Few- and Many-body Physics of Dipoles in Ion Traps and Optical Lattice Simulators

by

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BASc, University of Toronto (2008)

Submitted to the Department of Physics in partial fulfillment of the requirements for the degree of Doctor of Philosophy at the MASSACHUSETTS INSTITUTE OF TECHNOLOGY

February 2014

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Abstract

The presence of strong interactions in quantum many-body systems makes the analytical treatment of such systems very difficult. In this thesis we explore two possible proposals for simulating strongly correlated, quantum many-body systems: quantum simulations using trapped-ion quantum computers, and optical lattice simulators.

In the first part of the thesis we describe the recent advances in Quantum Information Processing. In particular, we focus on the trapped-ion quantum computer. One of the main experimental roadblocks for this architecture is the “anomalous heating”. This refers to the motional heating of the ion after being cooled to its ground state. In this thesis we present the first ab-initio and microscopic model for this noise. This model attributes the noise to fluctuating dipoles formed by adsorbates bound on the trap surface.

The second part of the thesis studies three different lattice boson systems. First, we study the Bose-Hubbard model for hard-core bosons, interacting via dipole-dipole interactions. The resulting extended Bose-Hubbard model can be experimentally realized by polar molecules, Rydberg atoms, or magnetic dipoles in optical lattices. We use quantum Monte Carlo simulations, using the two-worm algorithm to study the ground-state phase diagram of dipolar, hard-core bosons, trapped in a bilayer geometry. Each layer is a quasi two-dimensional lattice, the dipole are aligned perpendicular to the layer, and inter-layer hopping is suppressed. We present zero- and finite-temperature results.

Next we use a novel multiworm algorithm, along with bosonization, to study the ground-state phase diagram of bosons trapped in a stack of one-dimensional tubes. We study two different inter-particle interactions. First, we consider nearest-neighbor attractive interactions between the layers, and set the intra-layer interactions to zero. Next we study dipolar bosons with their dipole moments aligned perpendicular to the tube axis. Inter-layer tunneling is suppressed in both cases.

Finally, we explore the possibility of using few-body phenomena to create exotic quantum many-body systems. We present a novel scheme to realize a tunable, on-site, three-body interaction. We study the resulting extended Bose-Hubbard model
with a three-body on-site term using the Gutzwiller mean-field method, as well as quantum Monte Carlo simulations using the Worm algorithm.

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Acknowledgments

Throughout my PhD I have received help and guidance from many people. First, I would like to thank Hossein R. Sadeghpour for his continuing support, allowing me to join Institute for Theoretical Atomic and Molecular Physics (ITAMP), and being the catalyst for many projects and collaborations. I would like to thank Martin Zwierlein, for being an excellent advisor, and an amazing person. He has supported me through my PhD studies, and has helped me deal with many challenges.

My first project at ITAMP stemmed from discussions with Hossein and Peter Rabl. I would like to thank Peter for teaching me how to approach a complicated problem, and for patiently correcting the many mistakes I made along the way.

I owe a great deal to Barbara Capogrosso-Sansone. In addition to being a wonderful friend and mentor, she has taught me everything I know about quantum Monte Carlo simulations, and has spent many hours helping me debug codes, both in person and over Skype. Her meticulousness and enthusiasm have motivated me to be a better, and more careful scientist, and to try to understand the details of each problem.

I would like to thank Seth Rittenhouse for being a caring friend, and patiently teaching me about few-body phenomena. I received a great deal of encouragement from Seth throughout my PhD, and even gained some intuition about few-body physics.

Throughout the past year Misha Lemeshko has been a great friend and collaborator. He has helped me edit various fellowship applications, improve my talks, and has listened to me complain about almost everything. I would like to thank him for all of the above and his patience with me.

I would like to thank all my scientific collaborators. In particular, Dorte Blume, Anatoly Kuklov, Gunes Söyler, and Javier von Stecher have generously spent many hours teaching me new techniques and concepts. They have provided the guidance that has allowed me to complete a variety of projects.

This thesis would not have been possible without the training and education I
received prior to entering MIT. I would like to thank Young-June Kim at University of Toronto, for allowing me to work in his lab. His encouragement led me to study physics, as opposed to electrical engineering. My interest in quantum optics is largely due to working with Daniel James. He is an insightful and caring supervisor who has had a great impact on my life. I cannot thank him enough.

I have gotten to know many great people at MIT and ITAMP. I would like to thank Amanda Zangari, William Leight, Greg Little, Alexander Leder, Ariel Sommer, Jason Kovacs, Jeremy Lopez, and Hendrik Weimer for being great friends and playing board games with me. Alexander and Amanda, along with Benjamin Kaduk, and David Wilson have been great housemates as well. I would like to thank my friends Tout Wang, Jiayong Li, Kazuhiro Terao, Keigo Arai, Albert Chang, Elena Kuznetsova, Shannon X. Wang, Apratim Sahay, Elizabeth Sefton, Mohammad Faghfoor Magrebi, Golnaz Morad, Mona Hedayat and Yannan Zheng for the many fun gatherings and potlucks. I would like to thank Negar Elhami-Khorasani for hours of fun on Skype.

I am lucky to have an extremely supportive extended family. I would like to thank Reihaneh Safavi-Naini, Amir Safavi-Naeini, Hossein Safavi-Naeini, Gelareh Taban, Hamid Safavi-Naeini, Kasra Safavi-Naeini, Safieddin Safavi-Naeini, Marzieh Palizban, Daniel Franklin and Alvaro Cardenas. Most of all, I want to thank my parents Reza Safavi-Naini and Fattaneh Fatemi, and my sister Mitra Safavi-Naeini, for their endless love and support.
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The mathematical interpretation of a worldline. Between $\tau_{p-1}$ and $\tau_p$ the system is in state $\alpha$ with $E_\alpha$ given by Eq. (9.7). The off-diagonal matrix element $H_{1}^{\alpha\beta}$ is given by Eq. (9.8) which connects the state $\alpha$ to state $\beta$. The system stays in $\beta$ between $\tau_p$ and $\tau_{p+1}$ where a new kink changes the state of the system.

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10.1 Quantum phases of Fig. 10-1 and corresponding order parameters: structure factor $S(\pi, \pi)$; single-particle condensate $\psi_i^\alpha = \langle a_{i,\alpha} \rangle$ in each layer $\alpha$; pair-condensate order parameter $\Psi = \langle a_{i,\alpha} a_{i,\beta} \rangle$, with $\alpha \neq \beta$.
(See text) ................................. 156
Chapter 1

Introduction

The remarkable progress in atomic, molecular, and optical physics over the last quarter of century has provided new tools and prototypes to control interatomic and intermolecular interactions with precision, and to simulate strongly correlated systems. Due to the presence of correlations any exact analytical or numerical treatment of such systems is challenging, since one cannot treat the individual particles independent from each other. This focus of this thesis is two of the promising developments in simulating strongly correlated systems: quantum computing and optical lattice simulators. In particular, we will address one of the important roadblocks to realizing a universal quantum computer capable of simulating strongly correlated systems, and develop new computational techniques and generalize well-established analytical techniques for treatment of bosonic systems in optical lattices.

1.1 Quantum Information Processing (QIP): Motional Heating in Ion Traps

One of the aims of QIP is to carry out quantum simulations which further our understanding of strongly correlated quantum systems. The exact study of these systems is intractable on a classical computer, since the resources required to represent a quantum state on a classical computer scales exponentially with the system size.
However a quantum computer of tens of qubits allows us to study the equilibrium and dynamical properties of these systems exactly.

Any viable quantum computation device uses qubits that can be initialized, manipulated and read-out. Additionally, the device needs to satisfy the Di Vincenzo criterion [Div00] by providing

(i) well-characterized qubits

(ii) qubits with coherence times longer than the time scales of fundamental operations

(iii) a universal set of quantum gates

(iv) a qubit-specific measurement

(v) interconversion between stationary and flying qubits

(vi) the ability to faithfully shuttle flying qubits between specified locations.

Here flying qubits refer to quantum information transmitted over a physical distance.

So far, various implementations of qubits have been proposed. One of the earliest realizations of qubits, along with demonstrations of one- and two-qubit gates, and quantum algorithms, including Grover’s search and Shor’s algorithm used nuclear magnetic resonance (NMR) qubits [GC97, VSS+99, VSB+00, VSB+01]. In these experiments, the nuclear spin of the molecules in liquid solution are used as qubits, and radio frequency (rf) pulses are used to control the spin. However, these qubits cannot be initialized in the ground state with high fidelity, which limits the scalability of this architecture.

Another class of qubits use solid-state systems for quantum computation. Superconducting qubits are formed by the charge, flux, or phase of a Josephson junctions [SG08]. These qubits are particularly appealing since they are based on solid-state technologies and can be fabricated using the techniques developed in the transistor manufacturing. In addition to the ease of fabrication, these qubits provide coherence times up to three orders of magnitude larger than typical gate times [PSB+11],
as well as high gate fidelities [CGT+09], and the ability to perform various quantum algorithms [DCG+09a].

One of the most promising qubit candidates for the realization of a scalable quantum computer are trapped ions. In these systems the electronic, or nuclear spin states of the ion represent the qubits. The ions are trapped using electromagnetic forces in vacuum conditions. Hence these qubits are well-isolated and well-characterized. The qubit state is manipulated using laser pulses and can be initialized in the ground state with a fidelity of 0.9999 [RCK+06]. These qubits also fulfill the Di Vincenzo criterion of long coherence times. The phase coherence times of hyperfine qubits exceeds 10 s which is much longer than the typical gate times of 10-100 μs [LOJ+05]. Additionally, single qubit gates with fidelities exceeding 0.999 [RCK+06], as well as various quantum algorithms have been performed using trapped-ion qubits [GRL+03, BHL+05], have been demonstrated. The trapped-ion qubits can also be measured with fidelities exceeding 0.9999 [MSW+08].

It might be surprising that despite rapid experimental progress a universal quantum computer with trapped-ions has not been realized. This is in part due to issues of scalability. Many of the experiments cited above were performed in the conventional Paul traps, where trapping potential is formed by four rod electrodes. In these traps, the ions form a long chain along the trap axis. Due to Coulomb repulsion, the chain becomes more difficult to trap and control as it grows beyond tens of ions. The surface-electrode (planar) ion traps were proposed as an alternative to the Paul trap [CBB+05]. These traps allow one to use well-established microfabrication techniques, such as photolithography, to streamline trap manufacturing. Additionally these traps can be miniaturized, and allow for fast shuttling of ions, providing a scalable quantum computing structure.

However the surface-electrode traps present a new set of challenges in the way of realizing a universal quantum computer. In particular, a universal quantum computer needs to perform quantum algorithms in a fault-tolerant way. This requires quantum error correcting codes to correct for the errors accumulated after each gate operation. However the current error per gate operation, especially two-qubit gate operations,
exceeds the theoretical upper-bound required for fault-tolerant computation [Kni05]. In fact the best demonstration of two-qubit gates have achieved a fidelity of 0.995; a fidelity of greater than 0.9999 is needed for fault-tolerant schemes. The main obstacle in realizing high fidelities is the so-called "anomalous heating" in ion traps. Anomalous heating refers to the motional heating of the trapped ions, and is due to the fluctuations in the electric field at the location of the ions. In most two-ion entanglement gate proposals [BNS+94, CZ00, MSJ00, MW01, MS99, MLK+97, SM99, SDM04, Ste96], the motional states of the ions are used to mediate the interactions between the two ions. Hence any decoherence of the motional states will limit the fidelities of these gates. The scalability of the ion trap architecture relies on the miniaturization of the trap. However, since the heating scales as $1/d^4$, the miniaturization will make fault-tolerant computing impossible. It is vital to create theoretical models for the underlying causes of anomalous heating, as well as novel experimental methods to reduce the heating.

In this thesis, we present the first, \textit{ab-initio}, microscopic theory which attempts to describe the motional heating of the trapped ion [SNRWS11, SNKW+13]. This model attributes the noise to the presence of adatoms on the surface of the trap. The adatom moves in between the different bound states of the surface-adsorbate binding potential for emitting and absorbing surface phonons. Thus, the adsorbate creates a fluctuating dipole on the trap surface. The resulting dipole fluctuating spectrum displays the correct distance dependence, magnitude and frequency dependence for some choices of adsorbates. Further experimental investigations will allow for the development of better and more accurate models of the noise mechanism.

1.2 Simulating Many-body Hamiltonians Using Ultra-cold Atoms and Molecules in Optical Lattices

A system of weakly interacting, dilute bose gas can be treated analytically within the mean-field approximation, using the Gross-Pitaevskii (GP) equations (see Sec. 7.1 for
more detail). Using Bogoliubov theory, the GP equations can be extended to include quantum fluctuations as perturbations. In this limit, the gas satisfies the condition

\[ n a_s^3 \ll 1, \]

where \( n \) is the particle density, and \( a_s \) is the s-wave scattering length. This expression follows from the requirement that the interaction energy of the gas, \( E_{\text{int}} \sim \frac{4 \pi \hbar^2}{m} n \), should be small compared to its kinetic energy, \( E_{\text{kin}} \sim \frac{\hbar^2}{2mn^2/3} \) (see Sec. 7.1).

The remarkable success of the GP approach is limited to the weakly interacting, dilute gases. In the second part of this thesis, we explore the physics of strongly interacting systems, where the GP treatment does not apply. One key element in the realization of strongly interacting systems with ultra-cold gases, is the possibility of tuning two-body interactions in one of two ways: using Feshbach resonances [IAS+98, CGJT10], or changing the strength of the optical lattice confinement. An optical lattice is a periodic array of potential wells that is formed by counter-propagating laser beams. Feshbach resonances allow one to tune the bound energy levels of the two-body interaction potential, using an external magnetic field. The dependence of \( a_s \) on the applied field provides us with a method for tuning the interaction strength. While the efficacy of this method suffers due to the presence of three-body losses, the unprecedented control over ultra-cold atoms in optical lattices has opened up another possible path for the exploration of the physics of strongly correlated systems. Once a weakly interacting bose gas is loaded into the lattice, its kinetic energy can be tuned by varying the optical lattice depth. In a deep lattice where the atoms are tightly confined near the well minima, their kinetic energy (tunneling) is strongly suppressed.

Optical lattices can be used to realize defect-free, many-body condensed matter Hamiltonians. These quantum simulators allow for a clean experimental realization of paradigmatic condensed matter Hamiltonians, such as the Bose-Hubbard (BH) model [JBC+98, BDZ08]. Moreover, they facilitate the exploration of a panoply of quantum effects beyond the standard BH model (see references [PMWD10, GPRS10, OOW+06, GSM+06, GPP+09, LSC11, KS03, SCSPS09, Sow12, KLM+08, BPM+10].
In the second part of this thesis we explore two extensions to the standard BH Hamiltonian. Our main analytical tools are the Gutzwiller mean-field approach [KCB92, RK91] (see Ch. 12), bosonization [Gia04] (see Ch. 11). Additionally we use Path-Integral Quantum Monte Carlo (QMC) simulations using the Worm algorithm [PST98a, PST98b] (see Ch. 9) to study the systems exactly.

First we study the quantum many-body phases of dipolar bosons in layered geometries. These systems realize the extended BH model in the presence of long-range, and anistropic dipolar interactions (see Ch. 8). Recent experimental breakthroughs in the realization of ultracold gases of atoms with large magnetic dipole moments [KLM+08, BPM+10, LBL12, AFM+12], highly excited Rydberg atoms [SWM10, CP10], and of ground-state polar molecules [CNM+12, dCN+11, LTD+11] hold considerable promise for investigations of many-body quantum systems where dipolar interactions can become dominant [LMS+09, CDKY09, TMCL11, BDPZ12]. The anisotropy of dipolar interactions combined with the possibility to confine particles in low dimensional geometries using optical lattices, allow for study of novel pairing mechanisms and the associated quantum phases in a setup where collisional losses are suppressed. This is particularly intriguing for the case of magnetic atoms, where confinement to lattices with spacings as small as 200 nm is possible [Lev], which favors inter-site dipolar interactions and pairing. In this thesis we present the first exact, theoretical study of the zero- and finite-temperature phase diagrams for hard-core dipolar bosons in bilayer and multilayer geometries. To this end, we have used the two-worm algorithm and developed a novel multiworm QMC algorithm which allow for efficient simulation of layered systems, where pairing (in the case of bilayers) or chain formation (in the case of multilayers) is favored (see chapter 9 for details of the algorithms). The zero- and finite-temperature phase diagrams for the bilayer and multilayer geometries are presented in chapters 10 and 11, respectively.

Additionally we investigate the effect of on-site, three-body interactions on the physics of the BH model. Recently, effective multi-body interactions have been experimentally observed [WBS+10, MHL+11]. The question that naturally arises is how these interactions affect the many-body behavior. Topological phases such as frac-
tional quantum Hall states appear as ground states of model Hamiltonians with strong three-body interactions. Moreover exotic quantum phases have been predicted for bosonic Hamiltonians with many-body interactions, such as the ring exchange model [Coo04, MS02]. An important first step in realizing these models using ultra-cold atoms was the realization that strong three-body losses lead to an effective hard-core three-body interaction that can be used, for instance, to stabilize the BH model with attractive two-body interactions [DTD+09]. Under these conditions, the system can undergo a first order MI to SF transition in the presence of strong pairing interactions [KPS04]. Despite these recent studies, lattice systems with three-body interactions remain largely unexplored. In chapter 12 we describe a novel scheme for realizing a tunable, on-site, three-body interaction, that can be both repulsive and attractive. We study the phase diagram of the resulting model, which is the BH Hamiltonian with an additional interaction term. The Gutzwiller mean-field results, and exact QMC results are presented in sections 12.2 and 12.3, respectively.

Outline

This thesis is divided into two parts. The first part focuses on ion trap technology and the anomalous heating in ion traps and consists of the following:

Chapter 2 presents the basics of ion trap operation. It starts by describing the basics of trapping of charged particles using radio frequency fields. Next it introduces the linear Paul trap, the 2D quadruple ion trap, and the planar ion trap.

Chapter 3 describes how the internal atomic and motional energy levels of the trapped ion can be used as the computational basis. These energy levels form the qubit. In this chapter we will use the Sr$^+$ ion to describe the experimental procedures used to initialize, manipulate and measure the state of the qubit.

Chapters 4 and 5 discuss the motional heating of the trapped-ion. In chapter 4 we describe the procedure for measuring the heating rate, and present the current experimental data and techniques for reducing the noise. In chapter 5 we present the different theoretical models which have been developed in an attempt to explain the
anomalous heating.

Finally, chapter 6 presents the conclusion and outlook of the first part of the thesis.

In the second part of the thesis we describe how ultra-cold atoms and molecules in optical lattices can be used to realize, and study novel quantum many-body phenomena. This part consists of the following

Chapter 7 begins by discussing the physics of dilute bose gases. In this chapter we show how using optical lattices we can move beyond this regime and into the strongly correlated regime. The BH model is presented as an experimentally realizable model. Since the many-body Hamiltonians studied in this thesis are all based on BH model, this chapter concludes by presenting a discussion on the physics of the BH Hamiltonian.

Chapter 8 introduces the extended BH model in the presence of dipolar interactions. The chapter begins by briefly introducing dipolar interactions, which is followed by a discussion of stable geometries for trapping dipolar atoms and molecules. Finally a derivation of the extended model is presented.

Chapter 9 discusses Path Integral Quantum Monte Carlo algorithm, which is one of the main theoretical tools used in this thesis. In particular it focuses on the Worm algorithm, as well as the two-worm and the novel multiworm algorithms developed for the study of dipolar bosons in layered geometries.

Chapter 10 presents the results of our study of the extended BH model, with dipolar interactions, for a system of dipolar bosons in a bilayer geometry. The bosons are trapped in quasi two-dimensional pancakes, with their dipole moments aligned perpendicular to the trapping plane. This configuration favors pairing and we employ the two-worm algorithm to study the many-body phases of these pairs. The two-worm algorithm allows us to efficiently sample the Hilbert space of pairs.

Chapter 11 presents the results of our study of a multilayer system of bosons with arbitrary, inter-layer attractive interactions. We first use the N-tube bosonization formalism developed in this chapter, as well as the multiworm algorithm to study the Renormalization Group (RG) flows of the system. This system favors the for-
mation of chains spanning across the layers. The multiworm algorithm allows for efficient sampling of the chained phases. We prove that these phases are stabilized for infinitesimal, inter-layer, attractive interactions.

Chapter 12 presents the results of our study of the BH model in the presence of a three-body, tunable, on-site interaction. We present a scheme to realize this interaction, which can be both repulsive and attractive. This is followed by the study of the system Hamiltonian using the Gutzwiller mean-field approach, as well as using Quantum Monte Carlo algorithm using the Worm algorithm.

Finally, chapter 13 presents the conclusion and outlook of the first part of the thesis.

Parts of chapter 5 has previously appeared in


Chapter 10 has previously appeared in


Chapter 12 has previously appeared in


Chapter 11 is new material, in preparation to be submitted.

The following papers were also published during my PhD studies. They do not appear in this thesis:

Part I

“Motional Heating in Ion Traps”
Chapter 2

Trapping Ions with Radio Frequency Fields

The first requirement for ion trap quantum computation is the ability to confine an ion spatially. It is only after this step that one can begin to address the ion so that it can be initialized to a well-defined state. The ion can then be used to perform a set of universal gates at high fidelity. This chapter discusses the mechanism behind trapping a charged particle using static and rf fields. Section 2.1.1 describes the mechanical problem of trapping a ball on a saddle potential. Section 2.1.2 describes the basics of trapping a charged particles with radio frequency (rf) fields, using the 2D quadrupole ion trap and linear Paul trap as examples. Finally section 2.2 describes how planar ion traps can be used to create a scalable architecture for trapped-ion quantum computation.

2.1 Theory of RF Traps

I was introduced to the basics of ion trapping through a demonstration of the Nobel prize speech of Wolfgang Paul, performed by my undergraduate adviser using a cricket ball. It turns out that trapping charges in rf fields has an analog in classical mechanics. This section first describes the problem of trapping a ball on a rotating saddle surface which will provide an intuitive description of rf traps. We will then describe the 2D
quadrupole ion trap and the linear Paul trap.

### 2.1.1 Ball on a Rotating Saddle

If a particle of mass \( m \) subject to a restoring force of form

\[
\vec{F}(\vec{r}) = -k\vec{r} \tag{2.1}
\]

where \( k > 0 \) and \( \vec{r} = (x, y, z) \) is the position of the particle, it can be confined to a point in space. Since \( \vec{F}(\vec{r}) \) is conservative it can be written in terms of a scalar potential \( U(\vec{r}), \)

\[
\vec{F}(\vec{r}) = -\nabla U(\vec{r}). \tag{2.2}
\]

Integrating Eq. 2.1, we find the potential:

\[
U(x, y, z) = -\frac{k}{2}(\alpha x^2 + \beta y^2 + \gamma z^2). \tag{2.3}
\]

We are free to choose \( \alpha, \beta, \) and \( \gamma. \) Here we will choose \( \alpha = -\beta = 1, \) and \( \gamma = 0 \) to mimic the electrostatic potential used in the 2D quadrupole mass filter, discussed in section (2.1.2). With this choice of parameters, the potential in Eq. (2.3) takes the form:

\[
U(x, y) = -\frac{k}{2}(x^2 - y^2). \tag{2.4}
\]

As it is shown in Fig. 2-1(a), this potential can only trap a particle along the \( x \)-direction, since the stable minimum is only along this direction. However the particle can always escape along the \( y \)-direction. We can trap a particle only if we add a time varying part to the potential. If we start rotating the \( U(x, y, z) \) about the \( z \)-axis with frequency \( \Omega, \) a time dependent potential of the form

\[
U(x, y, t) = \frac{c}{2} \left[ (x^2 - y^2) \cos(2\Omega t) - 2xy \sin(2\Omega t) \right]. \tag{2.5}
\]

This potential is known as the flapping potential. It can be pictured as the potential shown in Fig. 2-1(a) where the wings on the saddle flap at frequency \( 2\Omega. \) If one
Figure 2-1: A schematic representation of the rotating saddle potential. (a) The static saddle potential can only confine the particle long the $x$ direction. Rotating the potential about the $z$-axis creates a flapping potential that confines the particle along both $x$ and $y$ directions. The corresponding pseudopotential is shown in (b). The potentials used to trap ions are similar to the rotating saddle potential depicted here.

considers the pseudopotential corresponding to the flapping potential the confining action will become visible. In the pseudopotential approximation the time dependent flapping potential is replaced by an averaged, effective potential. The pseudopotential corresponding to the rapidly oscillating flapping potential is shown in Fig. 2-1(b). It is easy to see that if the potential rotates fast enough it can confine the particle in the $y$-direction as well, and that the confinement increases with increasing $\Omega$. It can be shown that the particle will follow stable trajectories on the saddle if [LBMW03]

$$\Omega \geq \sqrt{\frac{2e}{m}}.$$  (2.6)

As we will show in the next section, the actual trapping potential in ion traps is different from the rotating saddle described in this section. However the rotating saddle is a useful picture to keep in mind.
2.1.2 2D Quadrupole Ion Trap

The 2D quadrupole trap is one of the simplest geometries used to trap charged particles. In these traps, the particle is trapped at the potential minimum. In an analogy to the static saddle potential described above, Earnshaw's theorem tells us that static fields alone cannot be used to trap a charged particle. However as we will show below a combination of static and rf electric fields form a dynamically stable trap.

The 2D quadrupole trap is formed by four hyperbolic electrodes that are arranged around the trap axis, as shown in Fig. 2-2. The hyperbolic electrodes are defined as

\[ \frac{x^2 - y^2}{r_0^2} = \pm 1 \]  \hspace{1cm} (2.7)

where \( r_0 \) is the distance from the center of the trap, as shown in Fig. 2-2. The total potential in this trap with rf frequency \( \Omega \) is

\[ \phi(x, y, t) = \phi_{dc}(x, y) + \phi_{rf} \cos(\Omega t) \]  \hspace{1cm} (2.8)

where

\[ \phi_{dc}(x, y) = \frac{U}{2r_0^2} (x^2 - y^2) \]  \hspace{1cm} (2.9)
\[ \phi_{rf}(x, y) = -\frac{V}{2r_0^2} (x^2 - y^2). \]  \hspace{1cm} (2.10)

Here \( U \) and \( V \) are the dc and rf voltage amplitudes.

We will use Newton's second law to extract the equations of motion of a charged particle in the quadrupole field given by Eq. 2.8,

\[ \vec{F} = -\vec{\nabla} \phi(x, y, t). \]

We find that the dynamics of a particle of mass \( m \) and charge \( Q \) are described by the
Mathieu equations,
\[ \frac{d^2 x}{d\xi^2} + (a_x - 2q_x \cos(2\xi))x = 0 \]  \hspace{1cm} (2.11)
\[ \frac{d^2 y}{d\xi^2} + (a_y - 2q_y \cos(2\xi))y = 0, \]  \hspace{1cm} (2.12)
where \( \tau, q, \) and \( a \) are dimensionless quantities for time, rf voltage, and dc voltage respectively, and are given by
\[ \tau = \frac{\Omega t}{2} \]  \hspace{1cm} (2.13)
\[ q_x = -q_y = \frac{2QV}{mr_0^2\Omega^2} \]  \hspace{1cm} (2.14)
\[ a_x = a_y = \frac{4QU}{mr_0^2\Omega^2}. \]  \hspace{1cm} (2.15)

The solution to the Matthieu equation is well known [AS72] and it can be shown that the motion of the ion follows stable trajectories if \( a \) and \( q \) satisfy
\[ 0 \leq \sqrt{a + q^2/2} \geq 1. \]  \hspace{1cm} (2.16)
In particular if \( a, q^2 \ll 1 \) and \( a \ll q \), the solution to the Mathieu equations to the lowest order are given by,
\[ u(t) = u_0 \cos \left( \frac{\sqrt{a_u + q_u^2/2} \Omega t}{2} \right) \left( 1 - \frac{1}{2} \cos(\Omega t) \right), \]  \( u = x, y. \) \hspace{1cm} (2.17)

Hence, in this region in parameter space, the ion’s motion has two components; a slow, harmonic motion at frequency \( \omega = \frac{\sqrt{a + q^2/2} \Omega}{2} \), which is known as the secular motion, and a rapid oscillation at the rf drive frequency \( \Omega \). These driven oscillations have an amplitude \( \frac{q}{2} |r| \), where \( |r| = \sqrt{x^2 + y^2} \), is the distance between the rf potential minimum and the trapped ion. Once the ion is Doppler cooled, its secular motion amplitude would be \( \sim 100 \) nm and the amplitude of the micromotion will be a factor of \( q/2 \) smaller.

Even though the amplitude of the micromotion is negligible compared to that
of the secular motion, it can be shown that the secular motion and micromotion contribute equally to the average kinetic energy [BMB+98]. Hence it is important to reduce the micromotion by calibrating the rf potential minimum so that it coincides with the dc potential minimum. This is known as compensation. At this point it is worth noting that stray dc electric fields present in ion traps cause excess micromotion that need to be compensated by applying counteracting electric fields. Therefore eliminating micromotion improves the trapping performance, eliminates unwanted Doppler shifts and enhances Doppler cooling [BMB+98].

The quadrupole trap described above can only confine the ion in the x- and y-directions. In the next section we will introduce the linear Paul trap which can confined the ion in all three directions.

2.1.3 Linear Paul Trap

A functional ion trap should confine the particle along all three spatial directions. This can be achieved using the linear Paul trap shown in Fig. 2-2(a), which is the 3D analog of the quadrupole mass filter described in the previous section. In the linear Paul trap four intersected, cylindrical electrodes are used to confine the particles along the trapping axis, z, as well as the x- and y-directions. Similar to the quadrupole trap, the trapping potential consists of an rf potential \( \phi_{rf} \) and a dc potential \( \phi_{dc} \). The rf potential is

\[
\phi_{rf}(x, y) = -\frac{V}{2r_0^2}(x^2 - y^2),
\]

where \( V \) is the rf amplitude, \( \Omega \) is the drive frequency and \( 2r_0 \) is the diagonal separation between the electrodes. Near the center of the trapping region the dc potential is given by

\[
\phi_{dc} = \kappa U \left( \frac{2z^2 - x^2 - y^2}{2z_0^2} \right),
\]

where \( U \) is the dc voltage, and \( \kappa \) and \( z_0 \) depend on the trap geometry. Hence the total trapping potential near the center of the trapping region is

\[
\phi(x, y, z, t) = -\frac{V}{2r_0^2}(x^2 - y^2) \cos(\Omega t) + \kappa U \left( \frac{2z^2 - x^2 - y^2}{2z_0^2} \right).
\]
Using the procedure described in the previous section we find that the trajectory of the trapped ion in a linear Paul trap is given by

\[
u(t) = u_0 \cos\left(\frac{\sqrt{a_u + q_x^2/2} \Omega t}{2}\right) \left(1 - \frac{q_u}{2} \cos(\Omega t)\right)
\]

(2.21)

where

\[
a_x = a_y = -\frac{1}{2} a_z = \frac{4q\kappa U}{2mz_0^2\Omega^2}
\]

(2.22)

\[
q_x = -q_y = \frac{2qV}{mr_0^2\Omega^2}
\]

(2.23)

\[
q_z = 0.
\]

(2.24)

Since there is no rf field along the z-axis, i.e. \( q_z = 0 \), the ion undergoes harmonic oscillations at frequency \( \sqrt{a_z}\Omega/2 \) along the trapping axis, and is not influenced by micromotion. The motion along the x- and y- directions are the same as those discussed in the case of the quadrupole ion trap.

### 2.2 Planar Ion Trap

The implementation of large scale quantum algorithms involves the ability to trap, and control a large number of ions. One of the possible trap architectures involves the use of segmented traps where the ions are held in trapping regions and are shuttled to an interaction zone where the coupling between the string of ions is mediated by the Coulomb interaction. Gate operations as well as state manipulation and readout are performed in the interaction zone [CBB+05].

The architecture described above cannot be implemented by the trap designs described in the previous sections. The linear traps use three-dimensional configurations of electrodes and are somewhat bulky and are extremely time consuming and complex to construct. These factors limit the scalability of these traps. Planar ion traps provide a scalable alternative that are more streamlined in terms of production since one can use well-established microfabrication techniques such as photolithography and
evaporative metal deposition. Typically these traps use gold or aluminum electrodes that are plated on the aluminum oxide, quartz or silicon substrates.

The confinement in planar ion traps is still provided by an array of dc and rf electrodes. The rf electrodes confine the ion in the x and y directions and the dc electrodes provide the trapping potential along z. Figure 2-2(b) shows a schematic of a typical planar ion trap, known as the five wire geometry, with three dc electrodes (white) and two rf electrodes (blue) providing the confinement.

![Figure 2-2](image)

Figure 2-2: A schematic representation of two different trap designs (not to scale). (a) A segmented linear Paul trap. The ions are trapped along the trapping axis. The rf electrodes, shown in black, create the confinement in the x and y directions. The dc electrodes are shown in blue. The outer segments are the positive dc electrodes while the middle segments are the negative dc electrodes. Together they provide the trapping potential in the z direction. (b) A five wire planar ion trap with three dc electrodes, shown in blue, providing the confinement along the z-axis and the two rf electrodes, shown in white, trapping the ion in the x and y directions. The trap axes along x and z directions are shown. The axis along y points into the page.

While planar traps are scalable and can be easily fabricated, higher fidelities can be achieved in the linear traps. This is mainly due to the proximity of the ion to the trap surface in planar ion traps. The separation between the ion and the trap surface in these trap is \(~ 20 - 100 \, \mu m\), while in the linear traps the ion is trapped about \(500 \, \mu m\) away from the trap electrode. This proximity mainly manifests itself in the charging of the trapping electrodes and more importantly in the anomalous motional heating of the trapped ion which we will discuss in detail in chapters 4 and 5. The linear trap designs cannot be used in large scale quantum computation. The
planar ion traps on the other hand can be miniaturized and microfabricated. Once the technical difficulties, such as the anomalous heating are reduced or eliminated, the planar traps will be a viable, scalable architecture capable of implementing quantum computing algorithms.
Chapter 3

The Qubit

The previous chapter described the mechanism behind ion trapping. In principle, the micro-fabricated planar traps can be used to trap any species of ion. However, quantum coherent control can only be achieved with certain species of ions, since the implementation of a reliable cooling scheme that can cool the ion down to its ground motional state requires an ion with closed and fast cycling transitions.

Section 3.1 describes the motional states of a trapped-ion. Section 3.2 introduces the atom-laser interactions, which allow us to coherently couple the internal energy levels of the trapped ion to their external motional degrees of freedom. The motional states of the ion, and the coupling between the internal and motional degrees of freedom play an important role in the observed anomalous heating in ion traps which will be discussed in the next chapter. Section 3.3 explains the level structure of \(^{88}\text{Sr}^+\) ion. Using this choice of qubit, section 3.4 concludes the chapter by describing the experimental procedures used for state initialization and detection.

3.1 Motional States in an Ion Trap

After the ion is initially trapped, it is laser cooled so that it occupies the lowest energy state of the trap potential with secular frequency \(\omega_z\). The methods used for cooling the ion are discussed in section 3.4. Here we will focus on the motional states of the trapped ion. The trap potential can be modeled as a harmonic well with discretized
levels that are separated by $\sim 1$ MHz $\approx 50 \mu K$. The trap Hamiltonian is

$$H_{\text{trap}} = \omega_z \left(a^\dagger a + \frac{1}{2}\right) \quad (3.1)$$

We will use the number basis to describe the eigenstates of the trap Hamiltonian. The number basis are a set of state $|n\rangle$ which satisfy

$$a|n\rangle = \sqrt{n}|n-1\rangle \quad (3.2)$$

$$H_{\text{trap}}|n\rangle = \omega_z \left(n + \frac{1}{2}\right)|n\rangle. \quad (3.3)$$

The state of the trapped-ion is the tensor product of its internal state and its motional state. The next two sections focus on the internal states of the qubit, as well as the coupling between the internal and motional states.

### 3.2 Atom-laser interactions: Two-level Atom

This section describes the interaction between a two-level atom and a single-mode laser. The level structure of the trapped ions is more complicated, however the two-level approximation is an adequate description of most experimental situations. This is because the electromagnetic fields are chosen such that they couple two of the internal levels of the ion.

The effective Hamiltonian describing an ion trapped in a harmonic trap interacting with a single mode laser beam is given by,

$$H = H_0 + H_{\text{int}} \quad (3.4)$$

$$H_0 = \frac{\hbar}{2} w_0 \sigma_z + \omega_z a^\dagger a \quad (3.5)$$

$$H_{\text{int}} = \frac{\hbar}{2} \Omega (\sigma_+ + \sigma_-) \left(e^{i(kz-\omega t+\phi)} + e^{-i(kz-\omega t+\phi)}\right) \quad (3.6)$$

where $\sigma_z = |e\rangle\langle e| - |g\rangle\langle g|$, $\sigma_+ = |e\rangle\langle g|$, $\sigma_- = |g\rangle\langle e|$, and $\omega_0 = \omega_e - \omega_g$ is the energy splitting of the two-level atom. Here $\omega_z$ is the secular frequency, and $\Omega$ is the dipolar
Rabi frequency given by
\[ \Omega = \frac{e E_0}{\hbar} |\langle e|r^*\cdot \varepsilon|g\rangle| \] (3.7)
where \( E_0 \) and \( \varepsilon \) are the amplitude and polarization of the laser field respectively. The laser beam has a frequency \( \omega = \omega_0 + \delta \), where \( \delta \) is the detuning from the atomic transition. Finally \( k \) and \( \phi \) are the wavenumber and the phase of the laser beam respectively.

The description of the dynamics due to the atom-laser interactions is most intuitively described in the interaction picture, where the states become stationary in the absence of the laser field. The interaction picture Hamiltonian is given by,
\[ \tilde{H} = e^{i\hbar H_0 t}(H - H_0)e^{-i\hbar H_0 t} \] (3.8)
where \( H_0 \) its the free Hamiltonian given by Eq. (3.5). Applying the above transformation to the Hamiltonian \( H \), we find
\[ \tilde{H} = \frac{\hbar}{2} \Omega \left( \sigma_+ e^{i\omega_0 t} + \sigma_- e^{-i\omega_0 t} \right) e^{i\frac{k}{\omega_0}a^\dagger at} \left( e^{i(kx - \omega t + \phi)} + e^{-i(kx - \omega t + \phi)} \right) e^{-i\frac{k}{\omega_0}a^\dagger at}. \] (3.9)

If we apply the rotating wave approximation, neglecting the rapidly oscillating terms, and using the Lamb-Dicke parameter \( \eta = k\sqrt{\hbar/2m\omega_z} \), the interaction Hamiltonian can be written in terms of \( a \) and \( a^\dagger \),
\[ \tilde{H} = \frac{\hbar}{2} \Omega \sigma_+ e^{\phi - i\delta t} e^{\eta a(t) + a^\dagger(t)} + \text{h.c.} \] (3.10)
where \( a(t) = ae^{-i\omega_z t} \) and \( a^\dagger(t) = a^\dagger e^{i\omega_z t} \). The Lamb-Dicke parameter \( \eta \) allows us to compare the extent of the lowest harmonic oscillator state to the wavelength of the atomic transition. If \( \eta \ll 1 \), i.e. the Lamb-Dicke regime, the spread of the ion wavefunction is much smaller than \( 1/k \). Experimentally, the ion is in the Lamb-Dicke regime after it has been laser cooled (see sections 3.3 and 3.4). In this regime the interaction Hamiltonian takes the simple form
\[ \tilde{H} = \frac{\hbar}{2} \Omega \sigma_+ e^{\phi - i\delta t}(1 + i\eta (a(t)e^{-i\omega_z t} + a^\dagger(t)e^{i\omega_z t})) + \text{h.c.} \] (3.11)
This Hamiltonian contains only three terms,

\[
H_{\text{car}} = \frac{1}{2} \Omega (\sigma_+ e^{i\phi} + \sigma_- e^{-i\phi})
\]
(3.12)

\[
H_{\text{red}} = \frac{1}{2} \Omega \eta (a\sigma_+ e^{i\phi} + a^\dagger \sigma_- e^{-i\phi})
\]
(3.13)

\[
H_{\text{blue}} = \frac{1}{2} \Omega \eta (a^\dagger \sigma_+ e^{i\phi} + a \sigma_- e^{-i\phi}).
\]
(3.14)

Let states \(|n\rangle\) represent the motional state of the ion. Then the first Hamiltonian facilitates transitions of the form \(|n\rangle|g\rangle \leftrightarrow |n\rangle|e\rangle\) with Rabi frequency \(\Omega\), known as the carrier resonance (\(\delta = 0\)). The second Hamiltonian corresponds to the resonance at \(\delta = -\omega_z\), which is known as the first red sideband. This corresponds to the transition \(|n\rangle|g\rangle \leftrightarrow |n-1\rangle|e\rangle\) with Rabi frequency

\[
\Omega_{n,n-1} = \Omega \eta \sqrt{n}.
\]
(3.15)

Finally, the last Hamiltonian corresponds to the resonance at \(\delta = \omega_z\), known as the first blue sideband. This Hamiltonian gives rise to the transition \(|n\rangle|g\rangle \leftrightarrow |n+1\rangle|e\rangle\) at Rabi frequency

\[
\Omega_{n,n+1} = \Omega \eta \sqrt{n + 1}.
\]
(3.16)

The red and blue sideband Hamiltonians entangle the motional state of the trapped-ion with its internal states. Moreover, the blue sideband transitions violate conservation of energy and are absent from the Jayne-Cummings Hamiltonian. This means that trapped-ion experiments have richer dynamics compared to their atom-photon counterparts, such as cavity QED setups. Figure 3-1 is a schematic representation of the state of a trapped ion, which is the tensor product of the motional qubit and the internal qubit.
Figure 3-1: The complete Hilbert space of the trapped ion is spanned by states that are tensor products of the ion’s internal state and its motional state.

### 3.3 The $^{88}$Sr$^+$ Qubit

Any quantum computer architecture needs to provide a qubit with long coherence times that can be easily addressed, manipulated and reproduced. Strongly ionized alkaline-earth ions such as Be$^+$, Mg$^+$, Ca$^+$, Sr$^+$, and Ba$^+$ are popular choices for trapped-ion qubits, since they fulfill these criteria. This section focuses on $^{88}$Sr$^+$ ion, which is a hydrogen-like ion, with a single electron occupying the zero angular momentum. The atomic structure of the $^{88}$Sr$^+$ ion is shown in Fig. 3-2 and it gives us another clue why this is a particularly good choice for a qubit. All transition wavelengths for the $^{88}$Sr$^+$ ion are in the visible or near-IR range, and are easily accessible with diode lasers, which greatly simplifies the experimental setups.

The $^{88}$Sr$^+$ ion does not have any nuclear spin. However the presence of the low lying, metastable D states allows for two different methods of encoding a qubit. One can either use the S-D optical transition, connecting the $S_{1/2}$ and the $D_{5/2}$ state, or the two Zeeman sub levels of the $S_{1/2}$ ground state which are split when an external magnetic field is applied. In the following I will use the $S_{1/2}(m = -1/2) \leftrightarrow D_{5/2}(m = -5/2)$ transition as the qubit transition, which is marked on Fig. 3-2. As it was described earlier any realization of a qubit should also allow for a reliable cooling
Figure 3-2: The atomic structure of $^{88}\text{Sr}^+$. (a) The blue arrows show the electric dipole transitions that are used in Doppler cooling and detection. The gray arrows are the dipole transitions used in repumping. The qubit transition is shown in red. The level structure in the presence of a magnetic field is shown in (b). The $S_{1/2}(m = -1/2) \leftrightarrow D_{5/2}(m = -5/2)$ is the qubit transition at 674 nm with a lifetime of 390 ms.

Mechanism. When the ion first enters the trap, its temperature is of the order of hundreds of motional quanta. The ion is first Doppler cooled using the $S_{1/2} \leftrightarrow P_{1/2}$ transition, where upon it enters the Lamb-Dicke regime. Qualitatively Doppler cooling works as follows: the ion moving at velocity $v$ interacts with a traveling laser field with wave-vector $\vec{k}$ with detuning $\delta$. Since the ion absorbs photons of a specific momentum from the laser but emits photons to $4\pi$ steradians, it feels a net force from the laser. Furthermore the force on the ion is larger if the ion moves anti-parallel to $\vec{k}$, which on average slows the ion down. However this process cannot cool the ion below a finite temperature $T_D$ given by

$$k_b T_D = 4\hbar \rho_{ee} \Gamma_{eg},$$

where $\Gamma_{eg}$ is the spontaneous emission rate from $|e\rangle$ to $|g\rangle$, $\rho_{ee}$ is the steady state population of the excited state and $k_b$ is the Boltzmann constant. The cooling limit exists since below this temperature the energy loss due to the cooling mechanism is balanced by the energy gained due to photon recoil processes during photon scattering [REF]. Ideally Doppler cooling allows one to cool the $^{88}\text{Sr}^+$ to $\sim 10$ motional quanta.
at which point the ion is in the Lamb-Dicke regime and the motion of the ion needs to be treated quantum mechanically.

### 3.4 Quantum State Initialization and Detection

The $^{88}\text{Sr}^+$ ion $S_{1/2}(m = -1/2) \leftrightarrow D_{5/2}(m = -5/2)$ transition forms the atomic qubit. The motional quits can be used as additional quits necessary for certain entangling gates, such as the CNOT gate, or to mediate coupling between ions trapped in a chain. While a viable quantum computing architecture requires the demonstration of state initialization, detection and gate operations, we will focus only on the initialization and measurement aspects. These two aspects are important in measuring the anomalous heating rate present in ion traps.

#### 3.4.1 State Initialization

Once the ion is cooled to the Doppler limit, it still needs to be initialized to a well-defined motional state, with low $n$, to facilitate high-fidelity quantum operations. Typically the qubit is initialized to the ground motional state with $n = 0$. This is achieved by resolved sideband cooling on the $S_{1/2}(m = -1/2) \leftrightarrow D_{5/2}(m = -5/2)$ transition.

The ion is cooled by first driving the red sideband transition $|S_{1/2}, n\rangle \leftrightarrow |D_{5/2}, n-1\rangle$. The $|D_{5/2}, n-1\rangle$ state preferentially decays to the $|S_{1/2}, n-1\rangle$ state via the carrier transition. Hence these set of steps removes one motional quanta from the system. The experimental implementation is slightly more involved since the $D_{5/2} \leftrightarrow S_{1/2}$ carrier transition has a long lifetime. The cooling process is sped up by simultaneously and incoherently driving the $D_{5/2} \leftrightarrow P_{3/2}$ transition, transferring the population to the $P_{3/2}$ state, where the spontaneous decay rate to the $|S_{1/2}, n-1\rangle$ state is much faster. It is worth noting that the $|S_{1/2}, 0\rangle$ state does not couple to red sideband pulses, so the population in the ground state remains in the ground state even when more pulses are applied.
3.4.2 State Detection

Since a trapped-ion has both atomic and motional qubits, detection schemes need to be able to detect both the internal state of the ion as well as its motional state. In the case of $^{88}$Sr$^+$ ion, the internal state can be easily detected. The S state is coupled to the P state with a strong transition (see Fig. 3-2), which is used in Doppler cooling. This transition is driven continuously to cool the trapped ion, so if the ion is in the S state, it will fluoresce and its fluorescence can be detected. Conversely, an ion in the D state does not fluoresce.

The detection of the motional state of the ion can only be detected in conjunction with its internal state, using sideband transitions. Measuring the motional state of the trapped ion is analogous to measuring its temperature. Previously we noted that the population in the ground state $|S_{1/2}, 0\rangle$ does not couple to the red sideband pulse. This means that as the temperature of the ion decrease the population transfer on the red sideband should decrease. Hence the ratio of transition probabilities on the red and blue sidebands should give us an estimate of the ion temperature and motional state. If an ion is in the Lamb-Dicke regime the Rabi frequency on the red and blue sidebands depend on $n$ (see Eqs. (3.15) and (3.16)). The transition probabilities on the red and blue sidebands from the state $|S_{1/2}, n\rangle$, denoted by $P_{\text{BSB}}$ and $P_{\text{RSB}}$, are the sum of the transition probabilities on each sideband with $\Delta n = 0, \pm 1, \pm 2, \cdots$ and are given by

$$P_{\text{BSB}} = \sum_{n=0}^{\infty} P_{n+1} \sin^2 \left(\frac{\Omega_{n,n+1} t}{2}\right)$$

$$P_{\text{RSB}} = \sum_{n=0}^{\infty} P_n \sin^2 \left(\frac{\Omega_{n,n-1} t}{2}\right).$$

Here $P_n$ is the occupation probability of the $n$th motional state. If we fix the detuning of an applied pulse to $\delta = \omega_z$ and measure the transition probability $P_{\text{BSB}}$ as a function of time we can extract the population distribution of the motional states.

If the ion is in a thermal state a simpler procedure can be used to extract the average number of motional quanta $\bar{n}$. In this case $P_n = \frac{1}{\bar{n}+1} \left(\frac{\bar{n}}{\bar{n}+1}\right)^{n+1}$. Substituting
this expression in Eq. (3.18) we find

\[ P_{BSB} = \sum_{n=0}^{\infty} P_{n+1} \sin (\Omega_{n,n+1} t/2)^2 \]  \hspace{1cm} (3.20)

\[ = \frac{\tilde{n}}{1 + \tilde{n}} \sum_{n=0}^{\infty} P_{n} \sin (\Omega_{n+1,n} t/2)^2 \]  \hspace{1cm} (3.21)

\[ = \frac{\tilde{n}}{1 + \tilde{n}} P_{RSB} \]  \hspace{1cm} (3.22)

Hence by measuring the ratio \( R = P_{BSB}/P_{RSB} \), which is not a function of time or \( \Omega \), we can determine the average number of motional quanta \( \tilde{n} \).
Chapter 4

Heating Rates and Electric Field Noise

In chapter 2, it was shown that planar ion traps can be subsequently used to confine an ion spatially, and the motional and internal states of this ion can be used as qubits in quantum computation. Microfabricated traps are often presented as a scalable quantum computing architecture. However, the scalability of this architecture is limited by the presence of the anomalous heating which heats the ion out of its ground motional state after it is trapped. Trapped ion quantum computation relies on maintaining the quantum coherence of the motion of the trapped ions to perform two-qubit gates which is not possible in the presence of heating rates at present experimental levels. Anomalous heating limits the fidelity of the quantum operations in ion trap experiments. It is of utmost importance to characterize this noise and determine its source.

A variety of traps with different trapped-ion species have been used to characterize anomalous heating. For each trap, the secular frequency $\omega_z$ and its heating rate out of the ground state are measured, since these two are the only parameters that determine the behavior of the ion trapped near the ground state. All other variables, such as the trapping potential and electrode configuration, only affect how the ion is loaded into the trap or how easy it is to use the trap, e.g. by allowing for better optical access.
Section 4.1 describes the experimental procedure for measuring the heating rate of an ion trap. Section 4.2 establishes the connection between electric field noise and the heating rate. Section 4.3 presents an overview of the current experimental data on heating rates and the characteristics of the anomalous heating. Finally, section 4.4 presents the recent experimental techniques used to reduce the motional heating of the trapped ion.

4.1 Measuring the Heating Rate

The protocol used for measuring the heating rate of the ion depends on the number of motional quanta present. The heating rate of hot ions can be estimated using a variety of methods. It can be related to the time required for the loss of the ion through boil-off, extracted from the dynamics of Doppler re-cooling, or estimated through balancing the Doppler cooling rate against the trap heating rate. This section describes how the heating rate of low energy ions can be measured using the $|S_{1/2}, n\rangle \leftrightarrow |D_{5/2}, n - 1\rangle$ sideband transition. After cooling the ions to the Doppler limit, the ions are sideband cooled to the ground motional state on the $|S_{1/2}, n\rangle \leftrightarrow |D_{5/2}, n - 1\rangle$ transition. In section 3.4.2 it was shown how the population distribution of the different motional states can be extracted from the transition probabilities on the red and blue sidebands. In particular for an ion in a thermal state, the average number of quanta $\bar{n}$ can be determined from just two sideband measurements. The heating rate of the trap, $\dot{n}$ can be determined by measuring the growth of $\langle n \rangle$ as function of time after preparing the state with $\langle n \rangle < 1$.

4.2 Electric Field Noise and Heating of the Ion

The previous section presented a protocol for measuring the heating rate in an ion trap. In this section, we establish the relationship between the electric field noise and heating in the secular approximation, where we ignore the micromotion and develop a method for heating rate measurement independent of the species of the trapped ion.
and the secular frequency of the trap. This measure allows us to combine data from various experimental groups in the next section.

Within the secular approximation the motion of the ion can be modeled as a harmonic oscillator within a pseudopotential

\[ Q\phi_p = \frac{Q^2}{4m\Omega^2} |\nabla \phi_{rf}|^2 \]  
\[ = \frac{1}{2} m\omega_z^2 x_0^2 \]  
\[ x_0 = \sqrt{\frac{\hbar}{2m\omega_z}} \]  

where \( Q \) and \( m \) are the charge and mass of the ion respectively, \( \Omega \) is the frequency of the rf drive, \( \phi_{rf} \) is given by Eq. (2.18), and the secular frequency of the trap \( \omega_z \) is given by

\[ \omega \approx \frac{q\Omega}{2\sqrt{2}} = \frac{1}{\sqrt{2}} \frac{QV}{m\Omega x_0^2} \]  

where \( q \) is dimensionless parameter for the rf voltage given by Eq. 2.14. The total trapping potential is \( \phi(x, y, z) = \phi_{dc} + \phi_p \), where \( \phi_{dc} \) is the static trapping potential (see Eq. 2.19).

The motion of the trapped ion in the absence of the electric field noise and in the secular approximation is described by

\[ H_{trap} = \omega_z (\hat{a}^\dagger \hat{a} + \frac{1}{2}) \]  

(see section 3.1) where \( \omega_z \) is the secular frequency of trap. The electric field noise can be added as a noise term to the Hamiltonian

\[ H = H_{trap} + Q\delta E(t) x = H_{trap} + Q\delta E(t) x_0 (a + a^\dagger) \]  

and can be treated as a perturbation that causes transitions from the ground motional state to the first excited state. The transition rate from \( |0\rangle \rightarrow |1\rangle \) is given by [TKK+00]

\[ \Gamma_{0 \rightarrow 1} = \frac{1}{\hbar^2} \int_{-\infty}^{\infty} e^{-i\omega_z \tau} \langle \delta E(t) \delta E(t + \tau) \rangle |\langle 0 | q x_0 (a + a^\dagger) |1 \rangle|^2 d\tau \]  

It is useful to write the transition rate in terms of the spectral density of the electric...
field noise

\[ S_E(\omega) = 2 \int_{-\infty}^{\infty} e^{-i\omega z} \langle \delta E(t) \delta E(t + \tau) \rangle d\tau. \]  

(4.7)

Using the above equation, the transition rate is given by

\[ \Gamma_{0 \to 1} = \frac{Q^2}{4m\hbar\omega_z} S_E(\omega_z) \]  

(4.8)

It is worth noting that if one starts with the full dynamical trapping potential \( \Gamma_{0 \to 1} \) is given by [WMI+97],

\[ \Gamma_{0 \to 1} = \frac{Q^2}{4m\hbar\omega_z} \left( S_E(\omega_z) + \frac{\omega_z^2}{2\Omega^2} S_E(\Omega \pm \omega_z) \right) \]  

(4.9)

where the additional term represents the coupling between the noise fields and the rf trapping fields. However this term is suppressed by a factor \( \sim 0.05 \) for typical trapping parameters and can be safely ignored.

The formulation of \( \Gamma_{0 \to 1} \) in terms of electric field noise facilitates the comparison of the heating rates of two different traps. A direct measurement of the heating rate will depend on the mass and charge of the ion, as well as the secular frequency of the trap. On the other hand \( S_E(\omega_z) \) does not depend on the species of the trapped ion or the trap, and its only dependence on the secular frequency comes from the frequency dependance of the noise fields:

\[ S_E(\omega_z) = \frac{4m(2\pi\hbar)\omega_z}{Q^2} \dot{n}. \]  

(4.10)

### 4.3 Characterizing Anomalous Heating in Ion Traps

The trapped ion quantum computing architecture as envisaged in [CZ95] creates two-qubit gates using long-range Coulomb interactions between the trapped ions, combined with qubit state-dependent excitation of the ion motion. In this scheme, as well as other implementations of two-qubit gates [BNS+94, CZ00, MSJ00, MW01, MS99, MLK+97, SM99, SDM04, Ste96], it is vital to maintain quantum coherence
in the motion of the trapped ion. Ideally one can isolate the ion motion from the environment, which means that the average number of motional quanta \( \langle n \rangle \) will stay constant during the gate operation. However quantum error correction protocols can correct for a heating rate of \( \dot{n} \approx 10^{-4} \) quanta/\( \tau_{\text{gate}} \), where \( \tau_{\text{gate}} \) is the time required to perform a specific gate operation. Hence it is important to measure and characterize the heating rate of ion traps used in quantum computation. In the previous section

![Figure 4-1: A plot of the normalized electric field noise spectral density \( \omega S_E(\omega) \) versus the distance between the ion to the trap electrodes \( d \). The open symbols indicate low temperature data and the filled squares indicate data taken at room temperature. The dashed lines are the \( 1/d^2 \) fits to the low and high temperature data points. Reproduced from [HCW+12].](image)

the protocol for measuring the heating rate of an ion trap was described. Figure 4-1 is a plot of the normalized electric field noise spectral density, \( \omega S_E(\omega) \), as a function of \( d \), the separation between the ion and trap surface in \( \mu \text{m} \). This data is an aggregate of experiments done in different traps, with different types of electrodes. The electrode materials are indicated in the legend and the open and filled symbols correspond to low and room temperature experimental data, respectively.

Figure 4-1 illustrates why this noise is in fact anomalous. The intuitive lower limit for heating rate is the Johnson noise due to the thermal motion of the electrons in the bulk of the metal which in turn generates a fluctuating potential (see section 5.1). However the measured noise value at room temperature is five or-
ders of magnitude larger than the Johnson noise estimate for the trap (indicated by the red crosses in Fig. 4-1). In addition to the size of the electric field noise spectral density, the experiments measure the distance dependence of the spectrum and its frequency dependence. The distance dependence of the data is best described by $1/d^4$ and its frequency dependence follows $1/f^\alpha$ with $\alpha < 2$ (see for example [TKK+00, LGA+08, LGL+08, HCW+12]). In section 5.1 we show how the distance and frequency dependence of the observed noise is also not consistent with the Johnson noise model. These three factors have led to the creation of various models in an attempt to describe this anomalous heating. We will discuss these models in the next chapter.

4.4 Experimental Progress in Reduction of Anomalous Heating

Section 4.3 presented the wealth of data gathered to characterize anomalous heating in ion traps. The experimental observations and the subsequent theoretical investigations have been followed by the development of new techniques for reducing this noise. These techniques attack this noise on two separate fronts. The first involves disabling thermally activated processes responsible for the electric field noise by operating the trap at lower temperatures. The second is concerned with creating a pristine trap surface, free of any contamination.

Deslauriers et al. [DOS+06] were the first to demonstrate a reduction in heating rate as the ion trap was cooled down to $\sim 150$ K with liquid nitrogen using a “needle trap” with tungsten electrodes. More recently Labaziewicz et al. [LGA+08, LGL+08] demonstrated a further reduction in heating rates by operating a gold surface-electrode ion trap at cryogenic temperatures $\sim 6$ K. While cooling the trap does reduce the heating rate it is not a scalable solution and more importantly the observed heating rate is still several orders of magnitude larger than the expected Johnson noise.
The scatter in the data shown in Fig. 4-1, which is an aggregate of experimental data from a variety of surface electrode ion traps, indicates that the heating rate is not dependent on the choice of material and the fabrication method. The independence of the heating rate from the bulk properties of the material has led to recent experimental efforts to create a better trap surface. An ideal trap surface should have minimal variation in work function over an area sensed by the ion and should be free of contaminants (see chapter 5). The variations in the work function of a bare metal surface arise at the interface of crystalline domains or due to variable surface composition. Additionally the diffusion of adatoms on the surface cause fluctuations in the local work function which in turn causes electric field fluctuations at the location of the ion. However recent experimental data indicates that an even more important source of the anomalous heating is the accumulation of carbon contaminants [HCW+12, HCW+13] on the trap surface during the trap fabrication. This has lead to the development of the in situ cleaning procedures which are described below.

The first surface cleaning procedure involves the application of high-intensity laser pulses to remove the surface contaminants. In [AHJ+12] 3-5 ns pulses from a frequency tripled Nd:YAG laser were used to clean the trap surface which lead to a 2-fold reduction in the heating rate. The second in situ procedure involving bombarding the trap surface with Ar$^+$ was more successful, reducing the heating rate by a factor of 100 [HCW+12] (see Fig. 4-1). This experiment was performed on Au surface electrode ion traps at room temperature and the resulting heating rates rivaled those achieved by Labaziewicz et. al at cryogenic temperatures [LGA+08, LGL+08]. It is worth noting that the frequency scaling of the noise before and after the ion bombardment procedure remains the same. This indicates that the underlying noise mechanism is the same before and after the cleaning procedure.
Chapter 5

Sources of Electric Field Noise in Ion Traps

The previous chapter introduced the anomalous heating present in planar ion traps and presented the existing data on the characteristics of this noise. As it was discussed previously this noise which heats of the ion out of its ground motional state poses a challenge to the scalability of trapped-ion architectures. In particular, in order for this architecture to be scalable the traps need to be miniaturized. This reduces the distance between the ion and the trap surface. However the ion trap heating rate scales as $1/d^4$, where $d$ is the distance between the trapped ion and the trap electrodes. Therefore before attempting any large scale quantum computation we need to understand the mechanism behind the anomalous heating.

In the previous chapter we showed how electric field fluctuations cause the motional heating of the ion. This chapter focuses on the possible sources of the fluctuations that give rise to the heating. These sources can divided into two categories, depending on whether they have to be treated microscopically or macroscopically using lumped circuit models. Section 5.1 discusses thermal electric field noise due to the finite resistances of the trap electrodes and voltage sources. While the source of this noise is microscopic, lumped circuit models can be used as an adequate treatment.

The rest of the chapter will focus on noise sources that are due to fluctuations in microscopic regions on the trap electrodes. Since experiments indicate a reduction
in noise at cryogenic temperatures (see section 4.3) we focus on mechanisms that involve thermally activated processes. One such possible source is fluctuating potential patches which form on the trap surface due to the presence of adsorbates or crystal facets. The patch potential model is discussed in section 5.2. Section 5.3 introduces an ab-initio microscopic model which attributes the electric field fluctuations to fluctuating dipoles formed by surface adsorbates. Section 5.4 further refines this model by introducing a monolayer of impurities on the trap surface. Finally a brief discussion of diffusion noise models for electric field noise is presented in section 5.5.

Based on the current experimental data discussed in section 4.3, Johnson noise can be ruled out as a cause of the anomalous heating in ion traps. All other noise mechanisms discussed in this section may be responsible for the anomalous heating present in ion trap experiments and further study is needed to identify the underlying heating mechanism.

Sections 5.3 and 5.4 have been published in [SNRWS11] and [SNKW+13] respectively.

## 5.1 Thermal Electronic Noise: Johnson Noise Mechanism

The thermal electronic noise (Johnson noise) in ion traps is generated by two sources: noisy voltage sources and resistivity of the trap surface (electrodes). This section presents a discussion of models that have been used to explain Johnson noise in ion traps. Johnson noise is well understood and has been studied in great detail in [WMI+98, WMI+97]. Here we present a brief overview of the model and discuss the characteristics of this noise and its applicability to the motional heating of the ions.

Fluctuations in the trap voltages $U$ and $V$ (see Eq. 2.20) are one of the sources of the electric field noise. The voltage noise spectral density $S_V(\omega)$ can be related to
the electric field noise density by

\[ S_{E,\text{source}} = \frac{1}{d^2} S_V(\omega) \]  

(5.1)

where \( d \) is the characteristic length in the trap. In this case \( d \) is the distance between the ion and the trap electrodes (surface).

Johnson noise can also be caused by lossy or resistive elements. It is convenient to model this noise using a lump circuit model. While the source of this noise is microscopic, this treatment is justified because the relevant fluctuating field oscillate at \( \omega_z \). The corresponding wavelength of these fields is much larger than the relevant trap length scales, e.g. the size of the trap electrodes.

A resistor \( R \) at temperature \( T \) generates a voltage noise with spectral density \( 4k_B T R \). Hence the finite conductivity of the trap electrodes and the surrounding circuitry gives rise to an electric-field noise spectral density

\[ S_{E,\text{Johnson}}(\omega) = \frac{4k_B T R(\omega)}{d^2} \]  

(5.2)

where \( d \) is the distance between the trap electrodes to the ion, \( T \) is the temperature of the system and \( R(\omega) \) is the resistance seen by the ion due to the electrode and the surrounding circuitry. In a typical trap \( R(\omega) = \rho l/A(\omega) \) where \( \rho \) is the electrode resistivity and \( A(\omega) \) is the effective cross-sectional area of the resistive path and is proportional to the skin depth \( \delta \) at frequency \( \omega \). Rearranging equation 4.10, we find that the heating rate of the trap due to Johnson noise is given by

\[ \dot{n}_{\text{Johnson}} = \frac{Q^2 k_B T R(\omega_z)}{m \hbar \omega_z d^2} \]  

(5.3)

The Johnson noise due to the finite resistivity of the trap electrodes can also derived from a microscopic starting point. The detailed derivation has been carried out in [WMI+98, WMI+97] where the trap surface is approximated as an infinite metal surface with conductivity \( \sigma \). The component of the electric-field noise spectral
density parallel to the surface is given by

\[ S_{E, \text{Johnson}}(\omega) = \frac{k_B T}{8\pi \sigma d^2} \left( \frac{1}{2} + \sqrt{\frac{1}{4} + \frac{d^4}{\delta^4}} \right)^{1/2} \]  

(5.4)

where \( \delta = \frac{2}{\omega \mu \sigma} \) is the skin depth of the conductor. This expression reduces to Eq. 5.2 when \( d \ll \delta \), a condition which is satisfied for planar traps used in ion trap experiments.

Both types of Johnson noise scale as \( 1/d^2 \). While Johnson noise is a source of electric field noise, the magnitude of the electric field noise generated by this mechanism is three orders of magnitude smaller than the observed noise. This means that using typical trap parameters the motional heating rate due to Johnson noise, \( 0.1 \text{quanta/s} < \dot{n}_{\text{Johnson}} < 1 \text{quanta/s} \), is significantly smaller than the measured rate.

5.1.1 Johnson Noise Model: Frequency Dependence

Johnson noise has a white spectrum. This means that the spectrum of the electric field noise generated by this mechanism is independent of the frequency. Since the applied electrode potentials are low-pass filtered, Johnson noise mechanism would result in a \( 1/\omega^2 \) behavior for \( \omega \) larger than the filter cutoff. While the exact frequency dependence of the electric field noise in ion traps has not been conclusively established most experiments indicate that it behaves as \( 1/\omega^\alpha \) where \( \alpha < 2 \) (see section 4.3).

5.1.2 Johnson Noise Model: Temperature Dependence

Cryogenic experiments take advantage of the reduction of the heating rate at lower temperatures. Despite this, the temperature dependence of the heating rate has not been studied in detail experimentally. A theoretical prediction of the temperature dependence of each noise model will aid in narrowing the possible sources of anomalous heating.

The noise power spectral density of Johnson noise is given by \( 4k_B R(\omega, T)T \), where \( R(\omega, T) \) is the effective resistance of the sample at a given temperature \( T \). The spectral
Figure 5-1: The behavior of Johnson noise power spectral density can be extracted from the behavior of the resistivity of the sample $\rho$ as a function of its temperature $T$. In (a) we plot $\rho(T)$ for bulk gold. The corresponding noise spectral density is shown in (b). The dashed line is a fit of the form $S_0 (1 + (T/T_0))^{\beta}$. The values of $\beta$ and $T_0$ will be different for a micro fabricated trap where the plated film of gold contains impurities. Data taken from [Mat79].

The resistivity density has the same scaling behavior as $\rho(T)T$ where $\rho(T)$ is the resistivity of the sample at $T$. Hence for each trap we need to determine the behavior of $\rho$ in the operating range experimentally. Figure 5-1(a) shows the temperature dependence of resistivity of bulk gold as a function of temperature, which increases linearly for $T \gtrsim 30$ K [Mat79]. The corresponding noise spectrum is shown in Figure 5-1(b), and the dashed lines shows the fit $S_0 (1 + (T/T_0))^{\beta}$. While the functional behavior of bulk gold is similar to that of plated film of gold used in the ion trap, the fit exponent $\beta$ and the turnover temperature $T_0$ cannot be determined using the bulk gold data. The plated film is often contaminated with impurities which change the dependence of $\rho$ on temperature.

### 5.2 Patch Potential Model

In the previous section we established that thermal electric field noise (Johnson noise) is not consistent with experimental observations of motional heating in ion traps. An alternative explanation relies on the existence of patch potentials on metallic surfaces. These are microscopic regions arising from variations in the local work-function which
can occur at the interface of materials, crystalline domains or due to variable surface composition. The patch potential model relies on the existence of these microscopic regions on the trap electrodes due to the polycrystalline structure of the surface [REF], material composition [REF], charging of the trap [REF] or the presence of surface adsorbates to explain the electric field noise leading to the motional heating of the trapped ion.

In order to build the patch potential model, we need to first establish a fluctuation mechanism. Here we will consider tunneling processes and thermally activated mechanisms that lead to fluctuations in the potential. In the following we will follow the formalism developed in [TKK+00] and [DH81] to derive the distance dependence and the frequency dependence of the noise spectrum, and the resulting motional heating due to fluctuating patches without considering a specific physical source.

5.2.1 Distance Dependence

Following the derivation presented in [TKK+00], we use an approximate model to derive the dependence of anomalous heating in ion traps due to fluctuating patches on the trap surface. We consider the trap electrodes to form a spherical conducting shell of radius \( d \) about the ion. We model the patches by circular discs of size \( r_p \ll d \) and electric potential \( V_p(\omega) \). The electric field generated by the patch potential at the location of the trapped ion is given by

\[
E_p(\omega) = -3V_p(\omega) \frac{r_p^2}{4d^3} \tag{5.5}
\]

and is directed towards the patch. The number of patches on the trap surface contributing to the total electric field at the location of the ion is given by \( N \propto \frac{\sigma^2}{\tau_p^2} \). For uncorrelated patches

\[
\langle E_p^2(\omega) \rangle = N \left( \frac{3r_p^2}{4d^3} \right)^2 \langle V_p^2(\omega) \rangle \propto \frac{r_p^2}{d^4} \langle V_p^2(\omega) \rangle \tag{5.6}
\]
Hence, the electric field noise is related to the voltage noise as

\[
S_E(\omega) \propto \frac{r_p^2}{d^4} \langle S_V(\omega) \rangle
\]  

resulting in a heating rate \( \dot{n}_p \) which scales as \( 1/d^4 \).

While the distance dependence derived for the patches is independent of the source of the patches, in the following we will consider a specific case which will also be relevant to the discussion in section 5.3. We can model the patches as random distributions of point dipoles with dipole moment \( \vec{\mu} \), formed by surface adsorbates. We assume that the dipole moment can only point up or down, perpendicular to the trap surface. If the ion is trapped at distance \( d \) from the trap surface, the field due to a single dipole at \( \vec{r} = x\hat{x} + dy \hat{y} \) at the position of the ion is

\[
\vec{E} = \frac{1}{4\pi \epsilon_0} \left( \frac{3(\vec{\mu} \cdot \vec{r}^3 - \vec{p})}{r^3} \right)
\]

If the surface density of the dipoles is \( n_s \) there are \( N = \frac{2\pi}{x} n_s dx \) dipoles in a ring of radius \( x \) and thickness \( dx \) on the trap surface. If \( \langle \mu \rangle = 0 \), the expected magnitude of the electric field due to these dipoles at the position of the ion is given by

\[
\left\langle \left( \vec{E} \cdot \hat{x} \right)^2 \right\rangle = \frac{3n_s \langle \mu^2 \rangle}{4(4\pi \epsilon_0)^2 d^4}
\]

In order to extract the frequency dependence of the electric field noise, we Fourier transform the above equation to find

\[
S_E(\omega) = \frac{3n_s S_\mu(\omega)}{4(4\pi \epsilon_0)^2 d^4}
\]

where \( S_\mu(\omega) \) is the dipole spectral density. We will derive the explicit form of \( S_\mu(\omega) \) for two-level fluctuators in section 5.2.2, and for multi-level fluctuators in 5.3.
5.2.2 Patch Potential Model: Frequency Dependence

As we showed before the patch potential model can describe the distance scaling of the electric field noise without specifying a source for the fluctuations. To derive the frequency dependence we need to make further assumptions about the nature of the fluctuators. The derivation in this section closely follows the derivations in [DH81], which tries to provide a phenomenological model for the 1/f dependence of the spectrum observed in some experiments (see section 4.3). Here we assume that the noise process is due to two-level fluctuators, e.g. electric dipoles with dipole moment $\mu$ that are formed on the metal surfaces by adsorbates that can switch between pointing up or down through a Debye-type relaxation process with relaxation rate $\Gamma$. The dipole spectral density corresponding to this process is

$$ S_\mu(\omega) = \frac{2\mu^2\Gamma}{\Gamma^2 + \omega^2} \quad (5.11) $$

For a thermally activated process, $\Gamma = \Gamma_0 e^{-E/k_BT}$, where $E$ is the activation energy for the relaxation process. If the relaxation process has a single activation energy, we recover the dipole fluctuation spectrum of a single two level fluctuator

$$ S_\mu(\omega, E) = \frac{2\mu^2\Gamma_0 e^{-E/k_BT}}{\Gamma_0^2 e^{-2E/k_BT} + \omega^2}. \quad (5.12) $$

which has a Lorentzian frequency dependence.

The 1/f noise emerges in systems where the relaxation rates take on a range of values with a given distribution. Following [DH81] we assume a distribution $D(E)$ for the activation energies:

$$ S_\mu(\omega, T) = \int dE D(E) S(\omega, E) \quad (5.13) $$

The spectrum in Eq. (5.12) is strongly peaked at $E_{\text{max}} = -k_BT \log \omega/\Gamma_0$ with a width of order $k_BT$. We can evaluate the integral in Eq. (5.13) by expanding $D(E)$ about
\[ E_{\max} \text{. We find} \]
\[
S_\mu(\omega, T) = 2\mu^2 \frac{k_B T}{\omega} \left[ D(E_{\max}) + \sum_{n=1}^{\infty} \frac{\mathcal{E}_n}{(2n)!} \left( \frac{\pi k_B T}{2} \right)^{2n} \frac{d^{2n} D(E)|_{E=E_{\max}}}{dE^{2n}} \right]. \tag{5.14}
\]

where \( \mathcal{E}_n \) is the \( n \)th Euler number. If \( D(E) \) varies slowly compared to \( k_B T \), we can keep only the first term in the expansion, recovering the 1/f scaling,
\[
S(\omega, T) \propto 2\mu^2 \frac{k_B T}{\omega} D(E_{\max}) = A \frac{\mu^2}{f} \tag{5.15}
\]

where \( f = \omega/2\pi \) and \( A \) depends on the frequency spectrum of the oscillating dipoles. For thermally activated dipole relaxation processes, \( A \sim 1 - 10 \) [REF1,REF2] corresponds to the range of energy barriers through which relaxation occurs. We can now combine this result with Eq. 5.10 to write an explicit expression for the electric field noise due to patch potentials formed by adsorbate dipoles. The noise spectrum is given by
\[
S_E(f) = A \frac{3n_\delta \mu^2}{4f(4\pi\epsilon_0)^2d^4} \tag{5.16}
\]

For typical trap parameters 100 \( \mu \)m, \( f = 1 \) MHz, \( A \sim 10 \) and assuming \( \mu = 1 \) D, we find that a density of \( n_\delta \approx 6 \times 10^{19} \text{ m}^{-2} \) is needed to explain the observed heating rates at room temperature shown in Fig. 4-1.

### 5.3 Ab-initio Microscopic Model for Anomalous Heating

In this section, we develop a microscopic theory of anomalous heating in ion traps and other charged systems. The central assumption in this section is that the electric field noise in ion traps is produced by randomly-distributed fluctuating dipoles on the gold electrode surface, which in turn are formed by surface adsorption of atomic impurities, from the atmosphere or in fabrication. This assumption is in agreement with the experimental observations mentioned above and is supported by the fact
that in many traps the heating rate increases over time, especially in the trap loading zone [DNM+11].

In our model, fluctuations of the adatom dipole moment arise from phonon induced transitions between multiple bound surface states. We use analytic models supported by exact density functional calculations to analyze the adatom surface interaction potentials and the resulting time variations of the induced dipole moment. From this analysis we obtain the electric field fluctuation spectrum, and thereby the ion heating rate, as a function of the relevant microscopic parameters of the atom-surface interaction. Our calculations go beyond the standard scenario of two level fluctuators [DH81, CYM09, LGA+08, DNM+11] discussed in the section 5.2.2 and we show that the inherent multi-level structure of the surface potential leads to a characteristic frequency and temperature dependence, where even for a single atom a region with $1/f$ scaling emerges due to a distribution of different transition rates. The predicted distance dependence and heating rates are in good agreement with experimental measurements. More importantly, the characteristic features of our noise model could provide more insight into the microscopic origin of anomalous heating and be tested against other potential mechanisms [HH08a] which will be discussed in section 5.5.

5.3.1 Anomalous heating of trapped ions

Fig. 5-2 (a) shows a typical experimental setting where a single ion of mass $m_i$ and charge $q$ is trapped at a distance $d$ above a metal surface using combined static and inhomogeneous rf electric fields (Paul traps). For various designs of surface patterned micro traps [SCR+06, PLB+06, LGA+08, AUW+10, ASS+10, DNM+11, AHJ+12], the separation $d$ is between 20 to 100μm. When the ion is laser cooled the vibrational ground state fluctuating electric fields couple to the motion of the ion and lead to an increase of the average vibrational occupation number $\bar{n}$ with a characteristic rate [TKK+00]
Figure 5-2: a) Fluctuating dipoles associated with a random distribution of adsorbed atoms lead to heating of an ion trapped at distance $d$ above the surface. b) Dependence of the electric field fluctuation spectrum $S_E(\omega_t)$ (in arbitrary units) as a function of the trap-surface distance $d$. The results have been obtained from a numerical simulation of the electric field from $N = 100$ uncorrelated dipoles distributed randomly over an area of $100 \times 100 \times d_0^2$. $d_0$ is the minimum separation between two dipoles.
\[ \dot{n} = \frac{q^2}{2m_I \hbar \omega_t} S_E(\omega_t). \] (5.17)

Here \( \omega_t \) is the trapping frequency of the ion, typically in the range \( \omega_t/2\pi \approx 0.1 - 10 \) MHz, and \( S_E(\omega) = \int_{-\infty}^{\infty} d\tau \langle \delta E(\tau) \delta E(0) \rangle e^{i\omega \tau} \) is the spectrum of the fluctuating electric field \( \delta E(t) \) (projected onto the trapping axis) at the position of the trap. The heating rate (5.17) can be measured in experiments and thereby provides an accurate probe of the electric field noise over the accessible distance and frequency range.

In our model we consider electric fields originating from a distribution of fluctuating dipoles \( \tilde{\mu}_t(t) \) which are associated with individual atoms adsorbed on the surface at positions \( \tilde{r}_i \). In accordance with previous "patch potential" models [TKK+00, DCG09b] the assumption of uncorrelated noise sources leads to the expected distance dependence \( d^{-4} \). This is illustrated in Fig. 5-2 (b) where we have numerically evaluated the electric field noise of \( N = 100 \) randomly distributed dipoles on a surface. More explicitly, by averaging over a homogenous distribution of atoms with area density \( \sigma \) the electric field noise spectrum at the position of the ion can be written as

\[
S_E(\omega_t) = \frac{3}{8} \frac{\sigma}{(4\pi \epsilon_0)^2} \frac{S_\mu(\omega_t)}{d^4}, \] (5.18)

where \( S_\mu(\omega) = \int_{-\infty}^{\infty} d\tau \langle \delta \mu_z(\tau) \delta \mu_z(0) \rangle e^{i\omega \tau} \) is the spectrum of the fluctuating dipole of a single adatom. Our main goal in the remainder of this paper is to provide a microscopic derivation of the dipole-fluctuation spectrum \( S_\mu(\omega) \), which by using Eq. (5.17) and Eq. (5.18) allows us to establish a direct relation between the ion heating rate and the microscopic details of the atom surface interactions.

5.3.2 Atom-surface interaction

Atoms approaching a surface experience an attractive force which at large distances is the well-studied van der Waals (vdW) potential \( -C_3/\epsilon^3 \) which eventually becomes repulsive again when the electronic wavefunctions of the adsorbant and the bulk atoms overlap. An atom approaching the surface can lose energy by phonon in-
duced processes and get trapped in the resulting potential well. We develop a model, based on physical intuition, which captures the essential aspects of the atom-surface interaction. To this end, we present *ab initio* density-functional calculations (DFT) of hydrogen adsorption on Au(111) surface and obtain the interaction potential normal to the surface. This potential is used as proxy for our model atom-surface potentials which more closely mimic realistic impurity reactivity on gold surfaces. The utility in using a parametric model potential rests in its flexibility for tuning phonon transition frequencies, and range of both short-range and vDW interactions.

**Ab initio atom-surface potentials**

For the calculations to be manageable, we chose hydrogen adsorption on the gold surface. Clearly, surface contaminants are more than hydrogen atoms and contain atmospheric species. We incorporate such species by devising realistic interaction potentials 5.3.2 to model the adsorption of atmospheric or fabrication impurities on gold surfaces. For the H–Au interaction, all-electron scalar relativistic calculations of the total energy and optimized geometries of a H–Au surface model system were performed using the spin-polarized density functional theory as implemented in the DMol3 software [Del00]. The exchange correlation energy was calculated using the local gradient approximation (LDA) with the parametrization of Perdew and Wang (PWC) [PW92].

In Fig. 5-3, the H-Au(111) surface potential is shown. The long-range interaction of atom-conductor potential is given by $C_3/z^3$, where $C_3$ is proportional to the atomic electric dipole transitions, and $z$ is the normal to the surface. The coefficient $C_3 = \frac{1}{4\pi} \int_0^\infty \alpha(i\omega)d\omega$ can be obtained numerically by evaluating the dynamic atomic polarizability at imaginary frequencies. The value of $C_3$ for hydrogen is given in Ref. [MDB97] as $C_3 = 7.36 \times 10^{-5}$ a.u. Allowance is made for the fact that Au dielectric constant is not infinite, i.e. $C_3(Au) = \frac{\epsilon - 1}{\epsilon + 1}C_3$, where $\epsilon$ is the dielectric constant for Au. The fundamental transition frequency is more than 25 THz, many orders of magnitude larger than any frequency scale in the experiments. Heavier adatoms on the gold surface mass scale the interaction potentials, leading to lowering of the
Figure 5-3: Potential energy curve for a H atom interacting with a $2 \times 2$ Au(111) monolayer along the normal to the surface calculated using density functional theory within the local density approximation.
Figure 5-4: Surface potential with potential depth $U_0$ and minimum at $z_0$. The potential supports several bound vibrational states with energies $\hbar \nu_i$. The arrows represent the phonon mediated transitions between the bound states. The parameters used for this plot are $U_0 = 12$ meV, $z_0 = 6.05 \sigma_0$, $\beta = 0.95 \sigma_0^{-1}$ and an atomic mass of $m = 20$ a.u. These parameters correspond to the case of Ne on a gold surface.

transition frequencies.

Model atom-surface potentials

To describe the atom-surface interactions for wider range of atoms we use a model potential which is commonly referred to as exp-3 [Hoi80]. This potential is frequently used in surface science studies [Hoi80] and provides a suitable description for short and medium range distances. Our potential in this range is described by

$$U(z) = \frac{\beta z_0}{\beta z_0 - 3} U_0 \left[ \frac{3}{\beta z_0} e^{\beta z_0 (1-z/z_0)} - \left( \frac{z_0}{z} \right)^3 \right],$$

(5.19)

where $z_0$ is the equilibrium position, $U_0$ is the depth of the potential and $\beta$ is the reciprocal range of repulsion. The typical shape of this potential is plotted in Fig. 5-4. In the long range Eq. (5.19) reproduces the correct $-C_3/z^3$ form where $C_3 = \frac{\beta z_0^3}{\beta z_0 - 3} U_0$ in terms of the model parameters, and by adjusting these three parameters, we can modify $U(z)$ to fit realistic atom-surface potentials. The potential supports
several bound vibrational states with energies $E_i = \hbar\nu_i$ as indicated in Fig. 5-4. By using an harmonic expansion of $U(z)$ we find that for an adatom of mass $m$, the typical vibrational excitation frequency is approximately given by

$$\nu_{10} := \nu_1 - \nu_0 \approx \sqrt{\frac{U_0}{m z_0^2} \frac{3(\beta^2 - 4\beta)}{(\beta - 3)}},$$

(5.20)

where $\beta = \beta z_0$. From this result, we also find a rough estimate of the number of strongly bound vibrational states $N_b \approx U_0/\hbar\nu_{10}$.

From the exact H-Au potential shown in Fig. 5-3, we deduce $U_0 \approx 2$ eV, corresponding to a temperature of $T = 1.6 \times 10^4$ K, $z_0 \approx 1.6\text{Å}$ and $\beta \approx 3.91\text{Å}^{-1}$, as example for an adatom with a high reactivity with the Au surface. Because of the low mass of H, also the vibrational frequencies are in the range of $\nu_{10}/2\pi \approx 40$ THz. In general we expect a similar reactivity for other alkali atoms as can be seen for example for K-Ag where $U_0 = 1.79$ eV and $z_0 \approx 2\text{Å}$ [XLC+10]. However, due to the larger mass we obtain significantly lower vibrational frequencies $\nu_{10}/2\pi \approx 4$ THz. In contrast, for weakly interacting atoms, we find from the widely-studied noble gas-metal potentials (see for instance, Refs. [dSS08, Oss86]) that potentials can be wider and much shallower. For example, for Ne on a gold surface $U_0 \approx 0.012$ eV, $z_0 \approx 3.1\text{Å}$ and $\beta \approx 1.86\text{Å}^{-1}$. Within this typical range of potential parameters and adatom mass $m \sim 10 - 150$ a.u., we expect the relevant vibrational frequency scales to be in the $\nu_{10}/2\pi \approx 0.1 - 1$ THz regime. For our model potential in Fig. 5-4, and using the reduced mass of Ne-Au, we find $\nu_{10}/2\pi \approx 0.3$ THz.

In our model of atom-surface interactions we ignore the dependence of $U(z)$ on $x$ and $y$ due to surface roughness. However, for a metal surface, where the electrons are smeared out, this variation should be weak. Also, the random motion of an otherwise fixed dipole along the $xy$-plane would lead to a different, $d^{-6}$ scaling of the heating rate which is not supported by experimental data.
5.3.3 Fluctuating Dipoles

Adatom dipoles

Adatoms adsorbed on the surface exhibit a finite permanent dipole moment perpendicular to the surface. This induced dipole moment can be understood from the distortion of the electronic wavefunctions. It is commonly argued that the dipoles form, when the impurity adatom valence electrons penetrate into the surface conduction bands, modifying the surface work-function. Here, we calculate the magnitude of the electric dipole moments of the adatoms, by resorting to elementary electrostatics, using image charge techniques. The electrons and the ionic core interact with the surface electrons through their respective image charges, as depicted in Fig. 5-5. We begin by writing the potential seen by the orbital electron due to its image charge [Ant74],

\[ V = -\frac{e^2}{8Z_n^3} \sum_i \left(z_i^2 + \frac{1}{2} \rho_i^2\right) - \frac{3e^2}{16Z_n^4} \sum_i \left(z_i^3 + \frac{1}{2} z_i \rho_i^2\right), \]

where \( \vec{r}_i = (\vec{\rho}_i, z_i) \) is the position of the \( i \)-th electron and \( Z_n \) is the distance from the nucleus of the adatom to the metallic surface (see Fig. 5-5). In specifying the position of the electron, we use \( z_i \) to refer to the distance from the electron to the nucleus along the normal to the surface. The first term is the above-discussed vdW interaction with the surface. The second term in Eq. (5.21) vanishes in the first order of perturbation expansion, but contributes to the second order energy shift, \( \Delta E^{(2)} \).

Following Ref. [Ant74], we use a variational ansatz of the form \( \phi = (1 + \sum_i \lambda_i z_i) \psi_0 \), where \( \psi_0 \) are the unperturbed atomic wave functions, and calculate \( \Delta E^{(2)} \), by varying the parameters \( \lambda_i \). From the deformed electronic wavefunction \( \phi \), we find an approximated induced dipole moment of the atom near the surface, \( P(Z_n) = \langle \phi | \sum_i e \vec{r}_i | \phi \rangle \). For hydrogen atom \( P(Z_n) = \frac{4.5a_0^5}{Z_n^4} \), where \( a_0 \) is the Bohr radius. Since the numerical factor in the expression is just the static polarizability of hydrogen, \( \alpha_H = 4.5a_0^3 \), this expression can be generalized to a generic atom with polarizability \( \alpha \),

\[ P(Z_n) = 0.47ea_0^{1/2} \alpha^{3/2} \frac{1}{Z_n^4}. \]
Figure 5-5: The adatom nucleus is at a distance $Z_n$ from the surface. The electron is at a distance $r_i$ from the nucleus.

We use the numerically constructed wave functions $|i\rangle$, corresponding to the vibrational bound states of our model potential $U(z)$, to evaluate the average induced dipole moments

$$\mu_{z,i} := \langle i | P(z) | i \rangle. \quad (5.23)$$

We should note that due to the image charges the dipole moment seen by the atom will be twice the induced dipole moment in Eq. (5.22). In Fig. 5-6 we plot the resulting induced dipole moments $\mu_{z,i}$ for the model potential parameters shown in Fig. 5-4. These parameters represent a weakly bound adatom similar to the Ne-Au surface potential [Oss86]. Using this potential together with the polarizability of Ne, $\alpha(\text{Ne}) = 0.36\text{Å}^3$ [KM85], and $Z_n = z_0$, we obtain an induced ground state dipole moment of $\mu_{z,0}(\text{Ne}) = 0.005\text{D}$. Hence the dipole moment seen by the Ne atom is approximately 0.01 D which is in good agreement with 0.016 D calculated for Ne in [dSS08]. Note that $\mu_{z,i} \sim \alpha^{3/2}/z_0^4$ and in general the typical magnitude of induced dipole moments is $\sim 1\text{D}$. For example in [VP05, STW99], it is shown that the dipole moment for Cs absorbed on Cu(100) is 4D. Similarly in [RM91] the induced dipole
Figure 5-6: Magnitude of the average induced dipole moments $\mu_{z,i}$ for different vibrational states $|\tilde{i}\rangle$. The values are shown for the model potential parameters given in Fig. 5-4 and a polarizability of $\alpha(\text{Ne}) \approx 0.36\text{Å}^3$.

moments for K adsorbed on W, Ni and Pd ranges from 1.45 to 3.1 D.

**Phonon induced transition rates**

The emission and absorption of phonons in the bulk lead to transitions between different bound vibrational states and result in fluctuations of the induced dipole moment of the adatom. To evaluate the phonon induced transitions rates, we approximate the trap electrode surface by a semi-infinite crystalline slab. The position of an atom in the solid is given by

$$\mathbf{r}_i = \mathbf{r}_i^0 + \mathbf{u}_i,$$

where $\mathbf{r}_i^0$ is the equilibrium position of the $i^{th}$ atom and $\mathbf{u}_i$ is its deviation from the equilibrium. We can write the displacements $\mathbf{u}_i$ terms of bosonic operators $a_\lambda(\mathbf{q})$ for
the phonon eigenmodes,

$$\mathbf{u}_i = \sum_{q, \lambda} \sqrt{\frac{\hbar}{2NM\omega_{\lambda,q}}} c_{\lambda}(q)(a_{\lambda}(q)e^{iqq_0} + h.c.),$$  \hspace{1cm} (5.24)

where $q$ is the quasi-momentum, $N$ is the number of atoms in the bulk and $M$ is their mass. For each $q$ the normalized vectors $c_{\lambda}(q)$ describe the three orthogonal phonon polarizations.

In the presence of phonons, the adatom surface potential $U(z)$ which in Eq. (3) has been defined for a static surface, will in general depend on the fluctuating positions of the bulk atoms so that $U(z) \rightarrow U(z, \{r_i\})$.

Expanding this potential to first order in $u_i$ gives,

$$U(z, \{r_i\}) \simeq U(z, \{r_i^0\}) + \sum_i \nabla U(z, \{r_i^0\}) u_i.$$  \hspace{1cm} (5.25)

Since our potential is already averaged over the two transverse directions, we are only interested in the variations in the normal direction. Further, the dominant deformation of the potential arises from the closest surface atom and in the following, we restrict the sum in Eq. (5.25) to a single atom.

We use Fermi's Golden Rule to evaluate the phonon induced transition rate between two vibrational states $|i\rangle$ and $|f\rangle$,

$$\Gamma_{i \rightarrow f} = \frac{2\pi}{\hbar} \sum_q \left| \langle f | \frac{dU}{dz} | i \rangle \right|^2 \left( |\langle n_q + 1 | u_z | n_q \rangle|^2 \times \delta(\Delta E - \hbar\omega_q) + |\langle n_q - 1 | u_z | n_q \rangle|^2 \delta(\Delta E + \hbar\omega_q) \right),$$  \hspace{1cm} (5.26)

where $\Delta E = E_i - E_f$ is the difference between the vibrational energies $E_{i,f}$, $n_q$ are phonon mode occupation numbers and in this equation $q \equiv (q, \lambda)$ includes the polarization label. Assuming $\Delta E > 0$ and using the mode decomposition in Eq. (5.24), the resulting phonon emission and absorption rates can be written as
Awi - Figg = i \frac{d}{dz} U(z) |i| \Delta \omega_{if} \rho \left( f | \frac{d}{dz} U(z) |i| \right)^2 n(\Delta \omega_{if}) + 1, \quad (5.27)

\Gamma_{i \rightarrow f} = \frac{\Delta \omega_{if}}{2 \pi \hbar v_3 p} \left( f | \frac{d}{dz} U(z) |i| \right)^2 n(\Delta \omega_{if}) \rho, \quad (5.28)

where \Delta \omega_{if} = |E_i - E_f|/\hbar, n(\Delta \omega) = \left( e^{\hbar \Delta \omega/k_B T} - 1 \right)^{-1}, v is the averaged speed of sound in the surface material and \rho is its bulk density.

In the following, we denote by \Gamma_0 = \Gamma_{i \rightarrow 0}(T = 0), the zero temperature decay rate from the first excited to the lowest vibrational state. From a simple harmonic approximation of \( U(z) \) around its minimum at \( z_0 \), we obtain the scaling

\[ \Gamma_0 \approx \frac{1}{4\pi} \times \frac{\nu_{10} m}{v^3 \rho}. \quad (5.29) \]

Using \( v = 3962 \text{ m/s} \) and \( \rho = 19.3 \text{ g/cm}^3 \) for Au, and the model potential parameters given in Fig. (5-4), with \( \nu_{10}/2\pi = 0.3 \text{ THz} \), we find \( \Gamma_0/2\pi \approx 3.31 \text{ MHz} \). For K-Au where \( \nu_{10}/2\pi = 4 \text{ THZ} \) \( \Gamma_0/2\pi \) is approximately 67 MHz and in general we expect \( \Gamma_0/2\pi \) to range from about 1 to a few hundred MHz. Note that the validity of Eq. (5.27) and Eq. (5.28) is restricted to transition frequencies \( \Delta \omega_{if} \) smaller than the Debye frequency \( \omega_D \) of the bulk material, which for gold is about 3.6 THz.

**Dipole fluctuation spectrum**

We are interested in the fluctuation spectrum of the induced dipole moment of a single adatom, defined as

\[ S_\mu(\omega) = \int_{-\infty}^{\infty} d\tau \left( \langle \mu_z(\tau) \mu_z(0) \rangle - \langle \mu_z(0) \rangle^2 \right) e^{i\omega\tau}. \quad (5.30) \]

Summarizing the results from the previous sections we can write the dipole moment operator as \( \mu_z = \sum_i \mu_{z,i} \rho_i \), where \( \rho_i = |i\rangle \langle i| \) is the projection operator on the vibrational level \( |i\rangle \). Therefore, for given values of \( p_i \) the dipole fluctuation spectrum can be related to the set of two-point correlation functions \( \langle \rho_i(t) \rho_j(t+\tau) \rangle \) of the vibrational...
populations. The populations in turn evolve according to the master equation
\[
\frac{d}{dt} \langle \rho_i \rangle = \sum_j M_{ij} \langle \rho_j \rangle,
\] (5.31)
where the diagonal \( M_{ii} = -\sum_{j \neq i} \Gamma_{i \rightarrow j} \) and the off-diagonal elements \( M_{ij} = \Gamma_{j \rightarrow i} \) are determined by the phonon induced transition rates discussed above. We evaluate the dynamics of the correlations \( \langle \rho_i(t) \rho_j(t + \tau) \rangle \) by first introducing the condition \( \sum_i \langle \rho_i \rangle = 1 \) into the master equation. For \( N \) bound states we have,
\[
\frac{d}{dt} \langle \rho_i \rangle = \sum_{j \neq N} M_{ij} \langle \rho_j \rangle + M_{iN} (1 - \sum_{k \neq N} \langle \rho_k \rangle) = \sum_{j \neq N} (M_{ij} - M_{iN}) \langle \rho_j \rangle + M_{iN}.
\] (5.32)
Since we are only interested in level populations, all coherences, \( \rho_{ij} = |i\rangle \langle j| \), in the density matrix can be omitted. Using the quantum regression theorem, we find for \( i < N \),
\[
\frac{d}{dt} \langle \rho_i(\tau) \rho_k(0) \rangle = \sum_{j \neq N} (M_{ij} - M_{iN}) \langle \rho_j(\tau) \rho_k(0) \rangle + M_{iN} \rho_k^{(0)}
\] (5.33)
where \( \rho_k^{(0)} \) is the steady state population in level \( k \). For \( i = N \) we obtain
\[
\frac{d}{d\tau} \langle \rho_N(\tau) \rho_k(0) \rangle = \sum_{i=1}^{N-1} (M_{Ni} - M_{NN}) \langle \rho_i(\tau) \rho_k(0) \rangle + M_{NN} \rho_k^{(0)}.
\] (5.34)
All two-point correlation functions can be calculated from the above two equations, and the full noise spectrum is obtained by summing all the two-point correlations.

### 5.3.4 Results and discussion

In Fig. 5-7, we plot the typical behavior of the dipole fluctuation spectrum \( S_\mu(\omega) \) as a function of frequency. The spectrum has been evaluated for the model potential parameters given in Fig. 5-4 and for different temperatures \( T \). The lowest temperature
$k_B T = 0.02 U_0$ corresponds to a situation where the thermal energy is smaller than the vibrational energy $h \nu_{10} \approx 0.1 U_0$ and only transitions between the two lowest vibrational states contribute to dipole fluctuations. In this case, the dipole fluctuation spectrum resembles that of a thermally activated two level system [CYM09], where at low temperatures

$$S_\mu(\omega) \approx (\mu_0 - \mu_1)^2 \frac{2 \Gamma_0}{\omega^2 + \Gamma_0^2} e^{-\frac{h \nu_{10}}{k_B T}}.$$  \hspace{1cm} (5.35)

For frequencies below the fundamental phonon transition rate, $\omega < \Gamma_0$, the spectrum is frequency independent (white noise) while above $\Gamma_0$ the scaling changes to $1/\omega^2$ as one would expect for a two-level system [CYM09]. The noise is thermally activated with a characteristic temperature scale $T = h \nu_{10}/k_B$, which depending on the atomic species ranges from few Kelvin to above room temperature for light and tightly bound adatoms like hydrogen.

When the temperature exceeds the characteristic vibrational energy $T > h \nu_{10}/k_B$, more and more vibrational levels are populated and contribute to the dipole fluctuations (curves in red, green and blue in Fig. 5-7). An intermediate frequency regime appears where the noise spectrum exhibits a $1/f$ scaling. We emphasis that in contrast to standard models for $1/f$ noise, based on a random set of two level fluctuators with varying parameters [DH81, CYM09], this $1/f$ scaling occurs in our model even for a single dipole and emerges from a distribution of different vibrational transitions rates $\Gamma_{1f}$ which contribute to the dynamics. We find that the approximate crossover between the white noise and the $1/f$ noise regime occurs at $\omega \approx \Gamma_0 \times (n(\nu_{10}) + 1)$.

To check the validity of our model, we compare our spectrum to the measured values. Using Eq. 5.18 we can relate $S_\mu(\omega)$ to $S_E(\omega)$. Since $S_\mu \propto \mu^2$, we note that in the $1/f$ noise region, $10^{-11} < S_\mu(\omega) < 10^{-7} \text{ D}^2/\text{Hz}$. The value for $\Gamma_0 \sim 1 - 10 \text{ MHz}$, and the $1/f$ behavior sets in at $10 - 100 \Gamma_0$ which corresponds to $10 - 100 \text{ MHz}$. Using the coverage fraction $\theta = 0.1$ corresponding to about $\sigma \sim 10^{18} \text{ m}^{-2}$, we find $3.2 \times 10^{-8} < \omega S_E(\omega) < 0.0032 \text{ V}^2/\text{m}^2$ at $d_0 = 10 \mu\text{m}$. The experimentally measured values range between $10^{-7} - 0.001 \text{ V}^2/\text{m}^2$ [DNM+11].
Figure 5-7: The dipole fluctuation spectrum $S_{\mu}(\omega)$ is plotted for six different temperatures $T$ (given in units of the vibrational excitation frequency $\nu_{10}$) and the model potential parameters given in Fig. 5-4 and Fig 5-6. The frequency is scaled by the zero temperature transition rate $\Gamma_0$. The curves in black ($k_B T/\hbar \nu_{10} = 0.2, 0.3, 0.4$) correspond to temperatures where only the two lowest vibrational states are populated. At these temperatures the spectrum resembles that of a two level fluctuator (see Eq. (5.35)) and its size increases with increasing temperature. For higher temperatures (shown in red, green and blue) more and more bound states are thermally occupied and an intermediate regime emerges where the dipole fluctuation spectrum exhibits $1/f$ noise scaling. For all temperatures, the crossover from the flat (white noise) regime to a $1/f^2$ noise or $1/f$ noise scaling occurs at around $\omega_c \approx \Gamma_0(n(\nu_{10})+1)$. 
Temperature dependence

The temperature dependence of the ion heating noise is more succinctly displayed in Fig. 5-8 as a function of scaled temperature in units of $\nu_{10}$. At low frequencies, i.e. in the white noise regime, the fluctuations are thermally activated, showing a peak at $k_B T / h \nu_{10} \approx 1$, while for higher temperature they fall off again as $\sim 1/T$. The suppression of low frequency fluctuations with increasing temperature is in principle expected from a single two level fluctuator. In some models based on multiple two level systems with a distribution of activation energies noise increases with increasing temperature over the whole frequency range [CYM09]. In our model this behavior is recovered for frequencies within the “1/f region” of the spectrum, $\omega \approx 20 \times \Gamma_0$, where the temperature dependence matches some of the experimental findings described in [LGA+08] and fits an Arrhenius curve $F(T) = S_T e^{-T_0/T}$ with the parameters, $S_T = 10^{-13}$ D$^2$/Hz and $T_0 \approx 0.242 U_0 = 56.9$ K. Finally, for very large frequencies, $\omega \gg \Gamma_0$, i.e. in the $1/f^2$ regime, noise scales linearly with $T$.

5.4 Effects of Monolayer Coverage on the Electric Field Noise

In the previous section we introduced an \textit{ab-initio} model for the anomalous heating based on fluctuating dipoles formed by the surface adsorbates. It is likely that in the experimental system the fluctuators are not adsorbed directly on the clean trap surface, but on a surface coated with several monolayers of impurities. In this section we study the effect of the presence of a monolayer on the noise spectrum. In particular we focus on two extreme cases of weakly interacting physisorbed monolayers as well as strongly interacting chemisorbed monolayers.

5.4.1 Atom-monolayer-gold surface interaction

As we discussed in section 5.3.2 the asymptotic potential for a polarizable atom with dynamic polarizability $\alpha(\omega)$, which approaches a surface of dielectric constant $\varepsilon$ is
Figure 5-8: Temperature dependence of the dipole fluctuation spectrum vs. normalized temperature \( (k_B T / h \nu_{10}) \). The three curves show the temperature dependence evaluated for frequencies in the “white noise regime” \( (\omega \rightarrow 0) \), the “1/f regime” \( (\omega = 20 \times \Gamma_0) \) and the high frequency, “1/f^2 regime” \( (\omega = 100 \times \Gamma_0) \). The other parameters are the same as in Fig. 5-7.
\[ U(z \gg z_0) \simeq -\frac{(e-1)C_3}{(e+1)z^3}, \text{ where } C_3 = \frac{1}{4\pi} \int \alpha(i\omega) d\omega \text{ and } z \text{ is the normal to the surface.} \]

As the atom approaches the surface, the interaction energy increases and the energy cost of electronic exchange between the electrons of the adsorbate atom and the bulk atom becomes too great to overcome, leading to a repulsive wall in the interaction potential. Below, we present \textit{ab initio} calculations of the interaction potential energies normal to the substrate surface of H atoms with a ML of adsorbate atoms He and N on top of the Au(111) surface.

**ML surface interaction potentials**

Total-energy calculations of bulk Au and Au(111) surfaces, with and without He and N adsorbate atoms, were performed using the spin-polarized density functional theory as implemented in the Vienna \textit{Ab initio} Software Package (VASP) [KF96]. The exchange correlation energy was calculated using the local gradient approximation (LDA) with the parametrization of Perdew and Wang (PWC) [PW92].

The interaction between valence electrons and ionic cores was described by the Projector Augmented Wave (PAW) method [Blö94, KJ99]. The Au 5d^{10}6s^1, N 2s^22p^3 and He 1s^2 electrons were treated explicitly as valence electrons in the Kohn-Sham (KS) equations and the remaining cores were represented by PAW pseudopotentials. The KS equations were solved using the blocked Davidson iterative matrix diagonalization scheme followed by the residual vector minimization method. The plane-wave cutoff energy for the electronic wavefunctions was set to 500 eV.

All structures were optimized with periodic boundary conditions applied using the conjugate gradient method, accelerated using the Methfessel-Paxton Fermi-level smearing [MP89] with a width of 0.2 eV. The total energy of the system and Hellmann-Feynman forces acting on atoms were calculated with convergence tolerances set to \(10^{-3}\) eV and 0.01 eV/Å, respectively. Structural optimizations and properties calculations were carried out using the Monkhorst-Pack special \(k\)-point scheme [MP76] with \(11 \times 11 \times 11\) and \(7 \times 7 \times 1\) meshes for integrations in the Brillouin zone (BZ) of bulk and slab systems, respectively.

The supercell consisted of a three-layer thick gold slab with (111) orientation and
a \( p(2 \times 2) \) mesh unit, covered by He or N adsorbate atoms on one side of the slab model. The calculated lattice constant of bulk Au was 4.06 Å, in close agreement with the experimental value of 4.0780 Å at 25°C [DD63]. The lattice parameters of the \( p(2 \times 2) \) Au(111) surface constructed by cleaving the optimized bulk structure were \( a = b = 5.74 \) Å and \( c = 25.00 \) Å, with ca. 20.00 Å vacuum separating slabs, and \( \alpha = \beta = 90^\circ \) and \( \gamma = 120^\circ \). Although a large vacuum region (ca. 20 Å) was used between periodic slabs, the creation of dipoles upon adsorption of atoms on only one side of the slab can lead to spurious interactions between the dipoles of successive slabs. In order to circumvent this problem, a dipole correction was applied by means of a dipole layer placed in the vacuum region following the method outlined by Neugebauer and Scheffler [NS92].

The He/Au(111) and N/Au(111) interaction potentials were calculated by gradually moving a single He or N atom along the \( z \)-axis normal to the Au(111) surface.

**Atomic adsorption on Au(111)**

Four different atomic adsorption sites are possible onto a Au(111) surface: 1) a bridge site between two gold atoms, 2) on top of a gold atom, 3) in a hollow site between three gold atoms, termed an hexagonal close packed (hcp) site when there is a gold atom in the layer directly beneath the surface layer, or 4) termed a face-centered cubic (fcc) site when there is a hole in the layer directly beneath the surface layer.

Total-energy calculations indicate that a single He atom adsorbs preferentially at the bridge site \( (E = -48.760 \text{ eV}) \), slightly more energetically favorable than at the top site \( (-48.756 \text{ eV}) \), the fcc site \( (-48.755 \text{ eV}) \) and the hcp site \( (-48.749 \text{ eV}) \). The elongated equilibrium He–Au bond distance of 3.58 Å suggests that He at the bridge site is weakly physisorbed to the Au(111) surface. For the adsorption of a single N atom, the fcc site is energetically preferred \( (E = -70.393 \text{ eV}) \) over the hcp site \( (-69.792 \text{ eV}) \), the bridge site \( (-69.098 \text{ eV}) \) and the top site \( (E = -66.510 \text{ eV}) \). Contrasting with the He adsorbate, the N atom occupying the fcc site appears chemisorbed to the Au(111) surface with a short N–Au bond distance of 2.05 Å.
Fig. 5-9 shows the adsorbate potentials of H on the bare Au surface and in the presence of an additional ML of He and N. Note that we have shifted the potentials so that $E(z_0 \to \infty) = 0$. The presence of the weakly adsorbed He results in a much shallower potential while the chemisorbed N has the opposite effect, creating a deeper well that support more bound states.

![Graph showing binding potentials](image)

Figure 5-9: The binding potentials for H adsorbate atoms on bare Au surface (solid) and Au surface covered with one ML of He (dotted) or one ML of N (dashed). The peak of the local potential at the position of the first Au layer, in direct contact with the N(He) ML, does (not) vary appreciably indicating the formation of a sizable (negligible) dipole moment. 1 Hartree = 27.21 eV.

**Atomic diffusion on Au(111)**

Although our primary focus in this work is on dipole fluctuations induced by atomic motion perpendicular to the surface, the numerical data obtained in the previous part allows us with no additional effort to evaluate the diffusion rates of adatoms
parallel to the surface. Such data could be relevant to other, diffusion related noise processes [GS85a, TvdZ66, HH08b] under identical conditions.

The surface diffusion coefficient is given by \( D = \frac{\sqrt{3} r_0^2 \Gamma}{4} \) for an fcc(111) surface, where \( r_0 \) is the lattice parameter [2.87 Å for Au(111)] and \( \Gamma \) is the jump rate. Two different diffusion regimes exist, namely a thermally activated regime and a quantum tunneling regime.

In the thermally activated regime, the thermal jump rate, \( \Gamma_{\text{therm}} \), can be calculated through the Arrhenius formula [Arr89],

\[
\Gamma_{\text{therm}} = \gamma \exp \left( -\frac{E_a}{k_B T} \right),
\]

where \( E_a \) is the activation energy barrier, \( k_B \) is the Boltzmann constant, \( T \) the temperature, and \( \gamma \) is a prefactor which contains dynamical quantities; \( \gamma \approx 10^{12} - 10^{13} \) Hz for most surfaces [OBWL01]. The diffusion of a He atom on Au(111) is expected to be nearly barrierless due to their weak physisorption interaction.

For the diffusion of a single N atom between adjacent stable fcc sites on Au(111) the activation energy was calculated in this study to be \( E_a = 0.17 \) eV using the nudge elastic band method within the DFT framework. This result is comparable to the value of \( \approx 0.10 \) eV determined previously from experiment and theory for the diffusion of Cr on Au(111) surface [OBD+05]. Following a simple Redhead’s analysis of the migration temperature on solid surfaces [Mas96], we estimate the temperature necessary for a N adatom to overcome this energy barrier to be \( \approx 65 \) K [\( E = 0.06 \) T kcal mol\(^{-1}\) K\(^{-1}\)]. Let us note that Redhead’s law predicts the migration temperature of Cr adatoms on Au(111) to be 39 K, in excellent agreement with experimental findings [OBD+05]. The thermally-activated diffusion jump rate of N on Au(111) at 65 K is calculated to be \( \Gamma_{\text{therm}} = 0.3 \) Hz for an activation energy of 0.17 eV and a prefactor \( \gamma = 5 \times 10^{12} \) Hz; this corresponds to a surface diffusion coefficient \( D = 1.2 \times 10^{-16} \) cm\(^2\)s\(^{-1}\). At \( T = 300 \) K, \( \Gamma_{\text{therm}} = 7 \times 10^9 \) Hz and \( D = 2.5 \times 10^{-6} \) cm\(^2\)s\(^{-1}\).

Below \( T \approx 65 \) K, thermally activated hopping is strongly suppressed, but adatoms
can still diffuse via quantum tunneling. Although a full quantum treatment of surface diffusion is quite involved [PL00] a characteristic rate can be estimated from the tunneling rate between neighboring sites. For a one-dimensional parabolic double-well potential this rate can be approximated by [Mer70]

\[
\Gamma_{\text{tunnel}} = \frac{2\omega}{\pi^{3/2}} \sqrt{\frac{2E_a}{h\omega}} \exp \left( -\frac{2E_a}{h\omega} \right),
\]

where \(\omega = \sqrt{2E_a/mb^2}\) and \(b\) is the barrier width \([b = 0.8 \text{ Å for Au}(111)]\). Therefore, the activation energy \(E_a = 0.17 \text{ eV}\) corresponds to \(\Gamma_{\text{tunnel}} \approx 70 \text{ Hz}\), which dominates over thermal activated processes below temperatures of about 75 K. If the calculated \(E_a\) is considered to be accurate within \(\pm 10\) meV, \(\Gamma_{\text{tunnel}}\) can vary in the range \(\approx 30 - 150\) Hz.

5.4.2 Work functions and surface dipoles

The work-function, \(W\), is defined as the minimum energy required to remove an electron from a solid to the vacuum region in the vicinity of the solid surface and is given by:

\[
W = V(\infty) - E_F,
\]

where \(V(\infty)\) is the plane-averaged electrostatic potential in the vacuum at a distance where the microscopic potential has reached its asymptotic value and \(E_F\) is the Fermi energy.

The electrostatic potential \(V(x, y, z)\) on a grid in real space can be obtained from a self-consistent electronic structure calculation using a plane wave basis set. The plane averaged potential is

\[
\bar{V}(z) = \frac{1}{A} \int \int_{\text{cell}} V(x, y, z) dx dy,
\]

where \(A\) is the supercell surface area. The asymptotic value \(V(\infty)\) can be extracted by plotting the variation of \(\bar{V}\) as a function of \(z\), as shown in Fig. 5-10 for a clean Au(111) surface and for a Au(111) surface covered by 1 ML of He and N atoms.
Figure 5-10: Au(111) slab models covered by a one-sided monolayer (1 ML) of (a) He atoms and (b) N atoms. The variation of the corresponding plane averaged electrostatic potential $\bar{V}(z)$ along the $z$-axis normal to the surface is represented for (c) He-covered and (d) N-covered Au(111) slabs, together with a clean Au(111) slab reference. The Fermi energy $E_F$ (horizontal dashed line) and the work-functions (vertical arrows) of the clean and adsorbate-covered slabs, $W_{\text{clean}}$ and $W_{\text{ads}}$, respectively, are also represented.

The calculated Fermi energy and electrostatic potential in the vacuum for the clean Au(111) surface are $E_F = -2.36$ eV and $\bar{V}(\infty) = +3.21$ eV. This corresponds to a work-function $W_{\text{clean}} = 5.57$ eV, in good agreement with the experimental value of 5.50 eV recently measured by Bröker et al. for this Miller index plane [BBF+08].

Adsorption of one monolayer of He atoms at bridge sites and N atoms at fcc sites onto the Au(111) surface results in $\bar{V}(\infty) = +3.24$ eV and $\bar{V}(\infty) = +4.68$ eV, respectively. Thus, the work-functions of He- and N-covered Au(111) surfaces are $W_{\text{ads}} = 5.60$ and 7.04 eV.

In order to analyze the change of the work-function upon atomic adsorption, we define the variation $\Delta W = W_{\text{ads}} - W_{\text{clean}}$. For the weakly physisorbed He monolayer this variation is negligible ($\Delta W = 0.03$ eV), unlike in the case of the chemisorbed
N monolayer ($\Delta W = 1.47$ eV). The variation of the work function results from the change in the surface electric dipole caused by adsorption of the adatoms. Simple electrostatics gives the relation

$$\Delta W = \frac{e \Delta \mu}{\epsilon_0 A},$$

(5.40)

where $A$ is the surface area taken up by one adatom, $\epsilon_0$ is the electric permittivity of free space and $\Delta \mu$ is the change in surface dipole, and is normalized per adatom. Since four adatoms form 1 ML covering the supercell surface area, the surface area by adatom can be approximated by $A \approx A/4$. We can now estimate the induced dipole moment for the case of He and N adsorbates. Using a DFT unit cell area of $A \approx 41$ Å$^2$ we find $\mu_{\text{He}} \approx 0.03$ D while $\mu_{\text{N}} \approx 1.60$ D.

It should be noted that the major contribution to the surface dipole results from the charge reordering associated with the formation of the chemical bonds between the metal surface and the adatoms. This contribution is foremost determined by the nature of the chemical bonds, but can also be modified by the packing density of the adatoms.

**Phonon Density of States in Presence of the Monolayer Adsorbates**

Phonon density of states (PDOS) were calculated by solving the dynamical matrix for bulk Au, clean Au(111) surface, and adsorbates (e.g., He or N) on the Au(111) surface as shown in Fig. 5-11. A $(2 \times 2 \times 2)$ supercell was adopted to obtain the force constant matrix of bulk Au that can be derived from the Hellmann-Feynman forces obtained from the DFT calculations using VASP [KF96]. The calculated PDOS of the bulk Au shows two main peaks represented by “T” and “L” that are in good agreement with previous experimental results [LSN73]. The longitudinal (L) and transverse (T) phonon modes of bulk Au are 4.61 THz and 2.75 THz, respectively, at a high symmetry point (X) in the Brillouin zone [LSN73].

The calculated surface PDOS using the $(2 \times 2)$ supercells are depicted in Fig. 5-11(b) for a clean Au(111) surface as well as for 1ML of adsorbates (He or N) on the Au(111) surface. There are three prominent peaks in the calculated PDOS of the
Figure 5-11: Phonon density of states (PDOS): (a) bulk Au, (b) bare Au(111) surface, (c) 1ML He-covered Au(111) surface, and (d) 1ML N-covered Au(111) surface. The curves in black are the calculated total PDOS and the shaded areas in red, blue, and green represent the partial PDOS projected to the surface atoms, He atoms, and N atoms, respectively. The peaks labelled by “T” and “L” refer to the transverse and longitudinal PDOS, respectively.

clean Au(111) surface, mainly contributed by the partial PDOS projected onto the surface atoms (red shaded area). The previous experimental study has identified four surface modes (2.31 THz, 3.5 THz, 4.0 THz, and 4.3 THz) at a high symmetry point (K) in the surface Brillouin zone [PFvdGB03].

The calculated PDOS of the 1ML He-covered Au(111) surface suggests a very weak interaction between He and the metal surface, providing no evidence of stretching or wagging modes of He atoms with respect to the metal surface. However, the partial PDOS projected onto the He atoms (blue shaded area) reveals the possible lattice
modes of the 1ML He atoms physisorbed on the surface as shown in Fig. 5-11(c).

Contrasting with the 1ML He-covered Au(111) surface, two additional peaks appear at high frequency above 5 THz for the 1ML N-covered Au(111) surface due to the wagging and stretching modes of N atoms attributed to the strong interaction with the metal surface, as shown in Fig. 5-11(d). The green shaded area represents the partial PDOS projected onto the N atoms.

5.4.3 Noise spectrum with ML present

Let us now evaluate the potential impact of different types of MLs on the dipole fluctuation spectrum of adatoms discussed in section 5.3.3. We first note that due to the high reactivity and low mass of H adsorbates – chosen in the previous section to reduce the DFT computational cost – the depth of the binding potential $U_{0,\text{bare}} = 1.85$ eV and vibrational frequencies $\nu_{10,\text{bare}}/2\pi \approx 40$ THz are exceptionally high. Therefore, for H adatoms thermally activated processes at room temperature do not play a significant role. However, the same qualitative changes that occur in the surface potential for H are also expected for heavier adatoms or molecules and for the following estimates we simply use the potentials shown in Fig. 5-9 together with the mass scaling relations in Eq. (5.29) to evaluate the noise spectrum for a more relevant range of adsorbable masses $m \sim 100$ amu.

In Fig. 5-12 we plot the dipole fluctuation spectrum $S_{\mu}(\omega)$ for a bare Au surface and in the presence of a He and N monolayer. For these results we have assumed $m = 100$ amu and two different temperatures $T = 50$ K (solid) and $T = 150$ K (dashed). The spectrum is given in units of $\mu_0^2/\Gamma_{0,\text{Au}}$, where $\mu_0$ is the dipole moment of the adatom in the vibrational ground state and is typically around 1 Debye. $\Gamma_{0,\text{Au}}$ is the characteristic phonon induced relaxation rate for the bare Au surface, which we use in all plots as a common frequency scale. For the bare Au surface where $z_0 \approx 1.59$ Å these values correspond to $\nu_{10}/2\pi \approx 4.5$ THz and ratios $k_B T/\hbar \nu_{10} \approx 0.20$ and 0.70 respectively. The analytic estimate given in Eq. (5.29) predicts $\Gamma_{0,\text{Au}}/2\pi \approx 2.2$ THz, but from Fig. 5-11b), we see that for these large vibrational frequencies the simple quadratic scaling of the PDOS already overestimates $\Gamma_{0,\text{Au}}$ by about a factor 5-10
Figure 5-12: The dipole fluctuation spectrum $S_\mu(\omega)$ as a function of $\omega/\Gamma_{0,Au}$ for adsorbate of mass $m \sim 100$ amu on He monolayer (black), N monolayer (red) and bare system (blue). For each system the solid curve corresponds to $T = 50$ K while the dashed curve corresponds to $T = 150$ K. The frequency $\omega$ is scaled by $\Gamma_{0,Au}$, the characteristic rate corresponding to the bare surface. The spectrum is given in units of $\mu_0^2/\Gamma_{0,Au}$, where $\mu_0$ is the dipole moment of the adatom in the vibrational ground state.

and more realistic values for $\Gamma_{0,Au}$ lie in the hundred GHz regime (for concreteness a value of $\Gamma_{0,Au}/2\pi = 250$ GHz is used for the plots in Fig. 5-12). For the assumed temperatures the dominant contribution of the noise comes from thermal excitations of the first excited vibrational state and the spectrum can be approximated by the Lorentzian

$$S_\mu(\omega) = (\mu_1 - \mu_0)^2 \frac{2\Gamma_0}{\Gamma_0^2 + \omega^2} e^{-\hbar \nu_{10}/k_B T}.$$  \hspace{1cm} (5.41)

In section 5.4.1, we have found that due to its low reactivity, the He ML results in a significantly shallower well depth, $U_{0,He} = 14.9$ meV, shifting the minimum to $z_{0,He} \approx 5$ Å. Both effects lower the vibrational frequency, $\nu_{10,He} \approx 0.4$ THz, and lead to
a drastic reduction of the characteristic phonon transition rate $\Gamma_{0,He}/2\pi \approx 150$ MHz. From Eq. (5.41) we see that this results in an increase of the low frequency noise level, but reduces the noise at frequencies $\omega \gg \Gamma_0$. Interestingly, Fig. 5-11c) shows that the projected PDOS of the He ML exhibits a sharp gap at frequencies around 0.5 THz. Since the adatom will be mainly affected by vibrations of the surface atoms, strong variation of $\Gamma_{0,He}$ within this frequency range is expected.

The more reactive N monolayer results in a deeper potential well with $U_{0,N} = 3.8$ eV, while only slightly affecting the equilibrium distance, $z_{0,N} \approx 2$ Å. This leads to an increase of the vibrational frequency, $\nu_{10,N} \approx 5.3$ THz and in general one would expect a corresponding increase of $\Gamma_{0,N}$. However, as shown in Fig. 5-11c) the strong binding of N leads to drastic modifications in the projected PDOS since vibrations of the ML atoms are mismatched in frequency and strongly decoupled from the phonons in the bulk. At frequencies around a few THz the numerically evaluated projected PDOS for the N ML is about a factor 100 smaller than for the bare Au surface and $\Gamma_{0,N} \approx \Gamma_{0,Au}/100 \approx 2\pi \times 2.5$ GHz. This is in contrast to a ML of similar reactivity, but matched phonon spectrum, where decay rates of $\Gamma_0 \sim 0.5 - 1$ THz are expected.

5.5 Diffusion Noise Model

So far three possible explanations for the motional heating of the trapped ions were presented: Johnson noise, patch potential model with two-level fluctuators and the ab-initio model based on fluctuating dipoles. This section follows the derivations presented in [GS85b] and [Gom73] to show how surface diffusion of adsorbates on the trap surface generates a frequency dependent electron-current noise spectral density. These formulations were motivated by the earlier work which used diffusion processes to explain the contact noise in semiconductors which had a $1/f$ behavior.

We model the trap surface as an infinite plane with out any boundaries with patch potentials of radius $r_p$ which are formed due to variations in the local work-function $\phi$. Here the patch potentials are analogous to the probe area discussed in [Gom73]. The noise spectrum generated by these patches will have the $1/d^4$ behavior described
in section 5.2.1. However the diffusion mechanism leads to a different frequency dependence. The noise spectral density can be derived from the field-emission current autocorrelation. The field-emission current density is given by the Fowler-Nordheim equation,

\[ j = BF^2 \exp \left( \frac{-b\nu}{F} \phi^{3/2} \right) \]  

where \( b = -6.8 \times 10^7 \), \( F \) is the electric field and \( \nu \) is an image correction term and \( B \) is a field-insensitive term. The presence of an adsorbate modifies the emission by changing \( \phi \) or \( B \). The induced dipole moment of the adsorbate modifies \( \phi \), while its intrinsic dipole moment modifies \( B \). In the following derivation we do not consider the induced and intrinsic dipole moments of the adsorbate separately. The equilibrium current in the patch is

\[ \langle i \rangle = \langle j \rangle A_p \]  

where \( A_p = \pi r_p^2 \) is the area of the patch. Using Eq. 5.42 the current fluctuations \( \delta i(t) = i(t) - \langle i \rangle \) can be written as

\[ \frac{\delta i(t)}{\langle i \rangle} = e^{-a[\phi^{3/2}(t) - \langle \phi \rangle^{3/2}]} - 1, \]  

where \( a = b\nu/F \). The work-function \( \phi \) is dependent on the field \( F \) and the adatom density \( n = N/A_p \), where \( N \) is the number of adaptors per patch. The dependance of \( \phi \) on \( F \) and \( n \) is given by

\[ \phi(F, n) = \phi(0, n) + 2\pi \alpha Fn \]  

where \( \alpha \) is the polarizability of the adatom. If the work-function fluctuations, \( \delta \phi \ll \langle \phi \rangle \), the current fluctuations are given by

\[ \frac{\delta i}{\langle i \rangle} = \frac{3}{2} a \langle \phi \rangle^{1/2} \delta \phi. \]
Using Eq. 5.45 we can write $\delta \phi$ as

$$\delta \phi = \delta \phi(0, n) + 2\pi \alpha F \delta n,$$  \hspace{1cm} (5.47)

and the relative current fluctuation as

$$\frac{\delta i}{\langle i \rangle} = \left( \frac{3}{2} a \langle \phi \rangle^{1/2} \frac{2\pi \alpha F + \partial \phi / \partial n}{A_p} \right) \delta N$$  \hspace{1cm} (5.48)

where we have used $\delta \phi(0, n) = (\partial \phi / \partial n) \delta n$. Using this expression for the relative current fluctuations we find that the relative field-emission current autocorrelation is given by

$$R(t) = \frac{\langle \delta i(t) \delta i(0) \rangle}{\langle i \rangle^2} = \left( \frac{3}{2} a \langle \phi \rangle^{1/2} \frac{2\pi \alpha F + \partial \phi / \partial n}{A_p} \right)^2 \langle \delta N(t) \delta N(0) \rangle$$  \hspace{1cm} (5.49)

where $\delta N(t)$ is the equilibrium adsorbate number fluctuations per patch. The particle number in the patch can be expressed in terms of the local particle densities $n(\vec{r}, t)$,

$$N(t) = \int_{A_p} n(\vec{r}, t) d\vec{r}.$$  \hspace{1cm} (5.50)

Using Eqs. 5.49 and 5.50 we can express $R(t)$ in terms of two-point auto-covariance of the density fluctuations,

$$R(t) = \left( \frac{3}{2} a \langle \phi \rangle^{1/2} \frac{2\pi \alpha F + \partial \phi / \partial n}{A_p} \right)^2 \int_{A_p} \int_{A_p} \langle \delta n(\vec{r}_1, t) \delta n(\vec{r}_2, 0) \rangle d\vec{r}_1 d\vec{r}_2.$$  \hspace{1cm} (5.51)

Classically the integrand can be written as

$$\langle \delta n(\vec{r}_1, t) \delta n(\vec{r}_2, 0) \rangle = \int_{A_{\text{trap}}} d\vec{r}_3 G(\vec{r}_1, t; \vec{r}_3) C(\vec{r}_2, \vec{r}_3)$$  \hspace{1cm} (5.52)

where $G(\vec{r}_1, t; \vec{r}_3)$ is the Green function for the diffusion equation, $A_{\text{trap}}$ is the area of the trap surface and $C(\vec{r}_2, \vec{r}_3) = \langle \delta n(\vec{r}_1) \delta n(\vec{r}_2) \rangle$ is the two-point covariance function.
In the classical approximation we find the general expression for $R(t)$,

$$R(t) = \left(\frac{3}{2}2^{1/2}\frac{2\pi \alpha F + \partial \phi / \partial n}{A_p}\right)^2 \int_{A_p} d\vec{r_1} \int_{A_p} d\vec{r_2} \int_{A_{trap}} d\vec{r_3} G(\vec{r_1}, t; \vec{r_3}) C(\vec{r_2}, \vec{r_3}).$$

(5.53)

This expression is valid for any boundary conditions. If one imposes the boundary less plane conditions explicit expressions for the Green function and two-point covariance can be found. The details of these calculations can be found in [REF]. These expressions can be used to construct an analytical expression for $R(t)$ and using the Wiener-Khinchin theorem the spectral density can be extracted from $R(t)$. In particular in can be shown that the at low and high frequencies the noise spectral density $S(\omega)$ is given by

$$\lim_{\omega \rightarrow 0} S(\omega) \propto \langle (\delta N)^2 \rangle r_p^2 D^{-1} \ln(D/r_p^2 \omega)$$

(5.54)

$$\lim_{\omega \rightarrow \infty} S(\omega) \propto (\delta N)^2 D^{1/2} r_p^{-1} \omega^{-3/2}$$

(5.55)

where $D$ is the diffusion constant.

While the model considered in this section relied on patch potentials the mechanism for generation of the noise was different than that discussed in section 5.2. In fact the diffusion mechanism leads to noise spectral density that scales as $\omega^{-3/2}$ at typical trapping frequencies. Since the recent experimental data shows a similar behavior it is likely that the anomalous heating in ion traps is at least in part due to diffusion processes. However more experimental data is needed to establish the frequency and temperature dependence of the anomalous heating in ion traps. This will allow us to identify the cause or coexisting processes that are behind the motional heating of the trapped ion.
Chapter 6

Part I: Conclusions and Outlook

The first part of this thesis presented an overview of the motional heating of trapped ions. We reviewed the basics of trap design in chapter 2. Chapter 3 presented the criterion for choosing a qubit, focusing on the Sr⁺ ion. Chapter 4 presented the experimental data for motional heating of the trapped ion. The motional heating is caused by the electric field noise and is referred to as anomalous heating since its behavior differs from the expected Johnson noise present in the trap. In particular the anomalous heating is larger than the Johnson noise by several orders of magnitude, scales as $1/d^4$, where $d$ is the separation between the ion and the trap electrodes, and has a $1/\omega^\alpha$ frequency dependence with $\alpha < 2$ (see section 5.1 for a review of the Johnson noise mechanism).

The main focus was to present theoretical models which could identify microscopic sources for the anomalous heating. We reviewed the patch potential model (section 5.2), the ab-initio model with fluctuating dipoles (sections 5.3 and 5.4), and finally the diffusion model (section 5.5). The main contribution of this thesis to the current understanding of the motional heating of the trapped ion was presented in sections 5.3 and 5.4 where the microscopic, fluctuating dipole model was discussed.

In 5.3 we developed a microscopic model for electric field noise generated by fluctuating dipoles associated with adatoms on a metallic surface. We showed that phonon induced transitions between different bound vibrational states cause fluctuations of the induced dipole moments and generate electric field noise which can contribute to
the anomalous heating observed in surface ion traps. The analysis were largely based
on analytic model potentials for the atom-surface interactions and induced dipole mo-
ments, allowing us to characterize the resulting field fluctuation spectrum for a wide
range of atomic or molecular species in terms of a small set of microscopic parameters.

Additionally we presented calculations of the noise induced heating in ion traps
due to randomly-fluctuating adatom dipoles in the presence of a single monolayer of
atomic species on Au(111) surface. Precise DFT calculations of surface potentials for
physisorbed and chemisorbed ML species provided us with accurate data for surface
potentials and PDOS from which the effects on the noise could be evaluated. We
have found that within our noise model, the presence of surface contamination can
lead to drastic modifications and depending on the reactivity of the ML species, the
PDOS and the frequency range, either enhance or reduce the noise level.

Our model predicts several distinct features for the electric field noise spectrum
which appear at characteristics frequency and temperature scales of the adatom sur-
face interactions. In future experiments the development of new trap designs [MLB+09]
could allow for more targeted search for these predictions, e.g. by probing samples
where a clean metal surface is contaminated with a single, pre-specified atomic species.
To access the frequency regime of 10 to a few 100 MHz, similar heating experiments
could be done with nano-mechanical resonators or carbon nanotubes, for which ac-
curate optical and electrical readout schemes have been developed (see for example
Ref. [PvdZ12] and references therein).

Additionally, careful experiments are needed to probe the distance dependence,
as well as the frequency dependence of the electric field noise. As we discussed in
the previous chapter, the current data collection is an aggregate of the heating rate
measurements performed on different traps, operating at different temperatures, with
different ion species. The noise mechanism in each of these experiments, particularly
in the two different temperature regimes, may be different. Hence, a credible mea-
measurement of $S_E(\omega)$ versus $d$ and $\omega$ should be performed using a single trap. This will
eliminate the variations in trap, and trapped-ion species. If the trap is operated at a
variety of temperatures, the validity of the diffusion model can also be tested, since
this mechanism has a well-defined temperature dependence.

On the theoretical front, more detailed diffusion models are needed. Such models need to account for the movement of adsorbates between the surface patch potentials and provide a credible mechanism for the slow diffusion within the patches.
Part II

“Simulating Many-body Hamiltonians with Ultra-cold Atoms and Molecules”
Chapter 7

Bose Gas in Optical Lattices

The ability to trap atoms and molecules in optical potential wells is a recent development in atomic, molecular, and optical physics. This important achievement, has led to the creation of defect-free optical lattices, formed by counter-propagating laser beams. These lattices provide us with an extremely tunable system, where the lattice depth, and lattice constant can be controlled by varying the laser intensity and wavelength, respectively. Moreover, Feshbach resonances allow for the precise control of the interparticle interactions. Hence optical lattice systems allow for experimental realization of a variety of condensed matter Hamiltonians, with a variety of lattice geometries.

In this chapter we introduce the theory of dilute bose gases in optical lattices. Section 7.1 reviews the theory of dilute bose gases. In section 7.2 we describe how an optical lattice can be used to trap neutral particles. Section 7.3 reviews the single particle properties of a bose gas trapped in a periodic potential.

7.1 Dilute Bose Gases

In this section, we review the basic theory of a dilute bose gas of neutral particles of mass $m$. The particles can be either atoms or molecules. Once the gas is cooled below its degeneracy temperature $T_c$, the particles form a Bose-Einstein condensate
(BEC). For an ideal, non-interacting gas the transition temperature is given by

\[ T_c = \left( \frac{n}{\zeta(3/2)} \right)^{2/3} \frac{2\pi \hbar^2}{mk_B} \]

(7.1)

where \( n \) is the particle density and \( \zeta(3/2) \approx 2.6124 \) is the Riemann zeta function.

Eq. 7.1 implies that below the degeneracy temperature, the phase space density of the gas \( \rho_{ps} \) is given by

\[ \rho_{ps} = n \lambda_T^3 \geq \zeta(3/2) \]

(7.2)

where \( \lambda_T = \left( \frac{2\pi \hbar^2}{mk_BT} \right)^{1/2} \) is the de-Broglie wavelength.

In an interacting gas, with the exception of helium, the phase-space density condition given in Eq. 7.2 cannot be fulfilled at thermodynamic equilibrium unless a solid phase is formed. However, the BEC can form under metastable conditions. Metastability is achieved if the three-body recombination processes become very rare. These three-body collisions are essential in the formation of the equilibrium configuration and eliminating them prevents the system from solidifying. In a gas of particle density \( n \), this condition is fulfilled if the spatial extent of the particle is much smaller than the average volume per particle, \( n^{-1} \). In this regime, two-body interactions dominate three-body recombination processes and thermalization results if the relaxations times associated with the two-body interactions are much shorter than the duration of the experiment, which is in turn shorter than the inverse rate of three-body recombination.

Alkali atoms can be treated by the dilute gas formalism if the interparticle separation is \( \sim 100 \text{ nm} \), corresponding to \( 10^{15} \text{ atoms/cm}^3 \). At ultra-cold temperatures \( \sim 1 \mu\text{K} \), only s-wave scattering, characterized by a scattering length

\[ a_s = \frac{m}{4\pi \hbar^2} \int d^3 \vec{r} V(\vec{r}) \]

(7.3)

occurs. Here \( V(\vec{r}) \) is the interparticle interaction which depends on the interparticle separation \( \vec{r} = \vec{r}_1 - \vec{r}_2 \) and the internal states of the particles. The s-wave scattering length can be interpreted as the apparent radius of the atoms when the atoms are
modeled as billiard balls. This interpretation allows us to write the condition for a dilute gas as

\[ na_s^3 \ll 1. \]  \hspace{1cm} (7.4)

Additionally, we can use Eq. 7.3 to define an effective interparticle interaction for point-like particles,

\[ V_{\text{eff}}(\vec{r}) = g\delta^{(3)}(\vec{r}) \]  \hspace{1cm} (7.5)

where \( g = \frac{4\pi\hbar^2a_s}{m} \) and \( \delta \) is the Dirac delta function. The effective interaction depends only on the scattering length. For Alkali atoms, the scattering length can be tuned to be positive or negative by varying the applied magnetic field near a Feshbach resonance, creating a repulsive or attractive interparticle interaction respectively [IAS+98, CGJT10].

The physics of a weakly interacting atomic BEC is well described by the Gross-Pitaevskii (GP) equation which describes the dynamics of the BEC order parameter and treats the interparticle interactions at the mean-field level. The GP equations can be extended to include small fluctuations using the Bogoliubov theory allowing one to accurately describe phenomena such as collective excitations of the system and its response to rotations. However the GP treatment cannot be applied in the presence of strong interactions, strong rotations or certain trapping potentials. The systems studied in this thesis are strongly confined in one or two dimensions, creating quasi two-dimensional and quasi one-dimensional systems, respectively. The trapping potential, combined with the interparticle interactions in the systems studied in this thesis require us to go beyond the GP description.

### 7.2 Optical Lattices

Optical lattices are artificial crystals of light formed by two or more counter-propagating laser beams [REF]. For instance two beams with wavelength \( \lambda \), propagating along the \( \hat{x} \) direction set up a standing wave of intensity \( I(x) \) and wavelength \( \lambda/2 \). The dipole coupling of the atom to the oscillating electromagnetic field induces a second order
Stark shift in the internal energy keels of the atom. This creates a trapping potential composed of a periodic array of potential wells. This section derives the optical lattice potential resulting from this coupling between the atom and the electromagnetic field.

The external electric field setup by the counter-propagating laser beams is

$$\vec{E}(\vec{r}, t) = 2E_0 \cos(\vec{k} \cdot \vec{r} - \omega_L t)$$  \hspace{1cm} (7.6)$$

where $\omega_L$ is the frequency of the monochromatic laser beams and $\vec{k} = (k_x, k_y, k_z)$ with $k_i = \frac{2\pi}{\lambda_i} (i = x, y, z)$. In the dipole approximation, where $\lambda_i$ is much larger than the spatial extent of the atom, the interaction Hamiltonian is given by

$$H_{\text{int}}(t) = -\vec{d} \cdot \vec{E}(\vec{r}, t)$$ \hspace{1cm} (7.7)$$

where $\vec{d} = -e \sum_i \vec{r}_i$ is the electric dipole moment of the atom with its electron positions given by $\{\vec{r}_i\}$. The interaction Hamiltonian shifts the energy of the internal states of the atom. These shifts can be calculated perturbatively if

$$|\Delta_L| = |\omega_L - \omega_0| \gg \Omega_0$$  \hspace{1cm} (7.8)$$

where $\Delta_L$ is the detuning of the laser beam, $\omega_0$ is an optical transition and $\Omega_0$ is the corresponding Rabi frequency. This condition ensures that the laser beam does not induce significant population transfer between the two states separated by $\omega_0$. Using perturbation theory, it is easy to see that the first order corrections vanish since the dipole operator is odd under $\vec{r}_i \rightarrow -\vec{r}_i$ transformation. The second order corrections are given by

$$\Delta E(\vec{r}) = -\frac{1}{2} \alpha(\omega_L) \langle \vec{E}(\vec{r}, t)^2 \rangle_t$$ \hspace{1cm} (7.9)$$

where $\langle \ldots \rangle_t$ denotes the time-averaged quantity over $t = \frac{\pi}{\omega_L}$ and $\alpha(\omega_L)$ is the polar-
izability of the atom given by

\[ \alpha(\omega_L) = \sum_\beta |\langle \beta | \vec{d} \cdot \vec{e} | g \rangle|^2 \left( \frac{1}{E_\beta - E_g + \hbar \omega_L} + \frac{1}{E_\beta - E_g - \hbar \omega_L} \right). \]  

(7.10)

Here \(|g\rangle\) and \(|\beta\rangle\) are the ground and excited states of the atom respectively, \(\vec{e}\) is a unit vector in the direction of the electric field, and \(E_g\) and \(E_\beta\) are the unperturbed energies of the ground and excited states, respectively. The atoms are trapped in an optical lattice with \(\omega_L\) chosen far detuned from any optical transition. Since the photon scattering rate scales with \(1/\Delta^2\), a large detuning suppresses the spontaneous emission rate of the atom. This in turn reduces heating and we can treat the optical lattice as a non-dissipative system. Hence in a typical experiment, the laser frequency is only close to one of the unperturbed excited states with \(E_e = \hbar \omega_e\), and there is no significant transition. In this regime, the term with the denominator \(E_\beta - E_g - \hbar \omega_L\) dominates the sum in Eq. (7.10). For the optical transition \(\omega_0 = \omega_e - \omega_g\), the polarizability is given by

\[ \alpha(\omega_L) \approx -\frac{|\langle e | \vec{d} \cdot \vec{e} | g \rangle|^2}{\hbar \Delta L} \]  

(7.11)

Combining Eqs. (7.9) and (7.11), we find the energy shift due to the applied electric field,

\[ \Delta E(\vec{r}) \propto \frac{I(\vec{r})}{\hbar \Delta L} \]  

(7.12)

where \(I(\vec{r})\) is the intensity of the laser beam.

This energy shift can be interpreted as an effective potential \(V_{\text{eff}}\) which follows the spatial pattern of the laser beam. The effective potential exerts a force on the atom which is known as the dipole force

\[ F_{\text{dipole}} = -\vec{\nabla} V_{\text{eff}}(\vec{r}) \]  

(7.13)

which attracts the atom to regions of high intensity when the laser is red-detuned \((\Delta < 0)\) and to regions of low intensity when the laser is blue-detuned \((\Delta > 0)\).

If the electric fields of two counter-propagating laser beams are linearly polarized
in the $x$ direction, the total field is given by

$$E_x(x, t) = 2E_0 \cos(k_xx - \omega_L t) + 2E_0 \cos(-k_xx - \omega_L t)$$  
(7.14)

$$= 4E_0 \cos(k_xx) \cos(\omega_L t)$$  
(7.15)

The corresponding effective potential is

$$V_{\text{eff}}(x) = V_0 \cos^2(k_xx)$$  
(7.16)

where $V_0 = 2E_0^2 \alpha(\omega_L)$. Hence the standing wave sets up an optical potential with periodicity $\lambda_x/2 = \pi/k_x$. This can be easily generalized to higher dimensions. For example one can form a cubic lattice by adding counter-propagating laser beams along the $y$ and $z$ directions setting up a potential

$$V_{\text{OL}}(\vec{r}) = V_{0x} \cos^2(k_xx) + V_{0y} \cos^2(k_yy) + V_{0z} \cos^2(k_zz)$$  
(7.17)

The lattice depth and periodicity can be manipulated individually for each direction. In this thesis, we consider one- and two- dimensional lattices in single and layered geometries. In many experimental systems the trapping potential consists of the periodic optical lattice potential $V_{\text{OL}}$ as well as a magnetic harmonic confinement $V_{\text{HO}}$. The total trapping potential is given by

$$V_{\text{trap}} = \sum_{i=x,y,z} V_{0i} \cos^2(k_ir_i) + \frac{1}{2} \sum_{i=x,y,z} \omega_i^2 r_i^2$$  
(7.18)

where $\omega_i$ are the trapping frequencies of the harmonic trapping potential. In the following we assume that the harmonic confinement varies on a scale greater than the optical lattice potential such that the variation of $V_{\text{HO}}$ can be ignored over a single site.
7.3 Single Particle in a Periodic Potential

The solution to the Shrödinger equation for a single particle in a periodic potential is well known [AM76]. The spectrum forms bands of allowed energies separated by energy gaps. The single particle wavefunction is given by Bloch functions

$$\Phi_{\alpha k} (\vec{r}) = e^{-i\vec{k} \cdot \vec{r}} u_{\alpha k} (\vec{r})$$

(7.19)

where $\alpha$ refers to the band index and $\vec{k}$ labels the quasi momentum $\hbar \vec{k}$. Here $e^{-i\vec{k} \cdot \vec{r}}$ is a plane wave and $u_{\alpha k} (\vec{r})$ is a periodic function with the periodicity of the external potential. For a given periodic potential, the energy eigenvalues, which form the bands, have the periodicity of the reciprocal lattice vector.

In optical lattices where the lattice depth is several times larger than the recoil energy $E_R = \frac{\hbar k^2}{2m}$, that is the change in the energy of the atom after absorbing a photon with momentum $\hbar k$, the separation between the low lying bands is much greater than the bandwidth. In this limit the optical potential provides harmonic trapping for the particle at lattice site $i'$. The band gap in the harmonic approximation is of the order of $\omega_T \approx \sqrt{4V_0 E_R}/\hbar$ [JBC+98]. At low enough temperatures, we can only consider the lowest energy band provided that the interactions between the particles do not induce inter-band transitions. Under these conditions it is more useful to form the single particle basis using the Wannier functions [Wan37] which are formed by the superposition of Bloch functions in momentum space. These functions form a complete set of orthonormal real, and localized functions for each band and are given by

$$w_{\alpha} (\vec{r}) = \frac{1}{\sqrt{N_{\text{sites}}}} \sum_{\vec{k}} e^{-i\vec{k} \cdot \vec{r}} \Phi_{\alpha \vec{k}} (\vec{r}),$$

(7.20)

where $N_{\text{sites}}$ is the total number of lattice sites. Wannier functions are particularly useful for deep optical lattices where tight binding approximation applies and $w_{\alpha} (\vec{r} - \vec{r}_i)$ is localized about the lattice site at $\vec{r}_i$. In the tight binding approximation, the Wannier functions for the $\alpha$-th band resemble the $\alpha$-th excited state of the harmonic trap centered at site $\vec{r}_i$. 

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7.4 Bose-Hubbard Model

The systems studied here all share the same starting point, i.e. the Bose-Hubbard model. The Bose-Hubbard Hamiltonian is the minimal model for interacting bosons in a lattice potential and can be realized with ultra-cold atoms trapped in optical lattices, as described in [REF]. The Bose-Hubbard model is given by

\[ H = \int d^3 r \hat{\psi}^\dagger(\vec{r}) \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\vec{r}) + \frac{g}{2} \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}) - \mu \right] \hat{\psi}(\vec{r}) \]  \hspace{1cm} (7.21)

where \( \hat{\psi}^\dagger(\vec{r}) \) and \( \hat{\psi}(\vec{r}) \) are the bosonic field creation and annihilation operators respectively, satisfying the bosonic commuting relations

\[ \left[ \hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}') \right] = \delta^{(3)}(\vec{r} - \vec{r}') \] \hspace{1cm} (7.22)

\[ \left[ \hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}') \right] = \left[ \hat{\psi}^\dagger(\vec{r}), \hat{\psi}^\dagger(\vec{r}') \right] = 0. \] \hspace{1cm} (7.23)

Here \( V_{\text{ext}} \) is the external trapping potential given by Eq. (7.18), and the third term in the brackets is the interparticle contact interaction as defined in Eq. (7.5). The work presented in this thesis is done in the grand canonical ensemble and the chemical potential \( \mu \) fixes the total number of particles in the system. The field operators can be expanded in the single particle basis.

Using the Wannier functions introduced in section 7.3, these operators are given by

\[ \hat{\psi}(\vec{r}) = \sum_{\alpha, i} w_\alpha(\vec{r} - \vec{r}_i) a_{\alpha, i} \] \hspace{1cm} (7.24)

\[ \hat{\psi}^\dagger(\vec{r}) = \sum_{\alpha, i} w^*_\alpha(\vec{r} - \vec{r}_i) a^\dagger_{\alpha, i} \] \hspace{1cm} (7.25)

If we restrict the sums in Eq. (7.24) to the lowest band the Bose-Hubbard model simplifies to

\[ H = -\sum_{i, j} J_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i, j, k, l} U_{ijkl} a_i^\dagger a_j^\dagger a_k a_l - \sum_{i, j} \mu_{ij} a_i^\dagger a_j \] \hspace{1cm} (7.26)
where

\[ J_{ij} = -\int d^3r w^*(\vec{r} - \vec{R}_i) \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_{OL}(\vec{r}) \right] w(\vec{r} - \vec{R}_j) \]  
\( (7.27) \)

\[ U_{ijkl} = g \int d^3r w^*(\vec{r} - \vec{R}_i) w^*(\vec{r} - \vec{R}_j) w(\vec{r} - \vec{R}_k) w(\vec{r} - \vec{R}_l) \]  
\( (7.28) \)

\[ \mu_{ij} = \int d^3r w^*(\vec{r} - \vec{R}_i) [\mu - V_{HO}(\vec{r})] w(\vec{r} - \vec{R}_j). \]  
\( (7.29) \)

In the deep lattice limit, the Wannier functions are well-localized on lattice sites and only those centered on nearest-neighboring sites have significant overlaps. In this limit, the dominant terms in the Hamiltonian given in Eq. (7.26) are \( U_{ii}, \mu_{ii}, J_{ii}, \) and \( J_{(ij)} \) where \((ij)\) indicates nearest-neighbor sites. The nearest neighbor contribution is significant due to the presence of the second derivative in the Hamiltonian. Hence in the deep lattice limit, we finally arrive at the well-known form of Bose-Hubbard Hamiltonian

\[ H_{BH} = -J \sum_{(ij)} a_i^\dagger a_j + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) - \sum_i \mu_i \hat{n}_i \]  
\( (7.30) \)

where the first term in the Hamiltonian is the kinetic energy term with hopping coefficient \( J \), the second term is the on-site interaction term with \( U = g \int d^3r |w(\vec{r})|^2 \), and \( \mu_i = \mu - V_{HO}(\vec{r}_i - \vec{r}_0) \) where \( \vec{r}_0 \) is the minimum of the harmonic trapping potential. Hence \( V_{HO} \) creates a local variation in the chemical potential. \( \hat{n}_i = a_i^\dagger a_i \) is the number operator at site \( i \). Figure 7-1(a) shows a schematic of a one-dimensional optical lattices with \( V_{OL} = V_0 \sin^2(kx) \), on-site interaction \( U \) and tunneling \( J \). Figure 7-1(b) is reproduced from [JBC+98], where the values of \( U \) and \( J \) were numerically determined for various lattice depths. The values for \( U \) (solid line) and \( J \) (dashed line) are shown in terms of recoil energy \( E_R \). It is clear that in an optical lattice experiment, \( J \) can be tuned over a large range of values by varying \( V_0 \) by tens of \( E_R \) and leaving \( U \) unchanged. This allows one to take the system from a system of isolated lattice sites at \( V_0 \approx 25E_R \) to a regime where the particles tunnel easily between neighboring sites at \( V_0 \approx 5E_R \).
Figure 7-1: (a) A schematic representation of the Bose-Hubbard Hamiltonian in Eq. (7.30) in a one-dimensional optical lattice. (b) On-site interaction $U$ and tunneling strength $J$ in units of recoil energy $E_R$ as a function of the optical lattice depth $V_0$. The tunneling can be tuned over a large range of values. The figure is reproduced from [JBC+98].

7.5 Physics of the Bose-Hubbard Model

In the previous section, we introduced the Bose-Hubbard model and showed how it could be realized using ultra-cold atoms trapped in an optical lattice. In this section, we will discuss the superfluid (SF) to Mott-insulator (MI) phase transition which is a paradigmatic quantum phase transition [FWGF89]. As discussed previously the Bose-Hubbard Hamiltonian in the grand-canonical ensemble is given by

$$H_{BH} = -J \sum_{<ij>} a_i^\dagger a_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \sum_i \mu_i \hat{n}_i$$

The kinetic energy term favors the delocalization of the particles, while the potential energy term suppresses density fluctuations and consequently localizes the particles to reduce the repulsive onsite interaction. The competition between the terms in the Hamiltonian is responsible for the SF to MI phase transition.

The following discussion describes the MI and SF phases in sections 7.5.1 and

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7.5.2 respectively. The phase diagram of the system is presented in 7.5.3. Finally section 7.5.4 discusses the MI-SF quantum phase transition.

Figure 7-2: (a) A schematic representation of MI phase in the $J/U \approx 0$ limit. (b) A schematic of the SF phase in the non-interacting limit with $U/J \approx 0$. (c) The zero-temperature phase diagram of Bose-Hubbard model. The lobes of MI phase occur at integer filling $\nu$ and the boundaries are given by Eq. (7.39). The system is in the SF phase outside of the lobes. The dashed line indicates $(J/U)_c$ for the first lobe which corresponds to the special transition at the tip of the lobe which happens at constant $\mu/U$ while increasing $J/U$.

7.5.1 The Mott-insulating Phase

It is easiest to study the MI phase in the limit where $J/U \ll 1$ where the particles are well-localized. In this limit the ground state of the system can be approximated by a product of Fock states as,

$$|\Psi\rangle_{J/U=0} \propto \prod_i |n_i\rangle$$  \hspace{1cm} (7.31)

Hence in this limit each site is occupied by a fixed number of bosons $n_i$ (see Fig. 7-2(a)). In the limit, where $J/U \approx 0$, the Bose-Hubbard model simplifies to

$$H_{BH}|J/U\approx0 = \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) - \sum_i \mu_i \hat{n}_i$$  \hspace{1cm} (7.32)
which is diagonal in the Fock basis. The eigenstates of $H_{BH}|_{J/U=0}$ are given by Eq. (7.31) and the eigenenergies are

$$E = \sum_{i} E(n_i)$$

(7.33)

$$E(n_i) = \frac{U}{2} n_i(n_i - 1) - \mu n_i$$

(7.34)

The ground state of the system for any $\mu$ corresponds to the value of $n_i$ for which the energy is minimized, that is

$$n_i = \lfloor \mu/U \rfloor$$

(7.35)

where $\lfloor \ldots \rfloor$ is the ceiling of the quantity. Hence as $\mu/U$ is varied, a series of steps in $n_i$ are observed at each integer value of $\mu/U$ and $n_i$ stays constant between two successive integer values. Hence, in this limit it is easy to see that the MI phase is incompressible, that is $\partial \langle \hat{n}_i \rangle / \partial \mu = 0$ except at the points where $\mu/U$ is an integer.

More generally, at finite $J/U$ the ground state of the system in the MI regime is not given by Eq. 7.31. The lowest energy excitations due to the presence of a finite but small hopping $J$ creates quantum correlated particle-hole fluctuations which conserve the particle number but introduce non-vanishing onsite fluctuations in the particle number. In low-dimensional systems these number fluctuations are significant even in the MI phase.

Since the MI phase is incompressible particle-hole fluctuations have an associated energy cost. Hence the energy gap in the MI phase for particle-hole excitations is a direct consequence of its incompressibility. We will discuss the energy gap in more detail in section 7.5.3.

### 7.5.2 The Superfluid Phase

As the hopping amplitude increases, particle delocalization becomes more favorable. Finally at some critical $(J/U)_c$, the system will enter the SF phase. We begin by describing the SF phase in the non-interacting limit with $U/J = 0$. In this limit, the
ground state of the system is a BEC in the zero-momentum Bloch state,

\[ |\Psi\rangle_{U/J=0} \propto \left( \sum_i a_i^\dagger \right)^N |0\rangle \quad (7.36) \]

where \( N \) is the total number of particles. Hence in this regime the eigenstate of the system is a product of single particle states and the particles are delocalized over the entire lattice (see Fig. 7-2(b)). In the thermodynamic limit, the wavefunction can be written as a product of coherent states \(|\alpha_i\rangle\) [BDZ08],

\[ |\Psi\rangle_{U/J=0} \propto \Pi_i |\alpha_i\rangle \quad (7.37) \]

This state is characterized by large onsite number fluctuations since the variance in the occupation number is \( \sigma_i = \langle \hat{n}_i \rangle \). Additionally it exhibits off-diagonal long-range order (ODLRO) (see e.g. [Leg06]), i.e.

\[ \lim_{|i-j|\to\infty} \langle a_i^\dagger a_j \rangle \neq 0 \quad (7.38) \]

where \( \langle a_i^\dagger a_j \rangle \) is the single particle density matrix.

At finite interactions \( U/J > 0 \), the superfluid state is no longer described by the BEC wavefunction given in Eq. 7.36. The introduction of interactions reduces \( \sigma_i \) and SF phase may be present in the absence of long-range order. For instance for low-dimensional systems the single particle density matrix exhibits algebraic decay corresponding to a quasi long-range order [Gia04]. Hence, in the following we will characterize the SF phase by the presence of a finite superfluid fraction, and not by the presence of long-range order or Bose-Einstein condensation. In contrast to the MI phase the excitations in the SF phase are gapless [BDZ08]. These excitations are Nambu-Goldstone modes with phonon-like dispersion relations at low momenta.
7.5.3 The Zero-temperature Phase Diagram

A schematic representation of the zero-temperature phase diagram of the Bose-Hubbard Hamiltonian is shown in Fig. 7-2(c). The MI phase is found within the lobe boundaries where the filling factor $\nu = N/N\text{sites}$ is an integer. The system is SF everywhere else. At $J/U \approx 0$ the width of each lobe is $\mu/U$, resulting in the step structure described in section 7.5.1. The phase boundaries in Fig. 7-2 were obtained using the mean field results in [FWGF89]. The MI phase boundary is given by

$$\frac{\mu}{U} = \nu_0 - \frac{1}{2} - j \pm \sqrt{j^2 - j(2\nu_0 + 1) + \frac{1}{4}}$$

(7.39)

where $\nu_0$ is an integer filling factor and $j = dJ/U$ where $d$ is the dimensionality of the system.

The phase diagram provides information about two different excitation gaps. First, the particle-hole excitation gap $\Delta_{\text{MI}}$, which keeps the total number of particles constant, is given by the width of the MI in the $\mu/U$ direction at a given $J/U$. The second excitation which is relevant in the grand-canonical ensemble involves a particle or hole excitation. At any given $\mu/U$, the energy cost for creating a particle (hole) excitation is the distance to the upper (lower) boundary in the $\mu/U$ direction. At $\mu/U = 0$ where the two lobes with integer filling factors $\nu_0$ and $\nu_0 + 1$ are degenerate, there is no energy gap for adding extra particles or holes, and the system is a SF. As hopping is increased the energy cost of adding/removing particles is offset by the gain in energy due to delocalization and the width of the lobes shrink. Finally at $(J/U)_c$, the delocalization of the particles compensates the cost of adding/removing a particle.

7.5.4 The Superfluid to Mott-Insulator Phase Transition

The Bose-Hubbard model displays two types of SF-MI phase transitions: $\text{generic}$ and $\text{special}$. The generic transition corresponds to crossing the phase boundary at constant $J/U$ while varying $\mu/U$. This transition corresponds to the addition/subtraction of
a small number of particles which leads to the condensation of additional particles. The SF fraction $\nu_s = \nu - \nu_0$ can be described by a weakly interacting Bose gas. Hence the dynamics close to the phase boundary can be described using the time-dependent GP equation.

The special transition corresponds to crossing the tip of the lobe at constant integer density by varying $J/U$. As we described above, this transition occurs at $(J/U)_c$ where the delocalization of the particles compensates the cost of adding/removing a particle. This transition is described by an effectively relativistic theory and belongs to the $(d + 1)$-dimensional XY universality class [FWGF89].
Chapter 8

Dipolar Bosons in Optical Lattices

The many-body Hamiltonians studied in chapters 10 and 11 are Bose-Hubbard models with dipolar interactions. In this chapter we describe how the extended Bose-Hubbard model can be realized in optical lattice systems. We begin this chapter by reviewing the properties of dipolar interactions in section 8.1. Section 8.2 introduces the anistropic, harmonic trapping schemes used to trap dipolar bose gases. Finally in section 8.3 we describe the extended Bose-Hubbard model which is the starting point for the following chapters.

8.1 Dipolar Interaction

Consider two dipolar particles separated by $\vec{r}$ with their dipole moments aligned along unit vectors $\hat{\vec{e}}_1$ and $\hat{\vec{e}}_2$ (see Fig. 8-1(a)). These two particles interact through the dipole-dipole interaction, given by

$$V_d(\vec{r}) = \frac{C_{dd} (\hat{\vec{e}}_1 \cdot \hat{\vec{e}}_2) r^2 - 3(\hat{\vec{e}}_1 \cdot \vec{r})(\hat{\vec{e}}_2 \cdot \vec{r})}{4\pi r^5} \quad (8.1)$$

where $C_{dd}$ is the dipolar coupling constant and is given by $C_{dd} = \mu_0 \mu^2 (d^2/\epsilon_0)$ for magnetic (electric) dipoles. Here $\mu_0$ and $\epsilon_0$ are the vacuum permeability and permittivity, respectively. Two properties of dipolar interaction result in novel physical phenomena. First, the dipole-dipole interaction is anisotropic. For example if the
Figure 8-1: (a) Two dipoles are aligned along unit vectors $\hat{e}_1$ and $\hat{e}_2$. The relative position of the two dipoles is given by $\vec{r}$ and the interact via the dipolar interaction given in Eq. (8.1). (b) Two dipoles polarized along the $z$-direction interact via the dipolar interaction given in Eq. (8.2) which depends on the separation between the dipoles $r = |\vec{r}|$ and the angle $\theta$ between the polarization of the dipole and the interparticle separation $\vec{r}$.

dipoles are polarized in the $z$-direction, i.e. $\hat{e}_i = \hat{z}$ with $i = 1, 2$, the interaction reduces to

$$V_d(\vec{r}) = \frac{C_{dd}}{4\pi} \frac{1 - 3\cos^2 \theta}{r^3}$$

(8.2)

where $\theta$ is the angle between $\hat{e}_i$ and $\vec{r}$ (see Fig. 8-1(b)). The dipolar interaction is purely repulsive for $\theta = \pi/2$ and attractive for $\theta = 0$. It is easy to see that if the two dipoles are aligned such that they are antiparallel the situation will be reversed. The second property of the dipole-dipole interaction is its long-range character. In contrast to the typical van der Waals interaction between neutral particles which decays as $1/r^6$, dipolar interaction decays as $1/r^3$.

In the absence of dipolar interactions, the isotropic van der Waals interactions can be treated by replacing the scattering potential with the contact potential given in Eq. (7.5). The scattering properties are fully determined by the $s$-wave scattering length and the contact scattering potential. However this treatment cannot be applied to dipolar bosons. Due to the anisotropy and long-range character of dipolar interactions, the contributions of all partial waves as well as the coupling between different angular momentum channels need to be considered.
8.2 Trapped Dipolar Bosons

Due to the anisotropy of dipolar interaction, the stability of a BEC of dipolar bosons depends on the trap geometry. Figure 8-2 shows two extreme trapping geometries which confine a dipolar BEC polarized along the z-direction. The cigar shaped trap (see Fig. 8-2(a)) is formed by applying a strong confining potential along two directions. We characterize the trap by its aspect ratio $\lambda$. A cigar shaped trap elongated along the z-axis has an aspect ratio $\lambda = \omega_z / \omega_\rho \ll 1$, where $\omega_\rho = \omega_x = \omega_y$ and $\omega_z$ are the radial and axial trap frequencies, respectively. The cigar shaped trap creates a density distribution along the polarization axis, where dipole-dipole interaction is almost entirely attractive, which may lead to the destabilization of the dipolar quantum gas [KLM+08, LMS+09, BWR09]. The pancake trap (see Fig. 8-2(b)) is formed by strongly confining the cloud in one direction only. For example a strong confinement in the z-direction forms a trap with $\lambda \gg 1$. The pancake trap creates a quasi two-dimensional density distribution of dipoles aligned perpendicular to the pancake. In this case the dipole-dipole interactions is almost purely repulsive. One can alternate between the two cases by adjusting the trap frequencies to create a stable BEC for each value of $\lambda$ by tuning the scattering length $a > a_{\text{crit}}$. In this section, we closely follow the derivation presented in [TMCL11] to derive the stability condition for trapped dipolar bosons within the mean-field approximation.

![Figure 8-2: A schematic representation of cigar shaped and pancake shaped trapping potentials used to confined dipolar BECs. In order to consider two extreme cases we use (a) a cigar shaped trap with the dipoles arranged head-to-tail, and (b) the pancake shaped trap with the dipoles polarized perpendicular to the trapping plane. In (a) the interaction is purely attractive while the dipoles in (b) interact with a purely repulsive dipolar interaction.](image)
The Hamiltonian of a dipolar BEC is given by

\[ H = \int d^3r \hat{\psi}^\dagger(\vec{r}) \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\vec{r}) + \frac{g}{2} \hat{\psi}^\dagger(\vec{r})\hat{\psi}(\vec{r}) - \mu \right] \hat{\psi}(\vec{r}) \]  

(8.3)

\[ + \frac{1}{2} \int \int d^3r_1 d^3r_2 \hat{\psi}^\dagger(\vec{r}_1)\hat{\psi}(\vec{r}_2)V_{d}(\vec{r}_1 - \vec{r}_2)\hat{\psi}(\vec{r}_1)\hat{\psi}(\vec{r}_2) \]  

(8.4)

This is just the Bose-Hubbard model given in Eq. 7.21 with the dipole-dipole interaction. Using the mean-field approximation we can write the filed operator \( \hat{\psi}(\vec{r}) = \Psi_0(\vec{r}) + \delta \hat{\psi}(\vec{r}) \) where the classical field \( \Psi_0(\vec{r}) \) is the condensate wavefunction and \( \delta \hat{\psi}(\vec{r}) \) is the non-condensate fraction.

Neglecting the fluctuations \( \delta \hat{\psi}(\vec{r}) \) we find the energy functional for the BEC:

\[ E[\Psi_0] = \int \left[ -\frac{\hbar^2}{2m} \left| \nabla \Psi_0(\vec{r}) \right|^2 + V_{\text{ext}}(\vec{r}) \left| \Psi_0(\vec{r}) \right|^2 + \frac{g}{2} \left| \Psi_0(\vec{r}) \right|^4 \right] d^3r \]

\[ + \frac{1}{2} \int \left[ \left| \Psi_0(\vec{r}) \right|^2 \int V_d(\vec{r} - \vec{r}) \left| \Psi_0(\vec{r}) \right|^2 d^3r' \right] d^3r \]  

(8.5)

Using a variational ansatz for the condensate we can evaluate the energy of the BEC with the ansatz,

\[ \Psi_0(z, \rho) = \sqrt{\frac{N}{\pi^{3/2} \sigma_\rho^2 \sigma_z^3 a_{\text{ho}}}} \exp \left[ -\frac{1}{2a_{\text{ho}}^2} \left( \frac{\rho^2}{\sigma_\rho^2} + \frac{z^2}{\sigma_z^2} \right) \right] \]  

(8.6)

where \( a_{\text{ho}} = \sqrt{\hbar / (m\bar{\omega})} \) is the harmonic oscillator length with \( \bar{\omega} = (\omega_\rho^2 \omega_z)^{1/3} \), \( \sigma_z \) is the axial width of the Guassian, \( \sigma_\rho \) is the radial width of the Gaussian, and \( N \) the total number of particles. Inserting the expression for \( \Psi_0 \) into the energy functional in Eq. (8.5) we find

\[ E_0(\sigma_z, \sigma_\rho) = \frac{N \hbar \bar{\omega}}{4} \left( \frac{2}{\sigma_\rho^2} + \frac{1}{\sigma_z^2} \right) + \frac{N \hbar \bar{\omega}}{4\lambda^{2/3}} \left( 2\sigma_\rho^2 + \lambda^2 \sigma_z^2 \right) + \frac{\hbar \bar{\omega}}{\sqrt{2\pi} a_{\text{ho}} \sigma_\rho^2 \sigma_z} \frac{1}{a_\sigma} \]

\[ - \frac{\hbar \omega_{\text{add}}}{\sqrt{2\pi} a_{\text{ho}} \sigma_\rho^2 \sigma_z} f(\kappa) \]  

(8.7)

where thefirst term is the kinetic energy, the second term is the potential energy contribution due to the external trapping potential, the third term is the contact
interaction energy and the last term is the contribution due to the dipolar interaction. Here \( a_{dd} = C_{dd} m/(12\pi \hbar^2) \) is the dipolar length, \( \kappa = \sigma_\rho/\sigma_\varphi \) is the aspect ratio of the density distribution, and the function \( f(\kappa) \) is given by

\[
f(\kappa) = \frac{1 + 2\kappa^2}{1 - \kappa^2} - \frac{3\kappa^2 \tanh^{-1} \sqrt{1 - \kappa^2}}{(1 - \kappa^2)^{3/2}}
\]  

(8.8)

Figure 8-3 shows the \( f(\kappa) \) while varying \( \kappa \). For \( \kappa = 1 \), \( f(\kappa) \) vanishes which implies that for a spherical density distribution, the mean-field dipolar interaction averages to zero. The plot also implies that the interaction strength, and the sign of the interaction can be varied by adjusting the aspect ratio of the trap, \( \lambda \). The trapped dipolar gas is stable if \( E_{int} = E_{contact} + E_{dipolar} > 0 \). Hence the stability condition for the gas is

\[
\frac{a_s}{a_{dd}} - f(\kappa) > 0
\]

(8.9)

which can be reached by varying the trapping frequencies in the axial and radial directions. The critical scattering length \( a_{crit} \) required for the stability of the trapped gas at a fixed aspect ratio \( \lambda \), \( N \) and \( \omega \) can be determined by minimizing the energy functional with respect to \( \sigma_\rho \) and \( \sigma_\varphi \). The details of this procedure are given in [BWR09]. The validity of the procedure has been confirmed experimentally in [KLM+08].

### 8.3 Extended Bose-Hubbard Model

In this section, we derive the extended Bose-Hubbard model for dipolar bosons in optical lattices. The derivation follows the same procedure as in section 7.4. We begin by expanding the field operators in the basis of the Wannier functions and restricting the terms in the expansion to only the first band. The first part of Eq. (8.3) which contains the kinetic energy term, the contact interaction and the external lattice potential reproduces the Bose-Hubbard model given by Eq. (7.30). The contribution of the dipolar interaction takes the form

\[
H_{dipolar} = \sum_{i,j,k,l} \frac{1}{2} V_{ijkl} a_i^+ a_j^+ a_k a_l
\]

(8.10)
The function $f(\kappa)$ which is proportional to the contribution of the dipole-dipole interaction to the energy of the dipolar BEC in the mean-field approximation. $\kappa$ is aspect ratio of the density distribution. $f(\kappa)$ varies smoothly as $\kappa$ takes values ranging from 0.01 to 100 which allows one to create repulsive or attractive dipolar interactions. $f(\kappa = 1) = 0$ corresponding to a spherical density distribution.

where the matrix elements of the dipolar interaction are given by

$$V_{ijkl} = \int d^3r_1 d^3r_2 w^*(\vec{r}_1 - \vec{r}_i)w^*(\vec{r}_2 - \vec{r}_j)V_d(\vec{r}_1 - \vec{r}_2)w(\vec{r}_1 - \vec{r}_k)w(\vec{r}_2 - \vec{r}_l)$$

(8.11)

where $\vec{r}_1$, $\vec{r}_2$, $\vec{r}_k$ and $\vec{r}_l$ are the lattice sites. The Wannier functions are centered at the minima of the optical lattice wells. If the optical lattice is deep enough the spread of the Wannier function will be much smaller than the optical lattice spacing. Hence $w(\vec{r}_1 - \vec{r}_i)$ will be strongly peaked near $\vec{r}_i$ and will not have significant amplitude away from the lattice site. Hence $V_{ijkl}$ is significant only if $i = k \neq j = l$ or if $i = j = k = l$.

The first case is the offsite dipolar interaction which takes the form

$$V_{ijij} = V_d(\vec{r}_i - \vec{r}_j) \int d^3r_1 d^3r_2 |w(\vec{r}_1 - \vec{r}_i)|^2 |w^*(\vec{r}_2 - \vec{r}_j)|^2$$

(8.12)
where we have approximated the dipolar potential $V_d(\mathbf{r}_1 - \mathbf{r}_2)$ as a constant potential $V_d(\mathbf{r}_i - \mathbf{r}_j)$. This approximation makes use of the fact that the dipolar interaction varies very little on the scale of the spread of the Wannier function. Since the Wannier functions only have appreciable amplitude about $\mathbf{r}_i$ and $\mathbf{r}_j$, the contribution of the off-site term to the Hamiltonian is

$$
H_{\text{off-site}} = \sum_{i \neq j} \frac{1}{2} V_{ij} \hat{n}_i \hat{n}_j
$$

(8.13)

Here $V_{ij} = V_d(\mathbf{r}_i - \mathbf{r}_j)$ and $\hat{n}_i = a_i^\dagger a_i$ is the bosonic number operator at site $i$.

We cannot approximate the dipolar interaction as a constant when evaluating the onsite contribution. The dipolar interaction in this case is given by

$$
V_{iiii} = \int \int d^3 r_1 d^3 r_2 n(\mathbf{r}_1) V_d(\mathbf{r}_1 - \mathbf{r}_2) n(\mathbf{r}_2)
$$

(8.14)

where $n(\mathbf{r}) = |w(\mathbf{r})|^2$ is the particle density at $\mathbf{r}$. This integral can using the convolution theorem. The contribution of the onsite dipolar interaction to the Hamiltonian is given by

$$
H_{\text{onsite}} = \sum_i \frac{1}{2} V_{iiii} \hat{n}_i (\hat{n}_i - 1)
$$

(8.15)

where

$$
V_{iiii} = \frac{1}{(2\pi)^3} \int d^3 k \mathcal{V}_d(\mathbf{k}) \hat{\rho}(\mathbf{k})
$$

(8.16)

Here $\mathcal{V}_d(\mathbf{k})$ and $\hat{\rho}(\mathbf{k})$ are the Fourier transforms of the dipolar potential and density respectively.

In its most general form the extended Bose-Hubbard Hamiltonian is the sum of the Bose-Hubbard Hamiltonian and the two dipolar contributions:

$$
H_{dd} = -J \sum_{\langle ij \rangle} a_i^\dagger a_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \sum_i \mu_i \hat{n}_i + \sum_{i \neq j} \frac{1}{2} V_{ij} \hat{n}_i \hat{n}_j
$$

(8.17)
where $U$ is the effective onsite interaction and is given by

$$U = g \int d^3 |w(\vec{r})|^4 + \frac{1}{(2\pi)^3} \int d^3 k \vec{V}(\vec{k}) \rho^2(\vec{k}). \quad (8.18)$$

We will study the extended Bose-Hubbard model in layered geometries in chapters 10 and 11. At this point, we note that in this thesis we present our results for hard-core bosons where $a_s \to \infty$, corresponding to a large, repulsive on-site contact interaction. In this limit, the Hilbert space is constrained to states with maximum of one particle per site. The extended Bose-Hubbard Hamiltonian for hard-core bosons is given by

$$H_{\text{dd}}^{\text{hard-core}} = -J \sum_{\langle ij \rangle} a_i^\dagger a_j^\dagger - \sum_i \mu_i \hat{n}_i + \sum_{i \neq j} \frac{1}{2} V_{ij} \hat{n}_i \hat{n}_j \quad (8.19)$$
Chapter 9

Path Integral Monte Carlo and the Worm Algorithm

Quantum Monte Carlo is one of the most powerful methods of simulating a quantum many-body Hamiltonians. This is especially true in higher dimensional systems (d>1) where other numerical techniques like the Density Matrix Renormalization Group (DMRG) no longer apply. Quantum Monte Carlo algorithms allow us to study the equilibrium properties of many-body systems. Section 9.1 introduces the Path Integral Monte Carlo (PIMC) which is one of the existing Monte Carlo techniques. Section 9.2.1 discusses the Worm algorithm which is one of the implementations of PIMC. In sections 9.2.3 and 9.2.4, we introduce the two-worm and multiworm algorithms used in this thesis.

9.1 Path Integral Monte Carlo

We begin by deriving an expression for the partition function in the path integral representation which closely follows the derivation in [PS09]. To this end, we choose a basis state $|\alpha\rangle$ such that the system Hamiltonian $H$ can be written as

$$H = H_0 + H_1$$  \hspace{1cm} (9.1)
where $H_0$ is diagonal in this basis. For example, for the Bose-Hubbard Hamiltonian we can choose the Fock basis. In this basis, the potential energy will be diagonal and $H_1$ will contain the off-diagonal hopping terms.

The partition function is the trace of the density matrix operator. In the interaction picture the partition function is given by

$$Z = \text{Tr} \left[ e^{-\beta(H_0 + H_1)} \right] = \text{Tr} \left[ e^{-\beta H_0} T \tau e^{-\int_0^\beta H_1(\tau) \, d\tau} \right]$$

(9.2)

$$H_1(\tau) = e^{\tau H_0} H_1 e^{-\tau H_0}$$

(9.3)

where $H_1(\tau)$ is the $H_1$ in the interaction picture, Tr is the trace operator, $\beta = 1/T$ is the inverse temperature with $k_B = 1$, and $T_\tau$ is the time ordering operator. Here $\tau$ is the imaginary time which is defined as $\tau = it$ on the interval $[0, \beta]$. Hence $e^{-\beta(H_0 + H_1)}$ is just the time evolution operator.

The partition function can be rewritten using Feynman path integral formulation by expanding the exponential on the right hand side of the time ordering operator in Eq. (9.2):

$$Z = \sum_{\{\alpha\}} \langle \alpha | e^{-E_\alpha \beta} \left( 1 - \int_0^\beta d\tau H_1(\tau) + (-1)^m \int_0^\beta d\tau_m \cdots \int_0^{\tau_2} d\tau_1 H_1(\tau_m) \cdots H_1(\tau_1) + \cdots \right) |\alpha\rangle$$

(9.4)

Here $E_\alpha$ are the eigenvalues of $H_0$ and the integrals are time-ordered. The summation over $\{|\alpha\rangle\}$ is due to the trace operator in the definition of $Z$.

We can further simplify Eq. 9.4 using the completeness relation for $\{|\alpha\rangle\}$. Inserting $\sum_{\alpha'} |\alpha'\rangle \langle \alpha'|$ between the $H_1(\tau_i)$ operators we can rewrite the products of these operators as

$$\langle \alpha | e^{-E_\alpha \beta} H_1(\tau_m) \cdots H_1(\tau_1) |\alpha\rangle =$$

$$e^{-E_\alpha \beta} \sum_{\alpha_1 \cdots \alpha_m} H_1^{\alpha_{m-1}}(\tau_m) \cdots H_1^{\alpha_2\alpha_1}(\tau_2) H_1^{\alpha_1\alpha}(\tau_1)$$

(9.5)

where

$$H_1^{\alpha\beta}(\tau) = e^{E_\alpha \tau} H_1^{\alpha\beta} e^{-E_\beta \tau}$$

(9.6)
are the matrix elements of $H_1(\tau)$. Using Eq. 9.5 in Eq. 9.4, the partition function can be written in terms of the eigenvalues $E_\alpha$ and the off-diagonal matrix elements $H_1^{\alpha\beta}(\tau)$. The partition function in Eq. 9.4 provides the $(d+1)$-dimensional configuration space where the PIMC updates are performed. In short, using the completeness relations we have derived an expression for $Z$ involving only scalar quantities. However this has also enlarged the configuration space by adding the $d+1$ dimension of imaginary time. In other words, the procedure described in this section is an exact mapping of the $d$-dimensional quantum system to a $(d+1)$-dimensional classical system.

In this thesis, we are interested in Bose-Hubbard type of Hamiltonians. It is useful to describe the configuration space in the context of these systems. The Bose-Hubbard model in the grand-canonical ensemble is given by Eq. (7.30). The potential energy term is diagonal in the basis of Fock states with $|\alpha\rangle = |n_1...n_i...n_{N_{\text{sites}}}\rangle$, where $n_i$ is the occupation number of site $i$, and $N_{\text{sites}}$ is the total number of sites. The diagonal matrix elements are the eigenvalues of $H_0$ and are given by

$$E_\alpha = \frac{U}{2} \sum_i n_i(n_i - 1) - \sum_i \mu_i n_i \right) \tag{9.7}$$

The off-diagonal terms are

$$H_1^{\alpha\beta} = -J\langle \alpha|a_i^\dagger a_j|\beta\rangle = -J \sqrt{(n_i^{(\alpha)} + 1)n_j^{(\beta)}} \tag{9.8}$$

where the states $|\alpha\rangle$ and $|\beta\rangle$ differ only in their occupation numbers at sites $i, j$ by one with $n_j^{(\alpha)} = n_j^{(\beta)} - 1$ and $n_i^{(\alpha)} = n_i^{(\beta)} + 1$.

The partition function for the Bose-Hubbard Hamiltonian is given by

$$Z = \sum_{m=0}^{\infty} (J)^m A_m \int_0^{\beta} d\tau_m \ldots \int_0^{\tau_1} d\tau_1 \sum_{\alpha_0...\alpha_m=\alpha_0} \exp \left\{ - \sum_{p=1}^{m} E_{\alpha_p}(\tau_p - \tau_{p-1}) \right\} \tag{9.9}$$

where $A_m$ is the product of the $m$ square root factors in the off-diagonal term given by Eq. 9.8 and $E_\alpha$ is given by Eq. 9.7. In Eq. 9.9, $\alpha_0 = \alpha_m$ and $\tau_0 = \tau_m$ to satisfy the period boundary conditions imposed by the $Tr$ operator.
Figure 9-1: A schematic representation of the configuration space in the $CP$ space. The horizontal and vertical axes are the imaginary time and space respectively. The imaginary time axis is continuous while the space is discretized with $j, j + 1, \ldots$ representing the different lattice sites. The dashed, solid and thick lines represent $n$, $n + 1$ and $n + 2$ particles respectively and the kinks represent the hopping between the nearest-neighbouring lattice sites.

We can recast Eq. (9.9) in the form

$$Z = \sum_{\nu} W_{\nu}$$

(9.10)

where $W_{\nu}$ is defined to be the weight of a given configuration

$$\nu \equiv [m, \alpha_0(\tau), \alpha_1(\tau), \ldots, \alpha_{m-1}(\tau)],$$

defined by the Fock states $|\alpha(\tau)>$, and their distribution in $\tau$. Figure 9-1 depicts a configuration. The horizontal axis is the imaginary time and the lattice sites are
plotted along the vertical axis. The solid lines represent the worldlines of the particles. In this figure we used dashed black lines to represent $n$ particles, solid black lines for $n + 1$ particles, and thick, blue lines to indicate the presence of $n + 2$ particles. These lines form closed loops in imaginary time satisfying the periodic boundary conditions imposed by the $Tr$ operator in $Z$. The systems studied in the thesis have periodic boundary conditions in space as well. As a result one can imagine the configuration shown in Fig. 9-1 to be wrapped on a torus. We refer to such configurations as a closed path (CP) configuration space which are spanned by the PIMC algorithm.

A cut of configuration space at a given imaginary time corresponds to a specific quantum state of the system. The points in the configuration space at which the state of the system changes are referred to as kinks. In the Bose-Hubbard model the kinks appear when a particle hops from one site to its nearest neighbor. A configuration with $\bar{m}$ kinks correspond to the $\bar{m}$th order term in the Taylor expansion of the partition function which is the $m = \bar{m}$ term in Eq. (9.9). In the PIMC algorithm updating a configuration refers to changing the number of kinks or changing the location of kinks in imaginary time. Interpreting the configuration as a set of quantum states connected by kinks we can easily extract the weight of a configuration by evaluating each segment of the worldline. In Figure 9-2 we show an example of a world line with the terms corresponding to each segment. Using these mathematical expressions, we can easily extract the weight for each configuration.

### 9.2 The Worm Algorithm

In the previous section we described configurations in the CP configuration space. These configurations contribute to the estimator of the partition function. The Worm algorithm which was first developed by Prokof'ev, Svistenov and Tupitsyn [PST98a, PST98b] enlarges the configuration by allowing one disconnected worldline which is known as the worm. This section provides a brief discussion of the Worm algorithm as well as its utility. We follow this by presenting the two-worm and multiworm algorithms which allow for two and several disconnected worldlines and efficient simulation.
Figure 9-2: The mathematical interpretation of a worldline. Between $\tau_{p-1}$ and $\tau_p$ the system is in state $\alpha$ with $E_{\alpha}$ given by Eq. (9.7). The off-diagonal matrix element $H_{1}^{\alpha\beta}$ is given by Eq. (9.8) which connects the state $\alpha$ to state $\beta$. The system stays in $\beta$ between $\tau_p$ and $\tau_{p+1}$ where a new kink changes the state of the system.

of multi-component or multilayered systems.

**9.2.1 The Single-worm Algorithm**

The Worm algorithm enlarges the configuration space by introducing a *worm*, which is a disconnected worldline. We refer to the phase space of these configurations as the CP$_g$ space. The subscript $g$ is used since in this enlarged configuration space one can efficiently collect statistics for the Green function.

The Green function of the system is given by

$$G(j, \tau) = \langle T_{\tau} a_{i+j} (t+\tau) a_{i}^\dagger (t) \rangle$$  \hspace{1cm} (9.11)

where $\langle \ldots \rangle$ denotes the statistical average of the expectation of an operator. While the configurations contributing to $Z$ belonged to the CP space, the configurations contributing to $G$ all contain a disconnected worldline that starts at $(i, t)$ and ends
Figure 9-3: A schematic of a typical configuration space in the $CP_g$ space where a single disconnected worldline known as the worm is present. The worm is shown using a thick, red line and it is delimited using circles. The horizontal and vertical axes are imaginary time and space respectively.

At $(i + j, t + \tau)$ (see Fig. 9-3). Once the worldline closes back on itself through configuration updates one recovers the CP space.

**Single-worm Updates**

The updating procedures for the Worm algorithm are a series of drawing and erasing procedures which affect the endpoints of the worm. Apart from the update which creates the worm, all other updates are performed in the $CP_g$ space. Additionally all updates come in pairs, that is for every update there is one that can undo the update.

Each update belongs to one of the two categories: updates which conserve the number of kinks and those which do not. For example creating a worm or moving its end points in imaginary time belong to the first category (see Fig. 9-4), while creating a new kink or deleting an existing one belong to the second category (see
In figures 9-4 and 9-5, the dashed, solid and bold lines correspond to the occupation numbers $n$, $n + 1$, and $n + 2$, respectively. Each worldline is divided into a series of segments that are delimited by kinks or the endpoints of the worm. These segments are referred to as intervals. At each step of the Worm algorithm an update is randomly selected. The proposed update is accepted only if the acceptance ratio $R > 1$. The acceptance ratio is given by

$$ R \sim \frac{\tilde{W}_\nu}{\tilde{W}'_\nu} , $$

where $W_\nu$ is the weight of the configuration resulting from the proposed update and $\tilde{W}'_\nu$ is the weight of the pre-update configuration. Hence once the details of each update are described one can find the weights of the old and new configurations using the procedure shown in Figure 9-2.
Create/Delete Worm

Fig. 9-4(a), shows the "create worm" update which is performed in the CP space. The panel on the left hand side shows the configuration before the update. In this update, an interval of the configuration is selected at random (e.g. interval \( n_1 \)). In the figure, the endpoints of the interval are shown using \( \times \) symbols. The update then suggests drawing a new piece of worldline (bottom right) or deletion of a piece from an existing worldline (top right). This update splits the \( n_1 \) interval into three intervals by creating a new interval \( n_2 \) which is delimited by the worm end points at times \( \tau_1 \) and \( \tau_2 \), with \( \tau_{\text{min}} < \tau_1 < \tau_2 < \tau_{\text{max}} \). In the figure, the endpoints of the worm are represented using filled circles and correspond to the \( a \) and \( a^\dagger \) operators. In addition to the acceptance ratio condition, this update can only be accepted if the resulting configuration does not violate the Hilbert space. For instance a valid update does not erase a worldline off an empty interval or draw a new worldline on an interval which has reached its maximum occupation number.

The create worm update can be reversed by its counterpart, the "delete worm" update which can only by used in the \( \text{CP}_g \) space and only if the endpoints of the worm belong to the same interval.

Time Shift

The "time shift" is the last of the updates which conserve the total number of kinks and is shown in Fig. 9-4(b). This update randomly selects one of the endpoints of the worm. Next, the algorithm selects a random interval delimited by \( \tau_{\text{min}} \) and \( \tau_{\text{max}} \), chooses a random point within this interval and moves the chosen endpoint of the worm to this point. This may move the endpoint of the worm forwards or backwards in imaginary time, thus shortening or lengthening the worm.

Space Shift

The remaining updates all change the number of kinks in the configuration space. The first of these updates is the "space shift (left)" update which is shown in Fig. 9-5(a).
It consists of creating or deleting a kink at $\tau_{\text{kink}}$ such that $\tau_{\text{kink}} < \tau_{\text{max}}$, where the $\tau_{\text{max}}$ is the position of operator $a$. The algorithm randomly selects two neighboring worldlines at sites $i$ and $j$. Next, the algorithm chooses a random interval delimited by $\tau_{\text{min}}$ and $\tau_{\text{max}}$ based on the current position of the operator $a$ and in such a way as to not interfere with any existing kinks. The position of the kink, $\tau_{\text{kink}}$ is randomly chosen within this interval.

![Diagram](image)

Figure 9-5: Pictorial representation of (a) the space shift left, and (b) the space shift right updates. These single-worm updates increase the number of kinks by one. See text for more detail on these updates.

The final update is the “space shift (right)” which is shown in Fig. 9-5(b). This update is equivalent to space shift (left) with the kink is inserted to the right of operator $a$.

The updates described above are the full set of updates required by the Worm algorithm. It is straightforward to see that the Worm algorithm operates in the grand canonical ensemble where the chemical potential $\mu$ fixes the average particle number.
9.2.2 Advantages of the Worm Algorithm

The Worm algorithm uses *local* updates to update the configuration by drawing new worldlines and erasing existing worldlines, and by the insertion or deletion of kinks which facilitate hopping between the worldlines. Since the algorithm uses the enlarged configuration space $CP + CP_g$, it allows one to measure both the partition function and the Green function. The configurations belonging to $CP$ in the absence of the worm contribute to the estimator of the partition function. However unlike algorithms which operate only in the $CP$ space, the intermediate configurations in the presence of the worm allow for efficient collection of statistics for the Green function.

Unlike other algorithms which rely on local updates for moving between configurations, the Worm algorithm does not suffer from critical slowing down in the vicinity of the critical point. In the critical region, the system develops long-range correlations and as a result its relevant degrees of freedom become non-local. Hence an algorithms based on local updates is likely to be extremely inefficient in simulating the system in this regime. In fact in most cases, the autocorrelation time diverges with the system size. The Worm algorithm works in a configuration space which contains an open ended worldline. It uses updates to manipulate the endpoints of the worm which are directly linked to the critical modes (long range order in $G(j, \tau)$). These updates allow the algorithm to efficiently generate independent configurations in the critical region.

Additionally the Worm Algorithm can efficiently sample configurations that are topologically distinct or those separated by an energy barrier. The latter guarantees that ergodicity is maintained. Figure 9-6(a) is a sketch of the trajectory of a particle in one spatial dimension. The system is periodic in both space and imaginary time which means that the configuration spaces is wrapped on a torus. In Fig. 9-6(b) a discontinuity is introduced to the worldline of the particle. The two endpoints can now move on the torus (see Fig. 9-6(c)) until in Fig. 9-6(d) the worldline winds once in imaginary time. In this configuration, the *winding number* is equal to one. This evolution from $W = 0$ to $W = 1$, where $W$ is the winding number of the
configuration, shows how the topology of the system can be changed efficiently using only local updates. Once again this is possible because the algorithm operates in the enlarged configuration space. In fact the ability to sample configurations with different winding numbers is crucial for the study of systems displaying superfluidity. It was shown in [CP89] that the superfluid stiffness of a system is related to the winding number statistics through

$$
\rho_s = \frac{T\langle W^2 \rangle}{dL^{d-2}},
$$

(9.13)

where $T$ is the temperature, $L$ is the system size, $d$ is the dimensionality of the system, and $W^2 = \sum_{i=1}^{d} W_i^2$.

### 9.2.3 The Two-worm Algorithm

The two-worm algorithm is an extension of the Worm algorithm which allows for efficient sampling of the Hilbert space of pairs [SCSPS09]. This algorithm can be used
to simulate paired phases in two-component Bose-Hubbard model as well as a system of dipolar bosons in a bilayer geometry. The two-worm algorithm extends the Worm algorithm by allowing two open worldlines of two different types, each corresponding to one component/layer in the system. The two worldlines propagate simultaneously and allow one to measure two-particle off-diagonal correlation functions. The second worldline enlarges the configuration space which allows one to simulate paired phases characterized by the simultaneous winding of the two types of worldlines. If one does not have a way of accessing the two-worm sector the algorithm will no longer be ergodic.

Figure 9-7(a) is a schematic of paired worldlines in the pair superfluid (PSF) state which wind once in space. The A and B type bosons are represented by blue and red lines respectively and the arrows indicate the direction of the particle number flow in imaginary time. In the paired phase separating the two worldlines will be energetically suppressed. Hence an update which removes a part of the A-particle worldline should be followed by a similar update removing a part of the B-particle worldline. This sequence is illustrated in Figures 9-7(b) and 9-7(c).

![Figure 9-7](image)

Figure 9-7: (a) Pictorial representation of a paired worldlines in a pair superfluid state. The worldlines wind once in space and the arrows indicate the direction of particle number flow. (b) An update removes a part of one of the worldlines in the pair. This update will be immediately followed by (c) an update which removes the same part of other worldline in the pair. Note that the two worldlines are on the same spatial location but are drawn apart for clarity.

In the non-paired phase, the two worldlines are not correlated and the configuration space will look similar to that of a single superfluid. While the winding numbers
are non-zero the two worldlines span the space independent of one another.

The two-worm algorithm relies on a set of updates to move between different quantum states. It is important to note that the two-worm algorithm operates in the zero, one and two-worm sectors so the single worm updates described in the previous section are still present. In order to get access to the $CP_{g2}$ space which contains the configurations with two worms present we need to introduce a new update.

**Create Second Worm**

Once the configuration is in the $CP_g$ space, one worm of type A or B exists. This worm is updated according to the prescription in the previous section, plus the new "create second worm" update. We use $I_i$ and $M_i$, $i = A, B$ to label the endpoints of the two worms which correspond to operators $a_i^\dagger$ and $a_i$ respectively (see Fig 9-8).

The create second worm update follows the same steps as the create worm update described in section 9.2.1. In principle the interval on which the second worm is created can be chosen at random. However the efficiency of the algorithm increases if the spatial position of the second worm and one of the two endpoints of the worms A and B are matched. In the PSF phase, where the two worldlines wind together we choose $I_B = I_A$ both spatially and in imaginary time. The update is shown schematically in Fig. fig:c2w where the dashed, solid and bold lines represent $n$, $n + 1$ and $n + 2$ particles, respectively.

Once the second worm is created, we enter the $CP_{g2}$ space with two worms present in the configuration. The updates in the $CP_{g2}$ space are the single worm updates with two differences:

(a) Worm A or B is randomly chosen and the update is performed on the chosen worm.

(b) One of the ends of each worm is pinned in space and imaginary time and is not moved. In the PSF phase, the pinned ends are $I_A$ and $I_B$.

However we do need to be able to manipulate $I_A$ and $I_B$ to exit the $CP_{g2}$ sector and enter the $CP_g$ space again.
Figure 9-8: The create/delete second worm update. The second worm is created with \( I_A = I_B \) in time and space. This is an efficient choose for simulating the PSF phase.

**Delete Second Worm**

The "delete second worm" update is the only update performed on \( I_A \) and \( I_B \). In this update worm A or B is randomly chosen and is deleted in a procedure similar to the delete worm update described in section 9.2.1. Once the worm is deleted, we enter the \( CP_g \) space where the updates for the single-worm sector are performed.

### 9.2.4 The Multiworm Algorithm

The multiworm algorithm extends the Worm algorithm to include \( N \) disconnected worldlines. This extension allows us to efficiently sample the space of multimers (in the case of multi-component mixtures) or \( N \)-boson chains that form in multilayered systems of dipolar bosons. This algorithm differs markedly from the two-worm algorithm. First, the multiworm algorithm always operates in the enlarged \( CP_{gN} \) space which contains configurations with \( N \) worms present. This increases the efficiency of the algorithm and is achieved by calling the "create \( N \) worms" update at the start of the simulation.
Create N Worms

The create N worms update chooses a random interval in the configuration space and creates \( N \) worms with the same position in space and imaginary time for \( I_i, \ i = 1, \ldots, N \). The \( I_i \) are created at the same position to increase the efficiency of simulating chained phases or phases of multimers where the worms wind together.

The configuration is updated by randomly selecting a worm and applying one of the single-worm updates described in section 9.2.1, with the exception of the delete worm update, to the chosen worm. In fact, unlike the two-worm algorithm, the multiworm algorithm does not allow one to delete any of the worms which means the system is always in the \( CP_{gN} \) space. While this makes the algorithm more efficient in measuring the \( N \)-particle off-diagonal correlation functions, we can no longer access the \( Z \) space and consequently cannot measure the partition function. In chapter 11 we describe how one can use the \( N \)-particle correlators to study the equilibrium phases of a multilayered system of dipolar bosons.

Lastly the multiworm algorithm does not pin the \( I_i \) ends of the worms. Hence the single-worm updates that move the worm endpoints randomly choose either \( I_i \) or \( M_i \). However to increase the efficiency of the algorithm one artificially keeps together, in space and imaginary time, creation operators by means of an artificial configuration weight

\[
W \sim \exp\left[-\sum_{m,n}^{N}(|x_m - x_n|/\xi + |\tau_m - \tau_n|/\xi_r)\right]
\]

(9.14)

where \( x_m \) and \( x_n \) are the spatial positions of \( I_i \) in the lattice, \( \tau_m \) and \( \tau_n \) are the positions of \( I_i \) in imaginary time, and \( \xi \) and \( \xi_r \) are chosen in order to maximize efficiency. Clearly one needs to include the artificial configuration weight when calculating the expectation values. The expectation value of an operator \( O \) is given by

\[
\langle O \rangle = \frac{\sum_{\alpha} O^\alpha D_N^\alpha W^\alpha}{Z}
\]

(9.15)
where $\alpha$ is the generic index labeling configurations,

$$D_N = D_N(\vec{x}_1, ..., \vec{x}_N, \tau_1, ..., \tau_N; \vec{x}'_1, ..., \vec{x}'_N, \tau'_1, ..., \tau'_N)$$

is the N-body density matrix, and $Z = \sum_\alpha D_N^\alpha W^\alpha$ is the normalization.
Chapter 10

Many-body Phases of Polar Molecules in a Bilayer Geometry

In the chapter we study a system consisting of hardcore dipolar bosons confined to two neighboring two-dimensional (2D) layers of a 1D optical lattice (see figure 10-1(a)). The dipole moment of each particle is polarized perpendicular to the layers, which results in repulsive in-plane dipole-dipole interactions. This ensures collisional stability against short-range inelastic collisions in the strongly interacting gas. Out-of-plane dipolar interactions are dominantly attractive, which favors inter-layer pairing. In section 10.1 we introduce the system Hamiltonian. Section 10.2 presents exact theoretical, zero-temperature phase diagram of the system obtained using quantum Monte-Carlo methods [PST98a]. We demonstrate that the anisotropy and the long-range nature of interactions can induce crystallization of the dipolar cloud into a charge-density wave for a wide range of trapping parameters and interactions. Exotic quantum phases such as the pair-supersolid (PSS) phase and a pair-superfluid (PSF) are achieved under experimentally realistic trapping conditions. These phases can survive up to temperatures of the order of a few nK for a gas of polar molecules or strongly magnetic atoms. This chapter has previously appeared in [SNSP+13].
Figure 10-1: (a) A schematic representation of the setup consisting of two, two-dimensional layers of a 1D optical lattice with. Here we are showing one row in each layer. The separation between the layers is denoted by $d_z$ and $a$ is the lattice constant. We use $V_{dd}$ and $V_{dd}^{\perp}$ to denote the intralayer and interlayer dipolar interaction respectively. (b) Phase diagram of Hamiltonian (10.1) as a function of $V_{dd}/J$ and particle density $n$, computed via QMC simulations, for an interlayer distance $d_z/a = 0.36$ (see text). CB: Checkerboard solid; PSS: Pair supersolid; PSF: Paired superfluid; 2SF: independent superfluids. The phase boundaries in the dashed region are not resolved.

### 10.1 System Hamiltonian

The system we have in mind is described by the single-band tight-binding Hamiltonian

$$H = -J \sum_{<i,j>,\alpha} a_{i\alpha}^\dagger a_{j\alpha} - \frac{1}{2} \sum_{i\alpha j\beta} V_{i\alpha j\beta} n_{i\alpha} n_{j\beta}$$

$$= - \sum_{i,\alpha} \mu_\alpha n_{i\alpha}.$$  \hspace{1cm} (10.1)

Here $\alpha, \beta = 1, 2$ and $i, j$ label the layers and the lattice sites in each layer, respectively, while $a_{i\alpha}$ ($a_{i\alpha}^\dagger$) are the bosonic creation (annihilation) operators, with $a_{i\alpha}^{\dagger 2} = 0$ and $n_{i\alpha} = a_{i\alpha}^\dagger a_{i\alpha}$. The brackets $<>$ denote summation over nearest neighbors only. The first term in Eq. (10.1) describes the kinetic energy with in-plane hopping rate $J$. The second term is the dipole-dipole interaction given by $V_{i\alpha j\beta} = C_{dd}(1 - 3 \cos^2 \theta)/(4\pi|i_\alpha - j_\beta|^{3})$, where $\theta$ is the angle between particles at
positions $i, j$ and $C_{dd} = d^2/\epsilon_0 (C_{dd} = \mu_0 d^2)$ for electric (magnetic) dipoles of strength $d$. We denote the repulsive (attractive) nearest neighbor intra-layer (inter-layer) interaction by $V_{dd} = C_{dd}/(4\pi a^3) (V_{dd}^\perp = 2C_{dd}/4\pi d_z^2)$, with $a$ the in-plane lattice constant. The interlayer distance is $d_z$. The relative strength $V_{dd}/V_{dd}^\perp$ can be tuned over a wide range of values by changing $d_z/a$. The quantity $\mu_\alpha$ is the chemical potential which sets the number of particles in each layer. Here we fix $\mu_1 = \mu_2$, i.e. $N_1 = N_2$.

Hamiltonian (10.1) provides a microscopic description for the dynamics of, e.g., a gas of RbCs molecules ($d \approx 1.25$ Debye) at low-density $n$, such that the initial system has no doubly occupied sites [BMZ07]. Collisonal stability is ensured for $n^{-1/2} \gg (d^2/\hbar \omega)_{1/3} \approx 130$ nm with $\omega_{\perp} \approx 100$ kHz the frequency of transverse confinement provided by the in-plane optical lattice [BDL+07]. In addition, the choice $d^2/d_z^3 < V_0$ avoids interaction-induced inter-layer tunneling, with $V_0$ the depth of the optical potential in the transverse direction. Model (10.1) can also be used to describe the dynamics of a gas of strongly magnetic dipolar atoms, such as Dy ($d = 10\mu_B$). In this case the conservative estimate above for collisional stability is satisfied for $\omega_{\perp} \approx 1 \text{ kHz}$.

### 10.2 Quantum Monte Carlo Results

In the following, we present exact theoretical results based on path integral Quantum Monte Carlo simulations using a two-worm algorithm [SCPS09] which allows for efficient sampling of paired phases. We have performed simulations of $L \times L = N_{\text{sites}}$ square lattices with $L = 8, 12, 16, 20$ and 24. For computational convenience, we have set the dipole-dipole interaction cutoff to the third nearest neighbor and have checked that using a larger cutoff did not change the simulation results within error-bars. Lower cutoff values do not allow for stabilization of, e.g., supersolid phases, see below. In the following we choose $d_z/a = 0.36$ and $d_z \sim 200$ nm, which is experimentally feasible with, e.g., Cr or Dy atoms [BPM+10, LBL12]. We show below that this choice allows one to access a parameter regime where particles on different layers can
pair up to form a composite object. Below, we first discuss the phase diagram, and then discuss in more details the various phases.

The phase diagram of Eq. (10.1) at temperature $T = 0$ is shown in Fig. 10-1(b) as a function of $V_{dd}/J$ and the density $n$, in the parameter regime $0.31 > V_{dd}/J > 0.2$ and $0.1 < n < 0.9$, with $d_z/a = 0.36$. We expect this phase diagram to be representative of situations with $d_z/a \ll 2$, where interlayer pairing is favored (see figure 10-2 below).

At half-filling $n = 0.5$, an incompressible checkerboard solid of pairs (PCB) is stabilized for sufficiently large values of $V_{dd}/J$. Similar to the conventional checkerboard phase present in single-layers [CTL+10], here atoms in each layer occupy every other site of the lattice, due to in-plane dipolar repulsion. The checkerboard order is characterized by a finite value of the static structure factor $S(k)$ at the reciprocal lattice vector $k = (\pi, \pi)$, with

$$S(k) = \frac{1}{N} \sum_{r,r'} \exp[i k (r - r')] \langle n_r n_{r'} \rangle,$$

and the system displays zero superfluidity. We find that in the PCB phase atoms across the layers are strongly paired due to attractive interlayer interactions. As a result, the position of the two checkerboard solids is strongly correlated, i.e., they sit on top of each other. The system can be thus envisioned as a solid of pairs [TML09, Cap11], with an effective mass $m_{\text{eff}} \sim J^2/(2V_{dd} + zV_{dd})$, where $z$ is the coordination number. The PCB solid is stabilized at (much) lower values of $V_{dd}/J$ compared to the

<table>
<thead>
<tr>
<th>Phase</th>
<th>$S(\pi, \pi)$</th>
<th>$\psi_i^\alpha$</th>
<th>$\Psi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>PCB</td>
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<td>0</td>
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<tr>
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<tr>
<td>2SF</td>
<td>0</td>
<td>$\neq 0$</td>
<td>$\neq 0$</td>
</tr>
</tbody>
</table>

Table 10.1: Quantum phases of Fig. 10-1 and corresponding order parameters: structure factor $S(\pi, \pi)$; single-particle condensate $\psi_i^\alpha = \langle a_{i,\alpha} \rangle$ in each layer $\alpha$; pair-condensate order parameter $\Psi = \langle a_{i,\alpha} a_{i,\beta} \rangle$, with $\alpha \neq \beta$. (See text)
case of checkerboard solids in a single layer [CTL+10], in analogy with what found in [Cap11]. This is due to the higher effective mass of the pairs. A similar robustness of this phase is also found for melting at finite temperature.

Upon doping the PCB solid with extra particles or holes, a so-called pair-supersolid (PSS) phase is immediately stabilized. The latter displays both diagonal long range order with $S(\pi, \pi) \neq 0$, off-diagonal long-range order associated with a non-vanishing value of the pair-condensate order parameter $\Psi = \langle a_{i,\alpha} a_{i,\beta} \rangle \neq 0$ (with $\alpha \neq \beta$), and an associated finite superfluid stiffness for pairs (see below). The single-particle condensate order parameter $\psi_i^\alpha = \langle a_{i,\alpha} \rangle = 0$ is instead zero. The existence of off-diagonal order is consistent with a picture of delocalized defects [AL69, BP12], which here correspond to correlated pairs of holes or extra particles across the layers. The PSS phase forms a lobe structure in the $(V_{dd}/J - n)$-plane, around the PCB line. Away from the tip of the lobe, we find that by varying $n$ at constant $V_{dd}/J$ the PSS loses its diagonal long range order by melting into a pair superfluid phase (PSF), via an Ising-type transition (red continuous line). The PSF phase, with $\Psi \neq 0$ and $\psi_i^\alpha = 0$, is destroyed in favor of a 2SF (a phase with independent, though correlated, superfluids on each layer) for smaller values of $V_{dd}/J$. In particular, we notice that a tiny PSF-region should persist in between the PSS and 2SF phases even close to the tip of the PSS-lobe, however this is within errorbars for $V_{dd}/J \lesssim 0.2$. Exactly at filling $n = 0.5$, our results are consistent with a direct PCB-2SF transition, as discussed below, with no intermediate PSS phase. In particular we find no evidence of, e.g., possible micro-emulsion phases [SK04, PPBT10], within errorbars.

Finally, we notice that a host of other phases are present in the general phase diagram for two layers. In particular, we find that for stronger values of $V_{dd}/J \gtrsim 0.3$ the system displays a sequence of incompressible phases at various rational fillings of the lattice, similar to the so-called Devil’s staircase found in the case of a single layer. We also expect novel PSS phases to appear around lobes at, e.g., filling $n = 0.25$, in analogy with Ref. [CTL+10]. In addition, independent solids as well as supersolid phases can be achieved by increasing the layer distance, while mixtures of solid and superfluid phases can be stabilized by modifying the relative particle density in the
two layers. The discussion of some of these phases is however outside of the scope of the present work. In the remainder of the paper we discuss in more detail the various phases and their transitions at zero and finite temperature around $n = 0.5$.

**Stability of the PCB phase:** As discussed above, the PCB phase at $n = 0.5$ is characterized by a finite value of the order parameter $S(\pi, \pi)$ and no off-diagonal order. The latter is associated with superfluidity in a (2+1) dimensional interacting system, which can be measured straightforwardly within Monte-Carlo (see below). In addition, within the PCB phase inter-layer dipolar attraction strongly correlates the positions of particles in the two layers.

The stability of the PCB phase with respect to intra-plane interactions as well as inter-layer distance $d_z/a$ at zero temperature is analyzed in Fig. 10-2. There, we numerically determine the minimum dipolar interaction strength $V_{dd}/J$ required to stabilize the PCB phase at a given $d_z/a$. In order to establish whether the solid phase is paired we have performed several simulations with different initial conditions for each set of parameters and observed whether the equilibrium configuration was dependent on the initial choice or not. The figure shows that a PCB phase is stabilized for $d_z/a \lesssim 2$ and sufficiently large $V_{dd}/J$ (continuous line). In this parameter regime, the system above (below) the continuous line is a PCB (2SF) phase, respectively, that is, the continuous line visualizes the shift of the PCB-2SF transition point of Fig. 10-1 as a function of $d_z/a$. Instead, for $d_z/a > 2$ and large enough interactions the insulating phase above the (dotted) line corresponds to two independent checkerboard phases (2CB). This points to the possible presence of a tri-critical point in the phase diagram around $d_z/a \approx 2$. The shaded area in Fig. 10-2 shows the transition region where the PCB phase is replaced by the 2CB phase. The details of this phase transition are beyond the scope of this work. We have confirmed that the computed transition points are independent of the interaction cutoff that we use, within our errorbars, and should be thus quantitatively relevant to experiments.

In the following we focus on $d_z/a = 0.36$ to satisfy $V_{dd} \gtrsim 10J$ in the vicinity of the tip of the lobe. We find that this choice ensures pairing at $n \sim 0.5$ (in the vicinity of
the PCB phase) while keeping $V_{dd}$ relatively low. This corresponds to experimentally optimal conditions to observe PSS phase: a lower effective mass of pairs $m_{\text{eff}}$ results in a larger superfluid density which in turn results in higher critical temperatures (see also below).

![Diagram showing the plot of minimum $V_{dd}/J$ needed to stabilize the CB phase as a function of $dz/a$. Once the layers are separated by $dz/a > 2$ they behave as independent layers. The shaded area indicates the transition region between the PCB and 2CB phases.](image)

**Pair supersolid phase:** Figure 10-1 shows that a PSS lobe is immediately formed by doping the PCB solid with either vacancies (holes) or interstitials (extra particles). The hard-core constraint of Eq. (10.1) ensures particle-hole symmetry, and thus reflection symmetry of the lobe, around $n = 0.5$.

We characterize this pair supersolid phase in Fig. 10-3, for a specific choice of interaction strength $V_{dd}/J = 0.238$. In the figure, the order parameter for the diagonal checkerboard solid order $S(\pi, \pi)$ (continuous lines) and the superfluid stiffness of pairs...
\( \rho_{\text{PSS}} \) are plotted as a function of \( n \). The quantity \( \rho_{\text{PSS}} = T(W^2)/dL^{d-2} \) [PC87] is directly related to a pair condensate, and can be calculated within quantum Monte-Carlo, with \( W = W_1 + W_2 \) the sum of winding numbers in layer 1 and 2. The figure shows that for an extended range of densities, both the static structure factor and the pair superfluid stiffness are finite and system size independent, showing the existence of a stable supersolid phase in the lobe region. We note that, due to pairing across the layers, in the PSS phase the fluctuation of difference in winding numbers is zero \( \langle (W_1 - W_2)^2 \rangle \).

**Superfluid phases:** As the system is doped further, the PSS disappears in favor of a PSF phase. The latter displays pair-induced off-diagonal long range order, only [see, e.g., Table 1]. We find that the PSS-PSF transition is of the Ising type universality class in \((2+1)\)-dimensions, analogous to the case of a single-layer [CTL+10]. Critical points are determined using finite size scaling for the static structure factor with scaling coefficients \( 2\beta/\nu = 1.0366 \) [HPV99] (see Fig. 10-3(b) for the specific choice \( V_{dd} = 0.238J \)). In the figure the scaled quantity \( S(\pi, \pi)L^{1.0366} \) is plotted as a function of \( n \), and the crossing of the curves at \( n_{cr} = 0.573 \pm 0.002 \) corresponds to the quantum critical point where the finite size effects disappear [see also panel (a)].

We find in general that by lowering the interaction strength \( V_{dd}/J \) at constant \( n \) from the PSF phase, the system finally develops into two independent superfluids (2SF) with a finite value of the single-component condensate order parameters, \( \psi_i^\alpha = \psi_i^\beta \neq 0 \), via a second order phase transition in the \((2+1)\) XY universality class. The transition points between the PSF and 2SF phases in Fig. 10-1 are calculated using finite size scaling of \( \langle (W_1 - W_2)^2 \rangle \). The latter quantity is zero inside the PSF phase in the thermodynamic limit due to pairing across the layers, while it has a finite value in the 2SF phase. We note that the pair order parameter in the 2SF phase is instead trivially non-zero, \( \Psi \neq 0 \) (see also Table 1).

The phase diagram in Fig. 10-1 shows that the boundary of the PSF-2SF transition shifts downward approximately linearly in the \((V_{dd}/J - n)\)-plane, as the density becomes sufficiently smaller or larger than \( n = 0.5 \). This is easily understood in
the limit of very small densities, by noting that inter-plane dipole-dipole interactions always favor the existence of a two-body bound state, even for an arbitrarily small interaction strength. However, we find that many-body effects result in a threshold for the formation of pairs at finite density, where the magnitude of the interaction strength required to stabilize pairing increases with \( n \). This is explained by noting that, in the limit of low density, \( a_s \sqrt{n} \ll 1 \), PSF phase is composed of weakly interacting superfluid dimers. As the density is increased exchanges between dimers are favored. This destabilizes the dimers, inducing the transition to two independent superfluids in the 2SF phase. Eventually, the presence of diagonal order near \( n = 0.5 \) forces the PSF-2SF line to bend down, deviating from the linear dependence on \( n \).

We gain further insight into the structure of correlations in the condensed phases by studying the following four-point correlation function:

\[
 f_{jl} = \langle \psi_{1,i} \psi_{2,l} \psi_{1,j} \psi_{2,l} \rangle. \tag{10.3}
\]

Here \( i,j,l \) refer to sites, 1, 2 refer to layers, and \( \langle \rangle \) denotes a quantum and thermal average as well as site averaging over \( i \). In the presence of pair superfluidity, one expects this correlation function to be short ranged with respect to \( r_{jl} = |r_j - r_l| \), and simultaneously long ranged with respect to \( r_{il} = |r_i - r_l| \) and \( r_{ij} = |r_i - r_j| \). In the 2SF phase, instead, \( f_{jl} \) is obviously long ranged with respect to \( r_{il} \) and \( r_{ij} \), but it is independent of \( r_{jl} \).

Figure 10-4 shows \( f_{jl} \) (normalized to unity: \( \int_0^\infty f_{jl} dr_{jl} = 1 \)) as a function of \( r_{jl} \) for the PSS (green triangles, \( n = 0.48, V_{dd} = 0.25J \)), PSF (red dots, \( n = 0.40, V_{dd} = 0.25J \)) and 2SF phases (blue squares, \( n = 0.30, V_{dd} = 0.18J \)). As expected, we find that \( f_{jl} \) is independent of \( r_{jl} \) in the 2SF phase, where pairing is absent, while it is peaked at \( r_{ij} = 0 \) both in the PSS and PSF phase. The figure shows that an exponential ansatz of the form \( f_{0} e^{-r_{jl}/\xi_0} \) fits quite well the large-\( r_{ij} \) behavior of \( f_{jl} \) in these latter phases, and is essentially exact for all \( r_{jl} \) in the PSS phase with \( \xi_0 = 1.63a \). Here \( \xi_0 \) can be interpreted as the spread of the pair wavefunction, and is obtained
from Fig. 10-4 by fitting the tail of \( f_{ji} \), as obtained numerically. The inset in Fig. 10-4 shows \( \xi_0 \) as a function of \( n \), as the PSF-PSS phase boundary is crossed. The pair wavefunction is shown to be considerably more tightly bound in the PSS phase than in the PSF phase. The abrupt drop in \( \xi_0 \) locates precisely the transition point.

**Finite temperature:** We have studied the robustness of the quantum phases described above against thermal fluctuations. As expected for two-dimensional systems, we find in general that superfluidity in the PSS, PSF and 2SF phases disappears at finite temperature \( T \) via a Kosterlitz-Thouless (KT) type [KT73] transition. Diagonal long range order in the PCB and PSS phases is instead lost via a two-dimensional Ising-type transition. We have found that, when present, pairing still exists at the transition points, suggesting that the temperatures required for breaking pairs are higher than the critical temperatures measured here.

Figure 10-5 shows one example for the SF-normal transition in the 2SF phase. We plot \( \rho_s \) vs. \( T/J \) at \( V_{dd}/J = 0.20 \) and \( n = 0.3 \) for different system sizes. The inset shows the finite size scaling procedure [CP89] used to determine the critical temperature. We find \( T_{KT,2SF} = \frac{\pi^2 \rho_s(T_{KT})}{4} \approx 0.255J \). For the PSF-normal transition we find \( T_{KT,PSF} \approx 0.08J \) at \( n = 0.3 \) and \( V_{dd}/J = 0.25 \). The lower KT transition temperature compared to the 2SF-normal transition is due to a larger effective mass of the pairs, i.e., lower effective hopping, which results in a suppression of particle delocalization and consequently smaller \( \rho_s \). The disappearance of the PSS phase proceeds in two successive stages. At \( T_{KT,PSS} \) the PSS phase melts into a liquid-like phase reminiscent of a liquid crystal, with \( \rho_s = 0 \) and \( S(\pi, \pi) \neq 0 \). Upon further increasing the temperature \( S(\pi, \pi) \) becomes zero at a critical temperature \( T_c \) through an Ising-type transition \((2\beta/\nu = 1/4 \text{ in } 2D)\). For example, we find \( T_{KT,PSS} \approx 0.06J \) and \( T_c \approx 0.3J \) for \( n = 0.48 \), \( V_{dd} = 0.25J \). Similar \( T_c \) values are found for the critical temperature of the melting of the PCB phase into a featureless normal fluid, e.g., \( T_c \approx 0.35J \) for \( V_{dd} = 0.25J \). Clearly, for larger interaction strengths, i.e., away from the tip of the lobe, transition temperatures will increase.

**Experimental estimates:** Based on our results we estimate under which experi-
mental conditions the phases described can be observed. For example, with a gas of Dy \((d = 10 \mu_B)\) a choice of lattice parameters \(a = 500\ \text{nm}, d_z = 200\ \text{nm}, J = 50\ \hbar\text{Hz}\) results in \(V_{dd}/J \sim 0.21\) which stabilizes the PCB phase. In the case of Er\(_2\) Feshbach molecules [Fer, DPZ10]\((d = 14\mu_B)\) with \(a = 400\ \text{nm}, d_z = 200\ \text{nm}, J = 100\ \hbar\text{Hz}\) the PCB phase is stabilized at \(V_{dd}/J \sim 0.4\). In both cases the PCB phase can be observed at nk temperatures.

Using RbCs \((d = 0.3\text{D})\) and typical trapping parameters \(a = 500\ \text{nm}, d_z = 300\ \text{nm}\) and \(J = 150\ \hbar\text{Hz}\) we find \(V_{dd}/J = 0.7\), which is large enough to stabilize the PCB. The latter survives up to \(T_{c}^{PCB} \sim 4\ \text{nK}\). By doping away from filling factor \(n = 0.5\) the PSS phase can be reached with a KT transition temperature for PSF-normal transition of the order of nK.

In local density approximation, the presence of weak in-plane harmonic confinement as provided by, e.g., magnetic trapping, will essentially result in a scan of the phase diagram over the chemical potential, with coexistence of different phases. Similar to the single-layer case [CTL+10], because of their energy gaps, we expect the solid phases CB and PCB to be robust against, e.g., hole doping, and thus observable, in the presence of in-plane harmonic confinement.

All phases discussed above can be distinguished by monitoring the behavior of the order parameters of Table 1. Inter-layer particle correlations will be detected via in situ imaging [WES+11, SBM+11] as well as noise correlation measurements. In addition, inter-layer pairing may be measured via spectroscopic techniques.
Figure 10-3: (a) Structure factor $S(\pi, \pi)$ (solid lines, left y-axis) and superfluid stiffness $\rho_s$ (dashed lines, right y-axis) in the PSS phase for $L = 8$ (black squares), 12 (red circles), 16 (blue triangles) and 20 (green diamonds) at $T/J = 1/(1.5L)$ shown using black squares, red circles, blue triangles and green diamonds respectively. The PSS-PSF transition point is at $V_{dd} = 0.238J$. (b) Scaled structure factor $S(\pi, \pi)L^{23/\nu}$ vs. $n$ with $2\beta/\nu = 1.0366$ for $L = 8, 12, 16$ and 20.
Figure 10-4: Four-point correlation function $f_{jl}$ of Eq. (10.3) as a function of $r_{jl}$ for the 2SF (blue squares, $n = 0.30, V_{dd} = 0.18J$), PSF (red dots, $n = 0.40, V_{dd} = 0.25J$) and PSS (green triangles, $n = 0.48, V_{dd} = 0.25J$) phases. The dashed (dotted) line is the exponential fit, $f_0 e^{-r_{jl}/\xi_0}$, to the PSF (PSS) histogram, where $\xi_0$ can be interpreted as the extent of the pair wavefunction (see text). The inset shows $\xi_0$ across the PSF-PSS phase boundary.
Figure 10-5: Superfluid stiffness $\rho_s$ as a function of temperature $T/J$, at $V_{dd} = 0.20J$ and $n = 0.30$, corresponding to 2SF phase at $L = 12, 16, 20$ and $24$ shown using black squares, red circles, blue triangles and green diamonds respectively. As temperature is increased the 2SF phase undergoes KT phase transition at critical temperature $T_{KT,2SF} \approx 0.255J$, indicated by an arrow. The inset shows finite size scaling [CP89] where the dashed line is a linear fit of our simulation results (points).
Chapter 11

Quantum Phases of Bosons in Multilayer Tubes

Previous theoretical studies, using variational methods or classical Monte Carlo techniques, have shown that stacks of one-dimensional tubes of dipolar bosons allow for the formation of superfluids of multi-atomic complexes – chain superfluids (CSF) [PBW+10, CK11, TK12, VZF+11]. Moreover, an interesting opportunity for the emergence of exotic parafermions in these systems has been proposed in [Gia04, LN12].

In this chapter, we study the ground states of hard-core bosons interacting by dipolar forces and trapped in a stack of $N$, one-dimensional optical lattices (tubes) parallel to each other with no inter-tube tunneling. *ab-initio* quantum Monte Carlo simulations are performed by the novel multiworm Algorithm and are compared with the results of the bosonization method. In contrast to what was previously done, here we study the actual quantum Hamiltonian of hard-core bosons. Note that, in light of what mentioned above, our algorithm is equally relevant to atomic mixtures and coupled spin chains.

Section 11.1 presents the system Hamiltonian. The many-body phases that can be stabilized in the system are described in section 11.2. We find several non-trivial ground states: superfluids and countersuperfluids made of composites of particles from different tubes, 1D checkerboard insulators, and mixtures of these phases. As
it turns out, such phases have zero threshold in the interaction and can invoke any number \( M \) of tubes, \( 1 < M \leq N \), regardless of their geometrical positions. The inter-tube imbalance of filling factors is a "tuning knob" for inducing such phases and switching between them. Section 11.3 presents the bosonization formalism which is used to study a system of \( N \)-tubes with arbitrary interactions. Finally we use the Quantum Monte Carlo simulation results, using the multiworm algorithm described in chapter 9, to study multilayer systems with attractive inter-layer interactions, and with dipolar interactions. The results are presented in section 11.4.

11.1 Hamiltonian

We study a system of coupled one-dimensional lattice layers described by the single-band tight-binding Hamiltonian,

\[
H = -t \sum_{<x,x'>,z} a_{xz}^\dagger a_{x'z} - \frac{1}{2} \sum_{xx'zz'} V(x - x', z - z') n_{xz} n_{x'z'} - \sum_{xz} \mu_z n_{xz}. \tag{11.1}
\]

Here \( t > 0 \) stands for the intra-tube tunneling amplitude, \( a_{xz}^\dagger \) (\( a_{xz} \)) is the creation (annihilation) operator for a hard core boson at site \( (x,z) \), where \( z = 0, 1, 2, \ldots, N \) labels the tubes and \( x = 0, 1, 2, \ldots, L \) is the coordinate along a tube. Here the brackets \(<\rangle\) denote summation over nearest neighbors), \( n_{xz} = a_{xz}^\dagger a_{xz} \), and \( \mu_z \) is the chemical potential which sets the number on particles in each layer.

The interaction \( V(x - x', z - z') \) can be arbitrary. In our simulations we will first address the case where the interaction exists only between particles on the same site \( x \) and on nearest neighboring tubes. Then, we will apply the algorithm to the case of the dipole-dipole interaction, with the polarization axis being perpendicular to the tubes and belonging to the plane of the tubes. In this case, the dipolar interaction takes the form:

\[
V(x, z) = V_d \frac{x^2 - 2z^2}{(x^2 + z^2)^{5/2}}, \tag{11.2}
\]

where \( V_d > 0 \) is strength of the nearest neighbor in-plane repulsion. In this geometry,
the interaction along the \(zz\)-axis is attractive and will induce formation of superfluid quasi-molecular complexes [WLD06, PBW+10, CK11, Gia04, VZF+11, BDTGA08, ADCMB09, KDS10, BMRZ11, AZFJ12, HZ]. The repulsive part of the interaction along the \(z\)-axis, instead, favors solidification.

When dipoles are polarized perpendicular to the tubes plane, the interaction becomes purely repulsive:

\[
V(x, z) = V_d \frac{1}{(x^2 + z^2)^{3/2}}. \tag{11.3}
\]

In what follows we will first introduce the general low energy description of the expected phases in terms of Thouless approach to superfluidity and bosonization. Then, we will report on a new multi-worm algorithm which allows efficient \textit{ab-initio} simulations of such phases.

### 11.2 Imbalance Induced Quantum Phases in Layered Systems

A system of hard-core bosons, trapped in one-dimensional tubes form with no inter-tube tunneling, forms \(N\) independent superfluids. This phase is characterized by independent quasi-condensate order parameters \(\langle \psi_z \rangle \sim \exp(i\phi_z)\) with phases \(\phi_z, z = 0, 1, 2, \ldots, N - 1\). In this system, the hard-core nature of the bosons in each tube, plays a special role. As we will see below, any arbitrary small inter-tube interaction can induce multiplicity of various superfluid and insulating phases depending on filling factor \(\nu_z\) in each tube. We will describe these phases, which we call \textit{Imbalance Induced Composites}, in terms of quantities which exhibit either long- or quasi-long range orders. It is worth noting that various mixtures of such phases can exist as well. The counter-intuitive threshold-less nature of the phases simply means that observing them is possible on correspondingly large spatial scales.
11.2.1 Thouless Phase Twists and Windings

Before describing these phases, we introduce their convenient description in terms of the generalized (and renormalized) superfluid stiffness $R_{zz'}$ and superfluid compressibility $C_{zz'}$. These are defined through contributions to the system action as a response to imposing infinitesimal Thouless phase twists $\tilde{\phi}(z) = (\phi_x'(z), \phi_r'(z))$ on the space-time boundaries of the tubes. Such twists can be viewed in terms of the corresponding gauge potentials $A_x(z, x) = \phi_x'(z)(x/L)$ along space and $A_r(z, \tau) = \phi_r'(z)(\tau/\beta)$ along time, where $L, \beta$ stand for tubes length and inverse temperature in atomic units, respectively. Then, the infinitesimal contribution to the action becomes

$$E = \sum_{zz'} \left[ \frac{\beta}{2L} R_{zz'} \phi_x'(z) \phi_x'(z') + \frac{L}{2\beta} C_{zz'} \phi_r'(z) \phi_r'(z') \right]. \quad (11.4)$$

The quantities $R_{zz'}$ and $C_{zz'}$ can be expressed in terms of topological properties of the particle world-lines, windings $\tilde{W}(z) = (W_x(z), W_r(z))$, and can be measured numerically. Global gauge invariance of the system implies that the total partition function $Z = \text{Tr}(\exp(-\beta H))$ can be represented as a statistical sum over all possible winding numbers of closed world lines of particles as

$$Z = \sum_{\{\tilde{W}(z)\}} Z[\{\tilde{W}\}] \exp[i \sum_z \tilde{W}(z) \tilde{\phi}(z)], \quad (11.5)$$

where $Z[\{\tilde{W}\}]$ stands for a functional of windings in all tubes. The superfluid stiffnesses can be obtained as second derivatives of $E = -\ln Z$ with respect to $(\phi_x'(z), \phi_r'(z))$ and taking the limit $\tilde{\phi}(z) \to 0$. This gives

$$R_{zz'} = \frac{L}{\beta} [\langle W_x(z)W_x(z') \rangle - \langle W_x(z) \rangle \langle W_x(z') \rangle], \quad (11.6)$$

$$C_{zz'} = \frac{\beta}{L} [\langle W_r(z)W_r(z') \rangle - \langle W_r(z) \rangle \langle W_r(z') \rangle]. \quad (11.7)$$

As long as the tubes are identical, $R_{zz'}$ and $C_{zz'}$ depend on the difference $z-z'$, $R_{zz'} = R(z-z')$ and $C_{zz'} = C(z-z')$. Hence, the Fourier transform along $z$-axis can be used,
\[ \tilde{R}(q_z) = \sum_z R(z) \exp(iq_z z), \tilde{C}(q_z) = \sum_z C(z) \exp(iq_z z), \] where \( q_z = \frac{2\pi n_z}{N}, n_z = 0, 1, 2, \ldots, N - 1. \) Then, if we express Eq. (11.5) in terms of the Fourier transforms \( \tilde{\phi}_{x,\tau}(q_z) = N^{-1/2} \sum_z \phi_{x,\tau}(z) \exp(iq_z z), \tilde{W}_{x,\tau}(q_z) = N^{-1/2} \sum_z W_{x,\tau}(z) \exp(iq_z z), \) we find

\begin{align*}
\tilde{R}(q_z) &= \frac{L}{\beta} [\langle \tilde{W}_x(q_z) \tilde{W}_x(-q_z) \rangle - \langle \tilde{W}_x(q_z) \rangle \langle \tilde{W}_x(-q_z) \rangle] \tag{11.8} \\
\tilde{C}(q_z) &= \frac{\beta}{L} [\langle \tilde{W}_{\tau}(q_z) \tilde{W}_{\tau}(-q_z) \rangle - \langle \tilde{W}_{\tau}(q_z) \rangle \langle \tilde{W}_{\tau}(-q_z) \rangle] \tag{11.9}
\end{align*}

These equations represent an extension of the expression in [CP89] for the superfluid stiffness and compressibility.

In full analogy with the \( N = 1, \) dimension \( D = 1 + 1 \) case, the ratio \( V_s(q_z) = \sqrt{\tilde{R}(q_z)/\tilde{C}(q_z)} \) has the meaning of the speed of sound propagating along tubes with the dispersion along the \( z \)-axis. Extending the analogy, the product \( \tilde{R}(q_z) \tilde{C}(q_z) \) gives the Luttinger “parameter” (rather, Luttinger matrix) as

\[ \tilde{K}(q_z) = \pi \sqrt{\tilde{R}(q_z) \tilde{C}(q_z)}. \tag{11.10} \]

Thus, the Gaussian renormalized action of the translationally invariant (along \( z \)-axis) system becomes

\[ S_R = \int_0^\beta d\tau \int dx \sum_{q_z} \left[ \frac{V_s(q_z) \tilde{K}(q_z)}{2\pi} |\nabla_x \tilde{\phi}(q_z)|^2 + \frac{\tilde{K}(q_z)}{2\pi V_s(q_z)} |\nabla_{\tau} \tilde{\phi}(q_z)|^2 \right], \tag{11.11} \]

where \( \tilde{\phi}(q_z) \) are the Fourier components of the phases \( \phi_z \) along \( z \)-axis.

The speed of sound is not significantly renormalized compared to the strong renormalization of superfluid stiffness \( R \) and compressibility \( C \) [Mat07]. Thus, for all practical purposes the dispersion in \( q_z \) of \( V_s \) can be ignored so that \( R_{zz'} = C_{zz'} \) in units of \( V_s = 1. \) Then, the generalized linear response can be fully described by the following translationally invariant action \( S_R = \int_0^\beta d\tau \int dx \sum_{q_z} \frac{1}{2\pi} \tilde{K}(q_z) |\nabla \tilde{\phi}(q_z)|^2 \), or in general
as

\[ S_R = \int_0^\beta d\tau \int dx \sum_{z,z'} \frac{1}{2\pi} (\hat{K})_{z,z'} \nabla \phi_z \nabla \phi_{z'}, \quad (11.12) \]

where \( \hat{K} \) stands for Luttinger parameter matrix with dimension \( N \times N \).

### 11.2.2 N Atomic Superfluids

If the layers have different filling factors, and the system is away from the special commensurate fillings, then the ground state is described in terms of \( \langle \psi_z \rangle \). These means represent quasi-long range (algebraic) order, and are zero in 1D. The corresponding one-particle density matrix \( \langle \psi_z(x)\psi_z(x') \rangle \sim 1/|x-x'|^b, b > 0 \), exhibits algebraic decay corresponding to 1D superfluids. Clearly, in the absence of the intertube tunneling \( \langle \psi_z(x)\psi_{z'}(x') \rangle = 0 \) for \( z \neq z' \). In the following we use \( \langle \psi_z \rangle \neq 0 \) when referring to the algebraic order in the one-particle density matrix channel. In terms of \( R \) and \( C \) responses, this phase is characterized by finite eigenvalues of the matrices \( R_{zz'} \) and \( C_{zz'} \) in the thermodynamical limit. When coupling between tubes is turned off, these matrices are diagonal and with a single eigenvalue \( N \)-fold degenerate for systems uniform along the \( z \)-axis. When tubes are coupled, instead, these matrices are not diagonal.

### 11.2.3 Composite Superfluids

If \( M \) out of \( N \) tubes are characterized by the same non-commensurate filling factor \( \nu \), the nature of the superfluid correlations changes dramatically as long as there is an arbitrary small attraction between the tubes. Specifically, any one-particle density matrix defined for such tubes will exhibit exponential decay. In other words, \( \langle \psi_z \rangle = 0 \). The algebraic decay will be observed only in the corresponding \( M \)-body density matrix constructed from the product \( \Phi(x) = \psi_{z_1}(x)\psi_{z_2}(x) \ldots \psi_{z_M}(x) \), where \( z_1, z_2, \ldots, z_M \) label the tubes characterized by the same filling factor. The field \( \Phi(x) \) is naturally understood as a quasi-molecular operator — \( M \)-composite. Then, the algebraic order can be observed as \( \langle \Phi(x)\Phi(x') \rangle \sim 1/|x-x'|^c, c > 0 \). In other words, the ground state
corresponds to the quasi-condensate of the $M$-composite field $\langle \Phi \rangle \neq 0$. It is important to note that such composite superfluid can be formed between any layers regardless of their geometrical positions, provided they are coupled and have the same filling factor. The corresponding $K$-matrix will have as many zero eigenvalues as there exist restored $U(1)$ symmetries. This number is given by the degree of degeneracy of the quadratic form of the stiffness. As an example, if there is a $M$-composite superfluid in $N$ layers, the degree of the degeneracy is $M-1$.

A particular case corresponds to the situation when all layers have the same filling factor, i.e. $M = N$. The system will therefore feature superfluidity of complexes consisting of $N$ bosons, forming a chain superfluid (CSF) [PBW+10, CK11, TK12, VZF+11], and the $K$-matrix will have a single non-zero eigenvalue. In terms of superfluidity matrix $R$ and compressibility matrix $C$, when their Fourier transforms (11.8) and (11.9) can be used, one has that $\tilde{R}(0) \neq 0$ and $\tilde{C}(0) \neq 0$ while all other Fourier components are zero. In the approximation of weak renormalization of sound velocity and setting $V_s = 1$, we find $\tilde{K}(0) \neq 0$ while all other harmonics $\tilde{K}(q_z) = 0, q_z \neq 0$.

### 11.2.4 Composite Countersuperfluids

This phase can be viewed as a bound state between particles and holes belonging to different layers. It can occur if filling factors $\nu_z$ on a set of some layers are matched by the filling factors $1 - \nu_z$ on other layers. Then, the corresponding order parameter operator is a product of creation and annihilation operators from the corresponding layers, e.g., $\Phi(x) = \psi_{z_1}(x)\psi_{z_2}(x)\psi_{z_3}^\dagger(x)\psi_{z_4}^\dagger(x)$. Thus, in this case, if $\nu_z \neq 1/2$, superflows along the layers $z_1, z_2$ are matched by the counter-flows along the layers $z_3, z_4$. In this sense, similarly to the composite superfluid case, $\langle \Phi \rangle \neq 0$ while $\langle \psi_{z_1} \rangle = 0, \langle \psi_{z_2} \rangle = 0, \langle \psi_{z_3} \rangle = 0, \langle \psi_{z_4} \rangle = 0$. The case of $N = 2$ corresponds to super-counterfluidity of two-component bosonic systems [KS03].
11.2.5 Composite Insulators

A special role is played by the filling factor $\nu = 1/2$. In the following, we show that for $N = 2$, and $\nu = 1/2$, arbitrary small intra-layer repulsion induces a checkerboard solid, provided that the inter-layer interaction is smaller (in absolute value) than the intra-layer repulsion. Remarkably, for $N > 2$, a checkerboard solid can also be formed in the absence of intra-layer repulsion as well. While solids at other rational filling factors $\nu = 1/3, 1/5, 2/5, \ldots$ can be induced as well, they form once interactions exceed the corresponding thresholds determined by the denominators of the fractions. In the insulating state $R_{zz'} = 0$, $C_{zz'} = 0$ (or $K_{zz'} = 0$).

11.3 N-tube Bosonization

Within the bosonization approach [Gia04, Hal80], the bosonic field operator $\psi_z(x)$ is represented in terms of the superfluid phase $\phi_z$ and the density $\rho_z = |\psi_z|^2$. The density can be expressed as follows:

$$\rho_z(x) = (\nu_z + \frac{1}{\pi} \nabla_x \theta_z) \sum_{m_z = 0, \pm 1, \ldots} e^{2m_z i(\theta_z + \pi \nu_z x)}, \quad (11.13)$$

where $\nu_z$ is the filling factor for each layer, and $\theta_z(x)$ is Haldane’s density phase conjugate to the superfluid phase $\phi_z$. The term $m_z = 0$ describes the forward scattering (FS) interaction and the terms with $m_z \neq 0$ account for the backscattering (BS) events.

In the absence of inter-tube tunneling, the bosonized action corresponding to the Hamiltonian given by Eq. (11.1) is given by

$$S = \sum_z S_z^{(0)} + \sum_{z, z'} [S_{z,z}^{(FS)} + S_{z,z}^{(BS)}], \quad (11.14)$$
where

\[ S_z^{(0)} = \int_0^\beta d\tau \int dx \frac{1}{2\pi K} [(\nabla_x \theta(x, \tau))^2 + (\nabla_z \theta(x, \tau))^2], \]  

(11.15)

in units \( V_s = 1 \). In the following we use periodic boundary conditions along \( x- \) and \( z\)-coordinates. \( K \) is the unnormalized Luttinger parameter, in contrast to what discussed in section 11.2 where we have introduced the Luttinger matrix. For hard-core bosons and zero dipolar interaction \( V_d = 0 \), each tube is equivalent to a XXZ spin \( S = 1/2 \) chain with zero \( S_z \) coupling. Accordingly, \( K = 1 \) (see Ref. [Gia04]).

The second term in Eq. (11.14) describes the forward scattering

\[ S^{(FS)}_{z,z'} = \frac{1}{2\pi^2} \int_0^\beta d\tau \int dx \int dx' V(x - x', z - z') \nabla_x \theta(x, \tau) \nabla_{x'} \theta'(x', \tau). \]  

(11.16)

In the long wave limit \( q_x \to 0 \) of the space-time Fourier representation this term takes the form:

\[ S^{(FS)}_{z,z'} = \frac{1}{2} \sum_\vec{q} \tilde{V}(z - z') q_x^2 \tilde{\theta}_z(\vec{q}) \tilde{\theta}_z(-\vec{q}). \]  

(11.17)

Here, the summation is performed over the time-space harmonics \( \vec{q} = (\omega, q_x) \), along each tube and

\[ \tilde{V}(z) = \frac{1}{\pi^2} \int dx V(x, z), \]  

(11.18)

where we have used the long wave limit \( q_x \to 0 \). In particular, for the dipole interaction given by Eq. (11.2) one finds

\[ \tilde{V}(z - z') = -\frac{\gamma_1}{(z - z')^2}, \quad \gamma_1 \approx \frac{2.00V_d}{\pi^2} \]  

(11.19)

for \( |z - z'| = 1, 2, 3, \ldots \). For \( z = z' \), the dipolar interaction is purely repulsive, with \( \tilde{V}(0) = \int dx V(x, z = 0) \), and must be cut off at the shortest distance. Here we consider the same length scale along \( z \) and \( x \), and choose the cutoff at \( x = 1 \) such that \( \tilde{V}(0) \approx 2.40V_d/\pi^2 \). Thus, in the long-wave limit the inter-layer interaction is attractive and the intra-layer interaction is repulsive. In the case of the purely repulsive dipolar
interaction, given by Eq. (11.3)) the FS interaction given by Eq. (11.19) changes sign.

Next we introduce Fourier harmonics along the z-coordinate, \( \tilde{\theta}(\vec{q}, q_z) \) and \( \tilde{V}_{q_z} \), corresponding to \( \tilde{\theta}(\vec{q}) \) and \( V(z) \), respectively. The Gaussian part of the action is given by:

\[
S_0 = \sum_{\vec{q}, q_z} \left[ \frac{1}{2\pi \tilde{K}(q_z)} \vec{q}^2 + \frac{1}{2} \tilde{V}_{q_z} q_z^2 \right] |\tilde{\theta}(\vec{q}, q_z)|^2.
\]

(11.20)

Eq. (11.20) features the renormalization of the speed of sound \( V_s \rightarrow V_s \sqrt{1 + \pi K \tilde{V}_{q_z}} \), which is set to unity, as well as of the Luttinger parameter

\[
K \rightarrow \tilde{K}(q_z) = \frac{K}{\sqrt{1 + \pi K \tilde{V}_{q_z}}}.
\]

(11.21)

Both quantities depend on the wave-vector \( q_z \) counting the layers.

The FS sets the initial value of the Luttinger matrix which is translationally invariant. Further renormalization due to BS in the presence of non-uniform chemical potential generates translationally non-invariant K-matrix.

Finally, the third term in the bosonized action, given by Eq. (11.14), results from the backscattering harmonics in Eq. (11.13):

\[
S^{(BS)}_{z,z'} = -\int d\tau \sum_{m_z, m_{z'}} \sum_{z=0,1,\ldots,L} V_{m_z, m'_{z'}}(z, z') \cos[2(m_z \theta_z + m'_{z'} \theta_{z'}) + 2\pi (\nu_z m_z + \nu_{z'} m_{z'}) \tau z],
\]

(11.22)

where the amplitudes \( V_{m_z, m'_{z'}}(z, z') \) are induced by the interaction and satisfy the renormalization flow (to be derived below in the standard one-loop approximation). The amplitudes \( V_{m_z, m'_{z'}}(z, z') \) can become translationally invariant, that is, dependent on the difference \( z - z' \) instead of \( z \) and \( z' \).

In the limit \( V_d \rightarrow 0 \) the RG flows can be found exactly. First we note that for hard-core bosons, \( K_{zz} = 1 \) and \( K_{zz'} = 0 \) for \( z \neq z' \). In this case, the lowest non-trivial values of \( m_z, m_{z'} \), i.e. \( m_z = \pm 1, m_{z'} = \pm 1 \), can set \( \nu_z m_z + \nu_{z'} m_{z'} = 0, \pm 1 \). Hence the terms with \( m_z = \pm 1, m_{z'} = \pm 1 \) are the only relevant terms and the relevance of the backscattering for a particular pair \( z, z' \) of layers can be controlled by the
corresponding chemical potentials $\mu_z, \mu_{z'}$.

11.3.1 RG Equations For the Complex Superfluid

For small interactions and identical filling factors $\nu_z = \nu_{z'}$ away from commensurability, the only relevant harmonics are given by terms corresponding to $m_z = -m_{z'}$, with $z \neq z'$. Therefore, the lowest relevant harmonic is $V_{1;-1}(z, z')$. The standard renormalization procedure consists of integrating out small oscillations of the Haldane phases $\theta$ (from the partition function $Z = \int D\theta \exp(-S)$) within the spherical shell of $q$ between some cutoff $\Lambda/(1+s)$ and $\Lambda$, and further rescaling $x \to (1+s)x$ and $\tau \to (1+s)\tau$, with $s \to 0$. In the lowest order (one-loop approximation), this procedure implies independent renormalization of each harmonic as follows:

\[
\frac{dV_{m;-m}(z, z')}{ds} = \left[ 2 - \frac{2m^2}{s} \langle (\theta_z - \theta_{z'})^2 \rangle \right] V_{m;-m}(z, z')
\]

(11.23)

where $\langle \ldots \rangle$ implies Gaussian average, with the integration performed over the shell of the momenta defined above. In two-dimensions $\langle (\theta_z - \theta_{z'})^2 \rangle$ exhibits log-divergence, that is, $\langle (\theta_z - \theta_{z'})^2 \rangle \sim s$, and it is independent of $\Lambda \to 0$. This average can be represented in terms of the elements of the Luttinger matrix by inverting the matrix $\hat{K}^{-1}$ as

\[
\frac{dV_{m;-m}(z, z')}{ds} = \left[ 2 - m^2(K_{zz} + K_{z'z'} - 2K_{zz'}) \right] V_{m;-m}(z, z')
\]

(11.24)

where $K_{zz'}$ are elements of the matrix $\hat{K}$.

In the case of translational invariance along the $z$-axis this equation can be explicitly written in terms of the Fourier harmonics $\hat{K}(q_z)$ of the matrix $\hat{K}$ as

\[
\frac{dV_{m;-m}(z)}{ds} = \left[ 2 - \frac{4m^2}{N} \sum_{q_z} \hat{K}(q_z) \sin^2 \left( \frac{q_z z}{2} \right) \right] V_{m;-m}(z)
\]

(11.25)

In the above expression we have used $V_{m;-m}(z, z') = V_{m;-m}(z - z')$ and $(\hat{K}^{-1})_{zz'} = \cdots$
\( \hat{K}^{-1}(z - z') \), with the inverse Fourier for the Luttinger matrix defined as:

\[
K_{zz'} = K(z - z') = \frac{1}{N} \sum_{q_z} \hat{K}(q_z) e^{iq_z(z - z')}.
\]  

(11.26)

Similarly, the inverse Fourier of the inverse Luttinger matrix is given by:

\[
(\hat{K}^{-1})_{zz'} = \hat{K}^{-1}(z - z') = \frac{1}{N} \sum_{q_z} (\hat{K}(q_z))^{-1} e^{iq_z(z - z')}.
\]  

(11.27)

If one ignores the renormalization of the Luttinger matrix, the value of \( \hat{K}(q_z) \) from Eq. (11.21) can be used in Eq. (11.25). For small \( V_d \) one can expand Eq. (11.21) in powers of \( V_d \) and find

\[
\frac{dV_{m,-m}(z)}{dz} = \left[ 2 - m^2 (2K - \pi K^2 (\bar{V}(0) - \bar{V}(z))) \right] V_{m,-m}(z),
\]  

(11.28)

where \( \bar{V}(z) \) is given in Eq. (11.19). In the limit \( V_d \to 0 \) and for \( |m| = 1 \), the critical value of \( K \) is \( K_c = 1 \). Thus, since \( K = 1 \), for \( \bar{V}(0) > 0 \) and \( \bar{V}(z - z') < 0 \) as in the case of dipolar interaction, the harmonic \( \cos(2\theta_z - 2\theta_{z'}) \) becomes relevant for arbitrary small \( V_d \). In other words, renormalization leads to the power law growth of \( V_{1,-1}(z) \) with the system size. This implies that the superflow is only possible in the channel of the center of mass motion because relative density fluctuations are gapped. We also note that higher harmonics \( V_{m,-m}(z), m > 1 \), are irrelevant because the critical value for them in the limit \( V_d \to 0 \) is \( K_m = 1/m^2 < 1 \).

It is also interesting to note that, in the case of the purely repulsive interaction (11.3), where \( \bar{V}(z) > 0 \) for \( |z| > 0 \), the complex superfluid is also possible as long as \( \bar{V}(0) > \bar{V}(z) > 0 \). This binding caused by repulsion is a specific property of 1D geometry.

The renormalization of the BS amplitudes, Eq. (11.23), should be considered together with the renormalization of the matrix \( (\hat{K}^{-1})_{zz'} \) in the quadratic form given in Eq. (11.12). In the one-loop approximation, the main contribution is due to the same BS harmonic, \( \cos(2(\theta_z - \theta_{z'})) \). It is important to realize that the harmonic generates the term \( \sim (\bar{V}(\theta_z - \theta_{z'}))^2 \) upon the RG procedure. Thus, the contributions
to the diagonal elements \((\hat{K}^{-1})_{zz}\) and to the off-diagonal ones \((\hat{K}^{-1})_{zz'}\) where \(z \neq z'\), should be considered independently. In the case of translational invariance, where \(\nu_z\) does not vary with respect to \(z\), we follow the standard procedure described in [Gia04], and find:

\[
\frac{d(\hat{K}^{-1})_{zz'}}{ds} = -C[V_{1,-1}(z, z')]^2(K_{zz} + K_{zz'} - 2K_{zz'}),
\]

and, for the diagonal term:

\[
\frac{d(\hat{K}^{-1})_{zz}}{ds} = C\sum_{z'}[V_{1,-1}(z, z')]^2(K_{zz} + K_{zz'} - 2K_{zz'}),
\]

where the constant \(C > 0\) depends on the type of the short-distance cutoff. This constant can be absorbed into the definition of \(V_{1,-1}(z)\) by simple rescaling so that the shape of the RG equations does not change. Note that, only pairs \((z, z')\) such that \(\nu_z = \nu_{z'}\) are involved in Eq. (11.29) and Eq. (11.30).

In the case of the translational invariance (that is, \(\nu_z = \text{const with respect to } z\)) these equations become:

\[
\frac{d(\hat{K}^{-1})(z)}{ds} = -\frac{4C}{N}[V_{1,-1}(z)]^2\sum_{q_z} K(q_z) \sin^2 \left(\frac{q_z z}{2}\right),
\]

and

\[
\frac{dK^{-1}(0)}{ds} = \frac{4C}{N}\sum_{z, q_z}[V_{1,-1}(z)]^2\tilde{K}(q_z) \sin^2 \left(\frac{q_z z}{2}\right).
\]

### 11.3.2 RG Equations for Complex Countersuperfluid

If there is a pair of layers \(z, z'\) with filling factors \(\nu_z\) and \(\nu_{z'} = 1 - \nu_z\), the BS harmonic \(V_{1,1}(z, z') \cos(2\theta_z + 2\theta_{z'})\) can become relevant, while the \(V_{1,-1}(z, z')\) is irrelevant due to the mismatch of filling factors. As a consequence, the gapless superflow is possible only in the counter-flow channel. In other words, it is the difference between the two phases which remains gapless. If more than two tubes have filling factors complementary to unity, for example filling factor \(\nu\) in \(M > 1\) tubes and filing factor \(1 - \nu\) in some other
$M$ tubes, a simple count of phases shows that only one phase out of the $2M$ phases remains gapless. Such phase accounts for the counterflow between the two groups of tubes.

The RG equations for the counterflow can be written for each pair of tubes with the complementary filling factors by simply changing the sign in front of the $K_{zz'}$ term in the corresponding equations, Eq. (11.24), derived above for the complex superfluids. Specifically, one finds:

$$\frac{dV_{1;1}(z, z')}{ds} = [2 - (K_{zz} + K_{z'z'} + 2K_{zz'})] V_{1;1}(z, z'). \quad (11.33)$$

Here, the $V_{1;1}$ channel is gapped. For the case of more than 2 tubes in the counterflow regime, the dipolar interaction can induce an additional gap in the $\sim V_{1;1}$ channel in tubes with same filling factors. However, a simple count of the remaining gapless phases shows there is still one gapless phase for the $M$ tubes. This has a very simple interpretation: the gaps in tubes with equal filling factors imply formation of a pair of composite superfluids, one per each group of $M$-tubes. These composite superfluids further bind in the counterflow regime.

The flow equation for the off-diagonal elements of the Luttinger matrix is analogous to Eq. (11.29),

$$\frac{d(\hat{K}^{-1})_{zz'}}{ds} = C[V_{1;1}(z, z')]^2(K_{zz} + K_{z'z'} + 2K_{zz'}). \quad (11.34)$$

Similarly, the diagonal terms satisfy:

$$\frac{d(\hat{K}^{-1})_{zz}}{ds} = C \sum_{z'} [V_{1;1}(z, z')]^2(K_{zz} + K_{z'z'} + 2K_{zz'})C \sum_{z'} [V_{1;1}(z, z')]^2(K_{zz} + K_{z'z'} - 2K_{zz'}), \quad (11.35)$$

where the first sum is the contribution from tubes with filling factor complementary to a given $z$-tube, while the second sum is the contribution from tubes with the same filling factor, as shown in Eq. (11.30)).

Finally, we write the above equations for the particular case of even tubes (labelled by $z = 0, 2, 4, \ldots$) with filling factor $\nu$ and odd tubes (labelled by $z = 1, 3, 5, \ldots$)
with filling factor $1 - \nu$. Then, similar to the complex superfluid case, we use the translationally invariant solution:

$$\frac{dV_{1;1}(z)}{ds} = \left[ 2 - \frac{4}{N} \sum_{q_z} \tilde{K}(q_z) \cos^2 \left( \frac{q_z z}{2} \right) \right] V_{1;1}(z),$$  \hspace{1cm} (11.36)

where the distance $z = z - z' = 1, 3, 5, \ldots$ corresponds to pairs of tubes with the complementary filling factors. For distances $z = 2, 4, 6, \ldots$, that is, for layers with same filling factors, Eq. (11.25)) with $m = 1$ has to be used. Similarly the flow of the matrix of stiffnesses at odd distances $z$ is given by:

$$\frac{dK^{-1}(z)}{ds} = \frac{4C}{N} [V_{1;1}(z)]^2 \sum_{q_z} \tilde{K}(q_z) \cos^2 \left( \frac{q_z z}{2} \right),$$  \hspace{1cm} (11.37)

while at even, non-zero distances $z$ the flow is described by Eq. (11.31). The diagonal term $\tilde{K}(0)$ has contribution from all pairs, and its flow is given by:

$$\frac{dK^{-1}(0)}{ds} = \frac{4C}{N} \sum_{q_z} \tilde{K}(q_z) \left[ \sum_{z=1,3,5,\ldots} [V_{1;1}(z)]^2 \cos^2 \left( \frac{q_z z}{2} \right) + \sum_{z=2,4,6,\ldots} [V_{1;1}(z)]^2 \sin^2 \left( \frac{q_z z}{2} \right) \right].$$  \hspace{1cm} (11.38)

It is instructive to ignore Eqs. (11.37) and (11.38), and substitute the initial value (11.21) into Eq. (11.36). For $z \neq 0$ this gives

$$\frac{dV_{1;1}(z)}{ds} = \left[ 2 - 2K + \pi K^2 (\bar{V}(0) + \bar{V}(z)) \right] V_{1;1}(z).$$  \hspace{1cm} (11.39)

Thus, for purely repulsive interaction the harmonic $V_{1;1}(z)$ is relevant for arbitrary small $V_d$ (since $K = 1$ here). This induces a gap in the channel of fluctuations of $\theta_{z_1} + \theta_{z_2}$. It is also interesting to note that, in a direct analogy with the complex superfluid, the inter-layer attraction $\bar{V}(z) < 0$ also induces the complex counter-fluid as long as the intra-layer repulsion is strong enough: $\bar{V}(0) > |\tilde{V}(z)|$. 

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11.3.3 RG Equations for Insulators

In the absence of the inter-tube interactions, hard core bosons can form a checkerboard (CB) type insulator at filling factor $\nu = 1/2$ if the repulsive interaction is strong enough, so that the Luttinger parameter $K$ is reduced from $K = 1$ to $K = 1/2$. This can be seen from Eq. (11.32) written for $z = z'$, that is, for the intra-tube harmonic $\cos(4\theta_x + 4\pi \nu_x x)$. Eq. (11.32) becomes $dV_{1;1}(0)/ds = (2 - 4K_{zz}V_{1;1}(0)$. In the limit $V_d \to 0$, the matrix $K_{zz}$ becomes diagonal with a single N-fold degenerate eigenvalue, the Luttinger parameter $K$. In this limit we can rewrite Eq. (11.32) as $dV_{1;1}(0)/ds = (2 - 4K)V_{1;1}(0)$, so that it is clear that the critical value corresponds to $K = 1/2$.

The situation changes dramatically in the $N = 21$ case, where arbitrary small repulsion $\tilde{V}(0) > 0$ induces the insulating state as long as the inter-layer interaction $|\tilde{V}(z)|, z = 1, 2, ..$ is finite and smaller than $\tilde{V}(0)$. Indeed, at $\nu = 1/2$, both harmonics $\cos(2(\theta_x \pm \theta_z))$, with $z \neq z'$, become relevant, as Eq. (11.28) and Eq.(11.39) show. The corresponding critical value of $K$ in the limit $V_d \to 0$ is $K_c = 1$. A finite interaction with $\tilde{V}(0) > 0$ lowers $K$ below $K_c$.

A more interesting situation occurs in the case $N > 2$ and $\nu = 1/2$. In contrast to the $N = 2$ system (which will be extensively studied numerically, see below), channels $V_{1;1}, V_{1;-1}$ do not decouple from each other as one can see from the evolution of $\tilde{K}$ given by Eqs. (11.37), and (11.38). The insulating state must form regardless of sign of the inter-layer interaction as long as it is not exactly zero. As an example, let's consider purely attractive interactions with $\tilde{V}(0) = 0$ and $\tilde{V}(z) < 0, z = 1, 2, ...$ Then, the superfluid channel $V_{1;-1}$ becomes gapped with respect to relative fluctuations of the density. Such gap, however, does not affect the harmonic $\tilde{\theta}(q_z = 0)$ as Eqs.(11.31,11.32 indicate. Thus, $\tilde{K}(q_z = 0)$ is the only harmonic which may remain finite in the thermodynamical limit. Then, turning attention to Eq. (11.36), which describes the RG flow of the harmonic $V_{1;1}$, immediately shows that, since all harmonics $\tilde{K}(q_z)$ with $q_z \neq 0$ flow to zero, the remaining equation for $V_{1;1}$ becomes

$$\frac{dV_{1;1}(z)}{dS} \approx [2 - \frac{4}{N}\tilde{K}(0)]V_{1;1}(z)$$ (11.40)
in the long-wave limit with $\tilde{K}(0) \approx 1$. This means that, despite that inter-layer interaction is purely attractive the superfluid of $N$-bosonic complexes cannot exist at $\nu = 1/2$ as long as $N > 2$. Instead, CB-type insulator must form.

The situation with $N = 2$ is marginal, as Eq. (11.40) indicates. This case require separate analysis. Below we will discuss in greater detail.

Finally, we note that, in contrast to the filling factor $\nu = 1/2$, forming insulating states at other special filling factors $1/3, 1/5, 2/5$, etc. requires that interactions exceed certain thresholds so that initial values of the Luttinger parameter $K$ become significantly below unity. Particular dependencies of $K$ on $V_d$ are strongly non-perturbative and can only be established numerically.

### 11.4 Ab-initio Simulations

In this section we present ab-initio results based on path integral QMC by the multi-worm algorithm described in section 9.2.4. Unless otherwise specified, the results we will present in this section refer to the following simplified version of model (11.1):

$$H = -t \sum_{<x,x'>,z} a^\dagger_{xz} a_{x'z} - \frac{1}{2} V_d \sum_{x<z'} n_{xz} n_{xz'} - \mu \sum_{xz} n_{xz}$$ (11.41)

where we consider only attractive interaction $V_d$ between dipoles sitting on top of each other and neglect any intra-plane repulsion. The chemical potential $\mu$ is the same on each layers, thus ensuring that layers have the same filling factor. As previously discussed, in this geometry, bosonization predicts stabilization of a superfluid phase of $N$-long chains extending across the layers. In what follows we will extensively discuss the case of $N = 2$ and $N = 3$ layers. The former case has been studied by means of a two-worm algorithm described in section 9.2.3, the latter by means of a novel multi-worm algorithm described in section 9.2.4.

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11.4.1 QMC Study of the Bilayer System, $N = 2$ Case

Absence of the threshold for the phases discussed above is a remarkable property of the geometry. It implies that, in order to realize such phases, there is no need to pursue strong dipole-dipole interactions. Instead, the size of the system should be made large enough (and temperature low enough) so that the effects of small gaps are seen. Here we will address the issue of no threshold in great detail by \textit{ab-initio} simulations of the bilayer system. The goal of this study is to demonstrate this property explicitly.

We consider two identical layers located at $z = 0, 1$ with $\nu_0 = \nu_1 = \nu$. Then, the Luttinger matrix consists of just two elements $(\tilde{K}^{-1})_{00} = (\tilde{K}^{-1})_{11}$ and $(\tilde{K}^{-1})_{01}$. The Fourier representation along $x$-axis has just two harmonics with $q_z = 0, \pi$, so that Eq. (11.27) yields $1/\tilde{K}(0) = (\tilde{K}^{-1})_{00} + (\tilde{K}^{-1})_{01}$ and $1/\tilde{K}(\pi) = (\tilde{K}^{-1})_{00} - (\tilde{K}^{-1})_{01}$.

At $\nu \neq 1/2$ the only relevant harmonic corresponds to $V_{1;-1}$. Thus the RG flow only affects $\tilde{K}(\pi)$ and $V_{1;-1}$ and the corresponding RG equations follow from Eq. (11.28), (11.31), and (11.32) combined as:

$$\frac{dV_{1;-1}}{ds} = [2 - 2\tilde{K}(\pi)]dV_{1;-1}, \quad (11.42)$$

$$\frac{d\tilde{K}^{-1}(\pi)}{ds} = 2CV_{1;-1}^2 \tilde{K}(\pi). \quad (11.43)$$

The initial value of $\tilde{K}(\pi)$ at small scales is set by Eq. (11.21) as $\tilde{K}(\pi) = K/\sqrt{1 + \pi K \tilde{V}(\pi)}$, with $\tilde{V}(\pi) = \tilde{V}(0) - \tilde{V}(1)$. In the particular case $\tilde{V}(0) = 0$ and $\tilde{V}(1) < 0$, the channel $(V_{1;-1}, \tilde{K}(\pi))$ develops a gap because the initial value of $\tilde{K}(\pi)$ is below its critical value.

In the case $\nu = 1/2$, or in the case of complementary filling factors $\nu_0 = \nu$ and $\nu_1 = 1 - \nu$, the channel $(V_{1;1}, \tilde{K}(0))$ must be considered. The corresponding RG equations follow from Eqs. (11.36), (11.37), and (11.38) combined:

$$\frac{dV_{1;1}}{ds} = [2 - 2\tilde{K}(0)]dV_{1;1}, \quad (11.44)$$

$$\frac{d\tilde{K}^{-1}(0)}{ds} = 2CV_{1;1}^2 \tilde{K}(0). \quad (11.45)$$

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with the initial value set by \( \bar{K}(0) = K / \sqrt{1 + \pi K \bar{V}(0)} \), with \( \bar{V}(0) = \bar{V}(0) + \bar{V}(1) \).

The above two groups of equations show that in the case \( N = 2 \), the two channels are completely decoupled and are described by the same set of equations:

\[
\begin{align*}
\frac{du}{ds} &= 2(1 - g)u \\
\frac{dg^{-1}}{ds} &= gu^2,
\end{align*}
\]

(11.46)

where the pair \((u, g)\) can take the values \((\sqrt{2CV_1}, \bar{K}(\pi))\), or \((\sqrt{2CV_1}, \bar{K}(0))\). Here \(s = \ln l\), and is determined by the RG scale \(l\), which can be taken as the system size \(l = L\). This system describes the famous Berezinskii-Kosterlitz-Thouless (BKT) transition [KT73]. The identity between the two channels means that at \( \nu = 1/2 \), and for certain values of \( \bar{V}(1) \) and \( \bar{V}(0) \), e.g. when \( \bar{V}(1) < 0 \) and \( 0 \leq \bar{V}(0) < |\bar{V}(1)| \), the \( \pi \)-channel is gapped, while the 0-channel is gapless. This region includes the particular case studied in our simulations, where \( \bar{V}(0) = 0 \) and \( \bar{V}(1) < 0 \). This should be contrasted with the case \( N > 2 \) when all channels interact with each other so that there must always be an insulator at \( \nu = 1/2 \) as discussed in section 11.3.3.

The Eqs. (11.46) can be solved analytically and yield the solution:

\[
\begin{align*}
u^2 &= 2[\xi^2 - (1 - c_0)], \\
F(\eta) &= \ln(\xi^2(L) - \eta^2) + \frac{1}{\eta} \ln \left( \frac{\xi(L) - \eta}{\xi(L) + \eta} \right) = 4 \ln \left( \frac{L}{L_0} \right),
\end{align*}
\]

(11.47)

where \(c_0\) and \(L_0\) are real constants of integration, \(\xi(L) \equiv g^{-1}(L) - 1\), and \(\eta \equiv \sqrt{1 - c_0}\). Both integration constants \(c_0\) and \(l_0\) are determined by the interaction \(V_d\). The parameter \(\eta\) can be real or purely imaginary depending on the initial values of \(\xi, u\). The critical solution \((\xi = 0, u = 0)\), that is \((K = 1, V_d = 0)\), belongs to the separatrix, \(\eta \to 0, \xi(l) = \xi_s(l)\),

\[
\ln \xi_s - \frac{1}{\xi_s} = 2 \ln \left( \frac{L}{L_0} \right).
\]

(11.48)

The separatrix divides the parameter space into two domains, with and without fixed points. In the context of our system this implies that \(\eta\) must approach \(\eta = 0\) as long
as $V_d \to 0$. Finite interaction $V_d$ drives the system away from criticality so that $\eta$ depends on $V_d$ with $\eta \propto V_d$ at small $V_d$. Thus, in order to compare the numerics with the RG predictions one should find such functions $\eta(V_d), l_0(V_d)$ so that the numerical solution for $g(L)$ follows the analytical one given by Eq. (11.47) for wide range of system sizes $L = l$.

The value of $g$ can be expressed in terms of the renormalized superfluid stiffness and compressibility, as in the general case of Eqs. (11.6) and (11.7). If we ignore renormalization of speed of sound, the Fourier of the Luttinger matrix (11.10) should be considered. Thus, for $g = g(\pi) = \tilde{K}(\pi)$

$$\tilde{K}(\pi) = \pi \sqrt{\langle |\tilde{W}_x(\pi)|^2 \rangle \langle |\tilde{W}_\tau(\pi)|^2 \rangle}, \quad (11.49)$$

where we have used $\langle \tilde{W}_x(\pi) \rangle = 0$ and $\langle \tilde{W}_\tau(\pi) \rangle = 0$ due to full symmetry between layers. More explicitly, in terms of windings in real space:

$$\tilde{K}(\pi) = \frac{\pi}{2} \sqrt{\langle (W_x(0) - W_x(1))^2 \rangle \langle (W_\tau(0) - W_\tau(1))^2 \rangle}. \quad (11.50)$$

For $g = g(0) = \tilde{K}(0)$, we find:

$$\tilde{K}(0) = \frac{\pi}{2} \sqrt{\langle (W_x(0) + W_x(1))^2 \rangle \langle (W_\tau(0) + W_\tau(1))^2 \rangle}. \quad (11.51)$$

Since $\tilde{K}(\pi)$ can be extracted from windings, we have used the Worm algorithm [PST98a, PST98b], which has been designed for this purpose to determine the windings, and determine $\tilde{K}(\pi)$ for various $V_d/J$. We summarize our numerical results for $\tilde{K}(\pi)$, Eq. (11.50), in Fig. 11-1).

Fig. 11-2 shows $F(\eta)$ as a function of $X = 4 \ln(L/L_0)$, extracted from the data for $K(\pi)$ presented in Fig. 11-1. If the data obey the RG flow, the curve $F$ vs $X$ will be a straight line with a slope of one for all values of the interaction $V_d$. The slope of the line of best fit, (see the thin black line in Fig. 11-2) is $1.01 \pm 0.02$ and the insets show the values of the fit parameters $\eta$ and $4 \ln L_0$ as a function of the interaction strength.
\[ V_d/J = 1, V_d/J = 0.9, V_d/J = 0.8, V_d/J = 0.7, V_d/J = 0.5, V_d/J = 0.4, V_d/J = 0.3, V_d/J = 0 \]

Figure 11-1: Plot of $K(\pi)$ as a function of system size for different inter-layer interaction strengths $V_d/J$.

$V_d/J$. The data clearly obey the RG flow. Moreover we find that all $\eta$ are real and the separatrix, corresponding to the point $\eta = 0$, occurs at $V_d/J = 0$. This indicates that pairs are formed for infinitesimally small interaction strengths, and completes our proof of the threshold-less nature of the composite phases.

We have also analyzed the flow of $\tilde{K}(0)$ at $\nu = 1/2$ when both harmonics $V_{1;-1}(1)$ and $V_{1;1}(1)$ can be relevant. According to the RG prediction, while $V_{1;-1}(1)$ is relevant, the harmonic $V_{1;1}(1)$ should be irrelevant as long as $\tilde{V}(0) = 0$ and $\tilde{V}(1) < 0$ (see Eq. (11.39)). Hence flow of $\tilde{K}(0)$ must begin above the critical value $\tilde{K}(0) = K = 1$ and reach some stable fixed point at $\tilde{K}(0) > 1$. However, the simulations conducted at finite $V_d/J$ show that $\tilde{K}(0)$ tends to reach some stable fixed point, $K^* \approx 0.5$, that is below the critical value. Our numerical results for $\tilde{K}(0)$ are collected in Fig. 11-3. In the presence of a stable fixed point below the critical value, inspection of Eqs. (11.44) and (11.45) show that the harmonic $V_{1;1}(1)$ should drive $\tilde{K}(0)$ to 0. In analogy with
Figure 11-2: The master curve $F(\eta)$ vs. $4 \ln (L/L_0)$ for the $K_-$ flows shown in Figure 11-1. The line of best fit has a slope of $1.01 \pm 0.02$ and the insets show the fit parameters $\eta$ and $L_0$ as a function of interaction strength $V_d/J$. The plot confirms that the separatrix occurs at $V_d/J = 0$ indicating that the chains are formed at infinitesimally small values of $V_d/J$.

what done for $\tilde{K}(\pi)$, we have constructed the master curve, as shown in Fig. 11-4. Furthermore, as the top-left inset of Fig. 11-4 shows, as $V_d/J$ is increased from 0.3 to 0.7, the curves tend to approach the critical separatrix described by Eq. (11.48), where $\eta = 0$, $K_c = 1$. However, once $V_d/J > 0.7$ the curves display a fixed point behavior where $K_c = 1/2$. This results from the criticality of the terms $\sim \cos(4\theta_0) + \cos(4\theta_1)$, which correspond to the case of non-interacting tubes.

At the moment we don’t have a clear understanding of this behavior. It is possible that, in contrast to the channel $V_{1-1}$, the limiting behavior $\eta \propto V_d$ is reached at values of $V_d/J$ much smaller than $V_d/J = 0.3$. For interactions $V_d/J < 0.3$, though, no renormalization could be reliably detected for accessible sizes $L \leq 600$. Such a disparity between the two channels may be due to different roles played by irrelevant
Figure 11-3: The plot of $K(0)$ as a function of system size $L$ for different inter-layer interaction strengths $V_d/J$.

11.4.2 QMC Study of the Multilayer System, N=3 Case

Here we present QMC results of a novel multi-worm algorithm. The main purpose of this section is to demonstrate that this new algorithm works successfully. We consider $N = 3$ layers. We start by looking at the properties of the 3-body density matrix $D_3(x_1, x_2, x_3; x_1', x_2', x_3')$. Specifically, we have measured $f_1(x_1', x_2') \propto \int dx_1 dx_2 dx_3 dx_3' D_3 w$ and $f_2(x_1, x_1') \propto \int dx_2 dx_3 dx_2' dx_3' D_3 w$, where the weight $w$ has been previously introduced in section 9.2.4. As already discussed, in a CSF phase, one expects $f_1(|x_1' - x_2'|) \sim \exp(-|x_1' - x_2'|/\xi)$ (short-ranged) and, at the same time...
\( f_2(|x'_1 - x_1|) \sim \frac{1}{|x'_1 - x_1|^b} \) (\( b > 0 \), quasi long-range). In a insulating phase, both \( f_1 \) and \( f_2 \) are short-ranged. Indeed, our simulation results are in agreement with this expectation as shown in Fig. 11-5, where the histograms are QMC results and dashed lines are fits to the data. We plot \( f_1 \) (Fig. 11-5(a) and \( f_2 \) (Fig. 11-5(b)) for the CSF phase at \( L = 300 \), \( \nu = 0.47 \) and \( V_d/J = 1 \) (in blue) and the insulating chain-checkerboard phase at \( L = 300 \), \( \nu = 0.5 \) and \( V_d/J = 1 \) (in black). (Recall that for \( N > 2 \), the checkerboard phase can be stabilized even in the absence of in-plane repulsive interaction, see section 11.3.3).

Next we address the stabilization of insulating phases at densities other than \( \nu = 0.5 \). For this purpose we consider the anisotropic dipolar interaction Eq. 11.2 with a cutoff of three sites. Charge density wave insulators at fractional filling factors are expected for large enough dipolar interaction (see section 11.3.3). When the system is in an insulating phase one expects function \( f_2(|x'_1 - x_1|) \) to be short ranged. We have measured \( \langle |x'_1 - x_1| \rangle \) as a function of density and at fixed dipolar interaction \( V_d = 2 \) for \( L = 180 \). We have observed similar behavior at other \( L \). Our QMC results are reported in Figure 11-6. Two dips corresponding to insulating phases at densities \( \nu = 1/3 \) and \( \nu = 1/2 \) can be clearly seen. To further confirm the presence of charge density wave insulating phases, we have measured the structure factor \( S(k) = \sum_{x,x'} \exp[(x - x')k(\nu_x\nu'_x)/L, \) where \( k \) is the reciprocal lattice vector of the corresponding solid. \( S(k) \) will be finite at \( k = 2\pi/3 \) and \( k = \pi \) in the solid phases at density \( \nu = 1/3 \) and \( \nu = 1/2 \) respectively. Our QMC results for \( S(k) \) are reported in the inset of Fig. 11-6 as a function of \( L \) and \( V_d/J \). The solid lines correspond to \( S(\pi) \) measured at \( V_d/J = 0.75 \) (circles), \( V_d/J = 1 \) (diamond), \( V_d/J = 1.5 \) (triangle), and \( V_d/J = 2 \) (square). The dashed lines correspond to \( S(2\pi/3) \) measured at \( V_d/J = 1.5 \) (triangle), \( V_d/J = 2 \) (square), and \( V_d/J = 3 \) (diamond). While we do not significant dependence on the system size for \( L > 150 \), indicating the existence of the solid phases at these two filling factors, it is evident that the solid at \( \nu = 1/3 \) is stabilized at higher interaction strengths compared to the checkerboard solid at half-filling.
Figure 11-4: The master curve for the data $\tilde{K}(0)$ for $V_d/J = 0.7$ (green squares), $V_d/J = 0.5$ (red triangles), $V_d/J = 0.4$ (blue stars), and $V_d/J = 0.3$ (orange circles). Insets show $|\eta|$ vs $V_d/J$ and $L_0$ vs $V_d/J$. The kink on $|\eta|$ vs $V_d/J$ corresponds to switching from real $\eta$ to purely imaginary for $V_d/J > 0.4$. The best fit at $V_d/J = 0.7$ gives $\eta = 0$ which implies the separatrix. The data with $V_d/J > 0.7$ cannot be described by this master curve. It belongs to a different flow where $K_c = 1/2$ and $L_0 = \infty$. 
Figure 11-5: Results of the 3-worm algorithm for a) the decay of function $f_1(x'_1, x'_2)$ (see text for details) in the chain-superfluid phase (blue) and the chain-checkerboard phase (black). b) the decay of function $f_2(x_1, x'_1)$ (see text for details) in the chain-superfluid phase (blue) and the chain-checkerboard phase (black).
Figure 11-6: The plot of $\langle |x'_1 - x_1| \rangle$ as a function of the filling factor at $V_d/J = 2$ and $L = 180$. The dips indicate the formation of solids at $\nu = 1/3$ and $\nu = 1/2$. This is further studied in the insets which show QMC results for $S(k)$ as a function of $L$ and $V_d/J$. The solid lines correspond to $S(\pi)$ measured at $V_d/J = 0.75$ (circles), $V_d/J = 1$ (diamond), $V_d/J = 1.5$ (triangle), and $V_d/J = 2$ (square) and prove the existence of a checkerboard solid at half-filling. The dashed lines correspond to $S(2\pi/3)$ measured at $V_d/J = 1.5$ (triangle), $V_d/J = 2$ (square), and $V_d/J = 3$ (diamond) and show the existence of a solid phase at $\nu = 1/3$. 
Chapter 12

Bose-Hubbard Model with
Three-Body Interactions

Chapter 7 introduced the Bose Hubbard (BH) model and its second order superfluid (SF)-Mott-insulator (MI) transition as one of the paradigmatic examples of strongly interacting many-body physics in lattice structures [FWGF89].

In this chapter, we analyze how the many-body physics of the BH model is affected by the presence of local and tunable three-body interactions. In section 12.1, we propose a mechanism for engineering a three-body onsite interaction term, $U_3$, which is controlled by an external rf pulse that couples the triply occupied state with a three-body bound state associated with an excited hyperfine state. In section 12.2 we use a mean-field Gutzwiller approach to study the BH Hamiltonian in the presence of such three-body interaction in the $U > 0$, $U_3 < 0$ regime. Section 12.3 presents the Quantum Monte Carlo (QMC) simulation results, using the Worm algorithm [PST98a], which provide quantitative predictions of the phase diagram in two dimensions and discuss the finite temperature effects and experimental signature of the first order transition.

This chapter has previously appeared (with some modifications) in [SvCR12].
12.1 Bose-Hubbard Model with Tunable, On-site, Three-body Interaction

In this section we propose a scheme for engineering a local, on-site, tunable three-body interaction term, $U_3$. This local three-body interaction only affects triply occupied sites leading to a modified BH Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} a_i^\dagger a_j + \sum_i \left[ \frac{U}{2} n_i(n_i-1) + \delta_{n_i,3} U_3 - \mu n_i \right]$$

(12.1)

where $a_i^\dagger(a_i)$ is the bosonic creation (annihilation) operator, $n_i = a_i^\dagger a_i$, $J$ is the hopping matrix element, $U$ is the two-body onsite interaction, $U_3$ is the 3-body onsite interaction, $\mu$ is the chemical potential, and $\langle i,j \rangle$ denote sum over nearest neighbor sites only [see Fig. 12-1(a)]. Note that the three-body interaction considered here is different from the more conventional interaction of the form $U_3 n(n-1)(n-2)/6$.

To achieve a separately tunable, on-site, three-body interaction of the form shown in Eq. 12.1, we envision a system in which a universal three-body bound state is attached to an excited hyperfine threshold [Efi70, BH06, NM99, NFJG01] which is coupled to the identical boson ground state by an external rf field (shown schematically in Fig. 12-1(b)) [LOS+10, TR11]. In this scheme, identical bosons in two different hyperfine states (labeled $b$ and $x$ for the lowest state and an excited state respectively) sit on a single site which we model as an isotropic oscillator with oscillator frequency $\omega$ length $l_{ho}$.

For a three-body bound state to form in an excited hyperfine state, we consider a system with repulsive $bb$ non-resonant interaction ($0 < a_{bb} \ll l_{ho}$) and large $bx$ scattering length ($a_{bb} \gg |a_{bx}|$). In this situation, universal three-body Efimov states form attached to the $bbx$ three-body hyperfine state [Efi70, BH06, NM99, NFJG01].

To analyze this scenario, we explore two-, three- and four-body single site physics within the harmonic approximation using a model short range interactions and a correlated Gaussian basis set expansion [SV98, vS10]. We tune the interaction parameters to achieve a $bbx$ Efimov trimer whose binding energy ($E_b = E_{NI} - E$ where
Figure 12-1: Schematic representations of (a) the Bose-Hubbard Hamiltonian considered here [Eq. (12.1)] and (b) the rf field tuned three-body onsite interaction are shown. In (b) red and blue circles represent bosons in the lowest and (excited) hyperfine states \( (b \text{ and } x) \) respectively. The dotted line represents the energy the rf field is tuned to with respect to the excited two- and four-body states. (c) The wavefunction overlap between the non-interacting ground state and the lowest excited hyperfine state is shown as a function of \( l_{ho}/a_{\text{Bz}} \) for two-, three- and four-atoms (solid, dashed and dotted lines respectively). (d) The energy of the lowest two-, three- and four-body states (solid, dashed and dotted lines respectively) in the excited hyperfine state is shown in trap units with respect to the non-interacting energy \( E_{NI} \). Also shown is the energy of the first excited four-body state (upper dotted line) to demonstrate that the universal three-body state is in fact isolated. In both (c) and (d) the calculations are done for model Rb atoms described in the text.
$E_{NI}$ is the non-interacting energy of the trapped system) is comparable to the trapping energy $\hbar \omega$ (see Fig. 12-1(c)). This particular scenario is suitable for achieving the proposed Hamiltonian for two reasons. First, the two-, three- and four-body binding energies are well separated allowing to tune the rf pulse in resonance with a particular single site occupancy; and second, the large wavefunction overlaps [see Fig. 12-1(d)] imply an efficient rf transition probability. Our numerical calculations show that the lowest three-body energy in the $bbx$ configuration is lower than the two-body energy ($bx$ configuration), and that for each Efimov trimer state, there is a single four-body state ($bbbx$ configuration) bound below the trimer state. All other four-body states lie above the trimer energy. This is in contrast to the more commonly considered case of four identical bosons in free space in which there are both a deeply bound and a weakly bound tetramer associated with each Efimov state [FKB+09, vSG09, HP07, PHM04]. The energies for two-, three-, and four-body states are shown schematically in Fig. 12-1(b) along with the energies at which the rf field is tuned to (dotted lines).

By detuning the rf field to the red of the Efimov state for three body occupation, both the two- and three-body identical boson ground states are shifted down. However, because there is an energy difference between the two- and three-body transition energy the two-boson state is shifted significantly less than the three-body. For higher occupation numbers, the rf-field is far blue detuned from the bound states and thus the four- or more identical boson ground states experience a weak upward shift. One might expect an additional shift in the higher occupation number states (four or more) resulting from a three-boson and spectator particle like system. However, for these weakly bound universal Efimov states, the size of the three-body state is similar to the trapping length, and thus additional bosons on site interact with the Efimov state and shift the resulting N-body excited state energy off resonance with the rf field.

As an initial study we consider $^{85}$Rb. Since resonance structure for scattering between hyperfine state is not known, we will assume that there exists an s-wave scattering resonance between the lowest and first excited hyperfine states at some
external magnetic field strength. For simplicity, we consider that identical bosons are roughly noninteracting. Assuming that the energy of the Efimov state is determined by the Van der Waals length of Rb, \( r_{vd} \approx 82 \text{ a.u.} \) [Efi70, BH06, NM99, NFJG01], and a lattice site trapping frequency of \( \omega = 2\pi \times 10 \text{ kHz} \), an Efimov state will arise at \( E_{3B} \approx -2\hbar \omega \) with respect to the \( b \) \( b \) non-interacting energy. Under these circumstances, we predict that \( U_3 \) can be tuned to be attractive and of order \( U \) with a detuning of \( \Delta \sim 1000\text{kHz} \) from the Efimov state transition energy. This large detuning also serves to mitigate the generally short lifetimes of Efimov states(on the order of \( 10\mu\text{s} \) [Wer09, NSE02, Pen99]).

This initial investigations, presented above as a plausibility argument, indicates that using the above scheme is feasible with existing experimental techniques.

A more detailed study to determine the effects of rf coupling to an excited three-body state is left for future investigations. Additionally, direct rf association of universal trimer states has already been demonstrated in ultra-cold, three-component, Fermi and Bose gases [LOS+10] lending credibility to the experimental accessibility of this model.

### 12.2 The Gutzwiller Mean-field Analysis

We will now use Gutzwiller mean field theory to study the modified BH Hamiltonian described by Eq. (12.1).

The Gutzwiller mean field theory is constructed by replacing the full Hamiltonian by an effective local Hamiltonian subject to a self-consistency condition. We introduce the superfluid order parameter \( \psi = \langle a_i \rangle = \langle a_i \rangle \) and the Gutzwiller wavefunction \( |G\rangle = \Pi_{i=0}^{N} (\sum_{n=0}^{\infty} f_n^{(i)} |n_i\rangle) \), so that the effective Hamiltonian for a translationally invariant system, i.e. \( f_n^{(i)} = f_n \), takes the form,

\[
E[\psi] = -Jz\psi \sum_n \sqrt{n + 1} (f_{n+1}^* f_n + \text{c.c.}) + zJ\psi^2 + E_n \tag{12.2}
\]
Figure 12-2: Mean field phase diagram in the $\mu/U$ vs. $zJ/U$ plane for $|U_3| = 0$ where $z = 4$ is the number of nearest neighbours in two dimensions. (a), $|U_3| = U/2$ (b), $|U_3| = U$ (c), and $|U_3| = -3U/2$ (d). When $0 < |U_3| < U$ the $n = 2$ and $n = 4$ lobes visibly shrink in favor of the $n = 3$ lobe, until they completely disappear at $|U_3| = U$ (c). For $|U_3| > U$ the $n = 3$ lobe begins to overlap with the $n = 1$ and $n = 4$ lobes and a direct phase transition between MI lobes becomes possible. The dotted rectangle in (d) highlights the region examined in detail in Fig. 12-3.
where $z$ is the coordination number, $f_n$ are variational parameters, and $E_n = \frac{U}{2} n(n - 1) + \delta_{n,3} U_3 - \mu n$. The problem is now reduced to determining the set of coefficients $\{f_n\}$ which minimize $E[\psi]$ and satisfy the normalization condition $\langle G|G \rangle = \sum_n |f_n|^2 = 1$ [JBC+98, KCB92, RK91].

Figure 2 shows the ground state phase diagram of model (12.1) at different values of $U_3$. As we increase the magnitude of $|U_3|$ from 0 to $U$ the $n = 2$ and $n = 4$ Mott lobes shrink considerably while the $n = 3$ lobe increases in size [as seen in Fig. 12-2(b)]. In particular, for $U_3 \geq -U$ the $n = 2$ and $n = 4$ lobes completely disappear since it is now energetically more favorable to have occupation number $n = 3$ [Fig. 12-2(c)]. This can be easily understood in the zero hopping limit. At $\mu = \mu_{12} = U$ a doubly occupied site has the same energy as a singly occupied one. At $\mu = \mu_{13} = (3U + U_3)/2$, instead, a singly occupied site has the same energy as a triply occupied one. The condition $\mu_{13} \leq \mu_{12}$ sets the $U_3$ value for which the second lobe disappears, i.e. $|U_3| > U$ (at $|U_3| = U$, sites with occupation number $n = 1, 2, 3$ are degenerate in energy for $\mu = \mu_{12} = \mu_{13}$). Direct transitions from MI occupation numbers $n = 1$ to $n = 3$ survive at finite hopping [Fig. 12-2(d)] confirmed below using QMC (see section 12.3). The same argument shows that $|U_3| > U$ also implies the disappearance of the 4th lobe. One can easily see that upon further increasing $U_3$, all lobes other than $n = 3$ will eventually disappear, e.g. at $U_3 = -3U$, the $n = 1$ and $n = 5$ lobes disappear.

We have monitored the behavior of mean field energy [Eq. (12.2)] at fixed $\mu/U$ while varying $J/U$ to study the order of phase transitions described by model (12.1). The formation of double minima structure in the mean field energy functional $E[\psi]$ is a signature of first order phase transitions. We have observed such double minima structure at $U_3 = -1.5U$ for the $n = 1$ MI-SF and the $n = 3$ MI-SF transitions. The occurrence of first order transitions can be understood with a simple argument. At fixed small $J/U$, $|U_3| \sim U$, and upon increasing (decreasing) $\mu$ in order to dope the $n = 1$ ($n = 3$) MI with particles (holes), double occupancy will be suppressed in favor of triply occupied sites. At large enough $|U_3|$ such mechanism will eventually prevent a gradual addition (subtraction) of particles resulting in first rather than
Figure 12-3: First order phase transitions at $U_3 = -1.5U$. The dotted line corresponds to the first order phase transition from the $n = 1$ MI (blue) to $n = 3$ MI (pink) predicted by mean field theory. Solid lines refer to mean field first order transitions from MI to SF. Solid circles are QMC results from hysteretic curves. Dashed lines correspond to second order mean field MI-SF transitions. Open squares are second order transition points from QMC. Lower (upper) inset shows examples of hysteretic behavior for the $n = 1$ ($n = 3$) MI-to-SF transition.

Second order transitions. Second order transitions will be restored at large enough $J/U$ as the kinetic energy gain due to hopping of extra particles (holes) will again favor a gradual change in density.

### 12.3 Quantum Monte-Carlo Results

In order to confirm the mean-field predictions, we have performed QMC simulations on a square lattice of linear size up to $L = 24$ (and $L = 30$ in certain cases) for selected values of $J/U$, and at $\beta = \frac{1}{k_B T} = L/J$ which corresponds to effective zero temperature regime. Figure 12-3 compares the QMC results with the mean-field predictions of
the phase diagram for $U_3 = -3U/2$. As mentioned above, a direct transition from $n = 1$ MI (lower lobe) to $n = 3$ MI (upper lobe) survives at finite hopping. This first order transition is depicted by the dotted line, while solid lines refer to first order transitions from MI to SF. The solid and open symbols correspond to QMC predictions of the phase boundary with first and second order phase transitions.

To extract transition points, we have analyzed the particle density $n$ as a function of $\mu$. Additionally we have performed hysteresis analysis by sweeping back and forth in chemical potential and calculating the corresponding particle density. The hysteretic behavior of the system along the phase boundaries (solid symbols) further confirms that these are first order transitions. We show two examples of such curves for the $n = 1$ MI-SF and $n = 3$ MI-SF transitions, in the lower and upper inset respectively. Based on the energy argument previously discussed, we expect the phase transition to become second order as $J/U$ is increased. Indeed, larger kinetic energy will favor formation of particle/hole excitations on top of the MI. The energy gain due to hopping of the latter will compete with the attractive three-body interaction and will eventually restore the second order MI-SF transition driven by addition/subtraction of small number of particles from the MI regime.

We have used QMC simulations to benchmark the $J/U$ values at which first order phase transitions become second order. Second order MI-SF transitions are depicted in Fig. 12-3 by dashed mean field lines and open squares representing QMC results. For $z = 4$, the $n = 1$ ($n = 3$) MI-SF transition becomes of second order at $zJ/U = 0.20 \pm 0.02$ ($zJ/U = 0.133 \pm 0.02$). We estimate the position triple point using the mean-field approximation [Eq. (12.2)] where we truncate the Hilbert space to the $n_i = 1, 2, 3$ states. Using this approximation we find $(zJ/U)_{TP} = -(U + U_3)/10$. For $U_3 = -1.5U$ and $z = 4$ this gives $J/U = 0.05$.

First order phase transitions present in our model can be experimentally detected due to a loss of adiabaticity across the phase boundary even upon an arbitrarily slow ramping up or down of the optical lattice, as suggested in [FFR11] or by observing the hysteretic behavior. In addition, first order phase transitions are characterized by discontinuity in density profiles, a local observable easily accessible with state of
the art techniques [GZHC09].

Finally we have looked at how first order phase transitions are affected by finite temperature. Strictly speaking, the MI state exists only at zero temperature. In practice, MI features persist up to temperature $T \sim 0.2U$ [Ger07]. QMC results show that phase transitions are still of first order at temperatures of $T \sim J$, where MI features are still well defined. A more extensive study of the behavior of the system at finite temperature will be the subject of future investigations.
Chapter 13

Part II: Conclusions and Outlook

In this part of the thesis we presented a brief overview of simulations of quantum many-body Hamiltonians with optical lattice systems. In these systems, counter-propagating laser beams are used to create a periodic array of potential wells which can be used to trap ultra-cold atoms and molecules. This forms a defect-free crystal, where the interparticle interactions, lattice geometry and lattice depth can be tuned easily.

Following a brief discussion of dilute bose gases, we introduced the single-band, Bose-Hubbard model in section 7.4. This model is valid in the deep-lattice limit. We then focused extensions of the Bose-Hubbard model realized by dipolar systems and three-body interactions. We studied these systems by means of novel Path Integral Quantum Monte Carlo algorithms discussed in chapter 9. Below we present a brief summary of the main results.

In chapter 10, we studied the quantum phases of dipolar bosons in a bilayer lattice geometry described by the microscopic Hamiltonian in Eq. (10.1) for hard-core particles, in a situation where the number of particles in each layer is the same. Relevant to experiments with polar molecules and magnetic atoms, we established under which conditions pairing for two particles is stabilized across the layers. Our zero temperature study indicates that the system displays a rich ground state phase diagram including a novel pair-supersolid phase for hard-core dipolar bosons, in addition to pair superfluid and checkerboard-like solid phases. Our finite temperature results
indicate that these phases are experimentally observable at temperatures of the order of ~nK. A four-body correlation function can be used to characterize these phases and their transitions. This correlation function is also related to the spread of the wave-function of the pairs.

In chapter 11, we studied a system of \( N \) one-dimensional tubes of hard-core bosons with arbitrary inter-layer interactions, described by the Hamiltonian given by Eq. 11.1. We used \textit{ab-initio} quantum Monte Carlo simulations, using two-worm and multiworm algorithms described in chapter 9, and compared the results to those of the bosonization method. We found several non-trivial ground states, including superfluids and countersuperfluids made of composites of particles from different tubes, 1D checkerboard insulators, and co-existence of these phases. Additionally we showed that these phases have \textit{zero} threshold in the interaction, and can be stabilized at arbitrarily small values of interaction. Moreover, we can use the the filling factors of the tubes as a \textit{knob} to stabilize the different phases.

Finally, in chapter 12, we studied an extended version of the Bose-Hubbard model which includes an attractive three-body interaction term \( U_3 \), both at a mean field level and by means of quantum Monte Carlo simulations. The three-body term results from a universal three-body bound state attached to an excited threshold and can be tuned via an external rf field. We have found that at \(|U_3| > U\), where the \( n = 2 \) lobe disappears, there exists a first order phase transition separating the \( n = 1 \) from the \( n = 3 \) lobes which extends up to a triple point. A strong three-body attraction also affects the order of the MI-SF transition. We found first order transitions separating the \( n = 1 \) and \( n = 3 \) MI from the SF. We also analyzed the effect of finite temperature and found that transitions are still of first order at temperatures \( T \sim J \).

The algorithms developed in this thesis can be extended to study a variety of systems. In particular, a \textit{different} type of multiworm algorithm, with indistinguishable worms, can be used to study a system of aligned dipoles titled with respect to the trap axis. This setup allows us to explore the effects of the anisotropy of the dipolar interaction on the physics of the two-dimensional system. So far, most studies of titled dipoles have been limited to the few-body systems. The previous numerical studies
by means of path integral QMC refer to the continuum space, or have been performed by inadequate algorithms, incapable of sampling the chain Hilbert space. Using the multiworm algorithm with indistinguishable worms we can resolve the exact phase diagram of a dipolar lattice gas in a two-dimensions, with tilted dipoles. Additionally we can use a mutliworm algorithm with both distinguishable, and indistinguishable worms, to study a system where the symmetry between the layers is broken through the introduction of population and mass (hopping) imbalance. This can lead to the formation of multimers, for example, trimer formation in wires coupled via dipolar interaction with population imbalance or in two-component systems. The multiworm algorithm developed in this thesis allows us to study the quantum phases of these exotic multimers, both in one- and two-dimensional coupled layers.
Bibliography


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