.3, 6.7, and 6.9 the starting state of diagonalization with stripes all merged
and the highest-weight state in the ground state eigenvector, and observed that
stripes tend to be far apart in the ground state. We are interested in obtaining the
statistical average of stripe separation for all states in the ground state eigenvector.
Finally, as mentioned in the introduction, there is another approach to the stripe
problem, using quantum elastic strings in the continuum to model stripes [5]. We are
interested in comparing our diagonalization data to results from these macroscopic
studies.
Bibliography

Chapter 7

A Few Fermions: Shell Effect and T-Matrix

In this chapter, we return to the low-density limit and study the problem of a few fermions. In Chapter 3, we used lattice Green function to study the problem of two particles (bosons and fermions), and at the end of that chapter, in Sec. 3.10, we obtained the ground state energy of a few particles on a large lattice by summing up the energy of each pair of particles. This chapter contains a much more detailed study of the few-fermion problem: we will consider first the fermion shell effect and then we will study the interaction correction to energy (ground state and excited states) for a few fermions (three, four, and five) using the t-matrix.

In Chapter 4, we saw that the t-matrix for the two-particle problem is an exact formulation of the Schrodinger equation and is also equivalent to the lattice Green function formulation derived in Chapter 3. The interacting energy $E$ is related to the noninteracting energy $E_0 = \mathcal{E}(\mathbf{q}) + \mathcal{E}(\mathbf{q}')$ by the following implicit equation,

$$E = E_0 + T(E), \quad (7.1)$$
where $T(E)$ is an eigenvalue of the matrix $\mathcal{T}(E)$ (see Sec. 4.3.7) and depends on $\mathbf{q}$ and $\mathbf{q}'$. For fermions, we have seen that a small number of iterations using $E_{n+1} = E_0 + T(E_n)$ converges to the exact energy $E$ quickly at least for the low-lying states (see Sec. 4.5).

What about more than two particles? After we exactly solved the Kepler two-body problem, how about the three-body problem with the same gravitational force? After hydrogen atom, how about helium atom? How about three magnons? or three electrons in the Hubbard model? These three-body problems that we mention here apparently range from a no-exact-solution-but-still-textbook problem (the helium atom, see Ref. [1]) to a research paper problem (see Ref. [2] for a number of three-body problems on the lattice, e.g., three magnons, and Ref. [3] for three electrons in the Hubbard model) to a very difficult open question (three-body problem in planetary motion, see e.g., Ref. [4]).

Fortunately, in our problem of three or more fermions, if we are only interested in energy (not eigenstate), there is a straightforward method using the two-particle $t$-matrix. The two-particle $t$-matrix is useful because it neatly packages the effect of interaction as it contains two-body scatterings to all orders. For just a few particles, we will use the following formula to calculate energy,

$$E = \sum_\mathbf{q} \mathcal{E}(\mathbf{q}) + \frac{1}{2} \sum_{\mathbf{q}\mathbf{q}'} \tilde{T}(\mathbf{q}, \mathbf{q}'),$$  \hspace{1cm} (7.2)

which includes the noninteracting energies in the first sum and interacting corrections applied to each pair in the second sum. We have use $\tilde{T}(\mathbf{q}, \mathbf{q}')$ for the two-particle $t$-matrix, built from the noninteracting state $|\mathbf{q}, \mathbf{q}'\rangle$, and the tilde denotes modification by the presence of other fermions due to Pauli exclusion.\footnote{Because many bosons can occupy the same states, thus forming a condensate, we need to modify Eq. 7.2. We have not worked out the boson problem.}
Eq. 7.2 has appeared in the introduction to Chapter 4, and in this chapter, we show example fermion calculations using this equation for three, four, and five particles. But first we demonstrate the shell effect for the case of a few fermions.

7.1 Fermion Shell Effect

7.1.1 Fermion Shells Introduced

The fundamental difference between fermions and bosons is the Pauli exclusion principle, that while many identical bosons can occupy the same state, no two identical fermions can do so. At zero temperature, the ground state of noninteracting fermions is formed by filling the one-particle states one by one from the lowest to higher energies. A familiar example is from atomic physics where the notation $1s^22s^22p^2$ for the carbon atom for example denotes two electrons (one spin up and one spin down) in the $n = 1$, $l = 0$ state, two in the $n = 2$, $l = 0$ state, and two in the $n = 2$, $l = 1$ state, where the states we refer to are the eigenstates of a one-electron atom, i.e., the hydrogen atom states with appropriate mass and charge factors. Because of the existence of degeneracy in one-electron states (i.e., states with different $l$ but the same $n$ have the same energy) and the exclusion principle, we have the familiar shell structure: as we fill the one-electron states, the energy jumps abruptly as one moves from a closed “shell” to the next state, e.g., adding an electron to the $1s^22s^22p^5$ state (open shell) is different energetically from add one to the $1s^22s^22p^6$ state (filled shell), because in the latter case a $n = 3$ state must be filled. For our model of spinless fermions on a square lattice, we have the two ingredients for the shell effect: fermionic exclusion and degeneracies of one-particle states due to the form of our energy function and lattice symmetry (for example for
a rectangular lattice the state with momentum \((1, 0)\) has the same energy as that with momentum \((-1, 0)\). In this section we will demonstrate the shell effect in our model in the dilute limit.

7.1.2 Fermion Shells: Rectangular-Boundary

In Fig. 7.1 we show the exact and for comparison the noninteracting ground state energies for the \(5 \times 8\) lattice for up to seven particles. The total energy curve (top graph) shows slope change at \(M = 3\) and \(M = 5\), and the energy increment curve \(E(M) - E(M - 1)\) (bottom graph) shows clearly the shell effect. For example, adding the fourth particle increases the energy much more than adding the third particle. The numerical values are shown in Table 7.1, along with the noninteracting states.

We should be clear that except for the filled shells \((M = 1, 3, 5)\), there are degenerate noninteracting states. For example, for \(M = 2\), we have shown in Table 7.1 the state \((0,0)(0,1)\) (with total momentum \((0,1)\)), but it is degenerate with the state \((0,0)(0,-1)\) (with total momentum \((0,-1)\)). Here the exact energy for \(k = (0,1)\) is identical to that for \(k = (0,-1)\) because of lattice reflection symmetry. This is also the case for \(M = 4\), with two degenerate states \((0,0)(0,1)(0,-1)(1,0)\) (shown) and \((0,0)(0,1)(0,-1)(-1,0)\) and the exact energies for \(k = (1,0)\) and \((-1,0)\) are identical, also for \(M = 6\), with four degenerate states. There is however a problem with the \(M = 7\) case. In Table 7.1 we show the \((0,0)(0,1)(0,-1)(1,0)(-1,0)(1,1)(-1,-1)\) state, with total momentum \((0,0)\). This state is degenerate with the state \((0,0)(0,1)(0,-1)(1,0)(-1,0)(1,1)(1,-1)\), with total momentum \((2,0)\), but the two states are not related by symmetry. The exact energy for the \(k = (0,0)\) sector is \(-14.6400957578\) (ground state) while that for \(k = (2,0)\) is \(-14.4375052486\). To calculate the exact energy from a particular non-
Figure 7.1: Shell effect for $5 \times 8$ lattice. Exact, interacting groundstate energies are compared with noninteracting energies for up to seven particles. Total energy (top graph) and energy increment $E(M) - E(M - 1)$ (bottom) are shown, with four shells apparent. Numerical values are in Table 7.1.
Table 7.1: Noninteracting and exact groundstate energies for $5 \times 8$ lattice with one to seven particles. The noninteracting states in momentum space are drawn. The energy increment is $E(M) - E(M - 1)$ from adding the latest particle. $k$ is the total momentum vector from exact diagonalization. The noninteracting states are unique for the filled shells, $M = 1, 3, 5$, but there are degenerate states for other cases. In the latter case, the one with the same total momentum as the diagonalization $k$ is drawn. See text for a more detailed explanation of this degeneracy.

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<th>$E$ (noninter)</th>
<th>State</th>
<th>$E$ inc.</th>
<th>$E$ (exact)</th>
<th>$k$</th>
<th>$E$ inc.</th>
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interacting state with a few fermions, we will need the t-matrix technique that will be introduced later in this chapter.

7.1.3 Fermion Shells: Square-Boundary

We should also mention that the filled shells are at \( M = 3 \) and \( M = 5 \) because we have deliberately chosen a rectangular system with \( L_x < L_y \); the \( x - y \) reflection symmetry is broken, with \( E(0, 1) < E(1, 0) \), so we have a filled shell at \( M = 3 \). On the other hand, if we have \( L_x = L_y \), so \( E(0, 1) = E(1, 0) \), then \( M = 3 \) will not be a filled shell. In Fig. 7.2, we show the noninteracting and interacting energies for the square \( 7 \times 7 \) lattice. It is clear that here the shell is not filled at \( M = 3 \) but continues to \( M = 5 \). In Table 7.2 we show the numerical values and draw the noninteracting states.

Again in Table 7.2, when there are degenerate noninteracting states, we have shown the one with the same total momentum as \( \mathbf{k} \) from diagonalization. Two degenerate states that are not related by symmetry are the \( M = 3 \) state \( (0, 0)(0, 1)(1, 0) \) with total momentum \( (1, 1) \) (shown in Table 7.2) and \( (0, 0)(0, 1)(0, -1) \) with total momentum \( (0, 0) \). The exact energy for \( \mathbf{k} = (1, 1) \) is -10.073561201 (ground state) and that for \( \mathbf{k} = (0, 0) \), -10.15749377. T-matrix calculations are again needed to for a precise map from noninteracting to interacting states.

7.1.4 Bosons: No Shells

For comparison, we show boson energy plot for the \( 5 \times 8 \) lattice in Fig. 7.3. Because bosons can all be at the zero-momentum state, where energy is \(-4\), the noninteracting energy is \(-4M\). The exact energy curve shows smooth changes when \( M \) increases. There is no shell effect.
Figure 7.2: Shell effect for $7 \times 7$ lattice. Exact, interacting groundstate energies are compared with noninteracting energies up to seven particles. Total energy (top graph) and energy increment $E(M) - E(M - 1)$ (bottom) are shown, with three shells apparent. Numerical values for these two graphs are in Table 7.2.
Table 7.2: Noninteracting and exact ground state energies for $7 \times 7$ lattice with one to seven particles. The noninteracting states in momentum space are drawn. The energy increment is $E(M) - E(M-1)$ from adding the latest particle. $k$ is the total momentum vector from exact diagonalization. When there are degenerate noninteracting states, the one has the same total momentum as $k$ from diagonalization is drawn.

<table>
<thead>
<tr>
<th>$M$</th>
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<th>State</th>
<th>$E$ inc.</th>
<th>$E$ (exact)</th>
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Figure 7.3: Boson noninteracting and exact groundstate energies for the $5 \times 8$ lattice with one to seven particles. Because bosons can all be at the zero-momentum state, where the energy is $-4$, the noninteracting energy is $-4M$ (a straight line). The exact energy shows smooth changes when $M$ increases. There is no shell effect.
7.2 T-Matrix Review

Before we apply the t-matrix to study the problem of a few fermions, let us review the t-matrix approach for the two-particle problem, by including below the outline from Sec. 4.3.7.

1. Given \( \mathbf{q}_1 \) and \( \mathbf{q}_2 \), with the total noninteracting energy \( E_0 = \mathcal{E}(\mathbf{q}_1) + \mathcal{E}(\mathbf{q}_2) \) and total momentum \( \mathbf{P} = \mathbf{q}_1 + \mathbf{q}_2 \), form \( Q_I \) and \( Q_{II} \) (with \( N_1 \) and \( N_2 \) elements).

2. Solve for \( E \) in \( E = E_0 + \text{Eigenvalue}(\mathcal{T}(E)) \), where \( \mathcal{T}(E) \) is given by

   (a) Form the \( 4 \times 4 \) matrix

   \[
   \mathcal{G}_{ij}^{II}(E) = G^{II}(E, \mathbf{P}; \mathbf{R}_i, \mathbf{R}_j)
   \]

   using Eq. 4.11.

   \[
   G^{II}(E, \mathbf{P}; \mathbf{r}, \mathbf{r'}) = \frac{1}{N} \sum_{\mathbf{q} \in Q_{II}} \frac{e^{i\mathbf{q} \cdot (\mathbf{r'} - \mathbf{r})}}{E - \mathcal{E}(\mathbf{q}) - \mathcal{E}(\mathbf{P} - \mathbf{q})},
   \]

   (b) Invert \( I - \mathcal{G}^{II}(E)V \).

   (c) Form the t-matrix

   \[
   \mathcal{T}_{\mathbf{q}, \mathbf{q}'} = T(E, \mathbf{P}; \mathbf{q}, \mathbf{q}')
   \]

   for \( \mathbf{q}, \mathbf{q}' \in Q_I \), using Eq. 4.21,

   \[
   T(E, \mathbf{P}; \mathbf{q}, \mathbf{q}') = \frac{1}{N} \sum_{ij} e^{i\mathbf{R}_i} e^{-i\mathbf{R}_j} \left( V(I - \mathcal{G}^{II}(E)V)^{-1} \right)_{ij}.
   \]

   (d) If we have \( N_1 = 2 \) or \( N_1 = 4 \) with pair component exchange symmetry, we can find the eigenvalues of \( \mathcal{T}(E) \) easily, by forming the symmetry reduced t-matrices, e.g., for \( N_1 = 2 \), \( T_{1,1}(E) \) and \( T_{1,-1}(E) \), and for \( N_4 \), \( T_{1,1,1,1}(E), T_{1,1,-1,-1}(E), T_{1,-1,1,-1}(E) \), and \( T_{1,-1,-1,1}(E) \). Then we just need to solve a scalar equation \( E = E_0 + T(E) \), where \( T(E) \) stands for
the symmetry-reduced functions \( T_{1,-1}(E) \) for example. (For a general

case, we diagonalize \( \mathcal{T}(E) \), and \( T(E) \) is one of the eigenvalues.)

3. The corresponding eigenvector is \( g(\mathbf{q}) \) with \( \mathbf{q} \in Q_I \). \( g(\mathbf{q}) = g(\mathbf{P} - \mathbf{q}) \) is the

boson solution, and \( g(\mathbf{q}) = -g(\mathbf{P} - \mathbf{q}) \) the fermion solution.

4. For \( \mathbf{q} \in Q_{II} \), using Eq. 4.22,

\[
g(\mathbf{q}) = \frac{1}{E - \mathcal{E}(\mathbf{q}) - \mathcal{E}(\mathbf{P} - \mathbf{q})} \sum_{\mathbf{q}'' \in Q_I} T(E, \mathbf{P}; \mathbf{q}, \mathbf{q}'') g(\mathbf{q}''). \tag{7.5}
\]

For our case \( V = +\infty \), the t-matrix expression becomes,

\[
T(E, \mathbf{P}; \mathbf{q}, \mathbf{q}') = \frac{1}{N} \sum_{ij} e^{i\mathbf{q}\mathbf{R}_j} e^{-i\mathbf{q}'\mathbf{R}_j} \left( -\mathcal{G}^{II}(E)^{-1} \right)_{ij}. \tag{7.6}
\]

The t-matrix’s starting point is a set of momentum vectors \( Q_I \) that have the same
total momentum \( \mathbf{P} \) and are degenerate in noninteracting energy \( E_0 \). It calculates
the interaction correction \( T(E) \) by summing all two-particle scattering terms (to
momentum vectors in \( Q_{II} \)), described by the ladder diagrams in Chapter 4, resulting
in \( \mathcal{T}(E) \). The symmetric eigenvectors of \( \mathcal{T}(E) \) then correspond to bosons and the
antisymmetric ones fermions.

For the two-particle problem, the resulting equation \( E = E_0 + T(E) \) is exact
because with two particles, only two-body scatterings are possible and they are all
summed in the t-matrix. For more than two particles, a natural way is to sum all
binary scattering corrections each calculated using the t-matrix. (With \( M \) particles,
there are \( M(M-1)/2 \) terms in the sum.) This procedure ignores the three or more
particle interactions, but for the dilute limit, we expect the two-body scattering
terms give the largest contribution. In the following section, we will introduce the
modifications to the t-matrix for problems with more than two particles. In this
chapter, we will only develop the t-matrix formalism for dilute fermion systems.
The boson case is different because of the presence of a condensate. We wish to consider the boson case in a future work.

7.3 A Three-Fermion Example

7.3.1 Noninteracting Levels and States

We first compute the energy of three fermions \( M = 3 \) for the \( 8 \times 9 \) lattice with \( \mathbf{P} = 0 \). For this example calculation, we have chosen \( L_x \neq L_y \) to reduce the number of degeneracies in the noninteracting spectrum. In Table 7.3 we show the lowest five noninteracting levels and the corresponding states in momentum space.

7.3.2 Ground State

Let us consider the lowest noninteracting state in the \( 8 \times 9 \), \( \mathbf{P} = (0, 0) \), and \( M = 3 \) system, with three momentum vectors: \( \mathbf{k}_1 = (0, 1) \), \( \mathbf{k}_2 = (0, 0) \), and \( \mathbf{k}_3 = (0, -1) \). And let us first consider the interaction of the pair \( \mathbf{k}_1 \) and \( \mathbf{k}_2 \). The noninteracting energy of the pair is \( E_0^{12} = \mathcal{E}(\mathbf{k}_1) + \mathcal{E}(\mathbf{k}_2) = -7.682507 \) and the total momentum is \( \mathbf{P}_{12} = \mathbf{k}_1 + \mathbf{k}_2 = (0, 1) \). As usual, we use \( E_0^{12} \) and \( \mathbf{P}_{12} \) to form the set \( Q_1^{12} \). Here there are no other degenerate vectors so \( Q_1^{12} = \{(0, 0), (0, 1)\} \). The three-particle problem is different from the two-particle case in the choice of \( Q_{II} \), the set of momentum vectors that the two particles can scatter into. Due to the presence of the third particle and Pauli exclusion, the two particles at \( \mathbf{k}_1 = (0, 1) \) and \( \mathbf{k}_2 = (0, 0) \) cannot be scattered into the momentum vector \( \mathbf{k}_3 = (0, -1) \), so we must exclude \( \mathbf{k}_3 \) from \( Q_{II} \). Furthermore, even though there is no particle at \( \mathbf{P}_{12} - \mathbf{k}_3 = (0, 1) - (0, -1) = (0, 2) \), this momentum cannot be scattered into, because otherwise the other particle would be scattered into the occupied \( \mathbf{k}_3 \). That is to say, the momentum vectors that
Table 7.3: Lowest five noninteracting energy levels for the $8 \times 9$ lattice with $M = 3$ fermions and total momentum $\mathbf{P} = (0, 0)$. States in momentum space are drawn with number of degenerate states in each level. The program \texttt{noninteracting} described in Appendix F is used to find the lowest noninteracting energies and eigenstates.

<table>
<thead>
<tr>
<th>Energy</th>
<th>Deg</th>
<th>States</th>
</tr>
</thead>
<tbody>
<tr>
<td>-11.06417777</td>
<td>1</td>
<td>•</td>
</tr>
<tr>
<td>-10.82842712</td>
<td>1</td>
<td>•</td>
</tr>
<tr>
<td>-9.892604897</td>
<td>6</td>
<td>•</td>
</tr>
<tr>
<td>-8.694592710</td>
<td>1</td>
<td>•</td>
</tr>
<tr>
<td>-8.239901252</td>
<td>6</td>
<td>•</td>
</tr>
</tbody>
</table>
can be scattering into are $\tilde{Q}_{12}^{2} = \{ \mathbf{k} | \mathbf{k} \neq \mathbf{k}_1, \mathbf{k}_2, \mathbf{P}_{12} - \mathbf{k}_3 \}$, where we have used tilde to denote exclusion. The exclusion is shown graphically in Tab. 7.4.

After this consideration of exclusion due to the presence of other particles, we can turn to the t-matrix formalism using $Q_{12}^{12}$ and $\tilde{Q}_{12}^{12}$ and compute energy correction $\tilde{T}_{12}$ for the interaction of the $k_1$ and $k_2$ pair (here the tilde denotes modification due to exclusion). $\tilde{T}_{12}$ denotes the iteration solution of $E = E_{0}^{12} + \tilde{T}_{12}(E)$, i.e., using iteration $E_{n+1} = E_{0}^{12} + \tilde{T}_{12}(E_{n})$, find $m$ such that $|E_{m+1} - E_{m}| < Tol$, where $Tol$ is the tolerance (we choose $Tol = 10^{-15}$), then write $\tilde{T}_{12}^{2} = \tilde{T}_{12}(E_{m})$. The number of iterations used in such a calculation is in the order of tens. Also $\tilde{T}_{12}(E)$ here is the fermion function, corresponding to the antisymmetric eigenvector of the t-matrix $\tilde{\mathcal{T}}(E)$.

We can repeat this process for all pairs in the system, here $(k_2, k_3)$, giving correction $\tilde{T}_{23}^{3}$, and $(k_1, k_3)$, giving $\tilde{T}_{13}^{3}$. The energy calculated from considering the pair t-matrix interactions for this three-particle system is then

$$E_{tm} = \mathcal{E}(k_1) + \mathcal{E}(k_2) + \mathcal{E}(k_3) + \tilde{T}_{12} + \tilde{T}_{13}^{3} + \tilde{T}_{23}^{3}. \quad (7.7)$$

The numerical values of this calculation are given in Table 7.4.

### 7.3.3 Nondegenerate Excited States

Using the same procedure, we can also calculate the t-matrix energies for the non-degenerate excited states\(^2\) of the $M = 3$ system in Table 7.3: the $(-1,0)(0,0)(1,0)$ and $(0,2)(0,0)(0,-2)$ states. The results are shown in Table 7.5. Fig. 7.4 shows graphically the noninteracting energy levels, the t-matrix energies for the three non-degenerate states, and the exact energies from diagonalization, and the arrows link

\(^2\)We will discuss the degenerate states in Sec. 7.5 after we present two more examples.
Table 7.4: T-matrix calculation for the 8 × 9 lattice with \( M = 3 \) noninteracting particles \( k_1 = (0, 0), k_2 = (0, 1), \) and \( k_3 = (0, -1) \). The total noninteracting energy is \( E_0 = \mathcal{E}(k_1) + \mathcal{E}(k_2) + \mathcal{E}(k_3) \) and the total t-matrix correction is \( \hat{T} = \hat{T}^{12} + \hat{T}^{13} + \hat{T}^{23} \). The energy calculated using the t-matrix is then \( E_{tm} = E_0 + \hat{T} \) and the exact energy from diagonalization is \( E_{\text{exact}} \). \( E_{ij} = \mathcal{E}(k_i) + \mathcal{E}(k_j) \), is the noninteracting energy of the \((i, j)\) pair. States in momentum space are drawn. The crosses denote the states excluded due to the presence of the third particle. The computer program \texttt{tmatrix} described in Appendix F is used to carry out this t-matrix calculation.

<table>
<thead>
<tr>
<th>( Q_{ij} )</th>
<th>( P_{ij} )</th>
<th>( E_{ij} )</th>
<th>( Q_{H} )</th>
<th>( \hat{T} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( (0,0)(0,1) ) ( (0,1) )</td>
<td>-7.532088886</td>
<td></td>
<td></td>
<td>0.041528483</td>
</tr>
<tr>
<td>( (0,0)(0,-1) ) ( (0,-1) )</td>
<td>-7.532088886</td>
<td></td>
<td></td>
<td>0.041528483</td>
</tr>
<tr>
<td>( (0,1)(0,-1) ) ( (0,0) )</td>
<td>-7.064177772</td>
<td></td>
<td></td>
<td>0.113914035</td>
</tr>
</tbody>
</table>

\( E_0 = -11.064177772 \)
\( \hat{T} = 0.196971001 \)
\( E_{tm} = -10.867206771 \)
\( E_{\text{exact}} = -10.871031687 \)
the noninteracting energies $E_0$ with the t-matrix results $E_{tm} = E_0 + \tilde{T}$. The agreement between $E_{tm}$ and $E_{exact}$ is good.

Table 7.5: Lowest 15 noninteracting, exact, and t-matrix energies for $8 \times 9$ lattice with $M = 3$ and $P = (0, 0)$.

<table>
<thead>
<tr>
<th>$E_0$</th>
<th>$E_{exact}$</th>
<th>$E_{tm}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>-11.064178</td>
<td>-10.871031687</td>
<td>-10.86720677</td>
</tr>
<tr>
<td>-10.828427</td>
<td>-10.608797838</td>
<td>-10.60467748</td>
</tr>
<tr>
<td>-9.892605</td>
<td>-9.672121352</td>
<td></td>
</tr>
<tr>
<td>-9.892605</td>
<td>-9.519017636</td>
<td></td>
</tr>
<tr>
<td>-9.892605</td>
<td>-9.497189108</td>
<td></td>
</tr>
<tr>
<td>-9.892605</td>
<td>-9.462304364</td>
<td></td>
</tr>
<tr>
<td>-9.892605</td>
<td>-9.398345108</td>
<td></td>
</tr>
<tr>
<td>-9.892605</td>
<td>-9.345976806</td>
<td></td>
</tr>
<tr>
<td>-8.694593</td>
<td>-8.252919763</td>
<td>-8.261358231</td>
</tr>
<tr>
<td>-8.239901</td>
<td>-8.015024904</td>
<td></td>
</tr>
<tr>
<td>-8.239901</td>
<td>-7.946278078</td>
<td></td>
</tr>
<tr>
<td>-8.239901</td>
<td>-7.809576487</td>
<td></td>
</tr>
<tr>
<td>-8.239901</td>
<td>-7.800570818</td>
<td></td>
</tr>
<tr>
<td>-8.239901</td>
<td>-7.690625772</td>
<td></td>
</tr>
<tr>
<td>-8.239901</td>
<td>-7.615399722</td>
<td></td>
</tr>
</tbody>
</table>

7.4 A Five-Fermion Example

We now consider a $M = 5$ calculation, again for the $8 \times 9$ lattice. The noninteracting ground state is unique, with momentum vectors $(0,0), (0,1), (0,-1), (1,0), \text{and } (-1,0)$.
Figure 7.4: Noninteracting, t-matrix, and exact energies of the three-particle fermion system on the $8 \times 9$ lattice with $\mathbf{P} = (0,0)$. The bracketed numbers refer to the degeneracies of the level (see Table 7.3). The arrows associate the noninteracting states with the t-matrix results. We have worked on nondegenerate noninteracting states so far.
In Fig. 7.5 we show the exclusion involved for the t-matrix computation for the pair (0,1) and (1,0). The three other momentum vectors are of course excluded along with the three vectors that give the same total momentum (1,1) with the excluded vectors. The t-matrix results for all 10 pairs are presented in Table 7.6.

![Momentum space exclusion](image)

Figure 7.5: Momentum space exclusion in t-matrix $M = 5$ calculation for momentum vectors (0,1) and (1,0). The ground state is (0,0), (0,1), (0,-1), (1,0), and (-1,0) (the solid dots). The total momentum for the pair is (1,1) and due to the presence of the other three particles, six vectors (crosses) are excluded.

### 7.5 Degenerate States

In the two examples considered so far, the noninteracting states are all nondegenerate. In this section we consider degenerate states.

Let us study a state in the third lowest level (six-fold degenerate) of the $8 \times 9$, $M = 3$ problem: (0,1)(1,0)(-1,-1) (see Table 7.3). The pair (0,1)(1,0) has the same total energy and momentum as the (0,0)(1,1) pair, due to the pair component exchange symmetry (see Sec. 4.2).

In our $M = 5$ example in Sec. 7.4, because (0,0) is occupied, the (0,1)(1,0) pair cannot be scattered into the (0,0)(1,1) pair. In our present state (0,1)(1,0)(-1,-1), the pair (0,1)(1,0) is degenerate with (0,0)(1,1) and can be scattered into (0,0)(1,1).
Table 7.6: T-matrix calculation for the $8 \times 9$ lattice with five particles (0,0), (0,1),
(0,-1), (1,0), and (-1,0). The exclusions in $\tilde{Q}_{ij}$ for the pair (0,1)(1,0) are depicted
in Fig. 7.5. The computer program `tmat` described in Appendix F is used to carry
out this t-matrix calculation.

<table>
<thead>
<tr>
<th>$Q_{ij}^{ij}$</th>
<th>$P_{ij}$</th>
<th>$E_{0}^{ij}$</th>
<th>$\tilde{T}^{ij}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0) (0,1)</td>
<td>(0,1)</td>
<td>-7.532088886</td>
<td>0.044794382</td>
</tr>
<tr>
<td>(0,0) (0,-1)</td>
<td>(0,-1)</td>
<td>-7.532088886</td>
<td>0.044794382</td>
</tr>
<tr>
<td>(0,0) (1,0)</td>
<td>(1,0)</td>
<td>-7.414213562</td>
<td>0.056279982</td>
</tr>
<tr>
<td>(0,0) (-1,0)</td>
<td>(-1,0)</td>
<td>-7.414213562</td>
<td>0.056279982</td>
</tr>
<tr>
<td>(0,1) (0,-1)</td>
<td>(0,0)</td>
<td>-7.064177772</td>
<td>0.113914036</td>
</tr>
<tr>
<td>(0,1) (1,0)</td>
<td>(1,1)</td>
<td>-6.946302449</td>
<td>0.079309608</td>
</tr>
<tr>
<td>(0,1) (-1,0)</td>
<td>(-1,1)</td>
<td>-6.946302449</td>
<td>0.079309608</td>
</tr>
<tr>
<td>(0,-1) (1,0)</td>
<td>(1,-1)</td>
<td>-6.946302449</td>
<td>0.079309608</td>
</tr>
<tr>
<td>(0,-1) (-1,0)</td>
<td>(-1,-1)</td>
<td>-6.946302449</td>
<td>0.079309608</td>
</tr>
<tr>
<td>(1,0) (-1,0)</td>
<td>(0,0)</td>
<td>-6.828427125</td>
<td>0.123770663</td>
</tr>
</tbody>
</table>

$E_0 = -17.892604897 \quad \tilde{T} = 0.757071857$

$E_{tm} = -17.13553304 \quad E_{\text{exact}} = -17.145715214$
Following the two-fermion calculation with $N_1 = 4$ (see Sec. 4.3.6), the energy splitting of the degenerate pairs $(0,1)(1,0)$ and $(0,0)(1,1)$ should be calculated by putting the two pairs in the same $Q_I$, which means the two states $(0,1)(1,0)(-1,-1)$ and $(0,0)(1,1)(-1,-1)$ should be calculated together. Next, to calculate the energy of the pair $(1,0)(-1,-1)$ in $(0,1)(1,0)(-1,-1)$, we should also include the pair $(1,-1)(-1,0)$, which means calculating the states $(0,1)(1,0)(-1,-1)$ and $(0,1)(1,-1)(-1,0)$ together. Using this kind of reasoning, we see that the six degenerate states in the third lowest level in Table 7.3 should all be considered together to get the splittings correctly. We have not carried out such a calculation.

In general, in a nondegenerate state (nondegenerate in total energy for one total momentum vector), for any pair of fermions, any other pair that has the same total energy and momentum should be either fully or partially (the $M = 5$ example in Sec. 7.4) occupied (otherwise this state cannot be nondegenerate). Our t-matrix method can treat this nondegenerate case.

### 7.6 Many-Fermion T-Matrix Procedure

The two example calculations in Secs. 7.3 and 7.4 should have made clear the general t-matrix calculation procedure for many fermions. Let us summarize it here.

We want to compute the interacting energy for a nondegenerate noninteracting $M$-fermion state. (Nondegenerate in the sense that no other $M$-fermion state has the same total energy and momentum.)

The many-fermion t-matrix procedure is:

1. For each of the $M(M-1)/2$ pairs of fermions, $k_i$ and $k_j$, find the noninteracting energy $E_{ij}^0$ and total momentum vector $P_{ij}$. Set $Q_{ij} = \{k_i, k_j\}$.
2. Form the set \( \tilde{Q}_{ij} \), which is the complement of \( Q_{ij} \), with the other \( N - 2 \) momentum vectors \( k_m \) excluded along with \( P_{ij} - k_m \) (\( N \) is the number of sites, and the number of reciprocal lattice vectors in one Brillouin zone).

3. Use iteration to solve \( E = E_0 + \tilde{T}_{ij}(E) \) and get \( \tilde{T}_{ij} \), where \( \tilde{T}_{ij}(E) \) comes from the following procedure:

   (a) Use \( Q_{ij} \) and \( \tilde{Q}_{ij} \) to form \( G^{II}(E) \) (4 x 4) (Eq. 7.3) and \( \tilde{T}(E)_{\alpha\alpha'} \) (2 x 2) (Eq. 7.4).

   (b) Diagonalize \( T(E) \), and the eigenvalue that corresponds to the antisymmetric eigenvector is the fermion t-matrix \( \tilde{T}_{ij}(E) \).

4. Then the t-matrix energy is

\[
E_{tm} = E_0 + \sum_{i<j} \tilde{T}_{ij},
\]

where \( E_0 \) is the total energy of \( M \) noninteracting fermions.

We have written a C++ program \texttt{tmat} that can take a set of noninteracting momentum vectors, form degenerate levels, find energy corrections using t-matrix iterations, and obtain \( E_{tm} \). This program is described in Appendix F and is what we used to obtain the results in Tables 7.4, 7.5, and 7.6. At the present time, the program cannot handle degenerate noninteracting states (see Sec. 7.5).

### 7.7 Errors of the T-matrix

How good are the t-matrix results? From our example calculations on the \( 8 \times 9 \) lattice, in Table 7.4, 7.5, and 7.6, we see that \( E_{tm} \) and \( E_{exact} \) are close.

In Fig. 7.6 we plot the noninteracting, t-matrix, and exact energies for \( M = 3 \), \( P = (0,0) \) ground state on a series of near square lattices \( L \times (L + 1) \). The
noninteracting ground state momentum vectors are \((0,0)(0,1)(0,-1)\) for this series of lattices. We do not plot for \(L > 12\), because, as can be seen in the graph, the t-matrix energy \(E_{\text{tm}}\) approaches the exact energy \(E_{\text{exact}}\) rapidly. To see more clearly the error of the t-matrix result, we plot also \(E_{\text{tm}} - E_{\text{exact}}\), which decays very fast as the size of the lattice increases.

We have investigated a series of near square lattices \(L \times (L+1)\) with \(M = 3, 4, 5\) and \(L \times L\) with \(M = 4\), and to understand better the influence of the lattice shape, we also considered a series of one-dimensional-like, extended lattices, \(4 \times L\), with \(M = 3, 4, 5\). The noninteracting ground states for these cases are all nondegenerate and we list them in Table 7.7. In all cases, we observe rapid convergence of the \(E_{\text{tm}}\) and \(E_{\text{exact}}\), that is qualitatively similar to the graph in Fig. 7.6.

Table 7.7: Noninteracting ground states (all nondegenerate) for a series of lattices studied using the t-matrix. \(\mathbf{P}\) is the total momentum vector. For \(L \times (L+1)\) and \(L \times L\) (square or near-square) lattices and for \(4 \times L\) lattices (one-dimensional like).

<table>
<thead>
<tr>
<th>Lattice</th>
<th>(M)</th>
<th>(\mathbf{P})</th>
<th>Ground State</th>
</tr>
</thead>
<tbody>
<tr>
<td>(L \times (L+1))</td>
<td>3</td>
<td>(0,0)</td>
<td>((0,0)(0,1)(0,-1))</td>
</tr>
<tr>
<td>(L \times (L+1))</td>
<td>4</td>
<td>(1,0)</td>
<td>((0,0)(0,1)(0,-1)(1,0))</td>
</tr>
<tr>
<td>(L \times (L+1))</td>
<td>5</td>
<td>(0,0)</td>
<td>((0,0)(0,1)(0,-1)(1,0)(-1,0))</td>
</tr>
<tr>
<td>(L \times L)</td>
<td>4</td>
<td>(1,0)</td>
<td>((0,0)(0,1)(0,-1)(1,0))</td>
</tr>
<tr>
<td>(4 \times L)</td>
<td>3</td>
<td>(0,0)</td>
<td>((0,0)(0,1)(0,-1))</td>
</tr>
<tr>
<td>(4 \times L)</td>
<td>4</td>
<td>(0,2)</td>
<td>((0,0)(0,1)(0,-1)(0,2))</td>
</tr>
<tr>
<td>(4 \times L)</td>
<td>5</td>
<td>(0,0)</td>
<td>((0,0)(0,1)(0,-1)(0,2)(0,-2))</td>
</tr>
</tbody>
</table>
Figure 7.6: Noninteracting, t-matrix, and exact energies for $M = 3$, $\mathbf{P} = (0,0)$ ground state $\{0,0\}(0,1)(0,-1)$ on a series of $L \times (L + 1)$ lattices as a function of $L$ (top graph). $E_{\text{tm}} - E_{\text{exact}}$ vs $L$ (bottom graph).
7.8 Summary

In this chapter, we studied the problem of a few fermions. We first demonstrated the shell effect and showed the correspondence between noninteracting and interacting shells. We then used the exact two-fermion t-matrix developed in Chapter 4 to study the problem of a few fermions. The general idea is clear that with only a few particles, we can ignore three or more-body interactions and only consider two-body interactions using the t-matrix. The modification is that in the t-matrix, the momentum vectors corresponding to occupied states must be excluded (along with states forbidden by momentum conservation). This idea is clearly shown in Fig. 7.5. The resulting energy, after adding the pairwise interaction corrections to the noninteracting energy, is shown in this chapter to be close to the exact value.

We have written a computer program which can carry out this pairwise t-matrix calculation for a given noninteracting state (nondegenerate with others, see Sec. 7.5), in part answering satisfactorily the question first asked in Sec. 3.6: can we go from the noninteracting spectrum to the interacting spectrum? The idea of Fermi liquid theory, that the interacting states correspond one-to-one to noninteracting ones, is demonstrated from the energy spectrum for two (Fig. 4.8) and three particles (Fig. 7.4).

We have also studied briefly the errors of the t-matrix, from neglecting three or more-body terms. We see that the error decays very fast as the lattice size increases.

The work in this chapter and the two-particle t-matrix work in Chapter 4 appear to be the first systematic study of t-matrix calculations for a lattice model. These few-particle t-matrix calculations enable us to obtain t-matrix fermion energies (that are close to exact energy) for very large lattices.

We hope that in the future an appropriate formulation for the degenerate non-
interacting levels can be studied. Another important and interesting work left out is the t-matrix study for more than two bosons. There, scatterings in and out of a condensate should be considered (see Fetter and Walecka [5] for the treatment in diagrammatic calculations). We hope to study the boson problem in the future.
Bibliography


Chapter 8

The Dilute Limit: Energy Curves

In this chapter, we study the dilute limit of our model. In Chapter 7, we used a modified two-particle t-matrix to study the problem with a few fermions, e.g., three, four, and five. In this chapter we fit the energy vs particle density curves for dilute bosons and fermions.

The motivation for this chapter is the 2D Fermi liquid question described in Sec. 1.8.1. Specifically, we would like to know: are dilute fermions in our model described by the Fermi liquid theory? In Chapter 7 on the problem of a few fermions, we have shown that the energies correspond one-to-one for low-lying noninteracting and interacting levels (Fig. 7.4). In this chapter we will study the energy vs particle density curve at the dilute limit. Both boson and fermion problems have been studied using diagrammatic calculations in the continuum (which we will describe below). We will first check the boson result with diagonalization, and we observe a good fit. The fermion diagrammatic calculations predict a valid Fermi liquid description but are still controversial. By checking the energy curve obtained from diagrammatics with diagonalization results, we can infer whether the Fermi liquid description is valid.
8.1 Introduction to Dilute Bosons and Fermions

Classic 3D Continuum Papers

The problem of dilute fermion and boson gases at zero temperature with strong, short-range repulsion, has a long and distinguished history. In the 1940s, the energy spectrum of a dilute, weakly interacting boson gas was considered by Bogoliubov in the context of superfluidity [1]. Bogoliubov transformations were used to diagonalize the Hamiltonian in a perturbation theory, and a system of noninteracting quasiparticles was obtained. In the 1950s, fermion and boson gases with hard-sphere interactions were treated using a pseudopotential method by Huang, Yang, Luttinger, and Lee [2, 3, 4, 5]. Ground state energy expansion in terms of particle density was obtained. The fermion problem was also treated in the context of the Fermi liquid theory by Abrikosov and Khalatnikov [6], and quasiparticle effective mass and the Landau $f$-function were calculated. Also at this time, this problem of dilute quantum gases with strong, repulsive, short-range interactions was formulated in the language of diagrammatic field theory by Galitskii [7] for fermions and Beliaev [8] for bosons. And in addition to the quasiparticle, pseudopotential, and diagrammatic approaches, rigorous bounds have also been sought for the hard-sphere boson gas. The correct upper bound was found by Dyson [9] in 1957 and the correct lower bound by Lieb and Yngvason [10] in 1998.

Textbook Treatments

By now, the problem of dilute fermions and bosons has entered a number of classic textbooks, including Pines [11] (which also contains reprints of a number of classic papers mentioned above), Abrikosov, Gorkov, and Dzyaloshinski [12], Landau and Lifshitz [13], and Fetter and Walecka [14], as an example many-body system and
a showcase for diagrammatic calculations. The key physical concept in these field-theoretical calculations is that even though we have a complex many-body problem, in the dilute limit, two-particle interactions give the largest contribution. These strong two-body interactions are described by ladder diagrams which can be summed to infinite order, giving the t-matrix.

2D Continuum Results

All of the preceding work is for three-dimensional, continuum systems. For two-dimensional continuous systems, diagrammatic calculations in the spirit of Galitskii and Beliaev were done by Schick for bosons in 1971 [15] and Bloom for fermions in 1975 [16]. In particular, energy per particle expansion in terms of particle density $n$ was calculated, and the leading order correction to the noninteracting energy was found to be in the form of $n/\ln n$ for both fermions and bosons. Expansions with second-order coefficients different from the results of Schick and Bloom were found in Refs. [17, 18] for the boson case and in Ref. [19, 20] for the fermion case. There is no consensus at this time on the correct second-order coefficient for both the boson and fermion problems.

Recent Revival: High-Tc and BEC

More recently, in the 1990s, the problem of dilute fermions and bosons in two dimensions received new attention. For the fermion case, since the discovery of high-temperature superconductors, there has been intense interest in two dimensional strongly-correlated electronic systems. A controversy has persisted regarding the validity of the Fermi liquid theory in two dimensions (see Ref. [21]). The question is this: is the dilute Fermi gas in two dimensions a Fermi liquid, as is the case in
three dimensions, or is it something drastically different, like the Luttinger liquid state in some one-dimensional models? This question was addressed in a series of papers, Refs. [22, 23, 20], using the t-matrix in two dimensions, and the answer given in these papers leans toward the Fermi liquid picture. At the same time, the dilute boson problem received more recent attention partly because of the successful experiments in Bose-Einstein condensation. In particular, Lieb and Yngvason [24] have proved rigorously the leading-order expansion of the two-dimensional dilute boson gas found by Schick [15].

3D and 2D Lattice Results

Analytical calculations for dilute fermions on a lattice have been done using the t-matrix. Kanamori [25] treated a tight-binding model that is essentially a Hubbard model and obtained the t-matrix. Mattis [26] calculated the t-matrix for the three-dimensional Hubbard model explicitly and obtained Kanamori’s result. For the two-dimensional Hubbard model, Rudin and Mattis [27] obtained upper and lower bounds for energy as a function of density. As described in Sec. 4.1.3, the result of Rudin and Mattis for low-density fermions in two dimensions has not been checked, as far as we know, by numerical studies. On the other hand, the dilute boson problem on a two-dimensional lattice has been studied using quantum Monte Carlo by Refs. [28, 29], and they obtain good fit with Schick’s calculation.

Chapter Organization

This chapter is divided into two parts: one on bosons and one on fermions.

First we fit the energy vs particle density curve for bosons. We find that the leading-order correction to the noninteracting energy obtained by Schick [15],
\[ 4\pi n / |\ln(na^2)|, \] where \( n \) is particle density and \( a \) the scattering length, works well for our model. From curve fitting, we obtain a scattering length for our lattice model.

For fermions, plotting the difference between exact energy and the noninteracting energy, the shell effect is eliminated and we obtain a well-defined the curve at the dilute limit. We explain that for fitting we will need the p-wave scattering term for energy, which is work in progress. We will show from the case of three, four, and five fermions that the interaction correction to the fermion energy (p-wave) is much smaller than that for the boson energy (s-wave).

### 8.2 Dilute Bosons

#### 8.2.1 Analytical Results

In this section we study the dilute boson energy vs particle density curve using exact diagonalization results. For the three-dimensional hard sphere bosons, the energy per particle at the low-density limit from diagrammatic calculations is

\[
\frac{E}{M} = \frac{2\pi \hbar^2 a}{m} n \left( 1 + \frac{128}{15} \left( \frac{na^3}{\pi} \right)^{1/2} + 8 \left( \frac{4\pi}{3} - \sqrt{3} \right) (na^3) \ln(na^3) + \mathcal{O}(na^3) \right),
\]

(8.1)

where \( M \) is the number of particle, \( n = M/L^3 \) the particle density (\( L \) is length of the cubic box of the system), \( m \) the mass, and \( a \) the scattering length (the quantity that characterizes two-body collision and is finite even for an infinite potential). (This calculation is shown in detail in Fetter and Walecka [14], §22.)

The two-dimensional expansion for hard disk bosons in the continuum was first done by Schick [15], and the energy per particle formula he found is

\[
\frac{E}{M} = \frac{2\pi \hbar^2}{m} \frac{n}{|\ln(na^2)|} \left( 1 + \mathcal{O} \left( \frac{1}{\ln(na^2)} \right) \right),
\]

(8.2)
where $a$ is now the two-dimensional scattering length. The coefficient of the second-
order term, as mentioned in the introduction to this chapter, Sec. 8.1, has not been
settled.

### 8.2.2 Relevance to Our Model

These hard sphere and hard disk calculations were carried out using the kinetic
energy $\hbar^2 k^2/2m$. In our lattice model, our hopping energy dispersion is

$$\mathcal{E}(k) = -2t(\cos(k_x) + \cos(k_y)) \approx -4t + tk^2,$$ (8.3)

where we have Taylor-expanded the dispersion function near $k = 0$ because in the
dilute limit, at the ground state, the particles occupy momentum vectors close to
zero. Therefore if we use $t = \hbar = 1$ and the effective mass $m^*$ such that we have the
form $\hbar^2 k^2/2m^*$, then $m^* = 1/2$ for our system. So for our model, Schick’s expansion
(8.2) should become,

$$\frac{E}{M} = -4 + \frac{4\pi n}{|\ln(na^2)|} \left(1 + \mathcal{O}\left(\frac{1}{\ln(na^2)}\right)\right),$$ (8.4)

where we have used $a^*$ to denote the scattering length in our lattice system. There
is no straightforward correspondence between Schick’s scattering length $a$ in the
continuum and our $a^*$ on the lattice. With infinite nearest-neighbor repulsion, the
closest distance that our particles can come to is $\sqrt{2}$. We expect roughly $1 < a^* <
\sqrt{2}$, and will determine a more precise value from curve fitting.

### 8.2.3 Fitting the Boson Energy Curve

In Fig. 8.1 we show the boson energy per particle ($E/M$) vs particle per site ($M/N$)
curve for ten lattices, ranging from 25 sites to 42 sites, with three or more particles
\((M \geq 3)\). The data from all these lattices collapse onto one curve, especially in the low-density limit. (Numerical diagonalization values for these lattices are contained in Tables from D.15 to D.24.)

Eq. 8.4, Schick's result applied to our model, suggests the following leading order fitting form for \(E/M\) vs \(n\) at the low-density limit,

\[
\frac{E/M + 4}{4\pi n} = A + \frac{B}{|\ln(\eta a^*)|}.
\]  

That is to say, if we plot \((E/M + 4)/(4\pi n)\) vs \(1/|\ln(\eta a^*)|\), then, if Schick is correct, we should get a straight line, with intercept \(A = 0\) and slope \(B = 1\), with one adjustable parameter \(a^*\).

In Fig. 8.2, we plot \((E/M + 4)/(4\pi n)\) vs \(1/|\ln(\eta a^*)|\) (with \(a^* = 1\)) for the data in Fig. 8.1. In the low-density limit the data do appear to fall on a straight line. In Fig. 8.3, we limit to \(n \leq 0.15\) (\(n = 0.15\) corresponds to \(-1/\ln(n) = 0.527\) in Fig. 8.1) and plot with three choices of \(a^* = 1.0, 1.36, \sqrt{2}\).

For \(a^* = 1.36\) the fitted intercept is \(A = -0.016\) and the slope \(B = 0.959\). In Table 8.1 we show the fitted slope and intercept for a number of \(a^*\) choices. The slope is zero close to \(a^* = 1.34\) and the intercept is zero close to \(a^* = 1.39\). Our data thus suggest \(a^* = 1.36 \pm 0.03\).

In Fig. 8.1, the solid line is the function \(-4 + 4\pi n(A + B/|\ln(\eta a^*)|)\) using \(a^* = 1.36, A = -0.016,\) and \(B = 0.959,\) and we obtain a good fit up to \(n = 0.15\).

For bosons, quantum Monte Carlo can be used to obtain zero temperature energies for reasonably large systems. For a dilute boson gas on a square lattice with on-site hardcore but not nearest-neighbor interaction, Ref. [28] has fitted the first term of Schick's formula (8.2), and Ref. [29] has used higher-order terms and included the fitting of the chemical potential also. The agreement is good in both studies.
Figure 8.1: Boson energy per particle $E/M$ vs particle density $M/N$ data for ten lattices and $M \geq 3$. Data from different lattices collapse onto one curve. The solid line corresponds to the fitting function $-4 + 4\pi n(A + B/|\ln(na^*)|)$ with $a^* = 1.36$, $A = -0.016$, and $B = 0.959$, which is Eq. 8.5 with parameters from Table 8.1. Numerical diagonalization values for these lattices are contained in Tables from D.15 to D.24.
8.2.4 Fixed $M$ and Large $L$: $M = 3, 4, 5$

The analytical results, Eq. 8.1 in three dimensions and Eq. 8.2 in two dimensions, are for large systems $N \to \infty$ and large number of particles $M \to \infty$, with the ratio, the particle density $n = M/N$, fixed as a small, finite value. Of course, with diagonalization, we are limited to small lattices, but for just a few particles, we can diagonalize larger systems. In Sec. 3.10, we have studied the large-$L$ energy for the case of three, four, and five bosons on a large $L \times L$ lattice. Here in Fig. 8.4, we plot exact diagonalization results for $M = 3, 4, 5$ for $L \times L$ lattices with $L$ ranging from

Figure 8.2: Boson $(E/M + 4)/(4\pi n)$ vs $1/|\ln(na^2)|$ for the data in Fig. 8.1, with $a^* = 1$ (see Eq. 8.5). Data in the low-density limit appear to fall on a straight line.
Figure 8.3: \((E/M+4)/(4\pi n)\) vs \(1/|\ln(na^a)|\) plot to check Schick's formula for two-dimensional dilute bosons (Eq. 8.4). The data points are for \(M \geq 3\) and \(n \leq 0.15\) from those in Fig. 8.1, for lattices from \(5 \times 5\) to \(6 \times 7\). For the three \(a^*\) values, the \(a^* = 1.36\) choice gives \(A = -0.016 \approx 0\) and \(B = 0.959 \approx 1\).
Table 8.1: Intercept $A$ and slope $B$ in linear fitting $(E/M + 4)/(4\pi n)$ vs $1/|\ln(na^*)|$ for bosons, using Eq. 8.5. The slope is one close to $a^* = 1.33$ and the intercept is zero close to $a^* = 1.39$. So we get $a^* = 1.36 \pm 0.03$. The fitting for three choices of $a^*$ is plotted in Fig. 8.3.

<table>
<thead>
<tr>
<th>$a^*$</th>
<th>slope $B$</th>
<th>intercept $A$</th>
<th>$a^*$</th>
<th>$B$</th>
<th>$A$</th>
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<th>$B$</th>
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<td>-0.0043</td>
</tr>
<tr>
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<td>-0.112</td>
<td>1.34</td>
<td>0.995</td>
<td>-0.027</td>
<td>1.39</td>
<td>0.906</td>
<td>0.0013</td>
</tr>
<tr>
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<td>1.35</td>
<td>0.977</td>
<td>-0.021</td>
<td>1.40</td>
<td>0.889</td>
<td>0.0069</td>
</tr>
<tr>
<td>1.31</td>
<td>1.053</td>
<td>-0.044</td>
<td>1.36</td>
<td>0.959</td>
<td>-0.016</td>
<td>1.414</td>
<td>0.865</td>
<td>0.015</td>
</tr>
</tbody>
</table>

5 to 30 for $M = 3$, from 5 to 15 for $M = 4$, and from 5 to 10 for $M = 5$, along with the data from Fig. 8.1. Numerical values for $M = 3, 4, 5$ are in Tables D.3, D.4, and D.5 respectively.

We need to caution that the situation of a fixed number of particles (here $M = 3, 4, 5$ in Fig. 8.4) on increasingly large lattices gives $n \to 0$ instead of the desired fixed $n$ result to compare with diagrammatic results. Going from $n \to 0$ to finite $n$ is straightforward in three dimensions because the leading-order correction to noninteracting energy is linear in density for both bosons (Eq. 8.1) and fermions (as we will see in Eq. 8.6). In two dimensions, it is delicate going from a few-particle energy expression in terms of $\ln L$ (see Eq. 3.64 for a few bosons) to the density $n = M/L^2$. The nonlinearity of the logarithm factor is what makes the two dimensional boson problem (and the fermion problem, as we will see in Sec. 8.3), in E. H. Lieb’s words, a subtle one [32].

Fabrizio et al. [30] studies the problem of a few electrons on the Hubbard model and in particular the problem of going from density $n \to 0$ to finite density, by
Figure 8.4: Boson $M = 3, 4, 5$ exact diagonalization results for $L \times L$ lattices with data from Fig. 8.1. $L$ goes from 5 to 30 for $M = 3$, from 5 to 15 for $M = 4$, and from 5 to 10 for $M = 5$. Numerical values for $M = 3, 4, 5$ are in Tables D.3, D.4, and D.5 respectively.
considering the higher order contribution to the scattering amplitude. This work is quite involved and is beyond this thesis work.

8.3 Dilute Fermions

8.3.1 Analytical Results

For fermions, it customary to write the energy per particle expansion in terms of the Fermi vector \( k_F \) (of course, \( k_F \) is related to the density \( n \)). For three-dimensional dilute hard sphere fermions, the energy per particle from diagrammatic calculations, is,

\[
\frac{E}{M} = \frac{\hbar^2 k_F^2}{2m} \left( \frac{3}{5} + \frac{2}{3\pi} k_F a + \frac{4}{35\pi^2} (11 - 2 \ln 2)(k_F a)^2 + \mathcal{O}(k_F a)^3 \right),
\] (8.6)

for spin-1/2 fermions in three dimensions (see Fetter and Walecka [14]). The first term in Eq. 8.6 is the familiar kinetic energy per particle of noninteracting fermions. In two dimensions, Bloom showed [16] that the expansion for spin-1/2 fermions is

\[
\frac{E}{M} = \frac{\hbar^2 k_F^2}{4m} \left( 1 - \frac{1}{\ln(k_F a)} + \mathcal{O}\left( \frac{1}{\ln(k_F a)} \right)^2 \right),
\] (8.7)

where the first term is the kinetic energy of noninteracting fermions in two dimensions.

An interesting observation is that if we write Eq. 8.6 in terms of \( n = M/L^3 \), using \( k_F = (3\pi^2 n)^{1/3} \) for spin-1/2 in 3D, then we have, to the leading order in \( k_F a \),

\[
\frac{E - E_0}{M} = \frac{\hbar^2 k_F^2}{2m} \frac{2}{3\pi} k_F a = \frac{\pi \hbar^2 a}{m} n,
\] (8.8)

which is exactly half of the leading order term for boson \( E/M \) in three dimensions (see Eq. 8.1). And in two dimensions, using \( k_F = \sqrt{2\pi n} \) for spin-1/2, we get from Bloom’s result, Eq. 8.7, the following expression for the leading order term,

\[
\frac{E - E_0}{M} = \frac{\hbar^2 k_F^2}{4m} \left| \frac{1}{\ln k_F a} \right| = \frac{\pi \hbar^2 n}{m} \left| \frac{1}{\ln 2\pi n a^2} \right| \approx \frac{\pi \hbar^2 n}{m} \frac{1}{\ln n a^2},
\] (8.9)
where we have left out the factor $2\pi$ in the logarithm because we work in the large-$L$, low-density limit. Eq. 8.9 is half of the leading order term for boson $E/M$ in two dimensions (see Eq. 8.2), as in the three-dimensional case. We will return to this observation in Sec. 8.3.4 when we fit the fermion energy per particle curve.

### 8.3.2 Formulas for a General Spin

Both Eq. 8.6 and Bloom’s result Eq. 8.7 are for spin-1/2 fermions. For fermions with spin $s$, the three-dimensional result Eq. 8.6 becomes

$$
\frac{E}{M} = \frac{\hbar^2 k_F^2}{2m} \left( \frac{3}{5} + 2s \left( \frac{2}{3\pi} k_F a + \frac{4}{35\pi^2} (11 - 2\ln 2)(k_F a)^2 \right) + \mathcal{O}(k_F a)^3 \right), \quad (8.10)
$$

(see Ref. [14], p. 169) and the two-dimensional result Eq. 8.7 becomes

$$
\frac{E}{M} = \frac{\hbar^2 k_F^2}{4m} \left( 1 - 2s \frac{1}{\ln(k_F a)} + \mathcal{O} \left( \frac{1}{\ln(k_F a)} \right)^2 \right), \quad (8.11)
$$

(see Ref. [19] and Ref. [31]). This means that for our spinless fermions ($s = 0$), the leading order corrections to the noninteracting energy in Eq. 8.10 and Eq. 8.11 are zero.

These terms are zero because Eq. 8.10 and Eq. 8.11 (and Eq. 8.6 and Eq. 8.7) are derived for s-wave scattering. In our model, without spin, only antisymmetric spatial wavefunctions are allowed for fermions, and therefore the leading correction to the noninteracting energy should be from p-wave scattering. Fetter and Walecka (Ref. [14], p. 169) contains the p-wave result for hard sphere fermions in three dimensions,

$$
\frac{E}{M} = \frac{\hbar^2 k_F^2}{2m} \left( \frac{3}{5} + (2s + 2) \frac{(k_F a)^3}{5\pi} \right), \quad (8.12)
$$

where the leading order correction to the noninteracting energy does not give zero
for $s = 0$. Unfortunately, we are not aware of a two-dimensional version of Eq. 8.12 in the literature for the p-wave scattering contribution to fermion energy. We have not worked out this p-wave problem in two dimensions.

### 8.3.3 Shell Effect in Energy Per Particle Curve

In the following, we present some studies of the dilute fermion problem, using exact diagonalization. In Fig. 8.5 we show the exact diagonalization data from a range of lattices from 25 sites to 42 sites. Comparing with the boson data in Fig. 8.1, we see that the spread of the fermion curve is larger. (Numerical diagonalization values for these lattices are contained in Tables from D.15 to D.24.)

The spread in the fermion curve is due to the shell effect discussed in Sec. 7.1. In Fig. 7.1 and Fig. 7.2 we studied the shell effect manifestation in total energy $E(M)$ and energy increment $E(M) - E(M - 1)$ as a function of particle number $M$ for $5 \times 8$ and $7 \times 7$ lattices. The total energy curve shows slope changes at filled shells, and the energy increment curve shows clear steps. In Fig. 8.6, we show the energy per particle $E/M$ curve for the same $5 \times 8$ and $7 \times 7$ lattices, including the noninteracting energies for comparison. Shell effect creates a zig-zag pattern in the $E/M$ curves, and careful readers following the symbols for a particular lattice in Fig. 8.5 may notice a similar zig-zag pattern (the inset includes the $6 \times 6$ lattice only and shows more clearly the shell effect).

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1 Apparently, this p-wave problem is straightforward enough to appear only as an exercise in Ref. [14]: problem 4.7 on p. 169. See also problem 11.7 on p. 386.

2 Bruch, in Ref. [19], discusses spin degeneracy, but does not contain a formula for p-wave terms.
Figure 8.5: Fermion ground energies from exact diagonalization for $M \geq 3$ on lattices from $5 \times 6$ to $6 \times 7$. The spread in the fermion curve is greater than that of the boson curve in Fig. 8.1. The inset shows the $6 \times 6$ lattice only, demonstrating more clearly the zig-zag pattern due to fermion shell effect. Numerical diagonalization values for these lattices are contained in Tables from D.15 to D.24.
Figure 8.6: Manifestations of the shell effect in energy per particle $E/M$ curve for $5 \times 8$ lattice (top) and $7 \times 7$ (bottom) lattices. Exact groundstate energies are compared with noninteracting energies. The total energy curves in Fig. 7.1 ($5 \times 8$) and Fig. 7.2 ($7 \times 7$) show slope changes. The $E/M$ curves here show a zig-zag pattern.
8.3.4 Fitting the Fermion Energy Curve

Because the shells for both the exact and the noninteracting systems occur at the same $M$ (see Fig. 8.6), we may hope that $E - E_0$, where $E$ is the exact energy and $E_0$ the corresponding noninteracting energy, will show less shell effect. In Fig. 8.7 we plot the energy difference per particle $(E - E_0)/M$ vs $n$ for the fermion data in Fig. 8.5. We indeed observe that the data now lie on a well-defined curve.

In Sec. 8.3.1, we mentioned that in both 3D and 2D, $(E - E_0)/M$ for fermions is, to the leading order in $n$, half of the same expression for bosons. In the spirit of Fig. 8.4, we plot in Fig. 8.8, the fermion diagonalization data for $M = 3, 4, 5$ on $L \times L$ lattices, with $L$ ranging from 5 to 30 for $M = 3$, from 5 to 15 for $M = 4$, and from 5 to 10 for $M = 5$, along with the data from Fig. 8.5. For comparison, the bold curves are $(E - E_0)/2M$ (note the $1/2$ factor) for boson $M = 3, 4, 5$ data from Fig. 8.4. It is clear that at the low-density limit, the fermion result is less than half of the boson result.

We expect, as in Eq. 8.12 for three dimensions, the p-wave contribution to energy should be considerably smaller than that from the s-wave term. The fermion p-wave calculation is in progress. In Sec. 3.10, we have considered the case of a few fermions on a large $L \times L$ lattice, and in Fig. 3-8 we have studied the interaction correction to the noninteracting energy $\Delta E$. It was show there that $\Delta E$ for our spinless fermions is much smaller than that for bosons.

8.4 Conclusion

In this chapter, after introducing the long and distinguished history of the dilute boson and fermion problems, we studied the dilute regime of our model. We showed
Figure 8.7: The difference between exact and noninteracting energies per particle \((E - E_0)/M\) vs \(n\) for the fermion data in Fig. 8.5.
Figure 8.8: Fermion $(E - E_0)/M$ vs $M/N$ for $M = 3, 4, 5$ on $L \times L$ lattices (light curves, from diagonalization), along with data from Fig. 8.5, with $L$ going from 5 to 30 for $M = 3$, to 15 for $M = 4$, and to 10 for $M = 5$. The bold curves are half of boson $(E - E_0)/M$ data for $M = 3, 4, 5$ from Fig. 8.4. At the low-density limit, the fermion results are smaller than half of the boson result. Numerical values for $M = 3, 4, 5$ are in Tables D.3, D.4, and D.5 respectively.
that, for bosons, the energy per particle curve can be fitted using Schick’s formula. For fermions, after subtracting the noninteracting energy, the $(E - E_0)/M$ curve becomes a well-defined one, and we explained the necessity for calculating p-wave scattering contribution to energy for the spinless fermions in our model.

To connect back to the long history of dilute boson and fermion problems, we make the following comments. We have checked Schick’s dilute boson formula using exact diagonalization for a model with not only hardcore interaction but also infinite nearest-neighbor repulsion. We find good leading order fit as other works have found with lattice quantum Monte Carlo. For the fermion case, because of the fermion sign problem, quantum Monte Carlo is not straightforwardly available, and to our best knowledge, we are not aware of direct numerical checks on Bloom’s formula for dilute fermions. Our exact diagonalization work is therefore a solid step in understanding dilute fermions in two dimensions, and is of close relevance to the 2D Fermi liquid controversy. The difficulty in our model is that the leading order contribution to energy is from p-wave scattering; therefore, the series of results based on s-wave calculations by Bloom [16], Bruch [19], and Engelbrecht, et al. [20] are not directly available. Hopefully, the work in progress on p-wave scattering will be completed, and our diagonalization data can shed light to the interesting problem of two dimensional dilute fermions.
Bibliography

[29] G. Batrouni, (private communication); cond-mat/0110314.
Chapter 9

Conclusion and Outlook

What have we done? What is new? What have we contributed to human knowledge? What remains to be done?

9.1 What have we done?

Our Model

We have studied a two-dimensional model of strongly-interacting fermions and bosons. This model is a simplified version of the Hubbard model and is the simplest model of correlated electrons. It is very difficult to study two-dimensional quantum models with short-range kinetic and potential terms and strong interaction. There are very few reliable analytical methods, and many numerical methods are not satisfactory. With our simplified model of spinless fermions and infinite nearest-neighbor repulsion, we can use exact diagonalization to study systems much larger (in lattice size) than that can be done with the Hubbard model. In the past two years, from roughly January 2000 to now, January 2002, we have written an exact diagonalization program from scratch and made a detailed study of many aspects of our model.
The program and the subsequent study are the content of this thesis.

**Diagonalization**

The diagonalization program is described in detail in Chapter 2. The difficult part of the program is using the translation-symmetry basis set and keeping track of the fermion sign. At the technical side, we installed two packages for matrix diagonalization (LAPACK for full matrix and ARPACK for Lanczos style diagonalization), and wrote our own Lanczos (faster than ARPACK) to obtain ground state eigenvalue and eigenvector. We hope that Chapter 2 contains enough detail for a beginning student to write an exact diagonalization program in two and higher dimensions without too much trouble.

**Two Particles: Green Function**

The physics part of this research is divided into two parts: one on the dilute limit and one on stripes. For the dilute limit, we started with the two-particle problem, that is two bosons or fermions on an otherwise empty lattice. This problem belongs to a large class of analytically tractable two-body problems, e.g., the hydrogen atom, and the two-magnon problem, that are in standard textbooks. In Chapter 3, we reformulated the Schrodinger equation using lattice Green function which is a good starting point for analytical calculations. In particular, after using lattice symmetries, we obtained the two-boson ground state energy on a large lattice, which was used to obtain an expression for the ground state energy for a few bosons.
Two Particles: T-Matrix

We reformulate the two-particle problem again in Chapter 4, this time deriving a scattering matrix: the t-matrix, which becomes one of the most commonly used words in this thesis. The reason the t-matrix is important is that it is the sum total of all two-body scattering terms and therefore works when the interaction is strong. It not only enables us to solve the two-particle problem easily (we showed that the first t-matrix iteration is often very good for fermions) but also enables us to generalize to more than two fermions in a straightforward fashion (that is the work of Chapter 7).

One Stripe and Holes

We left the t-matrix temporarily and moved to the near-half-filled limit, where our model naturally supports an interest object: the stripe. Stripes are holes aligned, and following the movement of the holes, stripes can fluctuate. It is basically an emergent phenomenon, very much like phonons arising from lattice vibrations. In Chapter 5, we studied the problem with a single stripe, which as we showed is exactly mapped to a spin-1/2 chain. And we studied the problem of one and two holes on a stripe, where we considered additional motions enabled by the holes and the energy dependence on the two dimensions of the lattice. Using a double-well model, we calculated the stripe effective mass from diagonalization data.

More Stripes

Stripes have been quite important lately because of their observation in some cuprate high-temperature superconductors. We believe that our model is the simplest microscopic model of interacting stripes, and we studied in Chapter 5 stripe-stripe in-
teraction. We find that they repel and the energy dependence on stripe separation is a power-law decay with exponent 2. Using a particle-in-a-box model, we explained the power-law and the exponent and extracted stripe effective mass from two and three-stripe interaction data. We also studied the stability of an array of stripes using a Maxwell construction on exact diagonalization data at the intermediate-filling limit. We obtained the interesting result that the boson stripe-array is not stable against phase separation into hole-rich and particle-rich regions, and the fermion stripe-array is close to the stability limit.

More Fermions

In Chapter 7, we returned to the dilute limit and studied the problem of a few fermions. We first demonstrated the shell effect, and using the two-particle t-matrix constructed in Chapter 4 we studied problems with three, four, and five fermions, with the modification due to exclusion by the presence of other fermions. The correspondence with exact energy is good, and we studied the errors introduced by the t-matrix in neglecting three or more-body interactions, and found that they decay very fast as the size of the lattice increases, thus showing the validity of using the t-matrix in dilute fermion calculations.

Dilute Limit: Success and Problem

The dilute boson and fermion energy per particle curves were studied in Chapter 8. The boson curve was fitted nicely with a previous diagrammatic calculation, and we explained that for fermions because the existing calculations are all for s-wave scattering and our model of spinless fermions needs the p-wave term, more work need to be done and this work is in progress.
9.2 What is new?

Many of our problems discussed in this work have a long tradition.

2D Diagonalization Description

The diagonalization program in one dimension has been discussed nicely in two *Computers in Physics* Refs [1, 2] articles. In fact, our program follows that of Leung and Oppenheimer [1] rather closely. The new thing here is that we have written down a detailed description of a two-dimensional diagonalization program, with rectangular as well as skewed boundaries. There are a number of complications in two dimensions, e.g., representation of lattice, translation, and especially fermion sign, and we hope that as Refs. [1, 2] are a good starting point for coding one-dimensional diagonalization, our description can be a good starting point for two-dimensional diagonalization.

Two-Particle Problem with Nearest-Neighbor Interaction

The two-particle problem in the Hubbard model is described in Ref. [3], and that is the source of some of the fruitful ideas in our lattice Green function calculation in Chapter 3. The new part here is the extension to nearest-neighbor interactions, whereas in the Hubbard model, there is only on-site interaction. As seen in Chapter 3, our Green function $\mathcal{G}$ is a $4 \times 4$ matrix while the Hubbard Green function is a scalar, and we had to use lattice symmetry to reduce the $4 \times 4$ to $1 \times 1$. We do not think this is new, but we have not found a calculation in the literature where many of the interesting details are spelled out.
Systematic Study of the T-Matrix

It is somewhat puzzling that with much hype attached to the two-dimensional Fermi liquid theory and the essential role the t-matrix plays in almost every calculation (in the dilute limit with strong interactions), no systematic study of the t-matrix for a lattice model has been made (and Rudin and Mattis’s analytical result on the dilute limit of the 2D Hubbard model is still not checked [4]). We believe that our work on the two-particle t-matrix (Chapter 4) and the few-fermion t-matrix (Chapter 7) is first such study. Some approximations that are routinely made in t-matrix calculations are graphically presented, especially the use of first t-matrix iteration in calculating fermion energy. And we demonstrate the qualitative difference between the boson and fermion t-matrices. We believe that Chapters 4 and 7 form a solid starting point for discussions on 2D Fermi liquid.

Simplest Model of Stripes: Stripes Repel

We believe that we have the simplest microscopic lattice model of interacting quantum stripes, and we have used our diagonalization power to obtain many detailed properties about stripes that cannot be obtained using the Hubbard or $t-J$ models (because of computer limitation). These include hole motion on a stripe and especially stripe-stripe interaction and we extract the stripe effective mass. We believe that our study is one of the first diagonalization studies of stripes and the two and three-stripe interaction results are one of the first convincing numerical results on the repulsive nature of fluctuating quantum stripes in two dimensions.
Diagonalization Study of Bosons and More Fermion Shells

Our work on dilute bosons complements quantum Monte Carlo results [5]. For the fermion problem, the demonstration of shell effect is not new (see Ref. [6]), but in Ref. [6], only square-boundary lattices are used. We here can work with rectangular-boundary lattices and skewed lattices. We need more work on p-wave scattering, as explained in Chapter 8. So the 2D Fermi liquid question has not been settled, but more work is in progress.

9.3 What have we contributed to human knowledge?

Briefly,

1. Exact diagonalization is nice.

2. Green function is powerful.

3. T-matrix is very useful and interesting.

4. Stripes repel.

5. Dilute bosons and fermions in two dimensions are subtle.

6. Physics is fun.

9.4 What remains to be done?

Here is a wish list.
Two-Fermion Ground State Energy on a Large Lattice

In Sec. 3.9.4, using the lattice Green function, we obtained the two-boson ground state energy on a large lattice, which gives in Sec. 3.10 an expression for a few bosons (Eq. 3.64). The two-fermion calculation is useful because it can be employed to obtain the ground state energy for a few fermions on a large lattice (using Eq. 3.62, same as for the bosons). This should be a p-wave calculation, and the resulting expression for energy should be a good guide for an expression for energy per particle at finite density (due to p-wave scattering, not in Bloom's calculation).

The difficulty here, as mentioned in Sec. 3.9.5, is that for two fermions we need to compute for the total momentum $\mathbf{P} = (0, 1)$ so we cannot use the same symmetry-reduced Green function for bosons (which is developed for $\mathbf{P} = (0, 0)$). Our lattice Green function is more complicated than that for the Hubbard model because we have nearest-neighbor interaction.

Few Fermions: T-Matrix for Degenerate Levels

For the problem of two fermions, we considered degenerate noninteracting states from the beginning of our t-matrix formulation (the sets $Q_I$ and $Q_{II}$, Eq. 4.5), and in Sec. 4.3.6, two and four-fold degenerate levels were studied using symmetry. For more than two fermions, in Chapter 7, we used the two-fermion t-matrix to calculate the energy (using the computer program outlined in Appendix F) by summing up the energy for all pairs.

Our program works when for each pair of fermions, each other pair that has the same energy and total momentum is either fully or partially occupied (see Sec. 7.5). We have not considered the case when such pairs are unoccupied, which happens for degenerate many-fermion levels, for example, the six-fold states in Table 7.3.
Therefore, in Chapter 7, we were limited to the nondegenerate cases. We would like to treat properly the energy splittings of degenerate states also (see Fig. 7.4).

**Few Bosons**

In Sec. 3.10 we obtained the ground state energy of a few bosons on a large lattice (Eq. 3.64) using the two-boson energy obtained from the lattice Green function. But we have not developed the more precise t-matrix treatment of the few-boson problem as we have done for the few-fermion problem in Chapter 7. The t-matrix is also important for dilute boson diagrammatic calculation, so we should have a lattice version t-matrix calculation for a few bosons. One of the difficulties with bosons is the existence of a condensate. We would like to give the boson problem a more thorough study.

**Dilute Fermion Curve Fitting with P-Wave Terms**

One of our motivations for studying the two-particle problem and the t-matrix is our interest in the validity of the 2D Fermi liquid picture, as we explained in Sec. 1.8.1. With spinless fermions and infinite repulsion, we have more diagonalization results than that can be obtained for the Hubbard model, but our fermions, because they are spinless, can only have p-wave scattering. This means that the interaction correction to the noninteracting energy should be much smaller than that from s-wave scattering. (For two particles, this is demonstrated in Fig. 3.8.) This also means that a series of analytical results for two-dimensional fermions with s-wave scattering cannot be used for our model. As mentioned earlier in this section, we are working on the two-fermion p-wave calculation first, which we expect to be able to guide our study of the finite-density energy. We then hope to fit the fermion energy
per particle curve in Fig. 8.7 as we have done in Fig. 8.1 for bosons.

More on Stripes

In this thesis work, due to the author’s time constraint, problems related to stripes have not been studied as thoroughly as problems related to a few particles. For example, the map of a single stripe to the spin chain introduced in Chapter 5 and the exact solutions associated with the spin chain have not been used very much in this thesis work. In the near future, we would like to make a more detailed study of stripes, as we have a good model and now a easy-to-use computer program. A number of future projects related to stripes have been summarized at the end of Chapter 6, and in the following, we emphasize three points.

Excitations of Stripes

In Chapters 5 and 6 on stripes, we did not study the excited states very much (except in Sec. 5.1.5 where we used the single stripe excited state energy to extract stripe effective mass). Excitations of stripes are interesting, and, as we used simple one-dimensional models to calculate stripe effective mass, we would like to use simple models to understand the low-lying excitations of stripes.

Statistical Average of Stripe Separation

In Chapter 6, we presented diagonalization results for the problem of two, three, and (very briefly) four stripes. We showed in Figs. 6.3, 6.7, and 6.9 the starting state of diagonalization with stripes all merged and the highest-weight state in the ground state eigenvector, and observed that stripes tend to be far apart in the ground state. We then used energy information (see Fig. 6.5) to show the repulsive nature of the
stripes.

We would also like to study the statistical average of stripe separation from all states in the ground state eigenvector, which we can obtain using the Lanczos method. For each state we need to identify the position of the holes in each column, compute their separation, average it over the length of the stripe, and then use the weight from diagonalization for this state to average over all states. This is a straightforward process, which we also hope to apply to the problem of two holes on a stripe in Sec. 5.4, to study the average separation of holes.

In fact, in this thesis, we have focused on the eigenenergy while the eigenstate information has not been used very much (except very briefly in our treatment of the two-particle problem, see Figs. 3.3 and 3.4). There are many interesting expectations that can be obtained from the diagonalization eigenvectors, e.g., the root-mean-square fluctuation of a stripe and the overlap of an exact fermion state with the noninteracting Fermi sea.

**Macroscopic, Continuum Studies of Stripes**

In Chapter 5 we studied one or two holes added to a stripe. We found that the energy decays exponentially as the lattice size grows in the direction perpendicular to the stripe. We used a one-dimensional double-well model to study this behavior and obtained stripe effective mass $m^*$. In Chapter 6 we also used stripe-stripe interaction energy to obtain effective mass for short stripes. And the results from these approaches are consistent. (On the other hand, we do not yet understand the dependence of stripe repulsion on the length of the stripe.)

We mentioned in the introduction and conclusion of Chapter 6 that there are macroscopic approaches to stripes by treating them as quantum elastic strings in
the continuum. Just as we used diagonalization data in the dilute limit to check diagrammatic results done in the continuum, we would like to study the predictions from the macroscopic, continuum approaches more and possibly check them using our diagonalization data.

**Diagonalize (or DMRG) 100 × 100 Lattice with 2000 Particles**

Dagotto wrote in 1991 [7]: “If the sign problem would not affect so severely low temperature Monte Carlo simulations then I am convinced that computer simulations on, say, 20 × 20 lattices would have already answered the main questions concerning the Hubbard model in strong coupling.” So this wish of ours is maybe a bit too greedy.\(^1\)

### 9.5 Outlook

**The Two-Dimensional Quantum World**

In this thesis we studied the physics of the two-dimensional quantum (lattice) world with strong interactions. The two dimensionality (flatland) is interesting in part because it lies between two much-better-understood realms. In one dimension, there are exact solutions using Bethe ansatz and a host of related analytical techniques (e.g., conformal field theory, quantum groups), and there is a very accurate numerical method (DMRG). In three dimensions, Fermi liquid theory works well in many cases. From many studies, the physics in the two-dimensional quantum world appears to be quite subtle (see for example, the logarithm in the two-boson large-lattice energy expression in Sec. 3.9.4, and the boson and fermion gases in Chapter 8).

\(^1\)Note a so-called “meron-cluster” quantum Monte Carlo method [8] has recently been developed to deal with the sign problem and may be able to handle spinless fermions.
Two Limits: Dilute and Dense

There are no good analytical or numerical methods for two-dimensional quantum problems at the present time (see Sec. 1.7 for a table on models). In this thesis work, we find that there are two limits which can be studied better than other parts of the phase diagram. First, at the low-density limit, two-particle interactions dominate, and we can use the results from the two-particle problem to understand the problem of a few particles (see Sec. 3.10 on a few particles on a large lattice and Chapter 4 on many-fermion t-matrix).

Second, at the dense limit, where particle movement is severely restricted by interaction, we can map a two-dimensional problem to a one-dimensional one and then use the many results from the one-dimensional world (see the one-stripe-to-spin-chain map in Sec. 5.1.3 and the double-well potential for the hole-on-stripe problem in Sec. 5.3.4 for example).

Two Methods: Symmetry and Renormalization

What about other parts of the phase diagram? In Fig. 1.6, we showed the phase diagram of the Hubbard model in two and higher dimensions, and remarked on the great unknown interior. From a general point of view, besides relying on the increasing power of the computer, perhaps two methods are promising for exploring the two and higher-dimensional quantum world.

In Sec. 1.4, we mentioned a few exact symmetries of the Hubbard model, e.g., translation and pseudospin symmetries. In our diagonalization program we used translation symmetries to reduce the matrix dimension by $N$, where $N$ is the number of lattice sites (see Sec. 2.5.2). Symmetries are of fundamental importance in physics. Many of the most well-known physical systems have a great deal of symmetry (e.g.,
three-dimensional the hydrogen atom has a four-dimensional rotational symmetry), and a lot of our understanding about the physical world comes from studying in detail models with symmetries. Perhaps some reasonably realistic quantum models in two dimensions with a lot of symmetries can be studied, and this can be used as some kind of entry point into the difficult two-dimensional quantum world.

Another way to approach a complicated problem is to use the idea of renormalization, that is, the parameters of a complicated system can be gradually changed and eventually turned into those for a simpler system. This is the idea of the Fermi liquid theory, in which complicated interacting states arise adiabatically from simple noninteracting states as interaction is gradually increased (see Sec. 1.8.1). One of our main objectives for undertaking this study is to understand the two-dimensional Fermi liquid better. Using the scattering t-matrix, we have mapped the noninteracting energy spectrum to the interacting one for the case of a few fermions (see for example Fig. 4.8 for two fermions and Fig. 7.4 for three fermions).

Another way to use the powerful renormalization idea is in numerical studies, in particular the density matrix renormalization group idea we discussed in Sec. 1.5.3. A small, well-understood system is gradually enlarged to eventually approach the thermodynamic limit. In two dimensions, this is still, as we mentioned in Sec. 1.5.3, an immature computational method but it is very promising.

High-Temperature Superconductivity

As far as high-temperature superconductivity is concerned, in view of the more than forty-five years that elapsed from the first experimental discovery by Kamerlingh Onnes in 1911 to the satisfactory solution by Bardeen, Cooper, and Schrieffer in 1957, the fifteen years that have passed since Bednorz and Muller’s discovery of
high-Tc in 1986 do not seem that long. In this thesis we addressed two problems related to the high-Tc superconductors: the Fermi liquid picture in two-dimensions and a model for interacting quantum stripes. We made some interesting studies using the t-matrix for the Fermi liquid problem (see especially Fig. 4.6 for a two-fermion t-matrix plot and Sec. 7.6 for the many-fermion t-matrix summary). And for the stripe problem, we obtained a number of interesting numerical results (see especially Figs. 6.5 and 6.8 for stripe-stripe repulsion data and Tables 5.2 and 5.3 for stripe effective mass).

It is fair to say that nobody knows what will become of the high-Tc field, but considering a host of interesting and fruitful ideas that it has inspired so far, it is a worthy intellectual pursuit that we are happy to be part of.

**Farewell**

“Our revels now are ended.” And before our subject melts into thin air, we make a parting outlook in Fig. 9.1.
Figure 9.1: The Outlook.
Bibliography

Appendix A

Running the Diagonalization Program

This appendix explains the procedures for running the diagonalization program described in Chapter 2 (the general program) and Sec. 5.2 (building basis states from a starting state). This appendix contains a description of the command line options, a collection of examples, and a note on time and memory issues, and can be used as a handy reference for running the diagonalization program. Appendix B describes in detail the output from the examples included in this appendix, and Appendix C describes the program files and implementation issues.

The format of the command line is:

```
java [Memory] Lattice.Model bf R_{1x} R_{1y} R_{2x} R_{2y} M [Trans] [Eval] [States]
[Diag] [Precision] [< input.file] [> output.file]
```

`java` is the name of the computer language, `Lattice` the package name, and `Model` the program name; they have to appear as such. This command line is for a lattice with boundaries defined by $(R_{1x}, R_{1y}) \times (R_{2x}, R_{2y})$, with $M$ particles, and `bf`
is either \texttt{boson} or \texttt{fermion}. The other command line options enclosed in brackets [...] are optional. See Table A.1 for the options. Except the \texttt{[Memory]} option that has to appear right after \texttt{java}, the other options in brackets do not need to follow the specified order (the order of the options not in brackets must appear as specified). If an option is not entered in the command line, the default choice is used. We will first describe the basic idea of the program, followed by detailed description of the options, a collection of examples, and then a discussion on time and memory issues.

Table A.1: The options of the diagonalization program command line. If an option is not entered at the command line, the default choice is used.

<table>
<thead>
<tr>
<th>Memory</th>
<th>Trans</th>
<th>Output</th>
<th>State</th>
<th>Diag</th>
<th>Precision</th>
</tr>
</thead>
<tbody>
<tr>
<td>default</td>
<td>64 MB</td>
<td>notrans</td>
<td>eval</td>
<td>build</td>
<td>full</td>
</tr>
</tbody>
</table>
| others | -mx[MB]M | all | ground | read | lan | precision $N_P$
| | | sel | state $N_S$ | | | lannostore |
| | | k | $K$ | kvectors | | arp $N_A$ |

\section*{A.1 Basic Idea of the Program}

It is good to have a basic idea of the program before considering the many combinations of the command line options. The user can ask him or herself the following questions:

1. About the basis set:

   (a) Do I want to use translation symmetry?

   i. If no, use \texttt{notrans} (default).

   ii. If yes, use \texttt{all}, \texttt{sel}, or $k$ $K$ ...
(b) Do I want to enumerate all states or read in a state?
   i. If all states, use build (default).
   ii. If read in a state, prepare an input file, use read and < input.file.

2. About diagonalization (after building the basis set):

   (a) Do I want just eigenvalues or also eigenstates?
      i. If eigenvalues only, use eval (default).
      ii. If also ground state eigenvector, use ground.
      iii. If state number \( N_S \), use state \( N_S \) \( (N_S = 0 \) is ground state).}

   (b) Do I want information just about the ground state or also excited states?
      i. If excited state information is desired, use full (default) for all states
         or arp \( N_A \) for the lowest \( N_A \) states (Arnoldi method using ARPACK,
         can be used for large number of states, with translation symmetry).
      ii. If only ground state is desired, can use lan or lannostore for Lanczos
         method (with translation symmetry). Then there are three more
         questions:
         A. Do I want to complete my job fast? Time constraint. Use lan.
         B. Do I want to compute a large system? Memory constraint. Use
            lannostore.
         C. How accurate do I want my results to be? Use precision \( N_P \).

3. How much memory [Memory] do I need to specify?

   This will be explained in Sec. A.4.
A.2 Command Line Options

1. Memory

Specifying the maximum memory allocated to the program. For example, 
\(-m x 128 M\) means 128 megabytes. \(-m x 1880 M\) is the limit for our version of java 
(1.3.1_01). The default is \(-m x 64 M\).

2. Trans

Specifying whether to use translation symmetry, and if use, specifying the \(k\) 
vectors.

(a) notran

Do not use translation symmetry. This is the default choice. Lanczos 
and Arpack have not been implemented for this option.

(b) all

Compute for all \(N\) \(k\) vectors, where \(N\) is the number of sites.

(c) sel

A selected set of \(k\) vectors not related by reflection and inversion sym-
metries. Works for rectangular-boundary lattices \(L_x \times L_y\) only (not im-
plemented for tilted lattices).

If \(L_x \neq L_y\), compute for only one \(k\) vector from the following set: \((k_x, k_y)\), 
\((-k_x, k_y), (k_x, -k_y)\), and \((-k_x, -k_y)\), that are obtained from \(k = (k_x, k_y)\) 
by reflections with respect to \(x\) or \(y\) axis and inversion with respect to the 
origin. By symmetry, the eigenvalue spectra for these (maximally four) 
vectors should be identical. Roughly \(1/4\) of the \(k\) vectors are computed.

If \(L_x = L_y\), compute for only one from the following set: \((k_x, k_y), (-k_x, k_y), \)
\((k_x, -k_y), (-k_x, -k_y), (k_y, k_x), (k_y, -k_x), (-k_y, k_x), (-k_y, -k_x)\), that also include those obtained from \(k\) by reflections with respect to \(y = \pm x\) lines. Roughly 1/8 of the \(k\) vectors are computed.

The \texttt{sel} option is useful when we want to find the ground state energy of a fermion problem without knowing the ground state \(k\) vector. It reduces the number of \(k\) vectors to compute.

\textbf{(d) k K k_1x k_1y k_2x k_2y \ldots k_Kx k_Ky}

Compute for the \(K\) \(k\) vectors \((k_1x, k_1y), (k_2x, k_2y), \ldots, (k_Kx, k_Ky)\). For example, to obtain boson ground state energy, one just need to use \(k 1 0 0\).

\textbf{3. Output}

\textbf{(a) eval}

Compute eigenvalues only. Default.

\textbf{(b) ground}

Compute eigenvalues and show the ground state eigenvector. Eigenstates in the ground state eigenvector will be listed and plotted with decreasing probability.

\textbf{(c) state N_S}

Compute eigenvalues and show the \(N_S\)th eigenvector \((N_S = 0, 1, \ldots,\) where 
\(N_S = 0\) is the ground state).

\textbf{4. State}

\textbf{(a) build}

Build all basis states. Default.
(b) read

Read in a state from a file and find all states that can be obtained from this state by hopping. The option [input.file] should be used to read in the file.

5. Diag

(a) full

Full matrix diagonalization, using LAPACK. The requires storing the matrix in memory.

(b) lan

Fast way to do Lanczos diagonalization, with information for the Hamiltonian matrix stored. This option requires a great deal of memory, and can handle roughly up to 1 million states.

(c) lannostore

Lanczos diagonalization without storing matrix information. This option requires much less memory than lan, but it can be slow.

(d) arp $N_A$

Diagonalization using ARPACK, a commercially available package using the Arnoldi method, which is closely related to the Lanczos method. This finds $N_A$ lowest energies. It is useful when excited states are needed and full diagonalization cannot be used because of memory restriction. Currently, this option does not give eigenvectors.

6. Precision

(a) Default
The precision (or error tolerance) for full diagonalization is set by LA-
PACK (double precision). The ARPACK precision is set at $10^{-15}$. The
default for Lanczos with matrix information storage is $10^{-15}$, and for
Lanczos without matrix storage is $10^{-7}$ (because this last option takes
more time than the one with storage).

(b) precision $N_p$

Specifying the precision for Lanczos (both lan and lanstore) at $10^{-N_p}$.
For example, precision 5 sets the tolerance at 0.00001. Currently the
precision for full and arp cannot be changed.

7. [<input.file>]

This is needed for the read option and specifies the starting basis state from
which the basis set is built from all possible hoppings. It should be a picture
drawing of a state with $M$ particles. For example, a $M = 11$ state on a $4 \times 7$
lattice can be,

```
   0 1 2 3
 6
 5  *
 4  *  *
 3  *  *
 2  *  *
 1  *  *
 0  *  *
```

$M = 15$ on a tilted lattice, $(5,1) \times (0,7)$, can be,

```
   0 1 2 3 4
 7
 6  *  *
 5  *  *
 4  *  *
 3  *  *
```
8. [> output. file]

Send the eigenvalue and, if specified, eigenvector results to text file output. file.

The output of our program contains one part going to standard error, which
is normally the screen. This part contains time and memory information. The
other part of the output contains eigenvalue and eigenvector results, and goes
to output. file if specified. If output. file is not specified, the two parts of
the output will both go to the screen.

If the queue system is used, with the option [> output. file], then the eigen-
value results go to output. file as above, and the error output goes to a file
named by the queue. For example, if the queue file that contains the job is
called runit. txt, and the job is number 31891, then the error output goes
to a file with the name like the following runit. txt.e31891.14736, where
the letter e says it is from standard error output, and 14736 is a randomly
assigned number to distinguish this file from others.

A.3 Collection of Examples

The user can use this section as an example sheet for his or her calculations. Detail
descriptions of these examples, including explanations of their output, are in Ap-
pendix B. The memory and time issues related to the program will be discussed in
Sec A.4. The user may wish to use Tables A.2 and A.4 (using lan) and Tables A.3
and A.5 (using lannostore) as a guide for time and memory usage.
No translation

1. Fermion, \((4,0) \times (0,5)\) with \(M = 7\), no translation, full diagonalization, eigenvalues only:

```
java Lattice.Model fermion 4 0 0 5 7 > result.txt
```

2. \((4,0) \times (0,5)\) with \(M = 7\), no translation, full diagonalization, eigenvalues and ground state eigenvector:

```
java Lattice.Model fermion 4 0 0 5 7 ground > result.txt
```

3. \((4,0) \times (0,5)\) with \(M = 7\), no translation, full diagonalization, eigenvalues and 5th excited state eigenvector:

```
java Lattice.Model fermion 4 0 0 5 7 state 5 > result.txt
```

4. \((4,0) \times (0,5)\) with \(M = 7\), no translation, full diagonalization, eigenvalues only, and build the basis set from reading in the state in file \(4_{-5}_{-7}.state\):

```
java Lattice.Model fermion 4 0 0 5 7 read < 4_5_7.state > result.txt
```

where as an example, the file \(4_{-5}_{-7}.state\) looks like

```
0 1 2 3
4 * * *
3 * * *
2 * *
1 * *
0
```

5. Tilted lattices \((4,-1) \times (1,5)\) with \(M = 7\):

```
java Lattice.Model boson 4 -1 1 5 7 > result.txt
```

```
java Lattice.Model boson 4 -1 1 5 7 ground > result.txt
```
Translation with full diagonalization

1. $(5, 0) \times (0, 6)$ with $M = 4$ and $k = (0, 0)$, full diagonalization, eigenvalues only:

   java Lattice.Model boson 5 0 0 6 4 k 1 0 0 > result.txt

2. $(5, 0) \times (0, 6)$ with $M = 4$ and $k = (0, 0)$, full diagonalization, eigenvalues and ground state eigenvector:

   java Lattice.Model boson 5 0 0 6 4 k 1 0 0 ground > result.txt

3. $(5, 0) \times (0, 6)$ with $M = 4$ and $k = (0, 0)$, full diagonalization, eigenvalues and 5th excited state eigenvector:

   java Lattice.Model boson 5 0 0 6 4 k 1 0 0 state 5 > result.txt

4. $(5, -1) \times (1, 5)$ with $M = 4$ and all $k$ vectors, full diagonalization, eigenvalues only:

   java Lattice.Model fermion 5 -1 1 5 4 all > result.txt
Use the following to extract the ground state energy from full diagonalization results for many k vectors:

```java
Lattice.Extract < result.txt
```

5. \((5,0) \times (0,6)\) with \(M = 4\) and selected k vectors (excluding those due to reflection and inversion symmetries), full diagonalization, eigenvalues only:

```java
Lattice.Model fermion 5 0 0 6 4 sel > result.txt
```

Again use `Lattice.Extract` to extract the ground state eigenvalue.

6. \((5,0) \times (0,6)\) with \(M = 4\) and \(k = (1,0)\) full diagonalization, eigenvalues only, build basis set from reading in a state:

```java
Lattice.Model fermion 5 0 0 6 4 k 1 1 0 read < 5_6_4.state > result.txt
```

where the file `5_6_4.state` can, for example, be

```
0 1 2 3 4
5  *
4 *
3 *
2 *
1 *
0 *
```

**Lanczos with Matrix Storage: lan**

1. The ground state energy of \(M = 6\) bosons on the \(7 \times 7\) lattice, with \(k = (0,0)\), using Lanczos with storage of matrix information:
java -mx128M Lattice.Model boson 7 0 0 7 6 k 1 0 0 lan
> result.txt

2. The ground state energy and eigenvector of $M = 6$ bosons on the $7 \times 7$ lattice,
with $k = (0,0)$, using Lanczos with storage of matrix informaton:

java -mx128M Lattice.Model boson 7 0 0 7 6 k 1 0 0 lan ground
> result.txt

3. The ground state energy of $M = 5$ fermions on the $7 \times 7$ lattice, with selected
$k$ (not related by reflection and inversion symmetries), using Lanczos with
storage of matrix informaton:

java -mx256M Lattice.Model fermion 7 0 0 7 5 sel lan > result.txt

To extract the ground state eigenvalue from a number of $k$ Lanczos results
(notice ExtractLan for Lanczos results and Extract for full diagonalization
results):

java Lattice.ExtractLan < result.txt

4. The ground state energy of $M = 5$ fermions on the $7 \times 7$ lattice, with all $k$,
using Lanczos with storage of matrix informaton:

java -mx256M Lattice.Model fermion 7 0 0 7 5 all lan
> result.txt

Again use Lattice.ExtractLan to extract the ground state eigenvalue.
5. The ground state energy of $M = 11$ bosons on the $4 \times 7$ lattice, with $k = (0,0)$, using Lanczos with storage of matrix information, and building the basis set from reading in a state:

```java
Lattice.Model boson 4 0 0 7 11 k 1 0 0 lan read
< 4_7_11.state > result.txt
```

where the state `4_7_11.state` can for example be:

```
0 1 2 3
6
  *
4  *
  *
3  *
  *
2  *
  *
1  *
  *
0  *
```

or for a tilted lattice, $(5, 1) \times (0, 7)$ with $M = 15$,

```
0 1 2 3 4
7
6  *
  *
5  *
  *
4  *
  *
3  *
  *
2  *
  *
1  *
  *
0 *
```

6. The ground state energy of $M = 6$ bosons on the $7 \times 7$ lattice, with $k = (0,0)$, using Lanczos with storage of matrix information, and tolerance $10^{-6}$ (the default tolerance is $10^{-15}$):

```java
Lattice.Model boson 7 0 0 7 6 k 1 0 0 lan
precision 6 > result.txt
```
Lanczos without Matrix Storage: lannostore

The options are the same as lan except lan is changed in the command line to lannostore, e.g., \((7, 0) \times (0, 7)\) with \(M = 6, \mathbf{k} = (0, 0)\).

\begin{verbatim}
java -mx128M Lattice.Model boson 7 0 0 7 6 k 1 0 0 lannostore
> result.txt
\end{verbatim}

Arpack: arp \(N_A\)

\((7, 0) \times (0, 7)\) with \(M = 5\) and \(\mathbf{k} = (0, 0)\), using Arpack to find the lowest 4 energies:

\begin{verbatim}
java -mx128M Lattice.Model boson 7 0 0 7 6 k 1 0 0 arp 4
> result.txt
\end{verbatim}

Noninteracting fermion ground state energy

Noninteracting energies for \(5 \times 8\) lattice, with up to 7 fermions

\begin{verbatim}
java Lattice.Noninter 5 0 0 8 7
\end{verbatim}

A.4 Memory and Time Issues

Translation symmetry is needed for large system computations, so in this section we consider in more detail the different diagonalization options and their memory requirements.

We will use \(N\) to denote the number of basis states after considering translation symmetry (i.e., the number of representative states). \(N\) is also the dimensionality of Hamiltonian matrix for each \(\mathbf{k}\) vector. We first explain the storage requirement for the basis set, then for the four diagonalization methods.
A.4.1 The Basis Set with Translation Symmetry

For each state, the following three items are stored:

1. Positions of the $M$ particles as an array of lattice site index numbers. We use a Java `short` number for each index.\(^1\) Each `short` number takes 2 bytes, so this array takes $2M$ bytes.\(^2\)

2. Fermion signs for translating the representative state for all $N$ lattice vectors. Each sign takes one bit, so these signs take $N/8$ bytes for each state.

3. Normalization factors for each $k$ vectors. If there are $K$ vectors to compute, there are $K$ `double` numbers to store. Each `double` takes 8 bytes, so these normalization factors take $8K$ bytes.

The total storage requirement for each basis state with translation symmetry is then $2M + N/8 + 8K$ bytes.

A.4.2 Four Diagonalization Methods

With translation symmetry, after the basis set is constructed and stored, there are four ways to diagonalize the Hamiltonian.

1. full

   (a) Store matrix information, i.e., for each column, a set of $(p, j(m), \sigma_{j(m)})$ described in Sec. 2.6.2 that contains information about the nonzero en-

---

\(^1\)In Java, short numbers are signed integers from -32768 to 32767. As indices for lattice sites, they are good for lattices as large as $100 \times 300$.

\(^2\)Because at each site, there can be only zero or one particle, so instead of using $M$ `short` numbers ($2M$ bytes), it is possible to use an array of $N$ bits ($N/8$ bytes). We did not use this option for speed reason, as we require a great deal of translations for each basis state.
tries of the Hamiltonian matrix in this column. Storing the matrix information takes a great deal of memory, but it makes matrix diagonalization a lot faster (especially when a number of k vectors are needed or there are many Lanczos or Arpack iterations).

(b) For each k, store the Hamiltonian matrix (Hermitian) in memory, and use LAPACK to find eigenvalues and eigenvectors. This requires storing in the order of $N \times N$ matrix entries and is therefore limited to $N$ up to a few thousands.

2. lan:

(a) Store matrix information as above.

(b) Need two complex vectors of $N \times 1$ for Lanczos if only eigenvalues are desired; need three such vectors if ground state eigenvector is also desired. The memory requirement for Lanczos, if only computing ground state eigenvalue, is 4 doubles per basis state.

3. lannostore:

(a) Do not store matrix information. Calculate the matrix elements on the fly.

(b) Again need two complex vectors of $N \times 1$ for lanczos if only eigenvalues are desired; need three such vectors if ground state eigenvector is also desired.

4. arp $N_A$

This option has not been systematically investigated by the present author. The user is pretty much on his or her own.
\texttt{lann} and \texttt{lannostore} are the most commonly used options for this thesis work. In Tables A.2 and A.3 (at the end of the chapter) we show the time and memory usage for $7 \times 7$ lattice using \texttt{lann} and \texttt{lannostore} respectively. Using \texttt{lann}, the $M = 9$ case with 1 million states can be done in 45 minutes (for one \textit{k} vector, with tolerance $10^{-15}$, on \texttt{charming}), but it uses 1.5 GB of memory, mostly for matrix information storage. This is basically the limit of \texttt{lann}, with memory limit set by Java at about 2 GB. Using \texttt{lannostore}, with a larger tolerance $10^{-7}$ (and therefore fewer Lanczos iterations), we can handle the $M = 11$ case with nearly 2 million states. This takes much longer than using \texttt{lann}, about 10 hours, but it requires much less memory, less than 400 MB.

In Tables A.4 and A.5 we also include the time and memory information for a series of calculations for fixed $M$ and increasing $L$. The $M = 4$ on $20 \times 20$ lattice, with around 2.5 million basis states, has the largest matrix we calculated for this thesis work so far.

In short, for matrices with $N$ less than 1 million, it is faster to use \texttt{lann}. With $N$ greater than 1 million, it is necessary to use \texttt{lannostore}, but this takes considerably longer; and therefore it may be useful to set a larger tolerance value to reduce the number of Lanczos iterations. Tables A.2 ($M$ particles on the $7 \times 7$ lattice) and A.4 ($4$ particles on the $L \times L$ lattice) contain time and memory usage for \texttt{lann}, and Tables A.3 and A.5 that for \texttt{lannostore}. The user may want to check with these tables when running large matrix diagonalizations.
Table A.2: Time and memory information for 7 × 7 lattice computed for one k vector using lan (eigenvalues only), with matrix information storage. \( N_{\text{Lan}} \) is the number of Lanczos iterations, while the Lanczos precision is set at \( 10^{-15} \). The time for filling in the basis set (with translation symmetry), storing basis set and matrix information, and Lanczos iterations is shown (on charming, Pentium III 700). The memory usage for basis set plus matrix information and two Lanczos vectors are also included. The \( M = 9 \) case with 1 million basis states, using 45 minutes of CPU time and about 1.5 GB of memory, is approximately the maximum limit for the lan option. The command line (for boson with \( k = (0,0) \)) is java -mx1880M

<table>
<thead>
<tr>
<th>( M )</th>
<th>( N )</th>
<th>( N_{\text{Lan}} )</th>
<th>fill (sec)</th>
<th>store (sec)</th>
<th>lan (sec)</th>
<th>total (min)</th>
<th>basis+mat (MB)</th>
<th>lan (MB)</th>
<th>total (MB)</th>
</tr>
</thead>
<tbody>
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<td>0.2</td>
<td>0.0</td>
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<td>1</td>
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<td>2</td>
<td>0</td>
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</table>
Table A.3: Time and memory information for $7 \times 7$ lattice computed for one $k$ vector using `lannostore` (eigenvalues only), without matrix information storage. $N_{\text{Lan}}$ is the number of Lanczos iterations, while the Lanczos precision is set at $10^{-7}$ (larger than that in Table A.2 because this option takes longer). The $M = 11$ case with 1.9 million basis states uses about 10 hours of CPU time but less than 400 MB of memory, and has the largest $\mathcal{N}$ of the $7 \times 7$ system. The command line (for boson with $k = (0,0)$) is `java -mx600M Lattice.Model boson 7 0 0 7 11 k 1`.

```
0 0 lannostore > b_7_0_0_7_11_zero_lannostore.data
```

<table>
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<tr>
<th>$M$</th>
<th>$\mathcal{N}$</th>
<th>$N_{\text{Lan}}$</th>
<th>fill</th>
<th>store</th>
<th>lan</th>
<th>total</th>
<th>basis</th>
<th>lan</th>
<th>total</th>
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<td></td>
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<td>(sec)</td>
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<td>(sec)</td>
<td>(min)</td>
<td>(MB)</td>
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<td>(MB)</td>
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</table>
Table A.4: Time and memory information for $L \times L$ lattice with $M = 4$ particles, computed for one $k$ vector using lan (eigenvalues only), with matrix information storage. $N_{Lan}$ is the number of Lanczos iterations, while the Lanczos precision is set at $10^{-15}$. The time for filling in the basis set (with translation symmetry), storing basis set and matrix information, and Lanczos iterations is shown (on charming; Pentium III 700). The memory usage for basis set plus matrix information and two Lanczos vectors are also included. The command line for $L = 17$ is (for boson with $k = (0, 0)$) is `java -mx1880M Lattice.Model boson 17 0 0 17 4 k 1 0 0 lan

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<th>$L$</th>
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<th>store (sec)</th>
<th>lan (sec)</th>
<th>total (min)</th>
<th>basis+mat (MB)</th>
<th>lan (MB)</th>
<th>total (MB)</th>
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</table>
Table A.5: Time and memory information for $L \times L$ lattice with $M = 4$, computed for one $k$ vector using lannostore (eigenvalues only), without matrix information storage. $N_{Lan}$ is the number of Lanczos iterations, while the Lanczos precision is set at $10^{-7}$. The $L = 20$ case with around 2.5 million basis states uses about 10 hours of CPU time and 546 MB of memory, and it is the largest matrix we computed for this thesis work. The command line (for boson with $k = (0,0)$) is java -mx800M Lattice.Model boson 20 0 0 20 4 k 1 0 0

lannostore > b_20_0_0_20_4_zero_lannostore.data

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<th>store</th>
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<th>total</th>
<th>basis</th>
<th>lan</th>
<th>total</th>
</tr>
</thead>
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<td>(sec)</td>
<td>(sec)</td>
<td>(min)</td>
<td></td>
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<td>0.03</td>
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<td>0.1</td>
<td>0.1</td>
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<td>0.1</td>
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<td>0.2</td>
<td>0.1</td>
<td>0.3</td>
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<td>13</td>
<td>0.1</td>
<td>0.5</td>
<td>7</td>
<td>0.1</td>
<td>0.4</td>
<td>0.2</td>
<td>0.6</td>
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<td>6635</td>
<td>15</td>
<td>0.2</td>
<td>1</td>
<td>22</td>
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<td>16</td>
<td>0.5</td>
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<td>58</td>
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<td>2</td>
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<td>30494</td>
<td>17</td>
<td>1</td>
<td>15</td>
<td>133</td>
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<td>2</td>
<td>5</td>
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<td>1</td>
<td>40</td>
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<td>526</td>
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<td>53</td>
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<td>22</td>
<td>13</td>
<td>826</td>
<td>2684</td>
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<td>1555</td>
<td>4266</td>
<td>97.4</td>
<td>77</td>
<td>45</td>
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<td>905168</td>
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<td>30</td>
<td>2840</td>
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<td>158.3</td>
<td>124</td>
<td>66</td>
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<td>9932</td>
<td>249.0</td>
<td>181</td>
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<td>26</td>
<td>61</td>
<td>8443</td>
<td>14732</td>
<td>387.3</td>
<td>262</td>
<td>130</td>
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<td>89</td>
<td>14024</td>
<td>21541</td>
<td>594.2</td>
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</table>
Appendix B

Running the Diagonalization Program: Examples

This appendix describe in detail the output of the example command lines included in Sec. A.3

B.1 Full Diagonalization without Translation

Because translation symmetry is not used, this case applies to very small systems.¹

B.1.1 Eigenvalues Only

Doing $M = 7$ fermions on the $4 \times 5$ lattice, the following is the screen output, running on the machine charming (which has a Pentium III 700 processor, 4096-megabyte (4096M or 4G) of memory, with the Linux operating system).

charmimg> java Lattice.Model fermion 4 0 0 5 7 > result.txt

¹This option will be useful for systems without translation symmetry, e.g., with disorder, for a future project.
(4,0)*(0,5) fermion N=20 M=7
notrans eval build full

Setting up BasisSet (s) 0.028
Total Memory (MB) 2.032
Memory Used (MB) 0.128

Matrix dim=200

Setting up matrix (s) 0.061
Diagonalization (s) 0.058
Total Memory (MB) 2.032
Memory Used (MB) 0.290

This is the standard error part of the output and contains various information about the running of the program. The command line options are notrans (no translation symmetry, default), eval (compute eigenvalue only, default), build (build all basis states, default), and full (full matrix diagonalization, default).

The time used for setting up the basis set is 28 milliseconds (ms); the total memory available after basis set construction but before matrix computation is 2 MB (java allocates memory as needed); the memory used up to this point (mainly for basis set) is 128 KB.

The matrix is $200 \times 200$. Without translation symmetry, this is a real symmetric matrix. The time takes to fill in matrix entries is 61 ms, and the time used for diagonalization is 58 ms. The memory used including matrix storage is 290 KB.

Now let us look at the output file:

```
charming> more result.txt
(4,0)*(0,5) fermion N=20 M=7
Matrix dim=200

-3.0818310161636956
-2.9533439181905172
-2.953343918190515
-2.9071727027770535
```
-2.9071727027770526
-2.838790407879369
-2.838790407879366
-2.8169874232305885
-2.8169874232305885
-2.8008566427613
-2.8008566427612998
-2.8005409174907046
-2.800540917490704

....

The eigenvalues are listed, from the ground state (-3.0818310161635956) up.

### B.1.2 Eigenvalues and Eigenvectors

If we would like to print out the ground state, we use

```
java Lattice.Model fermion 4 0 0 5 7 ground > result.txt
```

The output is:

```
charming> more result.txt
(4,0)*(0,5) fermion N=20 M=7
Matrix dim=200

-3.0818310161635964
-2.953343918190517
-2.9533439181905163
-2.907172702777054
-2.9071727027770478
-2.838790407879367
-2.838790407879366
...
2.9909571537788353
2.9909571537788366
3.012368634162049
3.0123686341620495
```

Eigenvector 0 probabilities: in decreasing order
```
[basis state number] probability
state picture
```
[199] 0.006672772268812676
  0 1 2 3
  4 * *  
  3 * *
  2 *
  1 * *
  0 *

[112] 0.006672772268812675
  0 1 2 3
  4 * *
  3 * *
  2 *
  1 * *
  0 *

[128] 0.006672772268812653
  0 1 2 3
  4 * *
  3 * *
  2 *
  1 * *
  0 *

[60] 0.006672772268812632
  0 1 2 3
  4
  3 * *
  2 *
  1 * *
  0 * *
  ...

Here the eigenvalues are followed by the ground state eigenvector (0th eigenvector): the 199th state on the basis set list has one of the highest probabilities 0.006672772268812676, and the state is drawn, etc.

If the 5th excited state is wanted, simply do

```
java Lattice.Model fermion 4 0 0 5 7 state 5 > result.txt
```
B.1.3 Reading in a State

We can also read in a state and build basis set from that state:

```java
Lattice.Model fermion 4 0 0 5 7 read < 4_5_7.state > result.txt
```

The state file should be a drawing like the one printed out using `ground` and `state` $N_S$, for example,

```plaintext
charming> more 4_5_7.state
 0 1 2 3
 4 * * *
 3 * * *
 2 *
 1 * *
 0
```

B.1.4 Tilted Lattices

The preceding options also apply to tilted lattices. Here we show command lines for $(4,-1) \times (1,5)$ with $M = 7$ bosons.

```java
Lattice.Model boson 4 -1 1 5 7 > result.txt
```

```java
Lattice.Model boson 4 -1 1 5 7 ground > result.txt
```

```java
Lattice.Model boson 4 -1 1 5 7 state 3 > result.txt
```

```java
Lattice.Model boson 4 -1 1 5 7 read < 4_-1_1_5_7.state > result.txt
```

```plaintext
more 4_-1_1_5_7.state
 0 1 2 3 4
 4 *
 3 * * *
 2 *
 1 * *
 0 * *
-1
```
B.2 Full Diagonalization with Translation

This case applies roughly to $N$ up to a few thousands (see Sec. A.4); we can obtain information about ground state and excited states.

B.2.1 A Few k Vectors

For bosons, to obtain ground state energy, we just need to compute for $k = (0,0)$. The following calculates $M = 4$ bosons on the $(5,0) \times (0,6)$ lattice with one $k$ vector $(0,0)$. The screen output is:

charmimg> java Lattice.Model boson 5 0 0 6 4 k 1 0 0 > result.txt
(5,0)*(0,6) boson N=30 M=4
trans eval build full

Filling in TransBasisSet...
Now at state done.
Time used to fill basis set is (s) 0.039
After fill, number of states is 354

Store translation basis state and matrix info...
Now at state 0 done.
Store state and matrix info time (s) 0.163

Total Memory (MB) 2.032
Memory Used (MB) 0.425

Matrix dim=354

[0] k = (0,0)
Setting up matrix (s) 0.085
Diagonalization (s) 1.254
Total Memory (MB) 2.982
Memory Used (MB) 1.437

The messages “Filling in TransBasisSet...Now at state done” and “Store translation basis state and matrix info... Now at state 0 done” are from
printing state numbers (every 10000 states) on the screen as the calculation progresses (so that the user does not stare at an uneventful screen for too long). These lines are going to be helpful for a large number of basis states (with Lanczos and Arpack), as we will see in later examples (Sec. B.3.1).

The time used to fill the basis set is 39 ms, to store the basis state and matrix information is 163 ms, to set up the matrix is 85 ms, and to diagonalize the matrix is 1.25 s. The memory used for basis state and matrix information is 425 KB, and with matrix stored in memory just after diagonalization, it becomes 1.437 MB. (Note that the total memory increases from 2 MB to 2.9 MB. Java allocates memory as needed, up to 64 MB. Above that, the memory limit has to be specified by using -mx.)

And the output is:

```
charming> more result.txt
(5,0)*(0,6) boson N=30 M=4
Matrix dim=354

[0] k = (0,0)
-11.592615224323364
-8.456584108053068
-7.99710850493835
-7.780998122378207
-7.497348400911269
-7.068855050598833
...
```

For the ground state eigenvector also, we run:

```
java Lattice.Model boson 5 0 0 6 4 k 1 0 0 ground > result.txt
```

The output we get is

```
charming> more result.txt
(5,0)*(0,6) boson N=30 M=4
```
Matrix dim=354

[0] k = (0,0)
-11.592615224323373
-8.456584108053072
-7.997108504938332
...
8.483510705626355
8.522053344183119
10.482396626105523

Eigenvector 0 probabilities: in decreasing order
[basis state number] probability
representative state picture
[214] 0.019372241274533155
   0 1 2 3 4
   5
   4
   3 *
   2 *
   1
   0 *
[203] 0.01937224127453307
   0 1 2 3 4
   5
   4 *
   3 *
   2
   1 *
   0 *
[333] 0.015731676777423768
   0 1 2 3 4
   5
   4 *
   3 *
   2
   1 *
   0 *

Here the pictures are for the representative states of the basis set.

For 5th excited state, we run
java Lattice.Model boson 5 0 0 6 4 k 1 0 0 state 5 > result.txt

For two k vectors (0,0) and (1,0) and eigenvalues only, we run:

java Lattice.Model boson 5 0 0 6 4 k 2 0 0 1 0 > result.txt

B.2.2 All k Vectors

For a fermion problem, let us say that we want to compute the ground state energy of \((5,-1) \times (1,5)\) with \(M = 4\). We do not know in which \(k\) sector we can find the ground state, so we compute for all \(k\) vectors:

charm> java Lattice.Model fermion 5 -1 1 5 4 all > result.txt

\((5,-1) \times (1,5)\) fermion \(N=26\) \(M=4\)
trans eval build full

Filling in TransBasisSet...
Now at state done.
Time used to fill is \(s\) 0.023
After fill, number of states is 740

Delete translation related states...
Now at state 0 (740) 100 (442) done.
Delete state time \((s)\) 0.225
After delete, number of state = 187

Storing matrix info...
Now at state 0 100 done.
Time used to store \((s)\) 0.141

Total Memory (MB) 2.032
Memory Used (MB) 0.352

Matrix dim=187

\([0] \ k = (0,0)\)
Setting up matrix \((s)\) 0.057
Diagonalization \((s)\) 0.154
\([1] \ k = (0,1)\)
Setting up matrix \((s)\) 0.064
Diagonalization (s) 0.146
[2] k = (0,2)
Setting up matrix (s) 0.051
Diagonalization (s) 0.148
[3] k = (0,3)
Setting up matrix (s) 0.050
Diagonalization (s) 0.146
...
[23] k = (4,3)
Setting up matrix (s) 0.053
Diagonalization (s) 0.145
[24] k = (4,4)
Setting up matrix (s) 0.053
Diagonalization (s) 0.148
[25] k = (4,5)
Setting up matrix (s) 0.050
Diagonalization (s) 0.146
Total Memory (MB) 2.032
Memory Used (MB) 0.625

And the output file contains eigenvalues from all 26 k vectors:

```
charming> more result.txt
(5,-1)*(1,5) fermion N=26 M=4
Matrix dim=187

[0] k = (0,0)
-8.01949235501879
-7.407879701707916
-7.2288912441532
...
7.148527549209429
7.2288912441532025
7.407879701707925
8.019492355018766

[1] k = (0,1)
-9.33222886829876
-6.857635970112962
-6.753928923478621
-6.201134688176292
...
6.753928923478629
6.857635970112941
```
This output file says that the ground state in \( k = (0, 0) \) sector is \(-8.01949235501879\), in \( k = (0, 1) \) sector is \(-9.33222886829876\), etc. The question is which is the ground state. It is somewhat tedious to look through all these sectors, so we have a program that can extract ground state energies from each sector, and also output the absolute ground state energy:

```
class> java Lattice.Extract < result.txt
(5,-1)*(1,5) fermion N=26 M=4

[0] k = (0,0)
  -8.01949235501879
[1] k = (0,1)
  -9.33222886829876
[2] k = (0,2)
  -8.590289930581571
...
[23] k = (4,3)
  -7.508811380436049
[24] k = (4,4)
  -8.590289930581568
[25] k = (4,5)
  -9.332228868298763
```
Number of k vectors = 26  
Ground state energy = -9.3322886829877

The ground state is -9.3322886829877 and is in k = (0,1).

B.2.3 Selected k Vectors

For rectangular-boundary lattices, we can also use a selected set of k vectors:

java Lattice.Model fermion 5 0 0 6 4 sel > result.txt

There are 12 vectors used (instead of 30 for all), and we can use Lattice.Extract to obtain ground state energy for each sector and the absolute ground state energy.

java Lattice.Extract < result.txt

B.2.4 Read in a State

We can also read in a state and build the basis set from there:

java Lattice.Model fermion 5 0 0 6 4 k 1 1 0 read < 5_6_4.state  
> result.txt

The state 5_6_4.state is specified as before, for example,

charming> more 5_6_4.state
   0 1 2 3 4
   5   *
   4
   3
   2 *
   1   *
   0   *


B.3  Lanczos with Matrix Storage: lan

As explained in Sec. A.4, lan stores matrix information, is fast, but takes a lot of memory; lannostore does not store matrix information, is slow, but takes much less memory.

B.3.1  Ground State Eigenvalue Only

This is the most commonly used option of the program, for fast computation of ground state energy using Lanczos.

As an example, we compute the ground state energy of $M = 6$ bosons on the $7 \times 7$ lattice, with $k = (0,0)$ (see Table A.2).

charmimg> java -mx128M Lattice.Model boson 7 0 0 7 6 k 1 0 0 lan
> result.txt
(7,0)*(0,7) boson N=49 M=6
trans eval build lan

Filling in TransBasisSet...
Now at state 10000 20000 30000 40000 50000 60000 done.
Time used to fill basis set is (s) 4.600
After fill, number of states is 68958

Store translation basis state and matrix info...
Now at state 0 10000 20000 30000 40000 50000 60000 done.
Store state and matrix info time (s) 58.931

Total Memory (MB) 133.956
Memory Used (MB) 82.439

Matrix dim=68958

Lanczos...
[0] k = (0,0) Iterations
-11.682246053113890
-16.432981896510730
-17.346612988020740
-17.731707980879925
-17.86278816847292
-17.904718571461510
... 
-17.923150810729517
-17.923150810730757
-17.923150810731098
-17.923150810731197

Number of Lanczos iterations 27

Time used for Lanczos iterations (s) 53.035
Total Memory (MB) 133.956
Memory Used (MB) 87.423

Here \( \mathcal{N} = 68,958 \), which takes about 82 MB of memory for basis set and matrix storage, and 88 MB total with Lanczos (so all except 6 MB went into basis set and matrix storage). The time to build the basis set is 4.6 seconds, to store basis set and matrix is 59 s, and to carry out Lanczos is 53 s. The number of Lanczos iterations is 27, the default tolerance \( 10^{-15} \) is used (see Item 6 in Sec. A.2), and the series of iteration results are shown.

Because it takes 59 seconds to store basis state and matrix information, in order to avoid the user staring at an uneventful screen for too long, the state number is print out for every 10000 states. In this case, every 10 seconds, a basis state index number appears on the screen.

The output file is:

```
charming> more result.txt
(7,0)*(0,7) boson N=49 M=6
Matrix dim=68958

[0] k = (0,0) Iterations
-11.68224605313890
-16.432981896510730
-17.346612988020740
-17.731707980879925
-17.862788816847292
-17.904718571461510
...
-17.923150810730757
-17.923150810731098
```
-17.923150810731197

Note that this output file includes all iterations of Lanczos so we know the precision of the eigenvalues. The label Iterations is to remind the user that these are iteration results and are unlike the full diagonalization output where the spectrum is displayed from the lowest energy up. The ground state energy to use is -17.923150810731197.

B.3.2 Ground State Eigenvector

To find ground state eigenvector:

java -mx128M Lattice.Model boson 7 0 0 7 6 k 1 0 0 lan ground > result.txt

This takes twice the time as the case calculating the eigenvalue only, because after computing the eigenvalue, the Lanczos iterations must be repeated to obtain the ground state eigenvector (see Sec. 2.7). The output is

charming> more result.txt
(7,0)*(0,7) boson N=49 M=6
Matrix dim=68958

[0] k = (0,0) Iterations
-11.682246053113890
-16.432981896510730
-17.346612988020740
...
-17.923150810729517
-17.923150810730757
-17.923150810731098
-17.923150810731197

Ground state eigenvector probabilities: in decreasing order
[basis state number] probability
representative state picture
[59637] 3.470706330801482E-4
0 1 2 3 4 5 6
B.3.3 A Few k

To find ground energies for a few k vectors:

java -mx256M Lattice.Model fermion 7 0 0 7 5 sel lan > result.txt

The output is

```
charming> more result.txt
(7,0)*(0,7) fermion N=49 M=5
Matrix dim=15397

[0] k = (0,0) Iterations
   -6.605674487074924
   -10.714719439377053
   -12.302336004059578
   -13.296971612816849
   ...
   -15.437583600843482
   -15.437583600843785
   -15.437583600843887

[1] k = (0,1) Iterations
   -5.892647068514771
   -9.375420649867355
   -10.565673738129851
```
-11.213828202356638 
... 
-14.520662849033693 
-14.520662849034002 
-14.520662849034130 

[2] \( k = (0,2) \) Iterations 
-5.215672507210743 
-8.426250556190880 
-9.767143445094709 
... 
-13.194962190685114 
-13.194962190685330 
-13.194962190685390 

[9] \( k = (3,3) \) Iterations 
-5.151014616665942 
-7.886691320491881 
-8.844531526843687 
... 
-12.514220150338838 
-12.514220150338975 
-12.514220150339028 

For square-boundary lattice, the \texttt{sel} option selects about \( 1/8 \) of the \( k \) vectors (see Item 2c in Sec. A.2). The ground state energy in \( k = (0, 0) \) is -15.437583600843887, in \( (0,1) \) is -14.520662849034130, \..., and in \( (3,3) \) is -12.514220150339028.

To extract lowest energy from the previous result, a case with a few Lanczos \( k \) vector results:

\texttt{charming> java Lattice.ExtractLan < result.txt}
\( (7,0)*(0,7) \) fermion N=49 M=5
Number of \( k \) vectors = 10

The lowest energy is:
-15.437583600843887

Note that the extract program with Lanczos is \texttt{Lattice.ExtractLan} because the Lanczos output files are different in format from the full diagonalization file (where we used \texttt{Lattice.Extract}, see Sec. B.2.2).
To find ground energies for all \( k \) vectors:

```
java -mx256M Lattice.Model fermion 7 0 0 7 5 all lan > result.txt
```

### B.3.4 Reading in a File

To read in a state from \( \mathrm{with} \) to build basis states with hopping,

```
java Lattice.Model boson 4 0 0 7 11 k 1 0 0 lan read < 4_7_11.state
> result.txt
```

As an example, we have a one-hole-on-a-stripe state in \( 4_7_11.\)state:

```
charming> more 4_7_11.state
  0 1 2 3
  6
  5  *
  4  *  *
  3  *  *
  2  *  *
  1  *  *
  0  *  *
```

For a tilted lattice \( (5,1) \times (0,7) \) with a single stripe \( M = 15 \), we use the following input file:

```
charming> more 5_1_0_7_15.state
  0 1 2 3 4
  7
  6  *  *
  5  *  *
  4  *  *  *
  3  *  *
  2  *  *  *
  1  *  *
  0  *
```
B.3.5 Changing Tolerance

As stated in Item 6 of Sec. A.2, the default tolerance for \texttt{lan} is $10^{-15}$. We can change this value by using \texttt{precision $N_P$} to set the tolerance to $10^{-N_P}$. This will reduce the number of Lanczos iterations used, and therefore reduce the running time. We repeat the example in Sec. B.3.1 by setting the tolerance at $10^{-6}$.

\texttt{java -mx128M Lattice.Model boson 7 0 0 7 6 k 1 0 0 lan precision 6}

> result.txt

The output is:

\texttt{charm\textasciitilde> more result.txt}

(7,0)*(0,7) boson N=49 M=6
Matrix dim=68958

\begin{verbatim}
[0] k = (0,0) Iterations
-11.6822461
-16.4329819
-17.3466130
-17.7317080
-17.8627888
-17.9047186
-17.9171416
-17.9211777
-17.9225980
-17.9229917
-17.9230952
-17.9231310
-17.9231441
\end{verbatim}

13 iterations are needed, rather than the 27 iterations for $10^{-15}$ in Sec. B.3.1.

B.4 Lanczos without Matrix Storage: \texttt{lannostore}

The options for this case are the same for \texttt{lan}, except using \texttt{lannostore}, and the matrix information is not stored (it is calculated on the fly). We simply recalculate the example in Sec. B.3.1 with \texttt{lannostore}. 
charmging> java -mx128M Lattice.Model boson 7 0 7 6 k 1 0 0
lannostore > result.txt

(7,0)*(0,7) boson N=49 M=6
trans eval build lannostore

Filling in TransBasisSet...
Now at state 10000 20000 30000 40000 50000 60000 done.
Time used to fill basis set is (s) 4.540
After fill, number of states is 68958

Store translation basis state info...
Now at state 0 10000 20000 30000 40000 50000 60000 done.
Store state time (s) 15.919

Total Memory (MB) 12.947
Memory Used (MB) 7.179

Matrix dim=68958

Lanczos...
[0] k = (0,0) Iterations
-11.68224605
-16.43298190
-17.34661299
-17.73170798
-17.86278882
-17.90471857
-17.91714163
-17.92117767
-17.92269795
-17.92299173
-17.92309519
-17.92313105
-17.92314412
Number of Lanczos iterations 13

Time used for Lanczos iterations (s) 432.221
Total Memory (MB) 21.844
Memory Used (MB) 12.163

Let us compare lannostore with lan (in Sec. B.3.1) for this example calculation.

As explained in Item 6 of Sec. A.2, the tolerance for lannostore is 10^{-7}. Here we
need 13 iterations instead of 27 for lan (tolerance $10^{-15}$). The basis set uses 7 MB of memory, the Lanczos 5 MB, and from the lan output in Sec. B.3.1 we see that the basis set and matrix together use 82 MB which means that storing matrix information takes 75 MB. The time used is 53 seconds with matrix storage (lan) for 27 Lanczos iterations, and 432 seconds without matrix storage (lannostore) for 13 iterations. (These numbers enter into Tables A.2 and A.3.) We see clearly the memory and time tradeoff issues of lan and lannostore considered in Sec. A.4.

**B.5 Arpack: arp $N_A$**

We compute the lowest four energy levels for $7 \times 7$ lattice with $M = 6$ using ARPACK.

```
charming> java -mx128M Lattice.Model boson 7 0 0 7 6 k 1 0 0 arp 4 > result.txt

(7,0)*(0,7) boson N=49 M=6
trans eval build arp

Filling in TransBasisSet...
Now at state 10000 20000 30000 40000 50000 60000 done.
Time used to fill basis set is (s) 4.606
After fill, number of states is 68958

Store translation basis state and matrix info...
Now at state 0 10000 20000 30000 40000 50000 60000 done.
Store state and matrix info time (s) 59.473

Total Memory (MB) 133.956
Memory Used (MB) 82.439

Matrix dim=68958

Arpack...
[0] k = (0,0)
Arpack multiplications... 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38
39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60
61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82
83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103
104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120
121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137
138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154
155 156 157 158 159
Number of iterations = 14

If info=0, info=0, ierr=0, the result is okay.
znauqd: info = 0
znewud: info = 0
znewud: ierr = 0

Time used for Arnoldi iterations (s) 418.103
Total Memory (MB) 133.956
Memory Used (MB) 104.525

The user should look out for the output flags of ARPACK: if info = 0 for both
znauqd and znewud and ierr = 0 for znewud, the subroutines have been completed
successfully. Arpack multiplication numbers are displayed as the calculation pro-
gresses. The output shows the lowest four energies.

charming> more result.txt
(7,0)*(0,7) boson N=49 M=6
Matrix dim=68958

[0] k = (0,0)
-17.923150810731354
-15.335045351952058
-15.252212593786181
-15.06851225098613

The ground state energy matches that from Lanczos iterations in Sec. B.3.1.

B.6 Noninteracting Fermion Energy: Noninter

In our research work, we sometimes need to know the ground state energy of \( M \)
noninteracting particles \( E_0(M) \) (for example, in Sec 7.1 on shell effect, or in Sec. 8.3
for dilute fermions).

The noninteracting ground state energy for $M$ bosons is simple, $-4M$, whereas that for $M$ fermions on an arbitrary lattice is not hard but requires a little computation. In momentum space, we sort $\mathcal{E}(k)$ (energy dispersion, Eq. 3.14) for all $N k$ vectors in increasing order, and fill the lowest $M$ states (for spinless fermions).

The following simple program computes the ground state energy for up to $N_M$ spinless fermions on a $(R_{1x}, R_{1y}) \times (R_{2x}, R_{2y})$ lattice:

```java
java Lattice.Noninter R_{1x} R_{1y} R_{2x} R_{2y} N_M
```

As an example, we calculate for the $5 \times 8$ lattice, with up to 7 fermions:

```
charming> java Lattice.Noninter 5 0 0 8 7
(5,0)*(0,8) N=40
Noninteracting fermion energies
  1  -4.0
  2 -7.414213562373095
  3 -10.82842712474619
  4 -13.446461113496085
  5 -16.064495102245978
  6 -18.096742653368967
  7 -20.128990204491956
```

This means that the noninteracting ground state fermion energy is -4.0 for one fermion, -7.4142 for two fermions, and so on. These data enter into Table 7.1 in Sec. 7.1 on the fermion shell effect.
Appendix C

Diagonalization Program Files

In an object-oriented programming language such as Java, a class is a collection of data and methods that operate on that data. In Java, the classes are organized in packages, and they can have subclasses. The following is a list of the packages and classes for our diagonalization program described in Chapter 2, Sec. 5.2, and Appendices A, B.

1. Package Lattice

This contains basis set and Hamiltonian matrix construction, and the Lanczos method. The following are the classes in this package.

(a) Main classes:

i. Grid

   Represent the lattice

ii. BasisSet

   Build basis set without translation symmetry

iii. TransBasisSet

   Build basis set with translation symmetry
iv. **HamMatrix**

Build Hamiltonian matrix using `BasisSet` or `TransBasisSet`, Lanczos subroutines, and matrix diagonalization calling LAPACK, Lanczos, and ARPACK.

v. **Model**

Dispatch command line options to appropriate subroutines.

(b) Supporting classes:

i. **Array**

Array arithmetics: searching elements in an array, sorting an array, merging arrays, etc.

ii. **Vec**

Vector arithmetics: vector norm, adding two vectors, producing a random vector, etc.

iii. **Extract**

Extract ground state energy from full diagonalization results of a series of k vectors.

iv. **ExtractLan**

Extract ground state energy from Lanczos diagonalization results of a series of k vectors.

v. **Noninter**

Calculate ground state energy for noninteracting spinless fermions.

2. **Package Matrix**

Java matrix classes, and interfaces to LAPACK (Fortran) diagonalization subroutines.
(a) **GeneralMatrix**: General real matrix.

(b) **ComplexMatrix**: General complex matrix.

(c) **SymmetricMatrix**: Real symmetric matrix.

(d) **HermitianMatrix**: Complex Hermitian matrix.

(e) **LapackSymmetricMatrix**

   Interface to LAPACK symmetric matrix diagonalization subroutine *dspev*.

(f) **LapackHermitianMatrix**

   Interface to LAPACK Hermitian matrix diagonalization subroutine *zhpev*.

3. Package *Arpack*

   Class **ArpackHermitianMatrix**: interface to ARPACK Hermitian matrix diagonalization subroutines *znaupd* and *zneupd*. 
Appendix D

Diagonalization Data

In this appendix, we collect together important diagonalization data used in this thesis work. These data are the raw materials from which the tables and figures in this thesis are made. First, we list the notations used in the tables; second, we describe the relations of the tables in this chapter to results in other chapters of the thesis; then, we show the data.

\[ M \] \quad \text{number of particles}

\[ k \] \quad \text{reciprocal lattice vector from diagonalization}

\[ N \] \quad \text{matrix dimensionality for one } k \text{ vector}

\[ E^b \] \quad \text{boson energy from diagonalization}

\[ E^f \] \quad \text{fermion energy from diagonalization}

\[ E^f_0 \] \quad \text{noninteracting fermion energy} \quad (E^b_0 = -4M \text{ for bosons})

\[ E_{\text{stripe}} \] \quad \text{ground state energy of one stripe}

\[ E_{\text{hole}} \] \quad \text{ground state energy of one hole with a stripe}

\[ E_{2\text{holes}} \] \quad \text{ground state energy of two holes with a stripe}

\[ E_{2\text{stripes}} \] \quad \text{ground state energy of two stripes}

\[ E_{3\text{stripes}} \] \quad \text{ground state energy of three stripes}
Table D.1: Relations of the tables in this appendix to results in other chapters of the thesis.

<table>
<thead>
<tr>
<th>Table Number</th>
<th>Short Description</th>
<th>Figure Numbers in Thesis</th>
</tr>
</thead>
<tbody>
<tr>
<td>D.2, D.3, D.4, D.5</td>
<td>$M = 2, 3, 4, 5$</td>
<td>2.8, 3.6, 3.7, 3.8, 3.9, 8.4, 8.8</td>
</tr>
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<td>1 hole, $L_y$</td>
<td>5.8, 5.9</td>
</tr>
<tr>
<td>D.8</td>
<td>1 hole, $L_x$</td>
<td>5.11</td>
</tr>
<tr>
<td>D.9, D.10</td>
<td>2 holes, $L_y$</td>
<td>5.12, 5.13</td>
</tr>
<tr>
<td>D.11</td>
<td>2 holes, $L_x$</td>
<td>5.14</td>
</tr>
<tr>
<td>D.12, D.13</td>
<td>2 stripes</td>
<td>6.5, 6.6</td>
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<td>D.14</td>
<td>3 stripes</td>
<td>6.8</td>
</tr>
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<td>D.15-D.24</td>
<td>all fillings</td>
<td>6.11, 8.1, 8.2, 8.3, 8.4, 8.5, 8.7, 8.8</td>
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</table>
Table D.2: Two-particle $M = 2$ ground state energies on a $L \times L$ lattice. $k = (0, 0)$ for bosons and $k = (0, 1)$ for fermions.

<table>
<thead>
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<th>$N$</th>
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<th>$E^f$</th>
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</table>
Table D.3: Three-particle $M = 3$ ground state energies on a $L \times L$ lattice. $k = (0, 0)$ for bosons and $k = (1, 1)$ for fermions.

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</table>
Table D.4: Four-particle $M = 4$ ground state energies on a $L \times L$ lattice. $k = (0,0)$ for bosons and $k = (0,1)$ for fermions. The results for $L = 18,19,20$ have fewer significant digits because they are obtained from Lanczos without storing matrix information, using tolerance $10^{-7}$. Time and memory information for these calculations is in Tables A.4 and A.5.

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<tr>
<th>$L$</th>
<th>$N$</th>
<th>$E^b$</th>
<th>$E^f$</th>
<th>$E_0^f$</th>
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</table>
Table D.5: Five-particle $M = 5$ ground state energies on a $L \times L$ lattice. $\mathbf{k} = (0,0)$ for bosons and $\mathbf{k} = (0,0)$ for fermions.

<table>
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Table D.6: One-hole-with-a-stripe ground state energy for a $L_x \times L_y$ lattice, with the number of particles $M = L_x(L_y - 1)/2 - 1$. $\mathcal{N}$ is the number of Bloch basis states constructed by applying hopping to a starting state of one hole on the stripe. The increment of $\mathcal{N}$ is constant for a given $L_x$. This table is for $L_x = 4, 6, 8, 10$ and Table D.7 is for $L_x = 12, 14$.

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Table D.8: One-hole-with-a-stripe energy $E_{\text{hole}}$ on $(L_x, b) \times (0,7)$ lattices with $M = 3L_x - 1$ and $b = 0, 1, 2$. 

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<th>$E_{\text{hole}}$</th>
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Table D.9: Two-holes-with-a-stripe boson and fermion energy $E^{b,f}_{2\text{holes}}$ for $L_x \times L_y$ lattices, with number of particles $M = L_x(L_y - 1)/2 - 2$. This table is for $L_x = 4, 6$ and Table D.10 is for $L_x = 8, 10$.

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Table D.10: Continuation of Table D.9, for $L_x = 8, 10$.

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Table D.11: Two-holes-with-a-stripe energy $E_{2\text{holes}}^{bf}$ on $(L_x, b) \times (0, 7)$ lattices with $M = 3L_x - 2$ and $b = 0, 1, 2$.

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Table D.12: Two-stripe ground state energy $E_{2\text{stripes}}(L_x, L_y)$ with $L_x = 4, 6$. For a $L_x \times L_y$ lattice, the number of particles is $M = L_x(L_y - 2)/2$. $\mathcal{N}$ is the number of Bloch basis states constructed by applying hopping to a starting state with two merged stripes. $\mathcal{N}$ increases linearly.

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<th>$L_y$</th>
<th>$M$</th>
<th>$\mathcal{N}$</th>
<th>$E_{2\text{stripes}}$</th>
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Table D.13: Continuation of Table D.12 with $L_x = 8$.

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Table D.14: Three-stripe ground state energy with stripe length $L_x = 4$. For a $L_x \times L_y$ lattice, the number of particles is $M = L_x(L_y - 3)/2$.

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Table D.15: \((5, 0) \times (0, 5)\) lattice, ground state boson and fermion, and noninteracting fermion energies for all \(M\) with nonzero energy.

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Table D.16: \((5, -1) \times (1, 5)\).

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### Table D.18: \((5, 0) \times (0, 6)\).

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Table D.20: $(5, 0) \times (0, 7)$. 
### Table D.21: $(6, 0) \times (0, 6)$

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### Table D.22: $(6, -1) \times (1, 6)$

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Appendix E

Real Space T-Matrix

This appendix shows an alternative definition of the t-matrix in real space that runs in parallel to the momentum space t-matrix in Chapter 4.

E.1 Derivation

The derivation here follows the conclusion of Sec. 4.3.3.

When $q \in Q_I$, $E - \mathcal{E}(q) - \mathcal{E}(P - q) = E_0$, we have from Eq. 4.8,

$$(E - E_0)\mathcal{g}(q) = \frac{1}{N} \sum_{r'} e^{iqr'}V(r')\tilde{g}(r').$$  \hspace{1cm} (E.1)

Multiplying this equation by $e^{-iqr}$ and summing over $q \in Q_I$, we get,

$$(E - E_0) \sum_{q \in Q_I} e^{-iqr} \mathcal{g}(q) = \sum_{r'} \left[ \frac{1}{N} \sum_{q \in Q_I} e^{iqr'} \right] V(r')\tilde{g}(r').$$  \hspace{1cm} (E.2)

Let us define,

$$G^I(E_0, P; r, r') = \frac{1}{N} \sum_{q \in Q_I} e^{iqr'},$$  \hspace{1cm} (E.3)

then using the definition for $\tilde{g}^I$ (Eq. 4.12) we have,

$$(E - E_0)\tilde{g}^I(r) = \sum_{r'} G^I(E_0, P; r, r')V(r')\tilde{g}(r').$$  \hspace{1cm} (E.4)
We proceed by restricting to the nearest-neighbor repulsion potential (3.13). Then Eq. E.4 becomes,

\[
(E - E_0)\tilde{g}^I(r) = \sum_j G^I(r, R_j) V \tilde{g}(R_j),
\]

(E.5)

where we have shortened the notation \(G^I(E_0, P; r, R_j)\) to \(G^I(r, R_j)\). Next, we plug in Eq. E.5 the result of Eq. 4.19, which is

\[
\phi = (I - \mathcal{G}^H(E, P)V)^{-1} \phi^I
\]

(E.6)

where \(\phi_j = \tilde{g}(R_j)\). We get a set of equations on \(\tilde{g}^I\) only,

\[
(E - E_0)\tilde{g}^I(r) = \sum_{ji} G^I(r, R_j) \left(V(I - \mathcal{G}^H(E, P)V)^{-1}\right)_{ji} \tilde{g}^I(R_i).
\]

(E.7)

Restricting \(r = R_i\), this becomes a closed set of four equations, which can be written in a matrix form,

\[
(E - E_0)\phi^I = \mathcal{G}^I \left(V(I - \mathcal{G}^H(E, P)V)^{-1}\right) \phi^I,
\]

(E.8)

where we have used the definition for \(4 \times 4\) matrix \(\mathcal{G}^H\) in Eq. 4.17 and defined

\[
\mathcal{G}^I_{ij} = G^I(R_i, R_j).
\]

(E.9)

Eq. E.8 is an equation on the exact energy, because it says that the matrix on the right hand side of the equation has an eigenvalue \(E - E_0\) with eigenvector \(\phi^I\). Finally, we use the fact \(V = +\infty\) and get,

\[
E = E_0 + \text{Eigenvalue} \left( -\mathcal{G}^I \left(\mathcal{G}^H(E)\right)^{-1}\right),
\]

(E.10)

where we have dropped the dependence on \(P\) because we always calculate \(E\) for a \(P\) specified at the beginning.

Eq. E.10 is basically of the form of Eq. 4.24, the t-matrix equation in momentum space, except we here work in real space \(R_j\). We will call the matrix \(-\mathcal{G}^I(\mathcal{G}^H(E))^{-1}\)
the real space T-matrix. Note from the definitions (E.9, 4.17) both \( G^I(E) \) and \( G^{II}(E) \) are \( 4 \times 4 \) Hermitian, \( G^{II}(E)^{-1} \) is then also Hermitian, but the product \( -G^I(E)G^{II}(E)^{-1} \) is not necessarily Hermitian. We will consider this problem later in this appendix. Note also how the potential cancels from the numerator and the denominator, producing a well-defined t-matrix even for an infinite potential \( V \).

## E.2 Summary of Solution Procedures

This section is the real space version of the momentum space procedure in Sec. 4.3.7.

We can trace back the equations to get the following procedures for solving the two-particle problem using the real space t-matrix.

1. Given \( E_0 \) and \( P \), form \( Q_I \) and \( Q_{II} \).

2. Form \( G^I_{ij} \) and the matrix function \( G^{II}_{ij}(E) \).

3. Obtain \( E \) from Eq. E.10.

4. Obtain the corresponding eigenvector \( \phi^I \).

5. Using Eq. 4.18, \( V \phi = - (G^{II}(E))^{-1} \phi^I \).

6. Using Eq. E.5 to get,

\[
g^I(r) = \frac{1}{E - E_0} \sum_j G^I(r, R_j)(V \tilde{g}(R_j)).
\]

7. Using Eq. 4.15 to get,

\[
\tilde{g}(r) = \tilde{g}^I(r) + \sum_j G^{II}(E, P; r, R_j)(V \tilde{g}(R_j)),
\]

8. Finally, using Fourier transform (3.36) to get \( g(q) \).
E.3 Solving For Energy Using $-G^I G^{II}(E)^{-1}$

This section runs in parallel to Sec. 4.4 using the momentum space t-matrix.

To solve for energy $E$ in Eq. E.10, we plot $f(E) = E_0 + \text{Eigenvalues} \left( -G^I G^{II}(E)^{-1} \right)$ (for each $E$ plot all four eigenvalues) along with the line $y = E$. Their intersections are the desired energies.

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure1}
\caption{$f(E) = E_0 + \text{Eigenvalues} \left( -G^I G^{II}(E)^{-1} \right)$ vs $E$ for $10 \times 11$ lattice with $P = (0, 0)$ and $E_0 = -8.0$ (i.e., $E_0 = \mathcal{E}(0) + \mathcal{E}(0)$.) Three of the four eigenvalues of $-G^I G^{II}(E)^{-1}$ are zero. This plot is the real space version of the momentum space plot in Fig. 4.3.}
\end{figure}
Fig. E.1 is \( f(E) \) vs \( E \) for the \( 10 \times 11 \) lattice with \( \mathbf{P} = (0,0) \) and the noninteracting energy \( E_0 = -8.0 = \mathcal{E}(0) + \mathcal{E}(0) \). This is the real space t-matrix version of Fig. 4.3. We see in Fig. E.1 that out of the four eigenvalues of the matrix \(-\mathcal{G}^I(\mathcal{G}^{II}(E))^{-1} \) for any \( E \), three of them are zero, which form the horizontal line in the graph \( y = E_0 \).

This is because the matrix \( \mathcal{G}^I \) (E.3) when \( Q_I = \{(0,0)\} \), is a matrix with all entries equal to \( 1/N \). It therefore has three zero eigenvalues. Note that in general if a matrix \( A \) has a null vector \( q \), then \( AB^{-1} \) has a null vector \( Bq \). Because \( \mathcal{G}^I \) has three zero eigenvalues, \(-\mathcal{G}^I(\mathcal{G}^{II}(E))^{-1} \) also have three zero eigenvalues.

Another point about these zero eigenvalues is that looking at the t-matrix equation, Eq. E.10, we might have thought that we can simplify it by computing the eigenvalues of \(-\mathcal{G}^{II}(E)(\mathcal{G}^I)^{-1} \) and set them equal to \( 1/(E - E_0) \). This simplifies the computation because \( \mathcal{G}^I \) does not depend on \( E \), so we can do matrix inversion once and for all, instead of inverting \( \mathcal{G}^{II}(E) \) for each \( E \). Here we see that \( \mathcal{G}^I \) is singular, so this method does not work.

In Fig. E.2 we plot for the noninteracting energy \( E_0 = \mathcal{E}(0,1) + \mathcal{E}(0,-1) = -7.365 \). Here \( \mathcal{G}^I \) has two zero eigenvalues corresponding to the horizontal line \( y = E_0 \).

In Fig. E.3 we plot \( f(E) \) for \( E_0 = \mathcal{E}(1,-1) + \mathcal{E}(-1,1) = \mathcal{E}(1,1) + \mathcal{E}(-1,-1) = -6.601 \). The two boson intersections closest to \( E_0 \) are \(-6.022 \) and \(-6.601 \). Note that the latter is also a noninteracting energy and it is the intersection of the horizontal line \( E = E_0 \) with \( y = E \). It is included in our derivation (see the discussion before Eq. 4.10) because this noninteracting energy comes from the four vectors, \((1,-1)(-1,1)(1,1)(-1,-1)\), none is in \( Q_{II} \).

The reason that all four eigenvalues of the t-matrix are meaningful in Fig. E.3 is that we have four vectors in the set \( Q_I \) and therefore expect to have four meaningful
Figure E.2: $f(E)$ vs $E$ for $10 \times 11$ lattice with $\mathbf{P} = (0,0)$ and $E_0 = -7.365$ (i.e., $E_0 = \mathcal{E}(0,1) + \mathcal{E}(0,-1)$). Here two of the four eigenvalues are zero. In the inset, the line $y = E$ intersects the fermion curve at $-7.311$ and the boson curve at $-7.299$. This plot is the real space version of the momentum space plot in Fig. 4.4.
Figure E.3: $f(E)$ vs $E$ for $10 \times 11$ lattice with $P = (0, 0)$ and $E_0 = -6.601$ (i.e., $E_0 = E(1, -1) + E(-1, 1) = E(1, 1) + E(-1, -1)$.) Here one eigenvalue is zero. This plot is the real space version of the momentum space plots Figs. 4.5 and 4.6.
eigenvalues to correspond to four basis states. This highlights the problem of the real-space formulation in Eq. E.10. The matrices $G^I$ and $G^{II}(E)$ have fixed dimensionality (four) that does not correspond to the dimensionality of $Q^I$. The situation in Fig. E.1 calls for a one-dimensional matrix, that in Fig. E.2 a two-dimensional matrix, and that in Fig. E.3 a four-dimensional matrix. Eq. E.10 works because the matrix $G^I$ has the right number of zero eigenvalues that cuts down the number of meaningful eigenvalues, but the symmetry properties are buried in the matrix product $-G^I(G^{II}(E))^{-1}$. We would like a better formulation of the t-matrix to employ the symmetries, and this is the momentum space formulation in Chapter 4.

On the other hand, the real space t-matrix $-G^I(G^{II}(E))^{-1}$, because it is always $4 \times 4$ may be computationally easier to handle if $N_1$ is very large (so the momentum space t-matrix is $N_1 \times N_1$). Following Feynman’s doctrine, “there are always more than one way to skin a cat,” we include this real space formulation here. However, we have not used the real space t-matrix elsewhere in this thesis work.
Appendix F

Few-Fermion T-Matrix Program

In this appendix, we describe the C++ program that we wrote to calculate the total energy of a few fermions, using the t-matrix, from a given noninteracting state, specified by $M$ reciprocal lattice vectors. Our computer program is the implementation of the procedures summarized in Sec. 7.6, for the many-fermion t-matrix. In this appendix, we will show calculations for the examples included in Sec. 7.3 and 7.4.

F.1 General

There are two steps. First, to find the lowest $N_N$ levels of $M$ noninteracting spinless fermions on the $L_x \times L_y$ lattice with total momentum $\mathbf{P} = (P_x, P_y)$, we use the following command line:

```
noninteracting L_x L_y M P_x P_y N_N
```

Second, to use the t-matrix to calculate the total energy of $M$ fermions on a $L_x \times L_y$ lattice.

---

$^1$Note: The program noninteracting is different from the program Lattice.Noninter described in Sec. B.6. The Java program Lattice.Noninter is used to find the noninteracting ground state energy for different $M$ and all $\mathbf{P}$. The C++ program noninteracting is used to find the lowest few noninteracting energies and states for a specified $M$ and $\mathbf{P}$.
lattice with the noninteracting fermions at $k_1 = (k_{1x}, k_{1y}), k_2 = (k_{2x}, k_{2y}), \ldots, k_M = (k_{Mx}, k_{My})$, we use the following command line:

$$\texttt{tmat } L_x \ L_y \ M \ k_{1x} \ k_{1y} \ k_{2x} \ k_{2y} \ \ldots \ \ k_{Mx} \ k_{My}$$

Currently both noninteracting and tmat apply to rectangular-boundary lattices $L_x \times L_y$ only. And the program tmat can only handle a nondegenerate noninteracting state, that is, no other states can have the same total energy and total momentum. See Sec. 7.5 for detail.

### F.2 Example $M = 2$

As we discussed in Chapter 4, the t-matrix for two particles is an exact formulation of the Schrodinger equation, and for fermions, a few iterations starting from the noninteracting energy converge to the exact energy. Let us as an example work on the $10 \times 11$ lattice with $P = (0,0)$. The results have appeared in Table 4.2 and Fig. 4.8.

#### F.2.1 Noninteracting Spectrum

To obtain the lowest 5 noninteracting energy levels of two spinless fermions $M = 2$ on the $10 \times 11$ lattice, we run:

```
noninteracting 10 11 2 0 0 5
```

And we get:

```
Lx=10, Ly=11, M=2, Px=0, Py=0, NN=5
E0 = -7.365014131324725
  0 1 0 10
E0 = -7.236067977499790
```
1 0 9 0
E0 = -6.601082108824515
1 1 9 10
1 10 9 1
E0 = -5.661660052007545
0 2 0 9
E0 = -5.236067977499790
2 0 8 0

This says that the lowest level has energy -7.365014131324725, corresponding to the two-fermion noninteracting state with momentum vectors \((0,1)\) and \((0,10)\) (the latter is equivalent to \((0,-1)\)). The first excited level has energy -7.236067977499790, corresponding to \((1,0)\) and \((9,0)\). The next excited level is two fold degenerate, with \((1,1)(-1,-1)\) and \((1,-1)(-1,1)\), etc.

**F.2.2 T-Matrix for Ground State**

For t-matrix calculation of the ground state \((0,1)(0,-1)\), we use:

```
tmat 10 11 2 0 1 0 -1
```

And we get

Lx=10, Ly=11, M=2, Px=0, Py=0

Kvecs:

\([1]\) = \((0,1)\)
\([2]\) = \((0,-1)\)

noninteracting energy E0=-7.365014131324725
Pair 1
E0=-7.365014131324725, Px=0, Py=0
Q1: \((0,1)(0,-1)\)
Q2: \([108]\)
E0=-7.365014130324725
E1 = -7.310598893175414
E2 = -7.311807221261775
E3 = -7.311779768591201
E4 = -7.311780391972222
E5 = -7.311780377816637
E6 = -7.311780378138079
E7 = -7.311780378130780
E8 = -7.311780378130945

== T1 = 0.053233753193784

Lx=10, Ly=11, M=2, Px=0, Py=0
noninteracting energy E0 = -7.365014131324725
interacting energy E = -7.311780378130941

The output says that $k_1 = (0, 1)$ and $k_2 = (0, -1)$, and there is only one pair.
The noninteracting energy $E_0 = -7.365014131324725$. The initial $E$ for the t-matrix
iteration is $E_0 + \delta$ with $\delta = 10^{-10}$ to avoid the zero denominator in the degenerate
state case (see Sec. F.3.4)\footnote{The program \texttt{tmat} is not designed to study the degenerate case, as explained in Sec. 7.5. $\delta$ is
used to avoid program freezing, and should not matter in a nondegenerate calculation.}. The set $Q_I = \{(0, 1), (0, -1)\}$ and the number of
elements in $\tilde{Q}_{II}$ is $N_2 = 108$ (tilde denotes exclusion due to the presence of other
particles). (For $10 \times 11$ lattice, with two $k$ vectors in $Q_I$, the rest is in $Q_{II}$.)

Here the first t-matrix iteration gives $E_1 = -7.310598893175414$, the fifth gives
$E_5 = -7.311780377816637$, and the final result is $E = -7.311780378130945$. (Ta-
ble 4.2 is obtained in this fashion.) The tolerance for iterations in \texttt{tmat} is set at
$10^{-15}$, and the result from diagonalization is -7.311780378130949.

We can use the same procedure for the nondegenerate excited states. The calcu-
lation for the degenerate states is not included in the program \texttt{tmat}. 
F.3  Example $M = 3$

We study the problem of three fermions $M = 3$ on a $8 \times 9$ lattice, with total momentum $\mathbf{P} = (0, 0)$. This is the problem that we investigated in Sec. 7.3. Table 7.3 contains the lowest five noninteracting states; Table 7.4 shows the $t$-matrix calculation for the ground state; Table 7.5 and Fig. 7.4, show $t$-matrix results for the ground state and two nondegenerate excited states.

F.3.1  Noninteracting Spectrum

To compute the 5 lowest noninteracting energy levels, we run:

```
noninteracting 8 9 3 0 0 5
```

And the output we obtain is:

- $E_0 = -11.064177772475912$
  0 0 0 1 0 8

- $E_0 = -10.828427124746190$
  0 0 1 0 7 0

- $E_0 = -9.892604897222101$
  0 0 1 1 7 8
  0 0 1 8 7 1
  0 1 1 0 7 8
  0 1 1 8 7 0
  0 8 1 0 7 1
  0 8 1 1 7 0

- $E_0 = -8.694592710667720$
  0 0 0 2 0 7

- $E_0 = -8.239901252555962$
  0 1 1 1 7 7
  0 1 1 7 7 1
Here, the lowest noninteracting level has energy $-11.064177772475912$, is non-degenerate, with $k_1 = (0,0)$, $k_2 = (0,1)$, and $k_3 = (0,8)$. The first excited level has energy $-10.82847124746190$, is also nondegenerate, with $k_1 = (0,0)$, $k_2 = (1,0)$, and $k_3 = (7,0)$. The third level has energy $-9.892604897222101$ and is six-fold degenerate, and so on. Using this output, Table 7.3 for noninteracting levels is obtained.

### F.3.2 T-Matrix for Ground State

To compute the total energy for the ground state $(0,0)(0,1)(0,-1)$, where $(0,-1)$ is equivalent to $(0,8)$, we use

```
tmat 8 9 3 0 0 0 1 0 -1
```

The output we get is:

```
Lx=8, Ly=9, M=3, Px=0, Py=0

Kvecs:
[1] = (0,0)
[2] = (0,1)
[3] = (0,-1)

noninteracting energy E0=-11.064177772475912
Pair 1
E0=-7.532088886237956, Px=0, Py=1
Q1: (0,0)(0,1)
Q2: [68]
E0=-7.532088885237956
E1=-7.490139670820531
E2=-7.490564694734343
```
E3= -7.490560359272070
E4= -7.490560403492911
E5= -7.490560403041867
E6= -7.490560403046468
E7= -7.490560403046421

>>> T1 = 0.041528483191535

Pair 2
E0= -7.532088886237956, Px=0, Py=-1
Q1: (0,0) (0,-1)
Q2: [68]
E0= -7.53208885237956
E1= -7.490139670820532
E2= -7.490564694734343
E3= -7.490560359272070
E4= -7.490560403492911
E5= -7.490560403041867
E6= -7.490560403046468
E7= -7.490560403046421

>>> T1 = 0.041528483191535

Pair 3
E0= -7.064177772475912, Px=0, Py=0
Q1: (0,1) (0,-1)
Q2: [69]
E0= -7.064177771475912
E1= -6.945493191858832
E2= -6.950469451355985
E3= -6.950254877309598
E4= -6.950264118087738
E5= -6.950263720105913
E6= -6.950263737246154
E7= -6.950263736507960
E8= -6.950263736539753
E9= -6.950263736538384
E10= -6.950263736538442

>>> T1 = 0.113914035937472

Lx=8, Ly=9, M=3, Px=0, Py=0
noninteracting energy E0= -11.064177772475912
interacting energy E= -10.867206770155370
This output is the source for Table 7.4. Using the notations there, we get \( k_1 = (0, 0), k_2 = (0, 1), \) and \( k_3 = (0, -1). \) For the interaction between \( k_1 \) and \( k_2, \) we have \( E_0^{ij} = -7.532088886237956, \) \( P_{12} = (0, 1), \) \( Q_t^{ij} = \{(0, 0), (0, 1)\}, \) and the number of elements in \( Q_t^{ij} \) is \( N_2^{ij} = 68 \) (4 momentum vectors are excluded from a total of 72, see Table 7.4). The t-matrix iterations are \( E_{n+1} = E_0^{ij} + \tilde{T}^{ij}(E_n). \) For \( k_1 \) and \( k_2, \) we have \( E_1 = -7.490139670820531, ..., E_7 = -7.490560403046421. \) As mentioned above, the tolerance is set at \( Tol = 10^{-15}, \) i.e., when \( |E_{m+1} - E_m| < Tol, \) we stop, and \( \tilde{T}^{ij} = T(E_m). \) Here \( \tilde{T}^{12} = 0.041528483191535, \) \( \tilde{T}^{13} = 0.041528483191535 \) and \( \tilde{T}^{23} = 0.113914035937472. \) The total noninteracting energy is \( E_0 = -11.064177772475912 \) and the final energy from t-matrix calculations is \( E_{tm} = E_0 + \tilde{T}^{12} + \tilde{T}^{13} + \tilde{T}^{23} = -10.867206770155370. \) Table 7.4 is therefore obtained.

### F.3.3 Nondegenerate Excited State

For the first excited state, we run:

```
tmat 8 9 3 0 0 1 0 -1 0
```

The output looks like the one in Sec. F.3.2, and it ends with the following three lines:

```
Lx=8, Ly=9, M=3, Px=0, Py=0
noninteracting energy E0=-10.828427124746190
interacting energy E=-10.604677479761003
```

These results go into Table 7.5.
F.3.4 Degenerate States

The program tmat has not been designed to treat degenerate noninteracting states (see the discussion in Sec. 7.5). Running the following

```
tmat 8 9 3 0 0 1 1 7 8
```
creates an error message

T doesn’t converge.

F.4 Example $M = 5$

Now let us treat briefly the five-fermion problem studied in Table 7.6. For the lowest three noninteracting energy levels on $8 \times 9$ lattice with $M = 5$, we run:

```
noninteracting 8 9 5 0 0 3
```

And we get:

Lx=8, Ly=9, M=5, Px=0, Py=0, NN=3

```
E0 = -17.892604897222103
0 0 0 1 0 8 1 0 7 0
E0 = -16.956782669698015
0 0 0 1 0 8 1 1 7 8
0 0 0 1 0 8 1 8 7 1
E0 = -16.721032021968291
0 0 1 0 1 1 7 0 7 8
0 0 1 0 1 8 7 0 7 1
```

For t-matrix calculation of ground state energy, we run the following:

```
tmat 8 9 5 0 0 1 0 8 1 0 7 0
```

This gives a lot of output, but the most crucial result is the last three lines:
Lx=8, Ly=9, M=5, Px=0, Py=0
noninteracting energy E0=-17.892604897222103
interacting energy E=-17.13533040191213

This is the final result of Table 7.6.

F.5 Description of Files

1. Main classes

   (a) Lattice

       Representation of the lattice, energy dispersion relation, lattice Green
       functions.

   (b) Kvecs

       Represent a set of noninteracting k vectors. Find lowest noninteracting
       energies and states.

   (c) Level

       The heart of the t-matrix calculation. One noninteracting energy pair,
       Q_I and Q_{II} for t-matrix calculations, matrix inversion for G^{II}, Fourier
       transform to get \hat{T}, diagonalize \hat{T}.

   (d) Levels

       Take in a set of noninteracting k vectors, organize them into pairs, and
       use Level to compute energy for each pair.

   (e) tmat

       Take in user input, form Lattice, Kvecs, and use Levels to compute
       energy.
2. Supporting classes

(a) General

General functions, e.g., complex number operations.

(b) Array

Array related functions, e.g., memory allocation and search.

(c) GeneralMatrix, ComplexMatrix, HermitianMatrix

Matrix subroutines, including inversion and diagonalization using LAPACK.