Quantum Phase Transitions in the Bose Hubbard Model and in a Bose-Fermi Mixture

Dissertation

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Abstract

Ultracold atomic gases may be the ultimate quantum simulator. These isolated systems have the lowest temperatures in the observable universe, and their properties and interactions can be precisely and accurately tuned across a full spectrum of behaviors, from few-body physics to highly-correlated many-body effects. The ability to impose potentials on and tune interactions within ultracold gases to mimic complex systems mean they could become a theorist’s playground. One of their great strengths, however, is also one of the largest obstacles to this dream: isolation. This thesis touches on both of these themes.

First, methods to characterize phases and quantum critical points, and to construct finite temperature phase diagrams using experimentally accessible observables in the Bose Hubbard model are discussed. Then, the transition from a weakly to a strongly interacting Bose-Fermi mixture in the continuum is analyzed using zero temperature numerical techniques.

Real materials can be emulated by ultracold atomic gases loaded into optical lattice potentials. We discuss the characteristics of a single boson species trapped in an optical lattice (described by the Bose Hubbard model) and the hallmarks of the quantum critical region that separates the superfluid and the Mott insulator ground states. We propose a method to map the quantum critical region using the single, experimentally accessible, local quantity $R$, the ratio of compressibility to local number fluctuations. The procedure to map a phase diagram with $R$ is easily generalized to inhomogeneous systems and generic many-body Hamiltonians. We illustrate it here using quantum Monte Carlo simulations of the 2D Bose Hubbard model.

Secondly, we investigate the transition from a degenerate Fermi gas weakly coupled
to a Bose Einstein condensate to the strong coupling limit of composite boson-fermion molecules. We propose a variational wave function to investigate the ground state properties of such a Bose-Fermi mixture with equal population, as a function of increasing attraction between bosons and fermions. The variational wave function captures the weak and the strong coupling limits and at intermediate coupling we make two predictions using zero temperature quantum Monte Carlo methods: (I) a complete destruction of the atomic Fermi surface and emergence of a molecular Fermi sea that coexists with a remnant of the Bose-Einstein condensate, and (II) evidence for enhanced short-ranged fermion-fermion correlations mediated by bosons.
To my parents, Nicholas Duchon and Suzanne Sands, who inspired and encouraged my love of science.
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I want to thank Professor Nandini Trivedi, my advisor, for helping me to understand how small-scale questions fit into ongoing research in the fields of ultracold atoms and condensed matter theory. I can only hope that I picked up some of her talent for reformulating overly narrow and overly broad questions into tractable questions with an appropriate scope. I am grateful for the opportunities to collaborate with theorists and experimentalists, and for support to attend major conferences.

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I thank my wife, Jennifer Yee, for her patience, camaraderie, and occasional reminders to go outdoors when I lost perspective. I will always remember the relaxing times I spent climbing with my sister Alice Duchon, and the love and encouragement of my grandparents Nicholas and Valeria Duchon, who inspired me to pursue my dreams. Finally, I am grateful for my parents’ love and support. More than anyone else, they taught me to examine both the forest and its trees, to search for mysterious fascinating facets, and then to ask “Why?”

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Chapter 1
INTRODUCTION

Ultracold atomic gases open the door to the creation and emulation of all manner of condensed matter systems. Experimental realization of weakly interacting, dilute and degenerate Bose and Fermi gases in highly tunable potentials were a milestone proof of concept and confirmation of atoms’ quantum statistics in a table-top experiment. Over 15 years, methods to create strongly interacting, many-body systems proliferated and experiments are on the brink of fully characterizing single species gases and lattice systems, and of creating spin-orbit-coupled continuum and lattice many-body condensed matter systems [5, 6, 7]. Universal fluctuations that depend on the system’s symmetry and dominate many-body systems near a phase transition link ultracold gases to field theoretic descriptions of the Higgs mode [8] and to string theory via the AdS-CFT correspondence and a predicted minimal viscosity [9]. In addition, ultracold atoms are a unique way to study few-body Efimov physics and low-temperature quantum chemistry [10].

Decades of effort culminated in the 1995 observation of a Bose-Einstein condensate (BEC) in a dilute, ultracold (∼ 1 µK) system by Cornell, Ketterle and Wieman. This achievement built on pioneering work in laser-based precision spectroscopy, laser cooling, magnetic and optical traps, and magnetic evaporation recognized by several Nobel prizes [11, 12, 13, 14]. As shown schematically in Figure 1.1, for a fixed density $n$ of atoms with an average inter-particle spacing $r_0 \sim n^{-1/3}$, the de Broglie wavelength $\lambda_{db} = h/\sqrt{2\pi mk_B T}$ increases as the temperature decreases, where $h$ is the Planck constant and $k_B$ is the Boltzmann constant. The the condition $\lambda_{db} \approx r_0$ estimates the critical temper-
Figure 1.1: The importance of particle statistics and quantum interactions increase as the temperature is decreased, shown schematically in (a-d). At low temperature, the de Broglie wavelength $\lambda_{db}$ becomes comparable to the interparticle spacing and eventually (d) bosons condense into a single state, the Bose-Einstein condensate, which can be thought of as a giant atom.

The fate of cold neutral atoms is decided by whether the number of neutrons in the nucleus is even or odd. $^{87}$Rb has 37 electrons, 37 protons and 50 neutrons, so the composite atom is a boson. The same is true for $^7$Li with 3 electrons, 3 protons and 4 neutrons, but $^6$Li, with one fewer fermion, is a fermion. This difference shows up beautifully as two atomic clouds, each composed of a single Li isotope, are cooled below their degeneracy temperatures. The distribution of the bosonic and fermionic clouds within a harmonic potential are separately captured by *in situ* imaging in Figure 1.2(c,d) and clearly show
that whereas the bosonic cloud shrinks in extent as temperature decreases (more and more atoms are in the zero momentum condensate), the fermionic cloud does not compress below a certain size. The finite size is due to the Fermi pressure that results from the requirement that the many-body wave function of fermions be antisymmetric with respect to interchange of two fermions. Another way to understand the fermion behavior is schematically shown in Figure 1.2(b). The Pauli exclusion principle restates the wave function antisymmetry as the requirement that no two fermions can share the same state; as fermions are added to the system, ever higher energy levels are populated. At zero temperature, the Fermi surface denotes the $N$ lowest energy levels occupied by $N$ fermions. The highest energy populated state, or the energetic cost to add a fermion at zero temperature, is the Fermi energy $\epsilon_F = k_B T_F$. $T_F$ is a good estimate of degeneracy temperature for the fermions, i.e. the temperature at which a Fermi surface forms. These are the canonical behaviors of non-interacting bosonic and fermionic systems.

The most important obstacle to characterizing ultracold systems and to exploring exotic states of matter in that context is their extreme isolation. Cooled and trapped using magneto-optical methods in an ultra-high vacuum, these quantum systems are quite stable because they are extremely weakly coupled to the rest of the universe. Unfortunately, this means that many otherwise ubiquitous measurements in condensed matter, such as the resistance or transport, are extraordinarily difficult to measure. Several observables that have traditionally been very difficult to precisely measure, on the other hand, are relatively straightforward in ultracold atom systems, including the local density, the momentum distribution, Bragg scattering and the dispersion relation. Sometimes traditional experiments have been emulated in ultracold atom systems, like Bragg scattering using atomic BECs, but often physicists have had to adjust their methods in order to squeeze the most possible information out of nonstandard or normally inaccessible observables. This issue is discussed in the context of the Bose Hubbard model in Chapter 2 and a generic method to identify quantum phase transitions using the local density and local compressibility is proposed.

The next important question is: what is the role of interactions? The major methods for introducing tunable interactions into these systems are Feshbach resonances that tune
Figure 1.2: Comparison of bosons (\(^7\)Li) and fermions (\(^6\)Li) near the condensation and Fermi temperature, respectively. (a,b) At zero temperature, bosons occupy the lowest allowed energy state while Pauli exclusion restricts one fermion to each energy level. (c,d) The atom density within a trap is imaged and the quantum statistics of each species revealed. For noninteracting particles, the extent of the boson cloud continues to shrink as the temperature decreases, while the fermion atom cloud has a minimal cloud size maintained by a Fermi pressure. Repulsive boson-boson interactions enlarge the zero temperature atom cloud whose size is otherwise given by the potential’s ground state [15].

In this thesis, we investigate quantum phase transitions instigated both by tuning Feshbach resonance in a continuum Bose-Fermi gas and by increasing the optical lattice potential for a bosonic system.

Feshbach resonances in ultracold gases are an amazing opportunity to control interactions that cannot be replicated in standard condensed matter experiments. In a normal material, the crystal structure, the electron and hole density, and any interactions are fixed
Figure 1.3: Counterpropagating laser beams impose periodic potentials on cold atom clouds. With the simplest laser arrangements, the atoms can be arranged onto two-dimensional pancakes, (a) one-dimensional tubes or (b) lattice structures. Additional, nonorthogonal lasers can create superlattices, graphene-like lattices, etc. Adapted from Reference [6].

and can usually only be slightly changed, for example by pressure (∼GPa), magnetic fields (∼T) or an electric potential (∼eV). In contrast, changing the magnetic field on the order of one percent of one Tesla can tune a quantum gas from having no interactions to having infinitely long ranged interactions at a Feshbach resonance. A resonance occurs whenever a two-body bound state energy $E_{\text{res}}$ is tuned to zero energy, i.e. to the energy of the surrounding system. Very roughly speaking, as $E_{\text{res}} \to 0^-$ the spatial extent of the bound state diverges, which is proportional to the scattering length scale $a$. A small attractive interaction develops between atoms for $E_{\text{res}} \to 0^+$ as well, even though no weakly-trapped bound state exists. It is normally convenient to parameterize the interaction by the inverse scattering length $1/a$, where $a \to \pm \infty$ or $1/a = 0$ is called unitarity and occurs at $E_{\text{res}} = 0$. Intra-species Feshbach resonances can tune systems into stable or unstable regimes and can
induce Efimov trimer states. Feshbach resonances between two hyperfine levels of fermionic atoms were used to map the BCS-BEC crossover from a “superconductor” of weakly bound Cooper pairs ($1/a \rightarrow -\infty$) to a condensate of tightly bound composite boson molecules ($1/a \rightarrow \infty$). Using numerical means, we investigate the analogous situation for a Feshbach resonance between a boson and a fermion atomic species.

Interacting Bose-Fermi mixtures have several interesting limiting cases and we choose to investigate the case of equal numbers of bosons and fermions near a wide Feshbach resonance, discussed in Chapter 3. At weak coupling, the bosons form a BEC and the fermions form a Fermi surface while at strong coupling, the bosons and fermions should all pair to create a molecular Fermi sea with neither a BEC nor a Fermi surface of the atomic fermions. In the intermediate to strong coupled regime, the bosons and fermions begin to pair into composite fermion molecules but cannot be modeled as a distinct species due to the molecules’ large spatial extent. Through zero temperature numerical methods, we find an interesting, unexpected phase where the atomic Fermi surface has been destroyed but not the BEC and evidence that boson-mediated fermion-fermion interactions are important.

Another method for inducing strong interactions in bosons and in fermions are periodic optical lattice potentials [18, 6, 19, 20, 21, 22, 23, 24, 25]. Creating these periodic potentials and characterizing the resulting phases are essential to successfully emulate and predict the properties of existing and new materials. In general, these potentials can be modeled by local and nearest neighbor interactions, and is known as the Hubbard model. For example, the Hubbard model is believed to model high-Tc superconductors. The boson analogue, the Bose Hubbard model, applies to $^4$He adsorbed into Vycor, to coupled Josephson junction arrays, and to certain superconductor-insulator transitions where disorder destroys systemwide Cooper pair coherence. With a zero temperature quantum phase transition from a superfluid to an insulator, it is also a strongly correlated system that is not analytically solvable, but in contrast to the Fermi Hubbard model, it is numerically tractable even at experimental scales of $10^6$ atoms. It has been an ideal vehicle to confirm theoretical and numerical methods and as a proving ground for experimental methods and probes (bosons are also easier to cool than fermions). Someday, these cold-atom systems
may even form the basis of high-precision sensors or of quantum computers. However, the biggest contemporary obstacle is full characterization of the phases within these extremely isolated experimental systems with minimal theoretical input.

In Chapter 2, we discuss our numerical results for the BHM in 2D and 3D, and propose two methods to map the finite temperature phase diagram. The first is a numerical tour-de-force that uses a trapped system’s characteristic density to identify all of the phases that coexist in a system at a given temperature. It agrees well with an experimental phase diagram constructed along similar lines and identifies finite temperature effects. The second phase diagram was also constructed via QMC but the method is very general and may be applied to ultracold atom experiments (and generic quantum many-body systems) with minimal reliance on theoretical or numerical results. We also discuss the limitations of a commonly used mapping from uniform to trapped systems and present numerically calculated spectral functions that form a platform for future experiments.

The field of ultracold atoms is exciting and offers great promise, although it is still a young and rapidly developing field. Perhaps no ultracold atom system has yet been fully characterized and every year sees innovative new proposals for novel systems to study and build. It is at the intersection of condensed matter physics and atomic, molecular and optical physics, and its highly tunable, strongly interacting systems enable exciting links to be made to nuclear physics and to field theories. Device applications, like using optical lattice systems to predict new superconductors or to build a quantum computer, are on the horizon. In this thesis, we contribute to knowledge about the Bose Hubbard model, develop and illustrate a general method to map finite temperature phase diagrams in ultracold atom systems and make specific predictions concerning equal-population Bose-Fermi mixtures near a broad Feshbach resonance.
Ultracold atomic gases loaded onto optical lattices have once again highlighted the Bose Hubbard model (BHM), a bosonic analogue of the Fermi Hubbard model that describes strongly correlated materials like high temperature superconductors. Initially, the BHM was investigated in the context of superfluid $^4$He adsorbed into a disordered medium like Vycor and coupled Josephson junction arrays [26], but these systems are difficult to characterize experimentally. Ultracold gases trapped on a highly tunable optical lattice are an ideal laboratory to test theoretical predictions for strongly-correlated many-body lattice systems. An eventual goal is to emulate real or possible materials and evaluate their phases and other properties without the need for difficult theoretical or time-consuming numerical calculations or for tedious and hit-or-miss attempts to grow novel materials. The extreme isolation of these systems, however, restricts the available experimental probes and, along with the difficulty of cooling, presents the largest obstacle. The bulk of the work in this chapter has gone toward numerical characterization of the BHM and to proposals that identify phases and phase transitions in experimental systems both with and without accompanying numerical simulations. Eventually, the ability to characterize both Bose and Fermi ultracold atom systems with minimal or no direct theoretical input could lead to the experimental emulation of theoretically intractable quantum many-body systems.

This chapter begins with basic facts and numerical and theoretical results about the BHM. The finite temperature phase diagram is constructed via two methods and compared with experiment, the effects of reduced dimensionality in trapped systems are discussed
and spectral functions are exhibited. The model overview describes the ground states and a simple mean field theory that qualitatively captures many features. The universal behavior near the quantum critical points is discussed and illustrated using results from QMC. Two QMC-constructed finite temperature phase diagrams for 2D systems follow, one based on the characteristic density of a trapped system and one based on the fluctuation-dissipation theorem that is applicable to both trapped and uniform systems. Finally, the effects of reduced dimensionality in a trap and spectral functions in 1D and 2D uniform systems are discussed.

2.1 Model Overview

We confine our attention to the two dimensional square \((d = 2)\) and three dimensional cubic \((d = 3)\) lattices, although other lattice geometries can easily be generated in experiments by modifying the number and orientation of the lasers forming the optical potential. The many-body physics of bosonic atoms with the coordination number \(n_c = 2d\) of nearest neighbors can be captured by the relatively simple Bose Hubbard Hamiltonian

\[
\hat{H} = -\frac{t}{n_c} \sum_{\langle ij \rangle} \left( \hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i \right) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i, \tag{2.1}
\]

where \(t\) is the boson hopping amplitude between neighboring sites \(\langle ij \rangle\), \(U > 0\) is the on-site repulsive interaction, and \(\mu\) is the chemical potential that controls the boson density. The number operator for particles on site \(i\) is \(\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i\), where \(\hat{a} \ (\hat{a}^\dagger)\) is the bosonic annihilation (creation) operator. As discussed in Appendix A, the energies \(t\), \(U\), and \(\mu\) are set by the optical lattice depth \(V_0\) and the lattice spacing \(a_{\text{latt}}\), such that \(t/U\) decreases as \(V_0\) or as \(a_{\text{latt}}\) increases [16]. In short, Bloch states form within the periodic lattice and a localized Wannier state \(W(|r - r_i|)\) at site \(r_i\) can be constructed from the lowest Bloch band. Then \(t\) is related to the overlap \(\int dr W(r - r_i) \nabla^2 W(r - r_{i+1})\) and \(U\) arises from the onsite density overlap \(\int dr W^4(r - r_i)\)\(^d\). In standard experiments, the harmonic curvature \(V_T\) of the laser’s intensity profile contributes to a site-dependent shift in the chemical potential \(\sim -V_T r_i^2\), where \(r_i\) is the distance from the trap center, and allows
several phases to coexist at equilibrium. This "trapped" system is often treated using the local density approximation and is discussed in Section 2.3.5. This Hamiltonian has $U(1)$ symmetry because it is invariant under the global gauge transformation $\hat{a} \rightarrow \hat{a} e^{i\theta}$ and $\hat{a}^{\dagger} \rightarrow \hat{a}^{\dagger} e^{-i\theta}$.

### 2.1.1 Ground States

**Mott Insulator**

Consider the limiting case of the BHM with average boson density $n = N_B/L^d$ ($N_B$ bosons with $L$ sites along each side) where $t \rightarrow 0$. The Hamiltonian $\hat{H}_U = \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) - \mu \sum_i \hat{n}_i$ is site-decoupled and diagonal in the Fock (boson number) basis, so the ground state has $n$ bosons on every site, determined by

\[
\frac{\mu}{U} < 0 \quad n = 0 \\
0 < \frac{\mu}{U} < 1 \quad n = 1 \\
1 < \frac{\mu}{U} < 2 \quad n = 2 \\
\vdots \\
(2.2)
\]

This state requires the number of particles to be commensurate with the number of lattice sites, so the density is quantized as illustrated in Figure 2.1(a). The ground state of this ideal Mott insulator with $n$ bosons per site is the product state

\[
|\Phi^{MI}\rangle = \prod_i L^d \left(\hat{a}_i^{\dagger}\right)^n |0\rangle.
\]

(2.3)

In a Mott insulator, a local phase $\theta_j$ can be applied to each boson as

\[
|\Phi^{MI}\rangle = \prod_j \hat{a}_j^{\dagger} e^{-i\theta_j} |0\rangle.
\]

(2.4)

Because the various $\theta_j$ are completely uncorrelated, the overall gauge symmetry is maintained in this state.

Excitations in a Mott insulator with density $n$ are gapped by the finite energy cost to add a particle $(Un - \mu)$ or to remove a particle $(U(n - 1) - \mu)$, so the Mott insulator is
Figure 2.1: Schematic of a Mott insulator state and a superfluid state in a lattice potential (a,b) and after time of flight expansion (c,d). At the start of the expansion, the lattice potential is switched off and the atoms’ crystal momenta are mapped onto the continuum momenta that govern the atom cloud expansion. (c) The atoms in the Mott insulator have random relative phases so they destructively interfere during expansion and a broad distribution results. (d) Each atom in the condensate has the same phase, so sharp peaks emerge at momenta that are multiples of the inverse lattice spacing, while uncondensed atoms contribute to a broad background. Adapted from [18].

The energy to add a particle in a Mott state with \( n \) particles per site is incompressible. The energy to add a particle in a Mott state with \( n \) particles per site is degenerate with the energy to remove a particle from a Mott state with \( (n + 1) \) particles per state at integer values of \( \mu/U \). Thus at small tunneling \( t \), superfluid order emerges near integer values of \( \mu/U \) where the gap to add or remove particles becomes the same order as \( t \). Any such transition point between the Mott insulator and the superfluid at zero temperature is a quantum critical point.

**Superfluid**

The competing superfluid state is described by the order parameter \( \langle \hat{a} \rangle = \sqrt{n_0}e^{i\theta} \) where \( n_0 \) is the condensate fraction and \( \theta \) is the phase of the complex order parameter. The superfluid breaks global gauge symmetry and picks the same phase for all sites, thereby generating a phase-coherent state. In a non-interacting \((U = 0)\) Bose-Einstein condensate (BEC), all
$N_B$ bosons occupy the same $k = 0$ state described by

$$|\Phi^{BEC}\rangle = \left(\hat{a}^\dagger_{k=0}\right)^{N_B}|0\rangle = \left(\sum_i \hat{a}^\dagger_i\right)^{N_B}|0\rangle.$$  \hspace{1cm} (2.5)

In real space, the BEC is described as a linear, \textit{coherent} superposition of configurations with fluctuating particle number at each site but with the \textit{same} phase. Particle number and phase are conjugate variables, so because the phase in a BEC is definite, the number of bosons at each site is completely uncertain. As interactions increase, one sees the depletion of the condensate fraction $n_0$ as well as increased phase fluctuations, even at $T = 0$. These observations about phase coherent and incoherent states are nicely summarized in the time-of-flight type of experiment that allows the atom cloud to expand according to its initial momentum and phase distributions, shown in Figure 2.1(c,d).

The kinetic part of the non-interacting Hamiltonian $\hat{H}_t = -t/z \sum_{ij}(\hat{a}^\dagger_i \hat{a}_j + \hat{a}_i \hat{a}^\dagger_j)$ can be diagonalized in momentum space through the standard Fourier transformation $\hat{a}_i = L^{-d/2} \sum_k \hat{a}_k e^{i k \cdot r_i}$ to yield

$$\hat{H}_t = -\frac{t}{n_c} \frac{1}{L^d} \sum_{kq} \sum_{i,\delta} \left(\hat{a}^\dagger_k \hat{a}_q e^{-i(k-q)\cdot r_i} e^{iq \cdot \delta} + \hat{a}^\dagger_q \hat{a}_k e^{i(k-q)\cdot r_i} e^{-iq \cdot \delta}\right) - \mu \sum_k \hat{n}_k$$

$$= \sum_k \hat{n}_k (\epsilon(k) - \mu)$$ \hspace{1cm} (2.6)

where $\delta/a_{\text{latt}} = \pm e_1, \pm e_2, \pm e_3$ denotes the unit vector to one of the nearest neighbors, the dispersion is $\epsilon(k) = -(2t/n_c) \sum_{\alpha=1}^d \cos (k\alpha a_{\text{latt}})$, and $k_\alpha = k \cdot e_\alpha$. The expectation $\langle \hat{a}_k^\dagger \hat{a}_k \rangle = n(k)$ is the momentum distribution function and will prove to be an important quantity. As mentioned above, $n(k) = N_B \delta(k)$ in a non-interacting BEC while both finite temperatures and interactions tend to depopulate the condensate. In superfluid $^4$He, only a fraction of atoms are in the condensate ($n_0 \sim 0.1$) at zero temperature.

The condensate fraction $n_0 = N_0/N_B$ can also be obtained from the correlation function $\lim_{r \to \infty} \langle \hat{a}_r^\dagger \hat{a}_0 \rangle = n_0$. A non-zero value of $n_0$ implies that the amplitude to remove a particle from the $N_0$-boson condensate at site $r = 0$ is phase coherent with the amplitude to add
a particle to the same condensate wave function very far away \cite{27}. Such off-diagonal long range order is characteristic of a superfluid. In the limit of \( r \to \infty \), the contributions to \( \langle \hat{a}^+_i \hat{a}_0 \rangle \) come exclusively from the condensate because the weight of transitions into or out of all other states add incoherently and vanish at long distances.

Another quantity of interest is the superfluid density \( \rho_s \), which is distinct from the condensate fraction \( n_0 \), and is a measure of the rigidity of the system under a twist or spatial gradient of the order parameter’s phase. In the ground state, a superfluid is phase coherent with a fixed phase \( \theta \) and does not have any net velocity. If a gradient in the phase is produced by, for example, rotating the superfluid, then the superfluid velocity \( v_s = \frac{\hbar m}{\rho_s} \nabla \theta(r) \) is obtained. The corresponding increase in free energy due to the kinetic energy of the superflow is

\[
\Delta F = \frac{1}{2} \int d^d r \, \rho_s v_s^2 = \frac{1}{2} \rho_s \left( \frac{\hbar}{m} \right)^2 \int d^d r \, (\nabla \theta)^2
\]

and provides a definition of \( \rho_s \propto \partial^2 F / \partial \theta^2 \). In two dimensions, \( \rho_s \) has units of energy. At \( T = 0 \) in superfluid \( ^4 \text{He} \), although the fraction of bosons in the lowest eigenstate is only 10\%, the superfluid density is equal to the the total boson density: \( \rho_s = \rho \). On a lattice with broken Galilean invariance it can be shown that \( \rho_s \leq \rho \) and is in fact bounded from above by the kinetic energy \cite{28}.

\subsection{2.1.2 Mean Field Theory}

**Formalism**

The superfluid to Mott transition of the BHM is captured by the single-site mean field theory introduced by Sheshadri, et al \cite{29}. With the definition of the order parameter \( \phi = \langle \hat{a} \rangle \), the annihilation and creation operators can be trivially rewritten as \( \hat{a}_j = \phi + (\hat{a}_j - \phi) \) and \( \hat{a}_i^\dagger = \phi^\ast + (\hat{a}_i^\dagger - \phi^\ast) \) and the kinetic energy expressed as

\[
\hat{a}_i^\dagger \hat{a}_j = \phi^\ast \hat{a}_j + \hat{a}_i^\dagger \phi - |\phi|^2 + [(\hat{a}_i^\dagger - \phi)(\hat{a}_j - \phi)].
\]
The mean field approximation is to assume that the phase fluctuations about the mean, denoted by $[\cdots]$, are small and can be neglected. The BHM reduces to a single-site mean field Hamiltonian as a function of the variational parameter $\phi$

$$\hat{H}^{MF}_i[\phi] = \frac{U}{2}\hat{n}_i(\hat{n}_1 - 1) - \mu\hat{n}_i - t\left(\phi^*\hat{a}_i + \hat{a}_i^\dagger\phi\right) + t|\phi|^2. \quad (2.9)$$

The mean field Hamiltonian can be solved by writing Equation (2.9) in the Fock basis with $n = 0, 1, \ldots, n_M$ bosons. The maximum number of bosons on a site, $n_M$, should be increased until the variational energy and parameter $\phi$ converge; $n_M \sim 10$ is usually sufficient for $\mu/U \lesssim 4$. By assumption, either $\phi$ is zero (in the MI) or $\phi$ is fixed at a finite value because the $U(1)$ symmetry is broken (in the SF). In both cases, we are free to fix the phase so that $\phi$ is real.

$$\begin{bmatrix}
|0\rangle & |1\rangle & |2\rangle & \cdots & |n_M\rangle \\
\langle 0| & t|\phi|^2 & -t\phi & 0 & \cdots & 0 \\
\langle 1| & -t\phi & t|\phi|^2 - \mu & -\sqrt{2}t\phi & \cdots & 0 \\
\langle 2| & 0 & -\sqrt{2}t\phi & t|\phi|^2 + U - 2\mu & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\
\langle n_M-1| & 0 & 0 & 0 & \cdots & -\sqrt{n_Mt}\phi \\
\langle n_M| & 0 & 0 & 0 & \cdots & \frac{t(|\phi|^2 - \mu n_M)}{U n_M(n_M-1)}
\end{bmatrix} \quad (2.10)$$

The variational energy $E^{MF}[\phi]$ [see Figure 2.2] is self-consistently minimized by the following procedure: (a) construct the mean field Hamiltonian matrix in Fock space (Equation 2.10) using a trial mean field $\phi$, (b) diagonalize the matrix and find the eigenstates $|\psi_i\rangle$ and eigenenergies $E_i$, (c) find the eigenstate $|\psi_0\rangle$ with lowest energy $E_0$, (d) update $\langle \hat{a}\rangle \rightarrow \phi$, and (e) repeat until the self-consistent condition $\phi = \langle \psi_0|\hat{a}|\psi_0\rangle$ is satisfied at the optimal $\tilde{\phi}$. The desired local properties are then evaluated within the lowest-energy eigenstate of $\hat{H}^{MF}_i[\tilde{\phi}]$. Local observables like the density can be estimated by $n = \langle \psi_0|\hat{n}|\psi_0\rangle$. 

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By modifying the self-consistency condition by the Boltzmann weight

\[
\phi = \frac{\sum_i \langle \psi_i | \hat{a} | \psi_i \rangle e^{-E_i/T}}{\sum_i e^{-E_i/T}},
\]

(2.11)

properties at finite temperature \(T > 0\) can be accessed with the estimator

\[
\langle \hat{O} \rangle = \frac{\sum_i \langle \psi_i | \hat{O} | \psi_i \rangle e^{-E_i/T}}{\sum_i e^{-E_i/T}}.
\]

(2.12)

**Mean Field Theory Results**

In the absence of inter-site tunneling, the density should increase in a stairstep manner as a function of \(\mu/U\) as outlined in Equation (2.2). Introducing a small tunneling \(t/U\) shrinks each step and opens a range of \(\mu/U\) over which the density deviates from integer values and the superfluid emerges in these regions [see Figure 2.3(c)]. At still higher coupling, number fluctuations cause the Mott plateaus to vanish entirely [see Figure 2.3(d)]. Within mean field theory, the superfluid density \(\rho_s = |\phi|^2\). At \(T = 0\) for large \(t/U\), the superfluid density \(\rho_s\) approaches the density \(n\), as for a Galilean invariant system. With decreasing tunneling \(t/U\) and especially near a quantum critical point, \(\rho_s\) is significantly suppressed
The superfluid density $\rho_s = \phi^2$ is zero in the vacuum $\mu/U < t/U$ and in the Mott insulator, while the density $n$ is quantized in the Mott insulator. A particle-hole symmetric quantum critical point occurs at the tip of each Mott lobe where the transition to the superfluid takes place at constant density. The color scales are the same in (a,b) so it is clear that as $t/U$ increases, $\rho_s \rightarrow n$. (c,d) The superfluid density and density profiles at $t/U = 0.05$ and $t/U = 0.15$, respectively. The stair-step increase in the density $n$ is characteristic for small values of $t/U$. At larger values of $t/U$, the superfluid density $\rho_s$ closely tracks $n$.

from $n$ by strong correlations even at zero temperature, and $\rho_s$ vanishes entirely within the Mott phase.

Upon raising the temperature, the order parameter $\phi$ and consequently $\rho_s$ are suppressed and vanishes at a critical temperature $T_c \propto t\phi$. As shown in Figure 2.4, the superfluid order is first destroyed near the Mott insulator and at low densities.

Several extensions of this basic mean field theory have been studied. Instead of decoupling to a single site model, several sites are kept in variational cluster perturbation theory [30]. This retains information about the lattice geometry and dimension and is sensitive to phases with multi-site ordering, which is essential for mean field investigations of
Figure 2.4: These finite temperature phase diagrams calculated within MFT qualitatively show the superfluid-Mott boundary at $T = 0$ and the superfluid-normal boundary at finite temperature, as determined by the vanishing of the superfluid density $\rho_s$. In both (a) the $t/U - \mu/U$ plane and (b) the $U/t - \mu/t$ plane, there is a vacuum with no particles at small $\mu$. It is clear that thermal fluctuations affect the lowest density superfluid phases the most. The classic picture of the tower of Mott lobes with increasing density and decreasing extent is shown in (a).

the BHM extended to include multiple species or to other lattices. Perturbative approaches describe the quantum phase transition from the superfluid [31] or from the Mott insulator [32, 33, 34] phase. Dynamical mean field theory models the BHM as a single impurity self-consistently coupled to a bath and works well in higher dimensions [35, 36].

Alternatively, the excitation spectrum can be evaluated within the random-phase approximation or from diagrammatic expansions [37, 38, 39]. In some situations, time-dependent extrapolations of MFT and time-dependent density matrix renormalization group (DMRG) methods have proven informative [40, 41, 42, 43]. These calculations hint that the gapped modes in the Mott insulator are still present at the quantum critical point and even survive into the superfluid phase with a finite weight. In the remainder of this chapter, the numerical results are obtained from a statistically exact world-line quantum Monte Carlo algorithm [see Chapter 4 for details].
Figure 2.5: The ground state phase diagram in $d = 1, 2, 3$ calculated via (a) DMRG and (b,c) QMC for the $n = 1$ Mott insulator to superfluid transition. The definition of the hopping energy is $J = t/n_c$ in (b) and (c). Adapted from [44, 45, 46].

2.1.3 Quantum Critical Phenomena

The MFT picture fails to even qualitatively estimate the properties of the quantum phase transitions in the BHM and more exact numerical methods must be applied. The zero temperature phase diagram has been exhaustively mapped numerically in $d = 1, 2, 3$ spatial dimensions (see Figure 2.5). In every dimension, as the tunneling $t/U$ increases, the Mott insulator-superfluid phase boundary tapers to a particle-hole symmetric quantum critical point for each of the $n = 1, 2, \ldots$ Mott states where $n(t/U)$ remains fixed across the quantum critical point [26]. This characteristic shape is called a Mott lobe and the quantum critical point at the tip of each Mott lobe is in the $d+1$ dimensional XY universality class, while in two and three dimensions all other quantum critical points along the MI-SF boundary are in the mean field universality class.

The quantum critical points (QCPs) in the BHM occur for $t/U$ of order unity and are extremely challenging to precisely locate within the phase diagram. Similar to classical critical points, large fluctuations arise near QCPs from new degrees of freedom that must form as the system transits from one phase to the other. These critical fluctuations leave a definite footprint in the thermodynamic and response functions for a large range of temperatures and parameter values near the QCP. They affect quantities like the density, superfluid density, compressibility and energy and cause them to scale with the temperature and the
distance from the QCP. The special symmetry at $d+1$ XY QCPs enables a mapping onto a $d+1$ dimensional classical spin system as well as onto quantum rotor models [47, 48, 49], which can make the investigation of quantum critical phenomena easier.

Near a quantum critical point, spatial fluctuations develop over a diverging length scale $\xi_x \sim \delta^{-\nu}$ and temporal fluctuations over a diverging time scale $\xi_t \sim \xi^z \sim \delta^{-z\nu}$, where $\nu$ and $z$ are critical exponents and $\delta = |t - t_c|/t_c$ or $\delta = |\mu - \mu_c|/\mu_c$ is the distance from a QCP at $(t_c, \mu_c)$. The divergent time scales correspond to vanishing energy scales $\Omega \sim \delta^{z\nu}$ at the QCP. Near the quantum phase transition, the thermodynamic and response functions show singularities characteristic of the transition’s universality class. Furthermore, the singular contributions to these functions exhibit scaling behavior that is independent of the details of the Hamiltonian. This aspect can be exploited to determine the location of QCPs in both simulations and experiments.

The scaling form of $\rho_s$, the superfluid order parameter, is particularly important in numerical investigations. We begin with the long-wavelength and low-energy effective action of the BHM at temperature $T = 1/\beta$ in imaginary time $\tau$

$$S_{\text{eff}} \sim \int_0^\beta d\tau \int_0^L d^d x \left( 2i n \partial_\tau \phi + \kappa |\partial_\tau \phi|^2 + \rho_s |\nabla \phi|^2 \right)$$

(2.13)
with coefficients of the density \( n \), superfluid density and thermodynamic compressibility \( \kappa_T = n^{-2} \partial n / \partial \mu \). Simple dimensional analysis shows that in the thermodynamic limit of \( \beta \to \infty \) and \( L \to \infty \)

\[
\rho_s \sim \xi^{-1}_\tau \xi_x^{2-d} = \delta^{\nu(z+d-2)}
\]

(2.14)

\[
\kappa \sim \xi_T \xi_x^{-d} = \delta^{\nu(d-z)}.
\]

(2.15)

But near a QCP, \( T_c \) must vanish according to \( T_c \sim \delta^{2\nu} \). Substituting for \( \delta \) in terms of \( \rho_s \) according to \( \delta \sim \rho_s^{1/\nu(z+d-2)} \) we obtain

\[ T_c \propto \rho_s^{z/(z+d-2)}. \]

(2.16)

which relates \( \rho_s \) at zero temperature to \( T_c \) [50, 51].

For finite \( \beta \) and lattice size \( L^d \), the diverging correlation lengths are cut off and \( \rho_s \sim \xi^{2-d-z} \) is replaced by

\[
\rho_s \sim L^{2-d-z} X (L/\xi_x, \beta/L^z) = L^{2-d-z} X (L g^\nu, \beta/L^z)
\]

(2.17)

\[
\kappa \sim L^{z-d} Y (L/\xi_x, \beta/L^z) = L^{z-d} Y (L g^\nu, \beta/L^z)
\]

(2.18)

where \( X \) and \( Y \) are universal scaling functions for \( \rho_s \) and \( \kappa \), respectively. Note that \( \delta = 0 \) at the QCP, so if the ratio \( \beta/L^z \) is fixed and \( L^{d+z-2} \rho_s(\mu) \) or \( L^{d-z} \kappa(\mu) \) are plotted for several values of \( L \) and \( \beta \), all the curves must intersect at the \((t_c, \mu_c)\) of the QCP. The mean field universality class is characterized by exponents \( z = 2 \) and \( \nu = 0.5 \) while the 3D XY universality class has \( z = 1 \) and \( \nu = 0.6717 \) [26, 52]. Once \( \mu_c \) or \( t_c \) is determined, the curves collapse onto the universal scaling function \( X \) or \( Y \) with the proper choice of the critical exponent \( \nu \), demonstrated in Figure 2.6. This type of finite-size scaling analysis for \( \rho_s \), the Mott gap and \( \kappa \) is the ideal method for determining the location of a critical point from numerical simulations [26, 46, 45].

A similar dimensional analysis of the singular part of the free energy density \( f_s \) leads
to [26, 53, 54, 55, 56]

\[ n_s(\mu, T) = n(\mu, T) - n_r(\mu, T) = T^{(d+z-1/\nu)/z} \chi \left( \frac{\mu - \mu_c}{T^{1/2\nu}} \right) \]  
(2.19)

\[ \kappa_s(\mu, T) = \kappa(\mu, T) - \kappa_r(\mu, T) = T^{(d+z-2/\nu)/z} \gamma \left( \frac{\mu - \mu_c}{T^{1/2\nu}} \right), \]  
(2.20)

with the singular part of the density \( n_s = -\partial f_s / \partial \mu \) and the singular part of the compressibility \( \kappa_s = -\partial^2 f_s / \partial \mu^2 \). The regular parts of the density \( n_r \) and compressibility \( \kappa_r \) can be estimated analytically [56]. This general scheme has recently been implemented in a 2D experiment at the superfluid to vacuum transition and a rough estimate of the critical exponents was obtained [57]. It is important to note that at a QCP above the upper critical dimension (i.e. mean field QCP in \( d = 3 \)), a modified finite size scaling must be employed. This incorporates a dangerous irrelevant variable that scales like \( L^{1-d} \) and is carefully justified in references [58, 59, 60].

At finite temperatures far from QCPs, the superfluid order is destroyed by thermal fluctuations. Phase fluctuations excited by thermal energy eventually destroy the superfluid as the temperature rises above the critical temperature, \( T_c \). This classical critical point is in the \( d \)-dimensional XY universality class. For \( d = 2 \), this transition is in the special Berezinskii-Kosterlitz-Thouless universality class where the phase fluctuations are vortex-antivortex pairs that proliferate and become unbound above \( T_c \). In the 2D superfluid, vortices cause correlations to decay algebraically and impose quasi-long-range order. In contrast, the Mott state experiences a smooth crossover to a normal state as temperature increases because it does not break any symmetry of the Hamiltonian. Particle-hole pair thermal fluctuations in the Mott insulator multiply as the temperature increases and give the state a finite compressibility.

As shown in Figure 2.7(a,b), one complication is identifying the data that should be scalable, i.e. in the quantum critical region. Neither the density \( n(\mu, T) \) nor the chemical potential \( \mu(n, T) \) is necessarily monotonic at intermediate temperatures and scaling such data may require extra experimental steps to estimate \( n, \mu \) and \( T \).

The non-monotonic behavior of \( \mu(n, T) \) can be understood in the following way. At
Figure 2.7: (a) Density \( n \) at fixed \( \mu/U \) at the \((2+1)d\) XY QCP (the Mott tip) \((t/U, \mu/U) \approx (0.2385, 0.375)\) \((+)\) and at a mean field QCP below \((t/U, \mu/U) \approx (0.15, 0.17)\) \((\square)\) and above \((t/U, \mu/U) \approx (0.15, 0.67)\) \((\times)\) the Mott lobe tip. The inset indicates each dataset’s parameters on a \( T = 0 \) phase diagram. (b) \( \mu/U \) as a function of \( \beta t = t/T \) for \( n = 1 \) and \( t/U = 0.2385 \).

low temperature, the system teeters between a Mott insulator and a superfluid, and both \( n(\mu, T) \) and \( \mu(n, T) \) are approximately constant. As the temperature increases, thermal effects overwhelm the boson-boson repulsion \( U \) and \( n(\mu, T) \) approaches the natural filling specified by \( \mu \): \( n > 1 \) for \( \mu > 0.5 \) or \( n < 1 \) for \( \mu < 0.5 \). Entropy trumps all other considerations at high temperatures and either drives \( n(\mu, T) \) to large values or moves \( \mu(n, T) \) toward the large negative values associated with a classical gas.

2.1.4 General QMC Results

Although MFT results are fairly accurate away from a QCP, the exact results from QMC are important for rigorous characterization and for estimates of any nonlocal properties, like the momentum distribution. QMC results confirm this expectation in two and three dimensions, as shown in Figure 2.8. The differences between QMC and MFT reflect the suppression of superfluid order by thermal and quantum phase fluctuations not included in MFT. The agreement is best in 3D and becomes progressively worse in 2D and 1D as phase fluctuations play an increasingly large role, shown in Figure 2.8(b). The entropy is estimated using the standard formula

\[
S(T) = \int_0^T dT' \frac{1}{T'} \frac{d \langle E \rangle}{dT'}. \tag{2.21}
\]
Several observables can play a role in identifying the phase or a quantum or thermal phase transition, as illustrated in Figure 2.9. The superfluid density is the most obvious because it is the superfluid's order parameter, but other observables show tell-tale features. As discussed above, the average density and compressibility will collapse onto a universal
Figure 2.9: (Upper panel) Local observables such as density $\langle n \rangle$, compressibility $\kappa = \partial \langle n \rangle / \partial \mu$ and local number fluctuations at site $i$, $\delta n_i^2 = \langle (\hat{n}_i - \langle \hat{n}_i \rangle)^2 \rangle$, across the superfluid-Mott quantum phase transition and across the superfluid-normal thermal phase transition in 2D. (Right panel) The superfluid density $\rho_s$ characterizes the thermal and the quantum phase transitions. $\kappa(\beta)$ clearly exhibits a kink at the superfluid-normal transition and careful analysis of $\kappa$, $n$ or $\rho_s$ would identify the quantum critical point. In contrast, $\delta n_i^2$ changes smoothly at all transitions. (Left panel) The $(t/U, \mu/U)$ parameters for each dataset are indicated on the $T = 0$ phase diagram. All results are from QMC simulations on at least $12^2$ site systems.

curve given the proper critical exponents and the location of a critical point. In addition, the compressibility $\kappa = \partial n / \partial \mu$ exhibits a distinct kink due to proliferating long-wavelength modes. On the other hand, the local number fluctuation $\delta n_i^2$ on site $i$, where $\delta n_i = \hat{n}_i - \langle \hat{n}_i \rangle$, is incapable of picking up any singular behavior.

The energy scales within each ground state are particularly important for estimating critical or crossover temperatures and identifying QCPs. In the Mott state, the energy cost to add ($\Delta_p(q)$) and remove ($\Delta_h(q)$) a particle at temperature $T = 0$ and momentum $q$ are the crucial energy scales. Away from the QCP, these two modes define the entire spectral
function in the Mott insulator

\[ A(\mathbf{q}, \omega) = -S_{h, \mathbf{q}} \delta(\Delta_h(\mathbf{q}) - \omega) + S_{p, \mathbf{q}} \delta(\Delta_p(\mathbf{q}) - \omega) \]  

(2.22)

where \( S_{p, \mathbf{q}} \) and \( S_{h, \mathbf{q}} \) are amplitudes for particle and hole modes. These gap scales are easily extracted from QMC simulations by the fit to the imaginary time Green function in momentum space

\[ \langle \hat{a}^{\dagger}(\mathbf{q}, 0) \hat{a}(\mathbf{q}, \tau) \rangle \approx S_{\mathbf{q}} e^{-\Delta_h(\mathbf{q})\tau} + (S_{\mathbf{q}} + 1) e^{-\Delta_p(\mathbf{q})(\beta - \tau)} \]  

(2.23)

where the coefficient \( S_{\mathbf{q}} \) is the spectral weight for the hole excitations shown in Figure 2.10(a). The spectral weight for the particle excitation must be \( S_{\mathbf{q}} + 1 \) to satisfy the sum rule \( \int_{-\infty}^{+\infty} d\omega A(\mathbf{q}, \omega)/2\pi = 1 \) for each \( \mathbf{q} \). These gap scales decrease and the spectral lines broaden as the QCP is approached. At the tip of the Mott lobe, both \( \Delta_h(0) \) and \( \Delta_p(0) \)
disappear, while at a QCP at \( \mu/U \) above (below) the tip, only \( \Delta_p(0) \) \( \Delta_h(0) \) continuously tends to zero. This is illustrated for \( \mu/U = 0.5 \) in \( d = 2, 3 \) in Figures 2.10 and 2.11.

Several related energy scales can be used to characterize the superfluid. The condensate fraction \( n_0 \) measures the occupation of the zero momentum state and is strictly bounded from above by \( \rho_s \). Within linear response theory, it can be shown that the kinetic energy \( E_{\text{kin}} = t \sum_{(i,j)} \left\langle \hat{a}^\dagger_i \hat{a}_j \right\rangle / L^d \) is a strict upper bound on \( \rho_s \), shown in Figure 2.10(b) \[28\]. Near the QCP and also as the dimension decreases from infinity in MFT to \( d = 3 \) and \( d = 2 \), interactions and quantum fluctuations increase in strength and suppress \( \rho_s \) and \( n_0 \), shown in Figure 2.10(b,c,d).

The momentum distribution \( n(k) \) is a very important quantity in both theory and experiment and is obtained by Fourier transform of the single body density matrix or the equal-time Green function

\[
G(r, \tau = 0) = \left\langle \hat{a}^\dagger(r) \hat{a}(0) \right\rangle.
\]

(2.24)
In these remarks we confine ourselves to $d = 2$ where $T_c \propto \rho_s(T \to 0)$ (Equation (2.16)). The Green function $G(x, \tau = 0)$ asymptotes to $n_0 \sim 1$ deep in the superfluid and decays exponentially in both the Mott and the high-temperature normal state in Figures 2.11(b,d). $n(k)$ shows that in the deep Mott state $[t/U \to 0]$ the momentum states become uniformly occupied while at high temperatures $n(k)$ is well approximated by the Maxwell-Boltzmann distribution, Figures 2.11(c,e). It is also clear that as $T$ decreases toward $T_c$, there is a significant occupation of low momentum states even before the system condenses.
### 2.2 Experimental Progress

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Table 2.1: A brief summary of common techniques to probe atoms in optical lattices.

Two broad categories of experimental measurements, local and global, have been developed to probe these isolated optical lattice systems. They are reviewed in Table 2.1. The first to be developed were global measurements that average over the entire system. These result in large signals from coherent components of the system but at the cost of losing detailed information about exactly which phases are present and where they are within the system. As mentioned above, the bosons are usually confined by a harmonic potential in addition to the lattice periodic potential, which allows multiple phases to coexist within a single system. The second class are *in situ* measurements that address single or small numbers of sites. The Mott state is easily characterized using these local density measurements, but the presence of the superfluid order is difficult to deduce. Another caveat is that in contrast to global-type measurements, many identical runs of the experiment must be averaged over to estimate the local average density and its fluctuations.
Figure 2.12: The microscopic optical lattice system is most easily characterized through a time-of-flight expansion. Upon the removal of all optical potentials, atoms occupying quasi-crystal momenta are projected onto continuum momenta and expand from \(25\mu m\) to \(500\mu m\). This matter field interferes according to each atom's original phase \(\theta_i\), captured in \(n(k)\). In the far-field (long expansion time), the interference pattern is a reliable indicator of the initial state in the optical lattice [20].

2.2.1 Mapping Momentum from the Lattice to the Continuum

Time-of-flight (TOF) experiments were some of the first to show evidence of superfluidity in optical lattices [20, 61, 62]. By switching off all potentials, allowing the cloud of bosons to freely expand and observing the bosons’ positions using resonant absorption imaging, these experiments probe phase coherence within the system. The interpretation proved more subtle than first expected, but the experiments were eventually well understood [72]. Direct comparisons between experiments and similar-sized QMC simulations of traps provided definitive proof that the BHM correctly describes these systems [63].

How the atom cloud expands is the crux of time-of-flight measurements and is sketched in Figure 2.12. If the cloud is imaged after a very short time \(t_{tof}\), the bosons have not had time to move and the small clouds are difficult to resolve using optical techniques. After slightly more time, the bosons move from their initial positions in the lattice but have not had time to expand according to their momenta into resolvable features. Optimally, the
cloud is imaged when it is much larger than the optical lattice and the interference pattern is far-field, but before it becomes very dilute. In this regime, the final distribution of boson positions \( r = \hbar t_{\text{tof}} k/m \) is directly proportional to the initial momentum distribution. The large confinement energy necessary to maintain the atoms in the optical lattice is released when the lattice is switched off so interaction effects are only a small perturbation during the ballistic expansion.

There are two essential components in the analysis of time-of-flight experiments [73]. The first is the equilibrium momentum distribution \( n(k) \) discussed in Section 2.1.4, which has a singular contribution at \( k = 0 \) in the superfluid and is a smooth function of all other momenta. The second aspect is the mapping from the momentum distribution within the optical lattice to real-space. This requires the Fourier transform of the Wannier function whose form is fixed by the lattice potential and the recoil energy [see Appendix A]. The resulting interference pattern is

\[
\tilde{n}(r) = \left( \frac{m}{\hbar t_{\text{tof}}} \right)^d \left| W \left( k = \frac{mr}{\hbar t_{\text{tof}}} \right) \right|^2 n \left( k = \frac{mr}{\hbar t_{\text{tof}}} \right). \tag{2.25}
\]

where it is important to remember that \( r \) in the TOF image is related to the initial \( k \). In three dimensions, the time-of-flight image records the column-integrated density \( \tilde{n}_{\text{col}} (k_x, k_y) = \int dk_z \tilde{n}(r = \hbar t_{\text{tof}} k/m) \). The primary subtlety to interpreting TOF images is that near a QCP, the small singular peak at \( k = 0 \) is difficult to distinguish from a large interaction-induced peak at small \( k \).

### 2.2.2 In Situ Experiments

Several experimental groups achieved single- or few-site in situ imaging of optical lattice systems nearly simultaneously using multiple techniques [68, 69, 67]. This breakthrough enabled detailed studies of the local density distribution within each phase in a trap, although the highest resolution techniques can only measure whether the onsite density is odd or even (Figure 2.13). Almost immediately, it became clear that similar systems could have radically different and unexpectedly long timescales for global equilibration. In these experiments, the lattice potential was ramped to a relatively large potential \((t/U \sim 0.05 - 0.1)\)
Figure 2.13: *In situ* density measurements (top column) and reconstructed site occupation modulo 2 (bottom row). Deep in the Mott state, hole and doubly occupied states are recorded as zero (modulo 2) and are tightly bound (left) while in the superfluid (right) the on-site occupation number has a much broader distribution. Adapted from [74].

and the equilibration timescales estimated by measuring \( n(r) \) at a series of times after the ramp and estimating how long it took to stabilize. Under some conditions, equilibration occurred in a fraction of the tunneling time \( \sim 0.1t^{-1} \) [71] but in others it took longer than the experimental timescale \( \sim 10t^{-1} \) [70].

Results from time-dependent MFT and DMRG simulations indicated how to resolve this discrepancy [42, 43, 75]. Instead of the tunneling timescale, it is the particle-hole timescale \( U^{-1} \) that sets the equilibration time in the superfluid. After a ramp, the amplitude of each occupation number \((0, 1, 2, \ldots)\) on each site fluctuates before being damped by the interaction \( U \). This result, valid in a superfluid in either a trap or a uniform system, is consistent with the former set of experiments. The longer timescale is directly related to the formation of Mott insulator shells within the trapped system. Since a Mott state has a very small compressibility at low temperatures, the mass transport of bosons across a Mott shell occurs very slowly and can hinder global equilibration if, to reach the equilibrium state, many bosons must be transported across a Mott shell. It is this trap-dependent distinction between fast equilibration within a superfluid shell but slow equilibration between superfluid shells that separated the experiments’ timescales so widely. At low temperatures, superfluid shells are isolated by the Mott shells and each can exhibit a distinct temperature and effective chemical potential.
2.3 Phase Identification by Local Observables

The two methods for mapping the finite temperature phase diagram discussed in the remainder of this chapter rely on local observables for phase identification. Because these methods are not rigorously found using scaling, they should be only be treated as good estimates. In addition, the Mott insulator has no order parameter and changes smoothly with temperature, so its crossover temperature $T_{\text{crossover}}$ is necessarily “squishy.” The development of in situ imaging [69, 71, 67] spurred theoretical work into the connections between experimentally measurable chemical potential and local density $\langle \hat{n}_i(\mu) \rangle$ and desirable information like temperature, characteristic energy scales and the phase of the system [56].

2.3.1 The Fluctuation Dissipation Theorem

The natural starting place is the fluctuation-dissipation theorem that exactly relates the compressibility

$$\kappa(\mu) = \frac{\partial \langle \hat{n}(\mu) \rangle}{\partial \mu} = \frac{1}{T} \frac{\delta N^2(\mu)}{L^d} = \frac{1}{T L^d} \sum_{ij} \langle (\hat{n}_i - \langle \hat{n}_i \rangle)(\hat{n}_j - \langle \hat{n}_j \rangle) \rangle$$

(2.26)

to the total number fluctuations $\delta N^2(\mu)$, where $\delta N^2(\mu) = \sum_{ij} \langle \delta \hat{n}_i \delta \hat{n}_j \rangle$ and $\delta \hat{n}_i = \hat{n}_i - \langle \hat{n}_i \rangle$. The “local” compressibility $\kappa$ is trivially related to the thermodynamic compressibility $\kappa_T = n^{-2}\kappa$. As discussed in Appendix B, the ratio of the compressibility to the total number fluctuations is equal to $1/T$ even when quantum effects are important. Furthermore, the local or on-site number fluctuations $\delta n^2 = \langle (\hat{n}_i - \langle \hat{n}_i \rangle)^2 \rangle$ can be explicitly separated out as

$$\kappa = \frac{1}{T} \left[ \delta n^2 + \frac{1}{L^d} \sum_{i \neq j} \langle (\hat{n}_i - \langle \hat{n}_i \rangle)(\hat{n}_j - \langle \hat{n}_j \rangle) \rangle \right]$$

(2.27)

The compressibility $\kappa$ and the total number fluctuations $\delta N^2$ can be independently measured: (a) $\kappa(\mu)$ is the change in the density due to a small change in the chemical potential around a reference value achieved, for example, by varying the characteristic length of the confining potential or the total number of atoms, and (b) $\langle \delta N^2(\mu) \rangle$ can be estimated through statistics generated by multiple experiment runs with the confining potential fixed.
at the reference value.

### 2.3.2 Compressibility

The superfluid is tricky to identify with *in situ* imaging because neither \( n_0 \) nor \( \rho_s \) are accessible. But the critical temperature \( T_c \) or critical chemical potential \( \mu_c \) is observable as a kink in \( \kappa = \partial \langle \hat{n} \rangle / \partial \mu \) as a function of \( T \) or \( \mu \), shown in Figure 2.9(upper panel)[76]. The kink is obvious in three dimensions but the Berezinskii-Kosterlitz-Thouless transition considerably damps its amplitude on the 2D optical lattice, illustrated by \( \rho_s(T) \) in Figure 2.9(right panel). On the other hand, the Mott insulating state has a commensurate filling and a gap to excitations, so it is identifiable at low temperatures by \( \kappa = 0 \), because \( \kappa \) is finite in all other states. The Mott insulator crossover temperature scale is typically and arbitrarily defined by \( \kappa(T_{\text{crossover}}) = \epsilon \) where \( \epsilon \) is some small number.

It is instructive to contrast \( \kappa_i = \partial \langle \hat{n}_i \rangle / \partial \mu \) evaluated at a single site \( i \) with the truly local compressibility \( \kappa_i^L = \partial \langle \hat{n}_i(\mu_i) \rangle / \partial \mu_i = \langle \delta n_i^2 \rangle / T \). The latter quantity \( \kappa_i^L \) measures the local change in density in response to a local change in the chemical potential at site \( i \). It is impossible for \( \kappa_i^L \) to pick up the singular behavior near a phase transition that is encoded within the long range behavior of correlation functions. In contrast, the “local” compressibility \( \kappa_i \) is a variation of \( \langle \hat{n}_i \rangle \) with respect to a global change in \( \mu \) and is clearly sensitive to the long-wavelength excitations associated with a phase transition.

### 2.3.3 Number Fluctuations

In a uniform system containing a single equilibrated phase, the number fluctuations are great indicator of the Mott insulator state. At \( T = 0 \) and \( t/U = 0 \), the number of bosons is perfectly commensurate with the lattice and both global and local number fluctuations are zero. Thermal or quantum fluctuations nudge number fluctuations to a nonzero but very small value as \( T \) or \( t/U \) increases, respectively. On the other hand, a superfluid system at fixed \( \mu \) exhibits relatively large local and global number fluctuations. Again, the distinction between a Mott-like state with small number fluctuations and a Bose liquid at finite temperatures is a fuzzy crossover. Site-resolved measurements in a trapped system
help to distinguish Mott state regions from normal or superfluid regions.

### 2.3.4 Thermometry

Temperature is another of the unexpectedly difficult quantities to measure in ultracold atom experiments but the fluctuation-dissipation theorem provides a clean measurement even when quantum effects dominate. Unfortunately, as outlined in Section 2.2.2, experimenters cannot always be confident that the system is in equilibrium, so they cannot necessarily rely on a temperature calculated from the ratio $\delta N^2(\mu)/\kappa$ to accurately estimate the temperature. Also, in a cold atom experiment the total number of particles in the system is fixed, so it is useful to consider a patch of the system of area $\Omega_{\text{patch}} = \xi_p^2$, with $L \gg \xi_p \gg a_0$, over which fluctuations are estimated [77].

Within an equilibrated patch, the ratio $\kappa(\mu)/\delta N_{\text{patch}}^2(\mu)$ provides an accurate estimate of the temperature [77, 78]. With local compressibility $\kappa_i$, the fluctuation-dissipation theorem can be specifically tailored for the patch $\Omega_{\text{patch}}$ around site $i$ by

$$
\kappa_i(\mu) = \frac{\partial \langle \hat{n}_i(\mu) \rangle}{\partial \mu} = \frac{1}{T} \left\langle \delta \hat{n}_i(\mu) \sum_j L^2 \delta \hat{n}_j(\mu) \right\rangle \\
\approx \frac{1}{T} \left\langle \delta \hat{n}_i(\mu) \sum_{|r_i - r_j| \leq \xi_p} \delta \hat{n}_j(\mu) \right\rangle = \frac{\delta N_{\text{patch}}^2(\mu)}{T}.
$$

Quantum Monte Carlo simulations using the directed loop algorithm show the nonlocal density correlations $\langle \delta \hat{n}_i \delta \hat{n}_j \rangle$ between sites $i$ and $j$ decay over a length scale $\xi_{nn} \lesssim 4a_{\text{Latt}}$ even near quantum critical points [see Figure 2.14], so $\xi_{nn}$ is driven by non-universal effects. As previously observed [77], this indicates that thermometry using the fluctuation dissipation theorem can be accurate even on a relatively small patch of size $\xi_p > \xi_{nn}$.

### 2.3.5 The Local Density Approximation

Many results from a uniform system with chemical potential $\mu$ can be directly mapped onto non-uniform systems with an effective local chemical potential $\mu_i^{\text{eff}}$ through the local density approximation (LDA). In a harmonically trapped system with curvature $V_T$, the
Figure 2.14: Nonlocal density correlations are negative and decay very quickly even near quantum critical points at inverse temperature $\beta t = 6$ and $t/U = 0.15$ with error $\sim 10^{-3}$.

LDA maps the position in the trap $r_i$ onto an effective chemical potential

$$\mu_i^{\text{eff}} = \mu_0 - V_T r_i^2 / a_{\text{latt}}^2,$$

where $\mu_0$ is the chemical potential at the trap center. This method is highly accurate for local observables like the number density and its fluctuations [see Figure 2.15] and also enables $\kappa_i$ to be extended to a trapped system

$$\kappa_i(\mu_i^{\text{eff}}) = -\frac{1}{2V_T r_i} \frac{\partial \langle \hat{n}(r) \rangle}{\partial r} \bigg|_{r \to r_i}.$$

As discussed below in Section 2.5, the LDA mapping is less reliable wherever $n(r)$ varies rapidly or near a transition between a superfluid and a normal or Mott state [4].

### 2.4 Numerical Phase Diagram using the Characteristic Density

This section\(^1\) studies the combined effects of a confining potential and finite temperature on the state diagram of the BHM in 2D, generalizing previous finite-T QMC work [79] at fixed density, and ground state QMC studies in the presence of a confining potential [80, 81]. This phase diagram is constructed in terms of experimental parameters – the particle number,

\(^1\)This section is published in Mahmud et al., PRB 84 054302 (2011) [4].
Figure 2.15: The local density approximation using the mapping (Equation 2.30) from a uniform system at chemical potential \( \mu \) onto a trapped system at position \( r = \sqrt{(\mu_0 - \mu)/V_T} \) in 3D. As a function of lattice site within the trap \( r/a_{\text{latt}} \), the density (blue stars) and local compressibility (red boxes) from within a trap compare well with the density (purple diamonds) and local compressibility (pink triangles) calculated in the equivalent uniform systems. For all the QMC simulations here, \( T/t = 0.1 \) and \( t/U = 0.15 \). The trap frequency was \( \omega = 2\pi \times 30 \text{Hz} \) and contained \( 10^5 \) bosons. From [76].

confining potential and interaction strength. We use an appropriately scaled measure of particle number, the ‘characteristic density’ \( \tilde{\rho} \), which allows systems of different sizes to be compared [81], to present the scale invariant finite temperature state diagram. We compare our state diagrams with the results of a recent NIST experiment on a harmonically trapped 2D lattice [Phys. Rev. Lett. 105, 110401 (2010) [82]], and identify a finite temperature effect in the experimental data. In addition to the trapped state diagram, the finite temperature phase diagram of the uniform 2D BHM is displayed. These results quantify the spatial inhomogeneity/phase coexistence which is created by the trap and the interplay of thermal fluctuations that give rise to a third, normal (N) liquid phase in addition to the usual ground state SF and MI phases of the Bose Hubbard model [26].

To obtain the phase diagram, we examine three local observables – the density \( n_i = \langle \hat{n}_i \rangle \), compressibility \( \kappa_i \) and the superfluid density \( \rho_s \). As discussed in Section 2.3, \( n_i \) and \( \kappa_i \) are able to distinguish the spatially separated phases in a trap. For a trapped system, a qualitative criterion for the appearance of a local MI is that the local density be an integer, as for the homogeneous case. At \( T = 0 \), a more precise criterion for identifying a local MI is to require that \( \kappa_i \) take on a value equal to the compressibility, \( \kappa = \partial n/\partial \mu \),
of a homogeneous system of commensurate filling [80, 81]. It is typically the case that an extended (more than 4-5 site) region of nearly constant, integer density has \( \kappa_i \) close to its value in the homogeneous MI, thus providing a rapid, visual means to identify a likely MI region. At finite temperatures the MI-N boundary is a crossover so there is no sharply defined phase boundary and drawing the boundary is somewhat arbitrary. In delineating the crossover boundary for the homogeneous and the trapped system at finite temperature, we have taken \( \kappa < 0.04/U \) to identify the Mott region. A superfluid region has a nonzero superfluid density in the equivalent uniform system, while the normal region is negatively identified as the region with \( \rho_s = 0 \), incommensurate filling and \( \kappa > 0.04/U \).

Defining a local superfluid density is not justifiable because \( \rho_s \) involves the response of the system to a global phase twist. While there are proposals to generalize \( \rho_s \) to a local quantity, we adopt the LDA approach [76] to estimate the state diagram for superfluids in confined systems, i.e. we assume the confined system is a superfluid if the equivalent uniform system is superfluid.

### 2.4.1 Uniform Systems at Finite Temperature

The zero temperature ground state phase diagram for the uniform BHM (\( V_T = 0 \)) in two dimensions has been worked out using strong coupling expansions [33], and using QMC [83, 79]. In Ref. [79], a finite temperature phase diagram for a constant occupation \( n = 1 \) was presented showing the boundaries of the SF and MI/N regions in the \( (T/t, U/t) \) plane. Mean-field theory has been used [29, 84, 85] to study different properties and to obtain the finite-T phase diagram in any dimension. Various other approximate methods have also been used to study the finite temperature BHM [34, 39]. We present the QMC uniform finite-T phase diagram in the \( (\mu/U, t/U) \) plane valid for the first two Mott lobes.

In Figure 2.16, \( n \) and \( \rho_s \) are shown as functions of \( \mu/U \) for two different temperatures \( T/t = 1/32 \) and \( T/t = 1/2 \) for a \( 32^2 \) lattice at \( t/U = 0.025 \). This lattice size is large enough so that finite size effects are minor. For \( T/t = 1/32 \), \( \rho_s \) is non-zero whenever \( n \) is incommensurate. For our purposes, this temperature is so low that it is effectively zero temperature and the system is either a MI or a SF. On the other hand, for \( T/t = 1/2 \),
Figure 2.16: Occupation \((n)\) and superfluid density \((\rho_s)\) as a function of the chemical potential \((\mu/U)\) for two different temperatures \(T/t = 1/2\) and \(T/t = 1/32\) at \(t/U = 0.025\) for the uniform 2D BHM calculated on a \(32^2\) lattice. A nonzero \(\rho_s\) corresponds to a superfluid (SF) phase, zero \(\rho_s\) with integer occupation \(n = 1\) to a Mott insulator (MI) phase, and zero \(\rho_s\) with non-integer occupation to a normal (N) phase. At the low temperature, wherever the density is incommensurate, the system is SF. Only at higher temperature do normal regions develop which have incommensurate filling and \(\rho_s = 0\). This is exemplified at the incommensurate density region near \(\mu/U = 0\) where a rise in temperature from \(T/t = 1/32\) to \(T/t = 1/2\) has destroyed the superfluid density and turned the SF to N.

This is no longer the case. There are substantial regions where \(\rho_s\) is zero even though \(n\) is incommensurate, which signifies a N liquid. Strictly speaking, the MI only exists at \(T = 0\) in a uniform system, however, Mott-like features can persist at finite temperatures with a small value of compressibility. As mentioned above, in drawing this MI-N crossover boundary at finite-T, we have taken \(\kappa < 0.04/U\) to identify the Mott region.

The QMC uniform system phase diagram for the 2D BHM at finite temperature was built up from sets of runs such as those shown in Figure 2.16 for different \(U/t\), and is presented in Figure 2.17. We show the phase boundaries for four different temperatures in panels (a)-(d): effectively zero temperature \(T/t = 1/32\), \(T/t = 1/4\), \(T/t = 1/2\) and \(T/t = 1\). At \(T/t = 1/32\) the system has only two phases – MI with an energy gap inside the lobe, and a gapless SF outside the lobe. The transition between them is driven by quantum fluctuations as \(t/U\) is varied. The lowest value of \(U/t\) for which the SF-MI transition can occur is \(U/t \approx 4.24\) (i.e. \(t/U \approx 0.236\)) [79], the location being at the tip of the first lobe. At
Figure 2.17: Finite temperature phase diagram for the homogeneous BHM in two dimensions in the $(\mu/U, t/U)$ plane for four different temperatures (a) $T/t = 1/32$, (b) $T/t = 1/4$, (c) $T/t = 1/2$ and (d) $T/t = 1$. (e) shows the phase diagram in a different representation, for fixed $T/U = 0.02, 0.04$ and $0.08$. The lines that demarcate the SF and N denote phase boundaries while those that demarcate MI and N denote crossovers. At finite temperature, normal phase regions appear between MI and SF.

At a finite temperature, thermal fluctuations play a part in reducing the MI lobes. For example, at $T/t = 1/4$ in Figure 2.17(b), we see that between the MI and SF phases, a region of normal phase has developed at the expense of reducing both the SF and MI regions. With further increase of temperature, the normal phase region widens. For $T/t = 1/2$, the N-SF phase boundary around $n = 1$ is no longer lobe-like; the SF region ceases to bend back inward to low $t/U$ at small density. With further increase of temperature to $T/t = 1$, the SF between the first two MI lobes is also replaced by N liquid.

In Figure 2.17(e) we present the finite-T phase diagram for temperatures in units of $U$, for $T/U = 0.02, 0.04$ and $0.08$. As temperature increases, the MI lobes shrink, and the N liquid phase region grows between the MI and SF region. For $T/U = 0.08$ we find that the compressibility $\kappa > 0.04/U$ near $t/U = 0$, which is therefore no longer a MI in our criteria. The pictorial representations of how the MI lobes behave, although different in the two representations of $T/t$ and $T/U$, are interchangeable. Now that $U$ is the unit of energy, the superfluid vanishes from integer $\mu/U$ first, rather than from the sides of the Mott lobe as for $T/t$. This is because $T/U$ remains a constant fraction of $U$ while thermal fluctuations at constant $T/t$ become less and less significant compared to $U$. Although
finite-T homogeneous phase diagrams are usually presented at constant \( T/U \) as in panel (e), phase diagram plots (a)-(d) for constant \( T/t \) values connect well to the confined system state diagram presented in Section 2.4.2 and provide a useful representation for optical lattice experiments where temperatures are often cited [86, 61, 82] in units of \( T/t \).

We conclude this subsection by noting that Figure 2.17 can be reinterpreted as giving the local density and SF profiles in a confined system, assuming the validity of the LDA. That is, each spatial site in a confined lattice is assigned the density and SF density of a uniform system with the same local chemical potential. The resulting sequence of LDA phases can most easily be understood by starting with the location \((\mu_0/U, t/U)\), where \(\mu_0\) is the chemical potential at the trap center, on the uniform phase diagram of Figure 2.17 and moving downwards at fixed \( t/U \) because decreasing \( \mu/U \) corresponds to increasing \( V_T r_i^2 \), i.e. moving outward from the trap center.

### 2.4.2 State Diagram at Finite Temperature

#### Characteristic Density

In the uniform case \((V_T = 0)\), the thermodynamic limit of the BHM is reached by increasing the linear lattice size \( L \) while keeping the density \( n = N_b/L^d \) constant, where \( N_b \) is the particle number, and \( d \) is the dimensionality. The standard phase diagram is a function only of \( U/t, T/t \) and \( n \) or \( \mu/U \), not of \( N_b \) and \( L \) separately. The generalization of this procedure for the harmonically confined system with \( V_T \neq 0 \) is to define a rescaled length,

\[
\xi_i \equiv x_i/\xi \quad \text{with} \quad \xi = \sqrt{t/V_T} \tag{2.32}
\]

and a “characteristic density”, \( \tilde{\rho} = N_b/\xi^d \) [81]. For the 2D model, \( \tilde{\rho} = N_bV_T/t \). The state diagram and the properties of the trapped system then depend only on the combination \( \tilde{\rho} \). Measurements at fixed \( U/t, T/t \) and \( \tilde{\rho} \) then approach a well-defined large \( L \) limit. Position dependent quantities match when plotted in units of rescaled length \( (x_i/\xi) \) and LDA-derived quantities like \( n \) or \( \rho_s \) trivially follow the rescaled distance or effective chemical potential.

The validity of characteristic density idea discussed in Reference [81] is illustrated in
Figure 2.18. For $T/t = 1/32$ (effectively zero temperature), (a) shows the QMC density profiles for two systems with the same characteristic density $\tilde{\rho} = 8.625$ but different trapping potentials and total number of particles, $V_T/t = 0.00625$, $N_b = 1380$ and $V_T/t = 0.0125$, $N_b = 690$. When plotted as a function of characteristic length scale $\xi = \sqrt{t/V_T}$, the density profiles are equivalent, as are all the position dependent local quantities [81]. (b) shows the actual density profiles for the two trap strengths in (a), clearly showing the different extent of the profiles and highlighting the concept of equivalence in the scaled plots in (a). The same holds true at finite-$T$, as shown in Figures 2.18(c) and (d) for $T/t = 1/4$. The density profile in (a) shows a constant integer plateau and an incommensurate ring with $n < 1$, calculated using QMC for a trapped system. In (c) the density profile at a higher temperature, $T/t = 1/4$, also shows a similar constant plateau and an incommensurate ring.

To determine whether the ring contains a SF or N liquid phase, we plot LDA-derived SF density across the trap. This shows that for Figure 2.18(a) the entire incommensurate ring is SF ($\rho_s \neq 0$), whereas in Figure 2.18(c) only a small part of the ring is SF and the rest is N, where $n$ is incommensurate but $\rho_s = 0$. This is how we identify trapped phases containing distinct combinations of MI, SF and N regions. Thanks to the scale invariance of $\tilde{\rho}$, the state diagram we obtain below is independent of the specific values of trap strength ($V_T$), number of particles ($N_b$) or lattice size. It only depends on the combination $N_bV_T/t = \tilde{\rho}$.

The state diagrams presented here were generated with up to $64^2$ site lattices.

**Zero Temperature State Diagram**

The state diagram for the harmonically confined system at zero temperature was presented in Reference [81]. In Figure 2.19(a), we reproduce the $T = 0$ state diagram in characteristic density – interaction strength ($\tilde{\rho}$, $U/t$) plane using QMC simulations in a trap, to higher values of $\tilde{\rho}$ than presented in Reference [81]. The three possible states are indicated in Figure 2.19(a), and illustrated in Figure 2.20. The region (I) corresponds to SF phase filling the trap. In region (II), a MI plateau with ($n = 1$) in the center is surrounded by a SF ring of $n < 1$. (III) is a state (see Figure 2.20(c)) where a local SF region at the center with $n > 1$ is encompassed by a MI domain with $n = 1$ and then by a SF ring with $n < 1$. 

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Figure 2.18: The validity of the characteristic density idea and the effects of temperature on spatially separated phases in a harmonically trapped system. For $T/t = 1/32$, (a) shows the density profiles for two systems with the same characteristic density $\tilde{\rho} = 8.625$ but different trapping potentials and total number of particles, $V_T/t = 0.00625$, $N_b = 1380$ and $V_T/t = 0.0125$, $N_b = 690$. All position dependent quantities are equivalent [81] when distance is rescaled by $\xi = \sqrt{t/V_T}$, as evident here in density matching. (b) unscaled density profiles for the two trapping strengths plotted in (a). The density profiles in (a) exhibit a constant integer plateau and an incommensurate ring with $n < 1$, calculated using QMC in a trapped system. (c) density profiles at a higher temperature $T/t = 1/4$ also show a similar constant plateau and an incommensurate ring. To determine whether the ring contains any SF, we plot the LDA derived $\rho_s$ that shows that for (a) the entire ring is SF, whereas in (c) only a portion of the ring is SF and the rest is N. (d) Unscaled density profiles for the two trapping strengths in (c).

This state diagram quantifies the parameter regimes for the appearance of these coexistent phases. Knowing the trap strength, total number of particles, and interaction strength we can predict the states in a trap. A MI is obtained for a $U/t$ that is always greater than the homogeneous system critical coupling of $(U/t)_c \approx 4.24$; only for a small window of $\tilde{\rho} \approx 5.75$ are the maximum critical couplings comparable. A recent determination of the critical coupling by a NIST group [86, 61] can be understood in terms of the characteristic density trajectory the experiment follows when $U/t$ ratio is increased [81]. Further experiments [82] validate the agreement with the QMC trapped system state diagram.

To go beyond the results of the zero temperature state diagram in Reference [81], we
Figure 2.19: State diagrams for a harmonically trapped system for (a) $T = 0$, (b) $T/t = 1/4$ and (c) $T/t = 1/2$. A schematic of all the phases according to their labels is shown in Figure 2.20. The phase boundaries indicate all of the phases that coexist in a trap and their ordering. For example, in (a), region (II) corresponds to a state which has a MI plateau in the center surrounded by a SF shell. For higher $T$, a normal (N) phase appears and there are states with many varieties of coexisting phases such as phase (IV) in (b) MI, N, SF and N from the center to the edge. At finite temperatures, the tail is always N. For higher $T$, the SF-N phase boundary shifts to a lower value of $U/t$, and the first appearance of a MI plateau occurs at a higher value of $U/t$.

compare the $T = 0$ trapped state diagram with the state diagram obtained by $T = 0$ LDA. The green line in Figure 2.19(a) is the LDA state diagram obtained from the uniform phase diagram by evaluating the density profiles and characteristic densities for specific values of $\mu/U$ at the phase boundaries [87]. The obvious disagreement between phase I (SF) and phase III (SF+MI+SF) arises from the finite gradients in the trapped systems. Specifically, the disagreement between the (I)–(III) boundary is related to the appearance of finite width MI shoulders within the trap. In the LDA picture, the MI appears at all $\mu/U$ or $\tilde{\rho}$ above the tip of the lobe $U/t$ in Figure 2.17. In a confined system, the Mott state takes up the center of the trap at the Mott lobe tip ($U/t_c$). At larger $\tilde{\rho}$ for fixed ($U/t_c$), the Mott state is pushed out from the center and the confined MI compressibility only equals that of a uniform system when the Mott shoulder or annulus is sufficiently wide. The trapped system (I)–(III) boundary therefore slowly deviates from the vertical LDA boundary. A recent 2D experiment done at NIST [82] has observed this deviation from the LDA. The transition from phase (II) to phase (III) requires the development of a superfluid bulge at the center of the trap. This occurs when it is favorable to put a particle at the center rather than at the outer edge of the atomic cloud. By an energy matching condition, it is possible
Figure 2.20: Schematic of all the phases for a trapped system at $T = 0$, $T/t = 1/4$, and $T/t = 1/2$, according to the labels shown in the state diagrams in Figure 2.19. At finite-$T$, part of the atomic cloud turns normal and forms rings between SF and MI regions. Three phases at $T = 0$ increase to seven different phases at $T/t = 1/4$ and five at $T/t = 1/2$. The furthest part of the tail is always N at a finite-$T$ as seen here in (d)–(o). Annular SF rings cannot form for a high enough temperature such as in (k)–(o).

This is indeed the case for both the LDA and trapped QMC data points. For MI shoulders with $n \geq 2$ at higher $\tilde{\rho}$, similar analytic phase boundaries exist with slopes $5\pi$, $9\pi$, etc.
Figure 2.21: The compressibility values and ways of distinguishing the N/MI phase boundary. We show panels (g) and (i) from Figure 2.20 for $U/t=10$ and $\tilde{\rho} = 16.1, 33.8$ respectively. Since N to MI is a crossover, there is arbitrariness in drawing the boundary and we have taken $\kappa < 0.04U$ to identify the finite-T Mott insulator-like region. (b) and (d) show the $\kappa U$ values in the systems from (a) and (c), respectively.

**Finite Temperature State Diagram**

Figures 2.19(b) and (c) show the finite temperature state diagrams at $T/t = 1/4$ and $T/t = 1/2$ respectively. The phase boundaries demarcate the distinct states that are possible when different parts of the atomic cloud are superfluid, normal fluid or Mott insulator. Figure 2.20 illustrates all the states of Figures 2.19 (b) and (c) according to their labels. In order to better understand all the phases, we start at a small $\tilde{\rho}$ at constant $U/t = 10$, and consider the impact of adding particles, thereby increasing $\tilde{\rho}$ along a vertical line at $U/t = 10$ in Figure 2.19(b). For $\tilde{\rho} < 0.34$, N phase extends all across the trap (phase I). Adding more particles introduces a SF region at the center of the trap while the tail stays normal (phase II). Even more particles introduces N liquid at the center while the SF+N regions of the previous phase remain as narrow annuli (phase III). With yet more particles, a Mott plateau forms at the center and pushes the N+SF+N region out (phase IV).
IV. Following the phase schematics of Figure 2.20 makes clear that adding more particles introduces a new phase region at the center and pushes the old phases outward and reducing their radial extent. This process explains the further appearance of phases V and VI with additional N and SF regions at the center. We can also think of varying $U/t$ while keeping a constant $\tilde{\rho} = 15$. At $U/t = 2.5$, we start with a SF+N phase we encountered earlier and as $U/t$ increases we reach phase VII, where the center is a SF surrounded by N+SF+N.

The appearance of different phases can also be understood in terms of LDA and the uniform phase diagram. At fixed $t/U$, going from high to low $\mu$ will traverse the same phases that would coexist in a trapped system at zero temperature with $\mu_0$ equal to the high $\mu$. This proceeds exactly as outlined in the MFT results Figure 2.3, except that $\mu$ in the uniform system is mapped onto the effective $\mu^\text{eff}_i$ in the trapped system a distance $i$ from the trap center. The order of appearance of phases coexisting in a trap can be understood by this effective chemical potential picture, in addition to the particle number discussed in the previous paragraph.

Figure 2.21 depicts the process of distinguishing between N and MI regions. Because the N/MI is a crossover boundary, we arbitrarily defined the boundary as $\kappa < 0.04U$, as as done recently in [55]. Figures 2.21(a,c) show the profiles of panels (g) and (i) from Figure 2.20 and Figures 2.21(b,d) show their respective $\kappa U$ values and the MI cutoff.

With further increase of temperature to $T/t = 1/2$ the state diagram in Figure 2.19(c) now has the five phases as shown in Figure 2.20. By focusing on a constant $U/t = 10$, and increasing characteristic density (by increasing particle number), we can visualize going through the phases for this state diagram as well. First we encounter phase I with N liquid all across the trap. Further increase in the number of particles introduces a MI at the center (phase II). Similarly, in phases III and IV, N and SF regions appear at the center pushing out the existing regions. If we start with N phase all across the trap (phase I) at a lower interaction $U/t = 5$ instead of $U/t = 10$, increasing $\tilde{\rho}$ would introduce a SF bulge at the center instead of a MI (phase V). Note that $T/t = 1/2$ is high enough that no SF rings appear in the trap in contrast to $T = 0$ and $T/t = 1/4$.

Some observations of finite temperature effects in a harmonically trapped lattice system
are summarized below:

(A) Thermal fluctuations always introduce a N phase region in the low density tail of the lattice gas. As temperature increases, N rings appear to surround MI and SF regions, which gives rise to more than three confined states – seven at $T/t = 1/4$ and five at $T/t = 1/2$. Thermal effects prevent SF rings from forming for high enough temperature, as seen from $T/t = 1/4$ and $T/t = 1/2$.

(B) Finite temperature causes a shift of the SF-N transition coupling $(U/t)_c$ to a lower value than for a zero temperature trapped system and to a higher value for the first appearance of a MI plateau. To see this, examine the zero temperature state diagram in Figure 2.19(a) where the phase boundary between states I and III denotes the appearance of MI shoulders. As we raise the temperature to $T/t = 1/4$ such as in Figure 2.19(b), this boundary (SF-MI) moves to bigger $U/t$ between the states VII and VI while another boundary (SF-N) appears between states II and VII at lower $U/t$, which signifies the appearance of N phase in the center of the cloud. For temperature range $T = 0$ to $T/t < 1/4$ as in the NIST experiment [82], the separation between these two boundaries is small, and the MI transition would pass through a narrow range in $U/t$ going through a SF-N transition first. In a $(T/t − U/t)$ phase diagram at $n = 1$, this lowering of $U/t$ for SF-N transition can be understood in terms of a downward shift of temperature as has been observed and explained in a recent experiment [63] in 3D.

(C) We identified and classified the trapped phases with QMC simulations but did not discuss the issue of their experimental signatures. However, we would like to make some comments in relation to the state diagrams. The two main ways of determining critical coupling in experiments are to analyze the momentum distribution with time-of-flight (TOF) experiments [86, 61] and by direct in situ imaging of density profiles [67]. The critical coupling $(U/t)_c$ for SF-MI transition at $T = 0$ corresponds to the appearance of a MI shoulder and is observed in TOF through reduced $n_0$. At finite-T, the difference between coherent and incoherent $n(k)$ is measured via $n_0$ and differentiates between SF and N/MI. However, the distinction between N and MI is difficult to detect with TOF imaging. Thermal or quantum fluctuations make distinguishing between SF-MI-SF and
SF-N-MI-N-SF-N very difficult with only $n_0$, and makes direct confirmation of the state diagrams in Figure 2.19 from TOF imaging quite demanding. *In situ* imaging may be a better method at finite temperatures because the distinction between the MI and the N is obvious. Single site resolution microscopes [68, 69] is a big step forward in this direction; detection of coexisting phases (including the superfluid) through density scanning has been discussed in Reference [76].

**Comparison with NIST Experiment**

A recent experiment at NIST [82] obtained the state diagram for a 2D harmonically trapped lattice system. They used TOF imaging to estimate $n_0$ and to determine the presence of superfluid regions in a trap as a function of atom number and lattice depth ($t/U$). By comparing to the $T = 0$ QMC state diagram, they confirmed the breakdown of LDA discussed for Figure 2.19(a) by finding MI shoulders only at higher values of $(U/t)_c$ (for larger $\tilde{\rho}$) than in the equivalent uniform system.

In Figures 2.22(a) and (b) we show respectively the $T = 0$ and $T/t = 1/4$ state diagrams of Figures 2.19(a) and (b) overlaid with the experimental data points of the NIST experiment; the circles represent MI and the triangles SF. We do not show the experimental phase boundary and its uncertainty reported in Reference [82]. Although the experimental comparison was done with a $T = 0$ state diagram, the temperature was reported to be $T/t = 0.23(5)$, considered a low enough temperature for such a comparison. However, as we have seen in Figures 2.19(a) and (b), the state diagram at $T/t = 1/4$ differs from $T = 0$ because of the appearance of normal phase regions in the cloud. Here we choose to overlay the experimental data both in our $T = 0$ and $T/t = 1/4$ state diagrams (same experimental data in both panels in Figure 2.22). It is visually quite clear that the experiment obtains SF points for low $U/t$ and MI points for high $U/t$. However, the transition to no superfluid does not occur at the same value of $U/t$ for every $\tilde{\rho}$, which signifies the breakdown of LDA.

We find that for MI points at low $\tilde{\rho}$, the data agrees more with the state diagrams at $T/t = 1/4$ than at $T = 0$. For low $\tilde{\rho}$ the measurement of different phases is difficult due to increased thermal fluctuations, and the measurement uncertainty is large. In Figure 2.22(a),
Figure 2.22: Comparison of theoretical state diagram boundaries with NIST experimental results of Reference [82]. Circles and triangles represent respectively MI and SF data points from the NIST experiment; same set of data is plotted in (a) and (b). Comparison is made with theoretical state diagram boundaries in (a) $T = 0$ and (b) $T/t = 1/4$. The types of coexisting phases for (a) and (b) are given in Figure 2.19. There are MI points for low values of $\tilde{\rho}$ in (a) that are below the state diagram boundary $\tilde{\rho} \approx 3.5$. For finite-T, the state diagram boundary goes down as in (b) containing many of these MI/N data points. We identify this feature as a finite temperature effect fully explainable with a finite-T state diagram.

many MI points are below the boundary of $\tilde{\rho} \approx 4.5$. In Figure 2.22(b), we see that the lower boundary for MI/N goes down to $\tilde{\rho} \approx 2.5$ and contains many of these points. We emphasize that the reported experiment temperature of $T/t = 0.23$ is the initial temperature, while the final temperature is unknown and could be higher. In that case, the boundary to (III) would descend to lower $\tilde{\rho}$ and contain all the experimental MI/N data points. We argue that the experimental result detected a finite temperature effect that is fully explainable with our finite temperature state diagram. It is important to note that the experimental phase diagram was not constructed in such a way that the MI and the N phases could be distinguished, although that may be possible with more detailed analysis or with direct comparisons to QMC.
Figure 2.23: (a) Density profile and local superfluid density for trapped atoms when the entire region is SF for parameters \( t/U = 0.00625, T/t = 1/32, V_T/t = 0.003 \) and \( \mu_0/U = 0.1 \). In (b) circles show the correlation decay between a point \( i = 10 \) and other points along the ring of radius \( i = 10 \), as a function of the arc distance \( d \). The pentagrams show correlation decay for a 2D uniform system for a chemical potential equal to that of the trapped system at \( i = 10 \). Because they match very well, we can conclude that the effect of trapping has not altered the long range correlations in this special case when the SF region is wide.

2.5 Limitations of LDA

The Green function or single-particle density matrix

\[
G(i,j) = \langle a_i^\dagger a_j \rangle
\]

is useful in identifying SF regions. Specifically, a \( G(i,j) \) that falls off sufficiently slowly as \( |i - j| \) becomes large signals the development of off-diagonal long range order and estimates \( n_0 \). Conversely, a rapid (exponential) fall-off of \( G(i,j) \) is consistent with a N or MI phase.

The phase boundaries for finite temperature (\( \rho, U/t \)) state diagrams in Figure 2.19(b) and (c) were obtained by determining the density profile and compressibility with QMC simulations of a confined system. In addition to these two quantities, and in the absence of a definition of the local superfluid, the LDA-derived \( \rho_s \) was used to determine the trapped superfluid region as has been standard practice in the literature [76, 88]. Here we study the bosonic Green function and, by comparing the correlations within trapped and uniform (LDA-equivalent) systems, we find that the LDA does not always correctly capture the trapped superfluid properties. For SF rings of narrow width, correlation decay do not match a 2D decay, and therefore assigning local \( \rho_s \) values from a 2D homogeneous system
has limited validity. The state diagram boundaries we have obtained previously give the upper limit boundaries for any confined superfluid phases. This effect does not alter the high temperature state diagram such as at \( T/t = 1/2 \) in Figure 2.19(c), where no SF rings can form. In Figures 2.19(a) and (b), for regions with SF rings the superfluid designation by way of the LDA-derived \( \rho_s \) has to be kept in mind. At \( T = 0 \) and \( T/t = 1/4 \), the SF rings appear to be quasi-1D superfluids or intermediate between 1D and 2D.

To be clear, there can be two obstacles to accurate LDA mapping; one is due to finite size effects and another is the description of superfluid properties in trapped rings with the LDA \( \rho_s \). Because QMC simulations in a trap were used for density and compressibility, we do not have the finite-size LDA issue related to the appearance of MI shoulders. It is the use of the LDA for \( \rho_s \) to designate the superfluid that requires qualification. A small finite width in the trap for a LDA-determined superfluid ring may prevent true long-range order or quasi-long-range order. In principle, this reduced dimensionality only affects relatively small systems and introduces a negligible correction for large systems. Unfortunately, experimental systems are on the order of “medium” sized so some care is required.

### 2.5.1 Correlation Function at Zero and Finite Temperature

To analyze the LDA and the trapped system in more detail, we study spatial correlations in the trap by looking at the Green function between bosons on site \( i \) and \( j \), \( G(i,j) = \langle a_i^\dagger a_j \rangle \).

As shown in previously, the harmonic trap creates a superfluid ring surrounding the Mott insulating or normal region at sufficiently low temperatures. A SF ring or annulus with a finite width and a relatively long circumference possesses a quasi-1D geometry.

For the parameters \( \mu/U = 0.1, \ t/U = 0.00625, \ V_T/t = 0.003, \) and zero temperature \( (T/t = 1/32) \), Figure 2.23(a) shows the density profile of trapped atoms where the whole region is SF. The red circles in (a) are local superfluid densities obtained by LDA. We plot the trapped \( G(i = 10, j) \) (circles) between a point at \( i = 10 \) and all points \( j \) along the ring at the same radius, as a function of the arc distance \( d \). Since the circular ring has the same local chemical potential at all points, we can make a meaningful comparison with the equivalent uniform system. The uniform system’s correlation decay, shown in
Figure 2.24: The effect of reduced dimensionality in a trapped superfluid ring. (a) A narrow SF ring only 4 sites wide exists for $t/U = 0.00625$, $T/t = 1/32$, $V_T/t = 0.0175$, and $\mu_0/U = 0.7$. (b) 3D plot of $G(i, j)$ for $i = 20$ where we see that $G(i, j)$ is nonzero all across the ring. (c) However, a comparison with the uniform system correlations reveals that correlations decay faster in a trap (circles) than in the equivalent uniform 2D system (pentagrams). We also compare trapped ring correlations with a 1D correlation decay (triangles) at the same parameters and temperature, and find that the 1D algebraic SF decay is faster. This demonstrates that the Bose gas in the incommensurate ring is in a crossover regime between 1D and 2D and that LDA estimates for $\rho_s$ cannot be trusted in such a narrow SF ring.

pentagram symbols, matches the trapped $G(i, j)$ decay very well. This implies that the effect of trapping (inhomogeneity) has not changed the behavior of long-range correlations.

In Figure 2.24, we investigate the zero temperature ($T/t = 1/32$) correlations for a narrow SF ring. Panel (a) shows the density profile and local superfluid density indicating that the ring is approximately 4 sites in width. Panel (b) shows a 3D plot of $G(i, j)$ for a point in the SF ring, between $i = 20$ and for all other sites $j$ in the lattice. It is evident that order persists around the narrow ring because $G(i, j)$ is nonzero along the circle, whereas it decays rapidly to zero radially from the SF region to the MI plateau. Similar to Figure 2.23(b), in Figure 2.24(c) we compare the trapped correlation decay for $i = 20$ along the ring (circles) to the equivalent uniform system’s correlations. The trapped SF decay matches the uniform system decay for only a short distance, after which it continues to deviate from a 2D SF decay. Thus the SF ring does not have 2D superfluid properties, rather it exhibits quasi-long-ranged correlations that are influenced by the ring width. We also compare the 2D trapped correlations along the ring with a 1D uniform system correlation decay (triangles) at the same density and temperature. In 1D, the decay is algebraic ($G(i, j) \sim |i - j|^{-p}$, $p > 0$ is the decay exponent) for superfluid and exponential
Figure 2.25: The behavior of spatial correlations for trapped superfluids at finite temperature. For the parameters $T/t = 1$, $\mu/U = 0.4$, $t/U = 0.0125$ and $V_T/t = 0.1$, (a) shows the density profile and local superfluid density, indicating a superfluid ring of finite width. (b) $G(i,j)$ between the point $i = 20$ and the rest of the lattice is plotted. Although $i = 20$ is SF according to LDA picture, there is no long-range order along the ring. (c) quantifies the decay in greater detail – the circles showing the correlation along the ring slowly going to zero at a large distance. $G(i,j)$ for a homogeneous 2D superfluid with the same parameters is given in pentagrams. The triangles, 1D correlation at the same density and temperature $T/t = 1/4$, decay much faster. However, the diamonds depicting 1D correlations at a much lower temperature ($T/t = 1/32$) are seen to be similar to that of the 2D trapped annular SF correlations at $T/t = 1/4$. (d) $G(i = 15, j)$ in the normal are the same in the trapped and in the uniform system.

$(e^{-|i-j|/\xi_x})$ for a Mott or normal phase [89, 90, 91]. We see that the 2D ring correlations decay slower than a homogeneous 1D algebraic SF decay but faster than a homogeneous 2D decay. We therefore conclude that the Bose gas in the SF ring is in a crossover regime between a 1D and 2D superfluid. As the width narrows, it would approach a 1D SF decay, and as the width increases, as we have seen in the earlier example, the trapped correlation decay approaches a 2D SF decay.

While all these may seem quite intuitive because of the quasi-1D nature of the ring, the significance of these results is that assigning the 2D LDA-derived $\rho_s$ to the ring is not always justifiable, in contravention of many recent papers [76, 55]. It indicates a breakdown
of LDA for local superfluid properties even as it continues to describe local density dependent quantities [76, 87]. It is well known that finite size effects can reduce the LDA’s applicability for every observable [81, 82], but we have shown here that the LDA accuracy is particularly suspect when used to identify reduced-dimensionality SF regions.

Figure 2.25 reiterates the behavior of spatial correlations at finite temperature which the key result of this section. For $T/t = 1/4$, $\mu/U = 0.4$, $t/U = 0.0125$ and $V_T/t = 0.1$, Figure 2.25(a) shows the density profile and the LDA-derived $\rho_s$ for a superfluid ring of finite width. Figure 2.25(b) plots $G(i, j)$ between the point $i = 20$ and other points on the lattice and clearly shows that although $i = 20$ is SF in a uniform system, the decay in a trap is reveals that the long-range order does not span the ring. Figure 2.25(c) quantifies the decay in greater depth – the circles showing the correlation along the ring slowly going to zero at a large distance. For a uniform 2D superfluid with the same $t/U$, $T/t$, and at the same $\mu$ as the spatial location $i = 20$, the correlation is shown in pentagons, where the decay is correctly that of a 2D SF. 1D correlation at the same temperature $T/t = 1/4$ and parameters, shown in triangles, decays much faster. However, the diamonds depicting 1D correlations at a much lower temperature $T/t = 1/32$ are seen to be qualitatively similar to that of 2D trapped annular ring at $T/t = 1/4$. This implies that as far as the long range properties are concerned, the annular ring is at a lower effective temperature than the 2D cloud. This may be due to reduced fluctuations induced by the finite width ring. In Figure 2.25(d) we show that correlations in a trapped normal region at $i = 15$ matches the correlations in the equivalent uniform 2D system.

To understand the trapped phases, we examined the spatial correlations of $G(i, j)$ around annular superfluid rings. We found that the correlation decay in narrow SF rings does not match the uniform 2D superfluid at the same parameters. At $T = 0$, the correlation decay is intermediate between 1D and 2D decay and at $T > 0$ the correlations in a trap decay much faster than the equivalent uniform 2D system. Although the correlations in a trap decay slower than the 1D decay at the same temperature, 1D correlations at a lower temperature match, indicating that the ring is at a lower effective temperature.
2.6 Mapping the Finite Temperature Phase Diagram using the Single Ratio $R$

One drawback to the finite temperature state diagram studied in Section 2.4 is the heavy reliance on QMC results even when interpreting experimental data. In this section, we propose a novel way to map the finite temperature phase diagram of the BHM that, in principle, can be used to analyze experimental data with no (or minimal) need for theoretical or numerical input. We illustrate this method using QMC results of the uniform BHM in 2D, but stress that it is applicable to generic many-body quantum systems.

2.6.1 Mapping the Quantum Critical Region

The insights gained from using the fluctuation-dissipation theorem for thermometry and from identifying the superfluid transition by kinks in $\kappa_i$ can be combined into a method to map the quantum critical region via a single observable $R$ [3, 2]. With this ratio, we can distinguish among the normal, Mott insulator and superfluid phases and furthermore estimate the high temperature limit of the quantum critical region. We restrict our finite temperature phase diagram to the uniform system and suppress the site index in $\kappa$ and $R$.

We discuss how to apply this method to a trapped system at the end of this section.

Consider the ratio

$$R = \frac{\kappa_i(\mu, T)}{\delta n_i^2(\mu, T)}$$

(2.34)

of the compressibility $\kappa_i = \partial \langle n_i \rangle / \partial \mu$ defined in Equations 2.27 and 2.28 to the local number fluctuations $\delta n_i^2 = \langle \delta \hat{n}_i \delta \hat{n}_i \rangle$. At high temperatures, the density-density correlations $\langle \delta \hat{n}_i \delta \hat{n}_i \rangle$ length scale $\xi_{nn}$ is negligible compared to $a_{\text{latt}}$ so $\kappa(\mu) \approx \beta \delta n^2(\mu)$ and $R(T) \sim \beta$ or $1/R(T) \sim T$ as required by the fluctuation-dissipation theorem in Equation 2.26. As the temperature decreases, $\xi_{nn}$ increases and $R(T)$ deviates from $\beta$ at a characteristic temperature $T^*$. We identify $T^*$ as an upper bound on the quantum critical region that can be read off of $R(T)$ in the upper panel in Figure 2.26. If a superfluid emerges at low temperature, the ratio

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Figure 2.26: (top panel) The ratio $R$ (Equation 2.34) across a quantum critical point from uniform 2D QMC calculations. At high temperature $T = 1/\beta$, $R \sim \beta$ (dashed line) while at low temperature, $R$ exponentially decays to zero in a Mott state or asymptotes to a finite value in the superfluid. (left panel) The parameters for each dataset are shown on a $T = 0$ phase diagram. (right panel) The superfluid density $\rho_s$ clearly shows the standard Berezinskii-Kosterlitz-Thouless-type transition for $\mu/U > 0.67$ at $t/U = 0.15$.

$R(T)$ peaks due to the kink in $\kappa_i$ at $T_c$ and $R$ asymptotes to a constant at low temperatures because $\kappa_i, \delta n_i^2 > 0$ at $T = 0$. In a Mott state, $R(T) \to 0$ as $T \to 0$ since $\kappa_i$ vanishes, while quantum fluctuations maintain $\delta n_i^2$ at a finite value. For both phases, $R(T)$ at fixed $\mu$ exhibits a peak at an intermediate temperature $T_{max}$ that corresponds to the characteristic energy scale of the phase, either $T_c$ in the superfluid or $T_{crossover}$ in the Mott, associated with vanishing $\kappa_i$.

The temperature $T_{max}$ of the peak in $R(T)$ and the temperature $T^*$ when $R(T)$ diverges from $1/T$ can be combined into a finite temperature phase diagram obtained from the single quantity $R$, shown in Figure 2.27. The superfluid and Mott lobes are clearly visible in Figure 2.27(a) at low temperature as are the general locations of the quantum critical points between the phases. Reassuringly, the temperature $T^*$ bounding the quantum critical region from above, which we associate with the onset of non-local quantum correlations, is independent of the underlying ground state or quantum critical point. In Figure 2.27(b) we
Figure 2.27: The finite temperature phase diagram at (a) $t/U = 0.15$ and (b) $t/U = 0.4$ constructed from characteristic energy scales of $R$ (Equation 2.34): $T^*$ (■) and $T_{\text{max}}$ (●) from $R(\beta, \mu)$. $T_{\text{max}}$ is in good agreement with $T_c$ (▲) and $T_{\text{crossover}}$ (▼) estimated from vanishing $\rho_s$ and $\kappa$, respectively. The temperature of the onset of quantum effects $T^*$ is independent of the underlying ground states and converges to $T_c$ far from quantum critical points. Note that the density plots of $R(\beta, \mu)$ have been normalized by the maximum value at $R(\beta_{\text{max}}, \mu)$ for each value of $\mu$ [from [3]].

see that $T^*$ converges to $T_c$ as $\mu$ increases away from the vacuum critical point, in line with the expectation that a quantum critical regime is only large near a quantum critical point. The uncertainty with which the peak position is identified in Figure 2.27(b) at large $\mu/U$ stems from the sharp transition from $R(T) = \beta$ (classical fluctuations) to $R(T) = \text{constant}$ (superfluid) and the corresponding vanishing of the peak near $R(T_c)$. Additionally, the Berezinski-Kosterlitz-Thouless transition rounds the kink or peak in both $\kappa$ and $R$.

### 2.6.2 Other Properties of $R$ and Finite Size Effects

The ratio $R$ contains several more pieces of information. Quantum critical points can be located using this ratio because $R(T)$ behaves like neither phase there. As shown in Figure 2.28(right panel), the singular part of $\kappa_i$ and $\delta n_i^2$ determine $R(T)$ at the generic and at the (2+1)d XY quantum critical points, respectively. In particular, at a generic quantum critical point, $\kappa$ is largely independent of $T$ and $R$ is determined by the smooth, slow decay of $\delta n_i^2$ with $\beta$. At a (2+1)d XY quantum critical point $\kappa \sim \beta^{-1}$ overwhelms $\delta n_i^2$ and causes $R(\beta) \sim \beta^{-1}$.

The deviation of $R^{-1}$ from linear $T$ behavior defines the temperature $T^*$ at which
Figure 2.28: Quantum critical points in two dimensions. Left panel: theoretical parameters for the particle-hole symmetric (2+1 dimensional XY) point at the tip of the $n = 1$ Mott lobe and for a generic point on the Mott-superfluid boundary at a lower $\mu/U$. Right panel: the ratio $R$ depends strikingly on the universality class. At the XY point $R$ (Equation 2.34) is determined by the singular behavior of $\kappa(\beta)$ while at a generic point, the non-universal behavior of $\delta n^2(\beta)$ overwhelms the $\kappa(\beta) \sim 1 + O(\ln \beta)$ singular behavior. From [2].

Figure 2.29: Boson bunching and anti-bunching. (a) Bunching ($R > \beta$) occurs at low temperatures for $t/U = 1.0$, $\mu/U = -0.95$. This system is not superfluid at the temperatures probed. (b) Anti-bunching ($R < \beta$) occurs at low temperatures for $t/U = 0.15$, $\mu/U = 0.05$. The error in $\beta^*$ is indicated by the horizontal bar. The large error in $\beta_{\max}$ (horizontal bar) is characteristic of the superfluid in the presence of strong interactions, where the peak in $R$ is difficult to resolve. The inset in each panel shows the density for the same parameters.

Quantum effects first become evident. In Reference [92], such deviations were observed for a uniform system near the normal-superfluid transition. The exact formula

$$R = \frac{\kappa_i}{\delta n_i^2} = \beta \left( 1 + \frac{\sum_{i \neq j} (\langle \hat{n}_i \hat{n}_j \rangle - \langle \hat{n}_i \rangle \langle \hat{n}_j \rangle)}{V\delta n_i^2} \right)$$

illustrates that any deviation of $R$ from $\beta$ is due to inter-site density fluctuation correlations.
At low density $n \lesssim 0.1$ and small interactions $U$, the quantum statistics of bosons leads to bunching (Figure 2.29(a)), or positively correlated density fluctuations, and manifests as $R > \beta$. For larger density and stronger interaction, the inter-boson repulsion overwhelms the bosonic tendency to bunch and density fluctuations between sites become anti-correlated, causing $R < \beta$ (Figure 2.29(b)).

The Mott gap suppresses the low energy excitations contributing to the compressibility and causes $\kappa$ to vanish exponentially with the $T = 0$ energy gap $\Delta_{ph}$ to add a particle or a hole, whichever is smaller [26], as $T \to 0$. The energy gap extracted by fitting a decaying exponential to $\kappa$ or $R$ agrees very well with QMC simulations [79] deep in the MI (Figure 2.30), but differ on approaching QCPs, which we attribute mainly to finite temperature and size effects. In spite of the Mott gap, the local number fluctuations remain finite down to the lowest temperatures due to local quantum fluctuations. With increasing temperature, the MI crosses over into the normal state with no transition and therefore shows no specific signature in $\kappa$, so the peaks of $R$ and $\kappa$ do not necessarily line up.

We briefly touch on the effect of finite size in the vicinity of and directly at MF quantum critical points. In both cases, the observables that probe long range correlations ($\kappa$, $\rho_s$ and
Figure 2.31: Finite size effects at the superfluid-normal transition at $t/U = 0.08$ and $\mu/U = 0.08$. We observe significant finite size effects in $R(T)$ (a) and superfluid density $\rho_s$ (b). As the system size increases, the peak in $R(T)$ becomes more pronounced and the system becomes less superfluid at a given temperature. The finite size effects are smaller for a system further from the QCP at $\mu/U \simeq 0.084$.

Figure 2.32: Finite Size Effects at the Mean Field Quantum Critical Point at $t/U = 0.15$ and $\mu/U = 0.172$. The local number fluctuations $\delta n_i^2$ (a) do not depend on the system size. The long-range observables like the compressibility $\kappa_i$ (b), superfluid density $\rho_s$ (c) and $R$ (d) do vary with the system size before converging for $48^2$ and $64^2$ site systems. Due to simulation time limitations, the error for the $64^2$ site system is larger than for the other system sizes.

$R$) exhibit large finite size effects while the local number fluctuations $\delta n_i^2$ are unaffected by the system size $L^2$. The superfluid-normal finite temperature transition (see Figure 2.31(b)) is in the Berezinski-Kosterlitz-Thouless universality class, so both $\kappa$ and $R$ are cusplike rather than singular at the transition. This cusp or peak becomes more pronounced in
larger systems, as shown in Figure 2.31(a). Increasing $L$ significantly suppresses both $T_c$ and $\rho_s$ (see Figure 2.31(b)), partly because of the nearby MF quantum critical point.

The finite size effects change somewhat at the MF quantum critical point. As expected, $\rho_s \to 0$ as $L$ increases, and $\delta n_i^2$ is unchanged, shown in Figure 2.32. For sufficiently large systems, the compressibility $\kappa$ converges to a constant at small temperatures. At a MF quantum critical point and for sufficiently large $L$, the ratio $R(T)$ is dominated by $\delta n_i^2$ at low temperatures and monotonically increases to a finite value, in stark contrast to its behavior at the BKT transition (Figure 2.31(a)) or at the 3D XY quantum critical point (Figure 2.28(right panel)).

2.6.3 Confining Potential Considerations:

The fluctuation-dissipation theorem is easily adapted to local thermometry within the local density approximation (LDA). As discussed in Section 2.5, applying the LDA to a harmonically trapped system reduces to mapping the position in the trap $r_i$ to an effective chemical potential $\mu_i^{\text{eff}} = \mu_0 - V_T r_i^2$, where $\mu_0$ is the chemical potential at the trap center. As in the uniform system (Figure 2.14(c)), QMC simulations have shown that $\xi_{nn}$ is on the order of several lattice spacings in the trapped system and that the prescription for local thermometry following Equation 2.28 should hold. The kinks in $\kappa_i$ are still visible in a trap but are slightly rounded by the finite size and reduced dimensionality that results from multiple phases coexisting in the same trap.

This coexistence means the finite temperature phase diagram is efficiently mapped using the ratio $R(T)$. As long as the trap is approximately uniform on the scale of $\xi_{nn}$ both $\kappa_i$ and $\delta n_i^2$ will accurately map onto a uniform system via the LDA and the phase diagram mapped using the ratio $R$. In other words, the uniform system phase diagram could be mapped from trapped experimental systems. In contrast to global methods like time-of-flight, the coexistence of phases within the trap actually enhances the efficiency of this method. A single realization would estimate $R(\beta, t/U)$ for many values of $\mu/U$. However, it is important to remember that the LDA mapping is less reliable wherever $n(r)$ varies rapidly or near a transition between a superfluid and a normal or Mott state.
2.7 Real-Frequency Response Functions and Scaling

Up to this point, we have considered only the static equilibrium properties of the Bose Hubbard model. In the remainder of this chapter, we discuss some preliminary results for response functions, namely the spectral function $A(k, \omega)$ and the dynamic structure factor $S(k, \omega)$. These quantities are important for scattering experiments and recent experiments have begun to probe them [93].

The spectral function

$$A(k, \omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i\omega t} \langle \hat{a}(k, t)\hat{a}^\dagger(k, 0) \rangle$$

$$= \langle \hat{a}(k, \omega)\hat{a}^\dagger(k, \omega) \rangle$$

$$= \sum_{m,n} \frac{e^{-\beta E_n}}{Z} \left| \langle m | \hat{a}^\dagger(k) | n \rangle \right|^2 \delta(\omega - (E_m - E_n))$$

(2.36) (2.37) (2.38)

describes the propagation of a single particle excitation with momentum $k$ from time 0 to time $t$. $A(k, \omega)$ is often written in second quantized notation and the spectral representation is shown in the latter equation, where $\hat{H} | \Psi_n \rangle = E_n | \Psi_n \rangle$. The width of each excitation indicates its lifetime. In a Mott insulator, the eigenstates of the Hamiltonian are in the Fock space so the low-energy excitations can be written as

$$A(k, \omega) \approx -A_- \delta(\omega + \Delta_-(k)) + A_+ \delta(\omega - \Delta_+(k))$$

(2.39)

where the Mott gap $\Delta = \text{Min} \Delta_-(k) + \text{Max} \Delta_+(k)$ and $A_- = |\langle m | \hat{a}(k) | n \rangle|^2$. At finite $t/U$, the peaks at $\Delta_\pm$ broaden. Note that the boson commutation relation yields the sum rule $-A_- + A_+ = 1$ or [see Section 4.4.1 for details]

$$\sum_{-\infty}^{\infty} A(k, \omega) d\omega = 1.$$ 

(2.40)

Another important sum rule relates $A$ to the momentum distribution

$$n(k) = \int_{-\infty}^{0} A(k, \omega) d\omega.$$ 

(2.41)

In contrast, the dynamic structure factor is a measure of density-density correlations,
given by

\[ S(k, \omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi N} e^{i\omega t} \langle \hat{\rho}(k, t)\hat{\rho}(-k, 0) \rangle \]

\[ = \frac{1}{N} \sum_{m,n} \frac{e^{-\beta E_n}}{Z} |\langle m | \hat{\rho}(-k) | n \rangle|^2 \delta(\omega - (E_m - E_n)) \quad (2.43) \]

where \( \hat{\rho}^\dagger(k) = \sum_{q} \hat{a}_{q+k}^\dagger \hat{a}_q = \hat{\rho}(-k) \). This is analogous to propagating a particle and hole with momentum \( q + k \) and \( q \), respectively, from time 0 to time \( t \). Some useful sum rules for \( S \) include

\[ \int_{-\infty}^{\infty} S(k, \omega) d\omega = 1 + n \int [g(r) - 1] e^{-i k \cdot r} dr = S(k) \quad (2.44) \]

\[ \int_{-\infty}^{\infty} \omega S(k, \omega) d\omega = \frac{k^2}{2m} \quad (2.45) \]

where \( S(k) \) is the static structure factor and \( g(r) \) is the (static) pair correlation function.

In general, \( A(k, \omega) \) and \( S(k, \omega) \) have no reason to show any correlation – the contributing \( |m\rangle \) and \( |n\rangle \) states in the spectral representation have the same number of particles on each site for \( S(k, \omega) \) and different numbers for \( A(k, \omega) \). Yet in the presence of a condensate, phonons dominate both response functions and they agree. Unfortunately, the number-number correlations are quite small and short ranged in the BHM and \( S(k, \omega) \) results are not shown in the preliminary results below (project is ongoing).

These sum rules are important checks on the numeric analytic continuation of imaginary time correlations from QMC simulations to the real frequency spectral function \( A \) or dynamic structure factor \( S \),

\[ G(k, \tau) = \int \left\langle \hat{a}(r, \tau)\hat{a}^\dagger(0, 0) \right\rangle e^{i r \cdot k} dr = \int \frac{d\omega}{\pi} \frac{e^{-\tau \omega}}{1 - e^{-\beta \omega}} A(k, \omega) \quad (2.46) \]

\[ \left\langle \hat{\rho}(k, t)\hat{\rho}^\dagger(k, 0) \right\rangle = \int \left\langle \hat{n}(r, \tau)\hat{n}^\dagger(0, 0) \right\rangle e^{i r \cdot k} dr = \int \frac{d\omega}{\pi} \frac{e^{-\tau \omega}}{1 - e^{-\beta \omega}} S(k, \omega) \quad (2.47) \]

The maximum entropy method we employ [see Section 4.4] reliably satisfies the sum rules.
Figure 2.33: The spectral function in the 1D BHM. (a,b) The vacuum and Mott insulator ($\mu = \pm 1.04t$) excitation spectra follow the characteristic dispersion relation in a square lattice. Note the gap $0.04t$ at $k = 0$ is too small to resolve on this scale. (c,d) On approach to the critical point at $\mu = t$, both particle and hole sound modes are visible at small $k$ for $\mu = 0.6t$ but the particle sound mode vanishes on approach to $\mu = t$, as shown in (d) for $\mu = 0.9t$. The green (orange) bars indicate the width of the particle (hole) excitation at each $k$.

2.7.1 1D Bose Hubbard Model Results

We study the 1D Bose Hubbard model with hard core interactions as a test for the reliability of our QMC plus analytic continuation methods. This model is particle hole symmetric about $\mu/t = 0$ and exhibits a quantum phase transition from superfluid to vacuum (Mott insulator) at $\mu = \mp t$. Several studies have been made of $A(k, \omega)$ and $S(k, \omega)$ in the regular 1D BHM using a variety of methods [94, 95]. Note that in the hard core case, the sum rule for $A(k, \omega)$ must be modified to $\int A(k, \omega)d\omega = 1 - 2n$ because bosons on the same site now
obey the anticommutation relation \( \{ \hat{a}(r), \hat{a}^\dagger(r) \} = 1 \).

The Mott state and vacuum states are the best place to start analyzing the spectral function, shown in Figure 2.33(a,b). In a vacuum, particles can only be added at \(+\omega\), while particles can only be removed at \(-\omega\) in the \(n = 1\) Mott insulator. As expected, the modes are very well defined and have a long lifetime. In addition, the hopping is still a relatively large energy scale so after a gap \(\Delta = 0.04t\), the particle and hole modes follow a free particle-like dispersion and \(~ k^2\) at small \(k\). \(A(k, \omega)\) has many more features in the superfluid, Figure 2.33(c,d). At the particle hole symmetric point \(\mu = 0\), the particle and hole excitation branches mirror each other. As \(\mu/t\) increases, fewer and fewer particle modes are available, spectral weight is redistributed to holes and the peaks acquire a finite width.

One last piece of information we obtain from \(A(k, \omega)\) is the speed of sound. Phonons are the primary excitation mode in the superfluid and they have a linear dispersion \(\omega = ck\) with speed \(c\). As shown in Figure 2.34, \(c\) decreases on approach to the quantum critical point at \(\mu = t\).
Figure 2.35: The spectral function $A(k, \omega)$ in the 2D BHM at $\mu/U = 0.5$, $t/U = 0.15$ and $\beta t = 40$. The positive and negative branches of $A(k, \omega)$ have been color coded and the particle and hole gaps are clearly visible. The overlaid lines result from the strong coupling expansion discussed in Reference [96].

2.7.2 2D Bose Hubbard Model Results

We briefly describe some preliminary results of the BHM in two dimensions. Away from quantum critical points, $A(k, \omega)$ in the superfluid and the Mott insulator is very similar to the results in the 1D BHM. The linear phonon dispersion in the superfluid is very obvious. Because the system is softcore, the $n = 1$ Mott insulator now has a particle excitation branch with sufficient weight to satisfy the standard boson sum rule for $A(k, \omega)$. We are particularly interested in the parameter regime around the quantum critical point, where higher energy excitations are likely to be observed as they are suppressed to zero along with all other energy scales. Figure 2.35 shows a preliminary result in this investigation: the spectral function within a Mott insulator. The particle and hole gaps are well defined, and the parameter point is deep enough within the Mott lobe that the spectrum agrees well with a strong coupling expansion [96].

2.8 Concluding Remarks

We have discussed detailed properties of the Bose Hubbard model in two and three dimensions, and highlighted quantities of experimental importance like the momentum distri-
bution and local observables. Although slightly beyond the reach of contemporary experiments, spectral functions are an important component of understanding both the excitations in a phase and the reorganization of the degrees of freedom on approach to a quantum critical point. The calculations shown above are little more than a proof of concept study that could be formalized and carried out at the XY critical point at the Mott lobe tip or in disordered systems.

Two very different approaches to mapping the finite temperature phase diagram were also implemented. The first relies heavily on QMC calculations, but the use of the characteristic density $\tilde{\rho}$ rather than the traditional chemical potential $\mu$ to indicate particle number makes it scale invariant and broadly useful for any system in a trap. Its chief drawback is its reliance on QMC calculations for construction; a phase diagram constructed entirely from experimental results would require many experiment runs and both in situ measurements to distinguish the Mott from the normal phase and time-of-flight imaging to diagnose the presence of a superfluid. The second method, based on deviations from the fluctuation-dissipation theorem, uses a single observable $R = \kappa / \delta n^2$ that can be estimated from in situ measurements. It roughly maps the energy or temperature scales of each phase and, as a bonus, estimates the high-temperature limit of the quantum critical region. It applies to both uniform and trapped Bose Hubbard models, and will work for any quantum phase transition between an ordered, gapless phase and a disordered, gapped phase.

In the context of the former phase diagram we also explored the limitations of the widely used local density approximation, which enables the properties of a trapped system to be directly compared to the properties of equivalent uniform systems. We found that the correlations embodied in the Green function in a trapped system match those of a uniform system when the phase is normal or Mott, or when the trap is mostly superfluid. A narrow ring of superfluid in a trap had distinctly suppressed correlations at long range even at $T = 0$ and narrowing the ring caused them to decay faster. Comparison with the Green function in 1D confirmed that a narrow ring imposed a reduced, quasi-1D dimensionality on such a confined superfluid.

The fundamental groundwork to identify and understand the phases and phase tran-
sitions of the BHM is in place both theoretically and experimentally, but the BHM has several other exciting directions. Calculating response functions is one of many challenging directions that studies of the BHM can take. Particularly near the particle-hole-symmetric QCP in two dimensions, the structure of the spectral density and whether the Higgs mode can be observed as a well-defined excitation are important questions being addressed through both analytic methods and analytic continuation of QMC correlations to real frequencies [47, 97, 98]. Experimentally, the first observations of the Higgs mode in an ultracold atom system has been made through periodic modulations of the optical lattice [8]. The phases of the disordered BHM are also becoming better understood using the strong disorder real-space renormalization group and large-scale QMC. These studies investigated the fate of the Mott insulator and the superfluid, the emergence of the Mott and Bose glass phases, estimated critical exponents and examined the universal DC conductivity value [99, 100, 101, 102, 49]. These could shed light on systems like $^4$He in Vycor, superconductor-insulator transitions, and disordered optical lattice experiments [103, 104].

An even greater variety of systems require only minor modifications of the basic BHM discussed here and explorations of them have begun both theoretically and in optical lattice experiments. The square or cubic lattice geometry can be altered to mimic the honeycomb structure of graphene or to triangular and other geometries [105]. Further manipulation can yield spin-dependent optical lattices so that with multiple species of bosons, novel phases emerge such as spin-ordered insulators and superfluids with a complex order parameter and non-trivial orbital symmetry [106, 107]. With multiple species comes the possibility to study spin textures and topological states in systems with an artificial gauge field [108, 48]. Frustration in an antiferromagnetic system is yet another branch of the BHM in an artificial gauge field [109]. As outlined above for the basic BHM, experimental and theoretical advances are continuing in the study, detection and characterization of these novel systems.
Chapter 3

BOSE-FERMI MIXTURES

Introduction. The problem of quantum phase transitions associated with Fermi surfaces is one of the most important open problems in modern condensed matter physics. It underlies the physics of high-Tc cuprates and of heavy fermion materials. Such quantum phase transitions defy simple theoretical treatment because the low energy excitations occur over the entire Fermi surface, in contrast to a single point as for a bosonic quantum criticality. The problem becomes even richer if the Fermi surface, being the locus of these low energy excitations, itself deforms across the quantum phase transition. We discuss, in this Chapter, possibly the simplest model that involves such changes of the Fermi surface induced by the coupling to a Bose-Einstein condensate (BEC), namely an equal population of spinless fermions and bosons with a tunable inter-species interaction.

Very recently, precisely such systems have been realised in $^{23}$Na-$^{40}$K [110], $^{23}$Na-$^{6}$Li [111] and $^{87}$Rb-$^{40}$K [112] mixtures and they have been cooled to quantum degeneracy temperatures [10, 113, 114]. What is exciting about these mixtures is their relative stability close to Feshbach resonance (about 100ms for $^{23}$Na-$^{40}$K mixture [110]), which should allow detailed experimental studies of the many-body physics and elucidate the questions raised above. With this intriguing possibility in mind, we investigate the quantum phases of a Bose-Fermi mixture as a function of the interaction between bosons and fermions with zero temperature quantum Monte Carlo (QMC) methods. Here are our findings:

This work was done in collaboration with Shizhong Zhang, Soon-Yong Chang, Mohit Randeria and Nandini Trivedi. This manuscript is in the final revision process before submission to a peer-reviewed journal.
(I) We find evidence for the anticipated weak and strong coupling phases, consisting of an atomic Fermi sea, characterised by a non-zero quasi-particle weight $Z_A$ and a Bose-Einstein condensate of bosons with condensate density $n_0 \neq 0$, a strong coupling phase of tightly bound molecular fermions ($Z_A = n_0 = 0$), respectively. Surprisingly we find an intermediate phase in which the atomic Fermi sea is completely destroyed ($Z_A = 0$) while the condensate still survives ($n_0 \neq 0$).

(II) Detailed calculations of various correlation functions in the intermediate phase reveal significant fermion-boson-fermion trimer correlations. These correlations indicate that strong boson-fermion attraction induces a boson-mediated fermion-fermion attraction, which suggests a mechanism for non-zero condensate fraction even at moderately strong coupling.

Our analysis is based on the one-channel model [115, 116, 117, 118], which is appropriate to the broad Feshbach resonance realised in experiments [110, 111]. Several experiments [15, 119, 120, 23, 121, 122, 123, 124] and theoretical studies investigated the weak coupling limit [125, 126, 127, 128] and also Bose-Fermi mixtures on optical lattices [22, 129, 130, 131, 132, 133, 134, 135]. Previous theoretical work has investigated the strongly coupled Bose-Fermi mixture in the narrow Feshbach resonance case [136, 137], where the tightly bound molecular states are well approximated by a two-channel model with an independent fermionic molecular field. In our case, however, the composite nature of the bound state is crucial and our variational wave functions interpolate between the weak and strong coupling limits.

3.1 The Bose-Mixture System

We consider a mixture of bosons and spinless fermions, each with total number $N (= N_B = N_F)$ and mass $m_B$ and $m_F$, confined in a box of volume $\Omega$ such that the density of each species is given by $n \equiv N/\Omega$. It is convenient to use the Fermi wave vector $k_F \equiv (6\pi^2 n)^{1/3}$ and the Fermi energy $\epsilon_F = k_F^2/(2m_F)$ to set the length and energy scales ($\hbar = 1$). The boson-fermion scattering length $a_{FB}$ parameterizes the inter-species potential $v(r)$ and can be tuned through an inter-species Feshbach resonance, at which $a_{FB} \to \pm \infty$. To stabilize
the system and prevent mechanical collapse, a repulsive boson-boson interaction must be included [138]. We model this boson interaction as a hardcore potential of the form $u(|r| < a_{BB}) = \infty$ and zero otherwise, where $a_{BB}$ is the boson-boson scattering length. Thus, the three dimensionless parameters in our model are $\zeta \equiv 1/(k_F a_{FB})$, $k_F a_{BB}$ and $\lambda \equiv m_B/m_F$.

We set $k_F a_{BB} = 0.8$ so the system remains stable for the entire range of values $\zeta \in (-\infty, \infty)$ and choose $\lambda = m_B/m_F = 0.575$, corresponding to $^{23}\text{Na}-^{40}\text{K}$ mixture [110]. We do not expect modification of $k_F a_{BB}$ to qualitatively change the physics, so long as $k_F a_{BB}$ is less than the close packing limit [117].

The Hamiltonian of the system is

$$
\mathcal{H} = -\sum_i \frac{\nabla_i^2}{2m_F} - \sum_j \frac{\nabla_j^2}{2m_B} + \sum_{ij} v(x_i - y_j) + \sum_{j<j'} u(y_j - y_{j'}) ,
$$

in which fermions (bosons) are labeled using coordinates $x$ ($y$) and particle indices $i$ ($j$). We employ the standard inverse-cosh potential used extensively in BEC-BCS crossover studies for the inter-species potential: $v(r) = -(8/[m_r R^2])V_0/\cosh^2(2r/R)$, where we have chosen $k_F R = 0.02$ and the reduced mass $m_r = m_B m_F/(m_B + m_F) = m_F \lambda/(\lambda + 1)$. The small value of $k_F R$ ensures that we obtain universal results, independent of the precise form of $v(r)$.

Two limiting cases of the system can be understood intuitively and are sketched in Figure 3.4(a) alongside the momentum distribution results that characterize them. For $\zeta \to -\infty$, the system consists of a non-interacting fermion gas that is only slightly perturbed by the bosons. Most fermions remain in the atomic Fermi sea characterized by a non-zero fermionic quasi-particle residue $Z_A$, and most bosons are condensed into a BEC with a condensate fraction $n_0$ slightly suppressed from unity by the hard-core repulsion. In the opposite limit of $\zeta \to +\infty$, tightly-bound boson-fermion molecules form a composite molecule Fermi sea and cause both the condensate and the atomic Fermi surface to be depleted: $n_0 = Z_A = 0$.

\footnote{We have checked the sensitivity of our results to $k_F R$.}
3.2 Feshbach Resonances

Feshbach resonances are generic features that arise whenever a low energy bound state (closed channel) hybridizes with a scattering state (open channel). Originally of interest in nuclear and atomic physics, Stwalley [139] posited their existence in ultracold gases. The basic idea is that if two incident particles in open channels scatter with a total energy \( E_0 \) near a bound state energy \( E_{\text{res}} \), they can occupy an intermediate state before decaying back into open channels. This process strongly affects the scattering within the open channels and gives rise to a Feshbach resonance where the scattering length \( a \) can be tuned from \( 0^+ \) to \( \pm \infty \) to \( 0^- \), although \( \zeta = 1/k_F a \) is a more common parameterization of interatomic interactions. Atoms weakly attract at \( \zeta \to -\infty \), strongly attract at \( \zeta = 0 \) (unitarity) and form molecules which are weakly repulsive at \( \zeta \to +\infty \).

The effect of a bound state on scattering states is often a second order process whose effect on the background scattering length \( a_{bg} \) can be estimated by [7, 10]

\[
\frac{4\pi \hbar^2}{m} a = \frac{4\pi \hbar^2}{m} a_{bg} + \left| \frac{\langle \Psi_{\text{res}} | P_{\text{closed}} \hat{H} P_{\text{open}} | \Psi_0 \rangle}{E_0 - E_{\text{res}}} \right|^2
\]

(3.2)

where \( \Psi_0 \) is the initial scattering state with incident energy \( E_0 \) and \( \Psi_{\text{res}} \) is the bound state with energy \( E_{\text{res}} \). The operators \( P \) project onto the indicated subspace. The scattering length becomes infinite as \( E_0 \to E_{\text{res}} \) and, crucially, can change sign. Feshbach resonances in ultracold atoms are usually tuned via homogeneous magnetic fields, but optical Feshbach resonances have been demonstrated.

For an elementary illustration, consider tuning a Feshbach resonance by a uniform magnetic field such that at \( B = B_0 \), \( a = \pm \infty \). The energy difference

\[
E_0 - E_{\text{res}} = (\mu_{\text{res}} - \mu_\alpha - \mu_\beta)(B - B_0)
\]

(3.3)

depends on the magnetic moment \( \mu_\gamma = -\partial E_\gamma / \partial B \), where \( \alpha \) and \( \beta \) are scattering states. Then the scattering length is

\[
a = a_{bg} \left( 1 - \frac{\Delta B}{B - B_0} \right)
\]

(3.4)
Figure 3.1: Schematic of the zero energy scattering state (solid red curve) of an attractive square potential with depth $V_0$ and a bound state at $V_c$. (a) The scattering length $a$ is negative for $V_0 > V_c$, (b) diverges as $V_0 \to V_c$ and (c) is positive once a bound state has formed for $V_0 < V_c$. Extrapolating the wave function to the $x$ axis yields the (negative) scattering length for $V_0 > V_c$. (d) The scattering length is plotted against the well depth.

with a resonance width

$$\Delta B = \frac{m}{4\pi \hbar^2 a_{bg}} \left| \langle \psi_{res} | P_{closed} \hat{H} P_{open} | \Psi_0 \rangle \right|^2.$$  \hspace{1cm} (3.5)

The zero energy scattering state is illustrated schematically in Figure 3.1 for a square well potential $V(r) = -V_0 \Theta(R - r)$ with depth $V_0$, range $R$ and a bound state at $V_0 = V_c$. At zero energy and with no angular momentum, the Schrödinger equation for the wave function $\psi(r) = u(r)/r$ can be recast as

$$\left[ -\frac{\hbar^2}{2m_r} \frac{d^2}{dr^2} + V(r) \right] u(r) = 0$$

(3.6)

where $u(r) = c_1 r + c_2$ for $r > R$, i.e. wherever $V(r) \approx 0$. With no potential, $u(r)$ is a line that terminates at the origin. A shallow attractive potential changes the scattering phase shift so more weight is located inside the potential. This shift is parametrized by a negative scattering length $a$ obtained by extrapolating $u(r > R)$ to its $x$-axis intercept. This phase shift is maximized for $V_0 = V_c$ where $a$ diverges. After a bound state has formed $V_0 > V_c$, the node $u(r = a) = 0$ gives the scattering length. Note that $a$ indicates the size of the bound state and can be much larger than the potential range when $V_0$ is near $V_c$. A many-body system interacting by such two-body potentials has two distinct regimes. At $a < 0$, particles in the gas are weakly attractive while at $a > 0$, the two-particle bound states are weakly repulsive in the sense that the potential can be modeled as a repulsive
potential with scattering length $a > 0$. Note that a positive potential must have $a > 0$.

The range $B$ of applicability of Equation 3.4 and the accuracy of the “universal” bound state energy $E_{\text{res}} = \hbar^2 / 2m_r a^2$ distinguishes between wide and narrow Feshbach resonances. In this sense, a wide Feshbach resonance is universal over a large range of $B$ or $a$ and contributions from scattering states dominate contributions from closed states, i.e. second-order perturbation theory is sufficient to quantitatively capture the physics of the scattering states. Near a wide resonance the molecules cannot be treated as distinct entities and the entire system must be treated within a single channel approach. On the other hand, near a narrow resonance the system the hybridization of the scattering states with the bound state is not well approximated by second-order perturbation theory. In this case, the mixture is well-described by a coupled channel theory with distinct atomic and molecular populations. In our treatment of the Bose-Fermi mixture, we focus on wide Feshbach resonances and use the inverse-cosh potential that has been successfully applied to the two fermion species BEC-BCS crossover [140, 141, 142, 143].

Experiments have identified many boson-fermion interspecies Feshbach resonances that are both wide and narrow, and have cooled Bose-Fermi mixtures to degeneracy temperatures. Very recently, ultracold mixtures of $^{23}\text{Na}^{40}\text{K}$ [110], $^{23}\text{Na}^{6}\text{Li}$ [111] and $^{87}\text{Rb}^{40}\text{K}$ [112] have been realized and several have been cooled to quantum degeneracy temperatures [10, 113, 114]. What is exciting about these mixtures is their relative stability near at least some Feshbach resonances (about 100ms for $^{23}\text{Na}^{40}\text{K}$ mixture [110]). This timescale should be long enough for equilibration and thereby enable detailed experimental studies of the many-body physics investigated below.

### 3.3 Wave Function Selection

The building blocks of the wave functions we considered are boson-boson $f_{BB}$ and boson-fermion $f_{FB}$ Jastrow factors, a boson-fermion pairing function $\varphi$ and a Slater determinant of the fermions coupled to plane waves with momenta $k$ from 0 to $k_F$. The Jastrow factors implement the correct short-range boson-boson and boson-fermion correlations and are
obtained with the lowest order constrained variational (LOCV) method with no externally adjustable parameters (see Appendix C for details and Figure 3.2(b)) [140]. We include the long-range boson-fermion correlations through the exact two-body bound state $\varphi^{2B}$ and through a variational form $\varphi^{var}$ in the wave functions $\Psi^{2B}$ and $\Psi^{var}$, respectively.

Significant depletion of the condensate requires an exponentially decaying pair function $\varphi$. A basic Slater-Jastrow wave function of the form

$$\Psi(\{x_i\}, \{y_j\}) = \prod_{ij} f_{FB}(x_i - y_j) \prod_{j<j'} f_{BB}(y_j - y_{j'}) \times \exp(ix_i \cdot k_j).$$

(3.7)

with Slater determinant $\ldots$ and short range boson-boson-fermion correlations built in through the $f_{FB}$ Jastrow term is insufficient to destroy the condensate. Even at $\zeta = 10$, the condensate fraction $n_0 \approx 0.6$. The boson-fermion paired state must decay exponentially at large separation to destroy the condensate, as is characteristic of bound states.

### 3.3.1 The Wave Function $\Psi^{2B}$

We began our investigations with the four-parameter wave function $\Psi^{var}$ [see next section] but discovered that the no-parameter wave function $\Psi^{2B}$ has similarly low energy in the $\zeta > 0$ regime. For clarity, we first describe $\Psi^{2B}$ and the long-range boson-fermion correlations built into it. The wave function is

$$\Psi^{2B}(\{x_i\}, \{y_j\}) = \prod_{j<j'} f_{BB}(y_j - y_{j'}) \times \left\| \varphi^{2B}(x_i) \exp(ix_i \cdot k_j) \right\|. (3.8)$$

This wave function form is symmetric and antisymmetric with respect to interchange of bosons and fermions, respectively. The last factor is modified from the usual Slater determinant by the pairing function $\varphi^{2B}(x)$ which is symmetric with respect to interchange of bosons. We give it the form

$$\varphi^{2B}(x) = \frac{1}{\sqrt{N_B}} \sum_j \varphi^{2B}(x - y_j),$$

(3.9)

where $\varphi^{2B}$ are the exact two-body bound states of the reparametrized inverse-cosh potential $v(r) = -(\hbar^2/2m_r)\alpha^2 \Lambda(\Lambda - 1)/\cosh^2(\alpha r)$ that models the boson-fermion interaction. These
Figure 3.2: Short range correlations in the wave function. (a) The exact two-body $\varphi^2_B(r)$ exhibits strong positive correlations at short distances and decays as $e^{-r/r}$ at large distances, with the decay rate increasing with $\zeta$. (b) The Jastrow factor $f_{FB}$ is indistinguishable from $\varphi^2_B(r)$ at short distance but asymptotes to 1 beyond the healing length that is self-consistently calculated via LOCV.

states are plotted in Figure 3.2(a) and given in terms of the hypergeometric function

$$\varphi^2_B(r) = \frac{(\cosh(\alpha r))^{2-\Lambda}}{\alpha r} _2 F_1 \left(2\Lambda - 2, -1, \Lambda - 1, \frac{1}{1 + e^{2\alpha r}}\right).$$

(3.10)

The pair function $\varphi^2_B$ includes both short and long range correlations. The absence of the Jastrow $f_{FB}$ is explained as follows in the strong coupling regime: either a boson and a fermion are close together, a situation favored by both $f_{FB}$ and $\varphi^2_B$, or they are far apart. The latter case corresponds to a boson and a fermion that are paired but not with each other. Both $f_{FB}$ and $\varphi^2_B$ treat those particles as not interacting with each other – they contribute no amplitude to the wave function. The primary difference is that only $\varphi^2_B$ imposes a severe penalty on a configuration where a fermion is not near any boson.

### 3.3.2 The Variational Wave Function $\Psi^{\var}$

We also consider the wave function $\Psi^{\var}$ because the wave function $\Psi^{2B}$ has a couple drawbacks. First, $\varphi^{2B}$ cannot be constructed for $\zeta \leq 0$ where there is no 2-body bound state, and second, $\Psi^{2B}$ has no variational parameters so its merit as a many-body state is unclear. In the variational wave function, we construct $\varphi^{\var}$ to tune the long-range correlations and include the short-range correlations of $f_{FB}$ because they should remain
accurate in the many-body system.

\[
\Psi^\text{var}(\{x_i\}, \{y_j\}) = \prod_{ij} f_{FB}(x_i - y_j) \prod_{j < j'} f_{BB}(y_j - y_{j'}) \times \left\| \phi^\text{var}(x_i) \exp(ik_i \cdot k_j) \right\| \tag{3.11}
\]

To preserve the short-range correlations we require \( \varphi^\text{var}(r) \to 1 \) for \( r \ll d \), where \( d \) is the LOCV healing length. We consider the parameterization

\[
\varphi^\text{var}(r) = \frac{1 + e^{-d/w_1}}{1 + e^{(r-d)/w_1}} \left( \frac{1}{1 + (r/w_2)^{1/p}} \right)^p \tag{3.12}
\]

With suitable choice of the four variational parameters \( \{d, w_1, w_2, p\} \), one can easily reproduce both weak and strong coupling limits. \( \varphi^\text{var}(r \ll d) \) minimally modifies the 2-body correlations while \( \varphi^\text{var}(r \gg d) \) can be constant (\( \zeta \to -\infty \)) or decay as \( \exp(-r/a_{BF})/r \) (\( \zeta \to \infty \)). Several representative curves for the optimized \( \varphi^\text{var}(r) \) are plotted in Figure 3.3 for various values of \( \zeta = 1/k_F a_{FB} \). The parameters were optimized by the variance minimization technique discussed in Section 4.1.2 and in References [144, 145]. We considered several other forms for \( \varphi^\text{var} \), including a decomposition into Fourier coefficients and into real-space splines, but the number of parameters required to satisfactorily obtain an exponentially decay in the long-distance tail was prohibitively large.

### 3.3.3 Comments on the Wave Function Form

This generic wave function form reduces to the expected form in both the non-interacting limit \( \zeta \to -\infty \) and the molecular limit \( \zeta \to \infty \). In the limit \( \zeta \to -\infty \), the functions \( f_{FB}, \varphi^\text{var} \) and \( \varphi^{2B} \) reduce to a constant so that each of \( \Psi^{2B} \) and \( \Psi^\text{var} \) become the wave function of a Bose condensate modified by the boson-boson interaction and decoupled from a non-interacting Fermi sea described by the Slater determinant. Note that \( \Psi^\text{var} \) has a lower energy than \( \Psi^{2B} \) for \( \zeta \leq 0 \) because only \( \varphi^\text{var} \) includes short range correlations. On
Figure 3.3: (a) The form of the variational wave function $\varphi_{\text{var}}(r)$ with (b) optimized parameters for a few selected values of $\zeta = 1/k_Fa_{FB}$. In the weak coupling limit $\zeta = -10$, the function is essentially constant ($\varphi_{\text{var}}(r) = 1$) and the wave function Equation 3.11 reduces to that of a non-interacting Fermi sea uncoupled from a BEC, as expected. In the strong coupling limit, the short-range value remains at $\varphi_{\text{var}}(r \to 0) = 1$ while $\varphi_{\text{var}}(r \to \infty) = e^{-r/w_1}/r$ decays like a bound state.

the other hand, when $\zeta \to \infty$, we can write

$$
\phi^{2B}(x_i) \exp(i k \cdot x_i)
= \sum_j \sum_q \phi_q^{2B} \exp(i q \cdot (x_i - y_j)) \exp(i k \cdot x_i)
= \sum_j \left[ \sum_q \phi_q^{2B} \exp\left(i \left(q + \frac{k}{2}\right) \cdot (x_i - y_j)\right) \right] \exp(i k \cdot \frac{x_i + y_j}{2})
$$

In the molecular limit, $\phi^{2B}(r)$ is short-ranged ($\sim a_{FB}$) and as a result, its Fourier transform is flat for $|k| \ll a_{FB}^{-1}$, which means that $\phi_q^{2B} \approx \phi_{q+k/2}^{2B}$ and the sum over $q$ in the square bracket simply reproduces the two-body wave function. The last factor gives the center of mass momentum of the fermonic molecules which fill up to $k_F$ as we expect on physical grounds. In the expansion of the Slater determinant, there are terms corresponding to a fermion which bonds with multiple bosons but these terms are strongly suppressed due to the strong boson-boson repulsion.

There are three length scale regimes in this simulation. The miniscule length scale is the
range of the potential and is on the order of \(0.02k_F^{-1}\). This scale is smaller than all others in this system. Small and large length scales are defined relative to \(k_F^{-1}\), to the LOCV healing length \(d\) or to the interparticle spacing. These length scales are all approximately \(k_F^{-1}\). Miniscule distances are on the scale of the potential range. Small length scales are larger than the potential range but less than the interparticle spacing and, for example, includes the molecule size at moderately strong coupling. Long-range effects occur on length scales at least as larger as the interparticle spacing.

### 3.4 Characterizing the Phase Transition Using VMC

We now present our results using the variational quantum Monte Carlo (VMC) zero temperature algorithm, based on the wave function of Equation (3.8) with \(N_B = N_F = 33\) particles. Throughout the computation, we fix \(k_F a_{BB} = 0.8\) and set \(\lambda = m_B/m_F = 0.575\). The basic picture from VMC simulations is summed up in Figure 3.4. At weak coupling, the system consists of a free Fermi gas with a perfect Fermi surface and a BEC slightly depleted by the hard core boson-boson repulsion. At strong coupling beyond \(\zeta_{c2}\), all fermions and boson pair into composite fermion molecules and create a Fermi surface. At intermediate couplings \(\zeta_{c1} < \zeta < \zeta_{c2}\), the atomic Fermi surface has been destroyed while a small but finite condensate fraction \(n_0 \sim 0.05 - 0.1\) persists. The condensate exists because of the tendency for two fermions to interact with a single boson that frees the excess boson to condense. The basic picture for the atomic species is built from momentum distribution calculations. The evidence for fermion-fermion-boson trimer-like states comes from pair correlation functions. After discussing these observables, we conclude with estimates of the energy and of the chemical potential, and some observations concerning the finite range of the boson-fermion potential and other possible trial wave functions.

#### 3.4.1 The Momentum Distribution

To locate the quantum phase transitions through quasi-particle weight \(Z_A\) and condensate fraction \(n_0\), we calculated the momentum distribution \(n_F(k)\) or \(n_B(k)\) of the atomic
Figure 3.4: (a) Schematic of the phases observed in this chapter. In addition to the expected noninteracting and fully paired limits at $\zeta \equiv 1/k_F a_{FB} \to \mp \infty$, we observe a state with no atomic Fermi surface and a finite but depleted BEC. In the latter state we find evidence of a three-body bound state or resonance, which has been shown to occur in few-body calculations [146, 147]. (b) VMC results: fermion momentum distribution $n_F(k)$ with the atomic quasiparticle weight $Z_A$. Each $n_F(k)$ is offset by 1 and labeled by the coupling $\zeta$. (c) Condensate fraction $n_0$ and $Z_A$ decrease as $\zeta$ increases with most change occurring beyond unitarity ($\zeta = 0$). $Z_A$ vanishes at a critical coupling $\zeta_{c1} \approx 2.0$ while an intermediate phase with finite $n_0$ exists between $\zeta_{c1}$ and $\zeta_{c2} \approx 10.0$.

fermions and bosons by Fourier transforming the single particle density matrix $\rho(x, x') = \langle \hat{a}_\sigma^\dagger(x) \hat{a}_\sigma(x') \rangle$ with respect to $x - x'$, where $\hat{a}_\sigma$ is the species-appropriate annihilation operator ($\sigma = \text{B,F}$). At weak coupling the Fermi surface is essentially intact and the jump $Z_A$ at $k_F$ is near unity while $n_0 = n_B(k = 0)/N_B$ is reduced from unity to about 0.95 by the hardcore repulsion. As we increase $\zeta$, $Z_A$ decreases rapidly between $0 < \zeta < 2$ and terminates at a critical point $\zeta_{c1} \approx 2.0$ (see Figure3.4(b,c)). We find the condensate fraction $n_0$ tracks the quasi-particle residue $Z_A$ for $\zeta < \zeta_{c1}$, but for $\zeta > \zeta_{c1}$, $n_0$ remains finite and slowly decays toward zero as $\zeta$ increases, becoming negligible for $\zeta_{c2} \approx 10$ which we identify as a second quantum critical point.
Figure 3.5: (a) The boson-boson pair distribution function $g_{BB}(r)$ defined in Equation 3.14 shows a sharp bosonic enhancement just beyond $a_{BB} = 0.8$ at $\zeta = 0$. At larger $\zeta$ the pair correlations are suppressed as the bosons pair with fermions and form a composite molecule Fermi surface. (b) The fermion-boson pair distribution exhibits a sharp enhancement at short distances at all $\zeta$ from the attractive $v(r)$ potential. (c) The fermion-fermion pair distribution follows the expected free fermion distribution at small $\zeta$. Unexpectedly, at large $\zeta$ a significant weight is observed at small separations.

3.4.2 The Pair Distribution Function

We reveal the nature of the intermediate $\zeta_{c1} < \zeta < \zeta_{c2}$ state through atom-atom and molecule-atom pair correlation functions

$$g_{\sigma\sigma'}(r) = \frac{\langle n_{\sigma}(r)n_{\sigma'}(0) \rangle}{\langle n_{\sigma} \rangle \langle n_{\sigma'} \rangle}, \quad (3.14)$$

where $\sigma, \sigma' = B, F, M$, a boson-fermion molecule. The atomic $g(r)$ are shown in Figure 3.5 for several $\zeta$. The $g_{\sigma,\sigma'}(r)$ is the probability to find a $\sigma$ particle a distance $r$ away from a $\sigma'$ particle, relative to the probability of finding a $\sigma$ particle infinitely far away from a $\sigma'$. The boson-boson pair correlation function $g_{BB}(r)$ is zero for $r < a_{BB}$ and at weak coupling, a peak is observed at short distances resulting from boson enhancement or statistics which has been observed in other hard core boson systems. At strong coupling, the short range correlations are significantly suppressed as would be expected if the bosons were pairing.
Figure 3.6: (a) The fermion-boson pair distribution function $g_{FB}(r)$ defined in Equation 3.14 shows weak correlations at $\zeta \ll 0$ which grow as $\zeta$ increases and the boson-fermion two-body bound state becomes more localized. (b) $N_{FB}(r)$ (Equation 3.15) is the average number of bosons (fermions) within a distance $r$ of a fermion (boson). It grows like $r^3$ at $\zeta = -10$ but at $\zeta \geq \zeta_{c1}$ it shows a quick rise to 1 followed by a plateau with no other particles at larger $r$. (c) We estimate the maximal molecule size $r_M$ by $N_{FB}(r_M) = 0.99$ and estimate the minimum distance $r_M^*$ to another molecule by $N_{FB}(r_M^*) = 1.01$. (d) The fermion-molecule $g_{FM}(r)$. (e) The probability $N_{FM}(r_M)$ that a fermion is a distance $r \leq r_M$ from a boson-fermion molecule. This agrees with $n_0$ for $\zeta > \zeta_{c1}$.

with fermions to form a weakly interacting composite-fermion gas with a molecular size smaller than the interparticle spacing. The basic behavior of the fermion-boson pair correlations is as expected: as the attractive potential $v(r)$ deepens and $\zeta$ increases, the short range correlations are enhanced. At large $\zeta$, the boson-fermion pair grows smaller than the interparticle spacing and a trough is observed near $k_{FR} \sim 0.8$. This is consistent with the existence of well-separated molecules, with the trough exacerbated by the hard core boson-boson repulsion. For all distances at weak coupling and at large distance for $\zeta > \zeta_{c1}$, the fermion-fermion $g_{FF}(r)$ conforms to expected behavior, while for $\zeta > \zeta_{c1}$, $g_{FF}(r)$ is unexpectedly enhanced at short distance. This suggests an effective attractive fermion-fermion interaction mediated by the bosons.

The size of the molecules and the relationship between boson-fermion-fermion (FFB)
trimer state and the existence of a finite $n_0$ can be quantitatively analyzed using $g_{FB}$ and $g_{FM}$ [see Figure 3.6]. We define the average number of $\sigma$ particles within a distance $r$ of a $\sigma'$ particle by

$$N_{\sigma\sigma'}(r) = \langle n \rangle \int_0^r g_{\sigma\sigma'}(r')d^3r'.$$  \hspace{1cm} (3.15)

We estimate the molecule size $r_M$ (a function of $\zeta$) by demanding that $N_{FB}(r_M) = 1$ or that, on average, there is one boson within a sphere of radius $r_M$ centered on a fermion. As expected, we find that $r_M$ decreases with $\zeta$ [see Figure 3.6(b,c)]. Note, however, that $r_M$ does not approach $a_{FB}/\sqrt{2}$ as expected for the average molecule size $\sqrt{\langle |r|^2 \rangle}$ because $r_M$ is an estimate of the maximum separation between the two atoms in a molecule. This estimate makes sense in the strong coupling regime, but is a fuzzy measure when the molecule size is on the order of the interparticle spacing. Nonetheless, the agreement between $r_M$ and $r_M^*$ (defined by $N_{FB}(r_M) = 0.99$ and $N_{FB}(r_M^*) = 1.01$, see Figure 3.6(c)) indicates that molecules have not become localized objects for $\zeta < \zeta_{c1}$, while at larger $\zeta$ there is a clear distinction between a molecule and the rest of the gas.

Once the molecular size $r_M$ is fixed, we then use $g_{FM}$ [Figure 3.6(d)] to estimate the fraction of FFB trimer states by $N_{FM}(r_M)$. In other words, we estimate the probability of a three-body trimer state within the radius $r_M$. Shown in Figure 3.6(e), this fraction of trimer states agrees quantitatively with the condensate fraction $n_0$ at $\zeta > \zeta_{c1}$. We interpret this result as follows: at intermediate coupling, most bosons and fermions have formed distinct pairs so $N_{FM}(r_M)$ is small, but occasionally a single boson interacts with two fermions, which leaves the excess boson in the condensate. As $\zeta$ increases, it becomes more and more favorable for the system to be fully paired and therefore both $N_{FM}(r_M)$ and $n_0$ decreases.

### 3.4.3 Energy and Chemical Potential

The energy is a useful way to locate the weak coupling limit and to understand the finite range effects of the boson-fermion potential. In the weak coupling limit, the energy per particle is determined by the mean field shift for fermions and by the Lee-Huang-Yang corrections for hard sphere bosons [126]. In the strong coupling limit, the system is composed of molecu-
lar fermions and the energy per particle is given by $\epsilon_b/2 = 0.5[\epsilon_F/(1 + \lambda)](3/5 - (\zeta^{\text{eff}})^2(\lambda + 1)^2/\lambda)$. In this simulation, the finite range $R^*$ of the potential $v(r)$ and finite energy of the bound state become important at $\zeta \gtrsim 5$ and drives $\epsilon - \epsilon_b/2$ negative. We estimate the energy-dependent effective scattering length by fitting $\varphi^{2B}$ to the 3D bound state form $A e^{-r/a^{\text{eff}}}/r$ with effective scattering length $a^{\text{eff}} = 1/\zeta^{\text{eff}}$. The effective scattering length and modified bound state energy follows the expected form for a weakly bound molecular state [148]

$$\frac{1}{a^{\text{eff}}(\epsilon_b)} = \frac{1}{a^{\text{bare}}} + 2m_r R^* \epsilon_b$$

(3.16)

In Figure 3.7(a), we compare to $\epsilon_b$ estimated from $\zeta^{\text{eff}}$ to the energy per particle $\epsilon$ from VMC. The molecules are identical composite fermions, so there is no $s$-wave interaction between them and we expect only weak molecule-molecule interactions.

The chemical potential is formally defined as

$$\mu_F = \frac{\partial E}{\partial N_F}, \quad \mu_B = \frac{\partial E}{\partial N_B}, \quad \mu_M = \frac{\partial E}{\partial N_M}$$

(3.17)

where $E$ is the total energy of the system. These are estimated for a system with $N_\sigma$
particles by taking the difference between the total energy of a system with \( N_\sigma + 1 \) and \( N_\sigma - 1 \) particles, so \( \mu_\sigma \) has a relatively large error bar. First consider the atomic chemical potentials \( \mu_F \) and \( \mu_B \). In the VMC simulation these are calculated by explicitly adding or removing a particle, measuring the energy difference and dividing by the difference in particle number. This works well for \( \zeta \to -\infty \), where \( \mu_F \to 3\epsilon_F/5 \), but fails for \( \zeta \gtrsim 0 \) for both atomic species. To understand why, consider the three possible VMC simulation cases illustrated in Figure 3.8: (1) a system with one excess fermion, (2) a system with equal numbers of bosons and fermions, (3) a system with one excess boson. A reasonable estimate for \( \mu_B \) or \( \mu_F \) requires a VMC simulation within both (1) and (3). For illustrative purposes in the strongly coupled regime, we assume an excess boson disappears into the condensate with no contribution to the energy while an excess fermion hybridizes with a boson-fermion pair with an energy \( \epsilon_{FFB} \). All other boson-fermion pairs then contribute the standard \( -\epsilon_b \). If the excess fermion simply occupies the lowest \( k \) states\(^5\) the energy \( \epsilon_{FFB} \) should approach \( -\epsilon_b \) (the original boson-fermion pair plus a low-energy atomic fermion) and so we expect \( \mu_F = \mu_B = \mu_M/2 = -\epsilon_b/2 \). However, the VMC simulation obtains \( \epsilon_{FFB} \approx 2\epsilon_b \) from \( \mu_B \approx -2\epsilon_b \) and \( \mu_F \approx \epsilon_b \). We will discuss in the next subsection why the wave function gives fermion-fermion-boson hybrid states such large weight in polarized systems such as (1) and (3).

The molecule chemical potential \( \mu_M \) is better behaved. Addition or subtraction of a molecule maintains equal numbers of bosons and fermions, so there are no excess particles of either species. Simple extrapolation from the schematic Figure 3.8 reveals that \( \mu_M = -\epsilon_b \) in the strong coupling limit. Shown in Figure 3.7(b), VMC simulations only qualitatively agrees with this expectation; the measured \( \mu_M \) is consistently higher than \(-\epsilon_b \). The higher than expected values of \( \epsilon \) and \( \mu_M \) indicate a combination of shortcomings in the wave function and relatively large molecule-molecule interactions.

\(^5\)All paired fermions are very localized in real space, so they must occupy the atomic \( k \) states relatively uniformly. This should allow the excess atomic fermion to occupy \( k < k_F \) states.
Figure 3.8: Energy accounting in the strongly coupled limit for chemical potential calculations. Small vertical dots indicate molecule pairs whose energies are presumably not affected by adding or removing a single particle. \( \epsilon_b \) is the magnitude of the boson-fermion bound state energy and \( \epsilon_{FFB} \) represents the energy of an excess fermion interacting with a boson-fermion bound state. The \( \mu^{\text{Both}}_{B(F)} \) is the appropriate add one and remove one red boson (blue fermion) method to estimate the atomic \( \mu \).

**Limitations on \( \mu_B \) and \( \mu_F \) imposed by the wave function**

We now discuss what role the wave function plays in the defective atomic chemical potential behavior and two ways to counter it. Recall that the wave function

\[
\Psi^{2B} = \prod f_{BB} \left\| \sum_{i'} \varphi^{2B}_{i'j} e^{i r_j k_i} \right\|
\]

(3.18) exponentially localizes every fermion be near some boson as \( \zeta \to \infty \). In that regime and for \( N_B = N_F \), we expect this wave function to successfully describe a gas of composite fermion molecules, each made up of one boson and one fermion, and bound together with a pairing wave function \( \varphi^{2B}(r) \). An excess fermion, however, is also constrained to be near to a boson, which forces the creation of a boson-fermion-fermion trimer. This clearly contrasts with the expected behavior of an excess fermion, which should occupy low-momentum states and more-or-less ignore the bosons. Note that an excess boson does not raise the energy significantly. \( \Psi^{2B} \) does enforce positive correlations with fermions but the extra boson is not strongly penalized if it delocalizes and joins the condensate.

A modification to the wave function might permit better estimates of \( \mu_F \) and \( \mu_B \) if it
enabled the excess fermion to interact minimally with the bosons. One possible form is

$$Ψ^{2B} = \prod f_{BB} \sum_{φ^0 \text{ row}} \begin{vmatrix}
\sum_{i'} φ^0_{i'1} e^{ir_1 k_1} & \sum_{i'} φ^0_{i'1} e^{ir_1 k_2} & \cdots & \sum_{i'} φ^0_{i'1} e^{ir_1 k_{N_F}} \\
\sum_{i'} φ^1_{i'2} e^{ir_2 k_1} & \sum_{i'} φ^2B_{i'2} e^{ir_2 k_2} & \cdots & \sum_{i'} φ^2B_{i'2} e^{ir_2 k_{N_F}} \\
\vdots & \vdots & \ddots & \vdots \\
\sum_{i'} φ^0_{i'N_F} e^{ir_{N_F} k_1} & \sum_{i'} φ^{2B}_{i'N_F} e^{ir_{N_F} k_2} & \cdots & \sum_{i'} φ^{2B}_{i'N_F} e^{ir_{N_F} k_{N_F}}
\end{vmatrix}$$

(3.19)

where $φ^0$ could be either constant or the boson-fermion Jastrow factor calculated from LOCV. This wave function would satisfy the atomic fermion statistics but only impose, at most, short range correlations between the excess fermion and the bosons.

### 3.4.4 The Effects of Potential Range and the Molecular Fermi Surface

We have also attempted to characterize the response of the system to the finite range of the boson-fermion potential $R^*$ and to roughly estimate the quasiparticle weight $Z_M$ of the molecular Fermi surface. As noted above, $R^*$ is large enough that at $ζ = 10$, the energy effective $a^{\text{eff}}_{FB}$ is significantly smaller than the zero-energy scattering length. Clearly, the effect will increase as $R^*$ increases. We investigate the impact on our results by examining $n_0$ and $Z_A$ for several different $R^*$ with optimized $Ψ^{\text{var}}$ in Figure 3.9(a,b). The only differences we observe are in the parameter regime near $ζ = 2$, where for $Ψ^{\text{var}}$, small $R^*$ appears to stabilize the Fermi surface and the condensate. This difference may be a sign that the $f_{FB}$ term is introducing some defect into the wave function or that as $R^*$ decreases, the variational parameter governing the width of the region with $~1$ weight near $r = 0$ is difficult to optimize. Because the energy of $Ψ^{2B}$ and $Ψ^{\text{var}}$ are so similar, another possibility is that the discrepancy in $n_0$ and $Z_A$ indicates that a completely different wave function would work best in the intermediate coupling regime, such as a boson-mediated $p$–wave fermion superfluid. Either way, we remind the reader that both $Ψ^{2B}$ and $Ψ^{\text{var}}$ have approximately the same energy over all $ζ > 0$ for $R^*k_F = 0.02$ as shown in Figure 3.7(a).

We conclude this discussion of VMC results with a rough estimate of the quasiparticle weight $Z_M$ of the molecular Fermi surface. Ideally, one would simultaneously track the suppression of $Z_A$ and the emergence of a molecular quasi-particle residue $Z_M$. Unfortunately,
it is difficult to formulate a precise definition of the molecular momentum distribution $n_M(k)$ because of the inherent ambiguity of a molecular state in this single-channel model. But note that the molecule size is very small for $\zeta \gg \zeta_{c1}$, so the composite nature of the molecule becomes irrelevant and a standard Fermi surface should result. To estimate $n_M(k)$, we calculate the two-body density matrix

$$
\rho_{FB}(x, x', \delta) \equiv \left\langle f^\dagger(x)b(x + \delta)b(x' + \delta)f(x') \right\rangle - n_0\langle f^\dagger(x)f(x')\rangle
$$

(3.20)

where $\delta$ is a fixed vector and $f(x)$ and $b(y)$ are destruction operators for a fermion at $x$ and a boson at $y$. The latter term removes the extraneous contribution from the condensate. To extract $n_M(k)$, we note that in the strong coupling limit, unless $\delta$ is within the molecular size, $\tilde{\rho}_{FB}(x, x', \delta)$ will be essentially zero. Furthermore, since the molecules must have $s$-wave character, we average over both the direction and length of $\delta$ to obtain an approximate definition for the one-body density matrix of the composite molecules $\rho_M(x, x') \equiv \int_0^{\delta_c} \tilde{\rho}_{FB}(x, x', |\delta|)\delta^2d\delta$, where the cutoff $\delta_c$ satisfies $k_F^{-1} > \delta_c > a_{FB}$. The Fourier transform of $\rho_M(x, x')$ with respect to the distance $x - x'$ then gives the momentum distribution $n_M(k)$ of the fermionic molecules and the jump $Z_M$ at $k_F$.

Figure 3.9: (a-c) The condensate fraction $n_0$, atomic quasiparticle weight $Z_A$ and molecular quasiparticle weight $Z_M$ for several effective potential lengths $R^*$. The error for $Z_M$ larger than the error for $n_0$ and $Z_A$ because it results from a four-body, rather than a two-body, correlator. The previous $\Psi^{\text{var}}$ and the $\Psi^{2\text{B}}$ results are at $R^*k_F = 0.02$. 
Along with \( N_{FB}(r) \), the jump at \( n_{M}(k_F) \) is the most direct evidence for composite molecules and a molecular Fermi surface at large \( \zeta \). As shown in Figure 3.9(c), \( Z_M \) increases from near zero at unitarity to about 0.7 near \( \zeta_{c1} \). Then it gradually approaches 1 as \( \zeta \) increases. This behavior appears to be almost independent of \( R^* \).

### 3.5 Diffusion Monte Carlo Results

Diffusion Monte Carlo (DMC) projects a trial wave function \( \Psi_T \) onto the ground state \( \Phi_0 \) and enables the ground state properties to be measured. An initial configuration obtained from \( \Psi_T \) is time evolved by the standard operator \( e^{-t(H-E_T)} \) for a time \( t \). After some time \( t \) and given a trial energy \( E_T \leq E_0 \), all excited states are exponentially suppressed and configurations should be distributed according to \( \Phi_0 \). For technical reasons reviewed in Section 4.2, the system is time-evolved using a very small time step \( dt \). We are currently applying DMC to this Bose-Fermi mixture, with \( \Psi^{2B} \) as \( \Psi_T \), but have not yet obtained results.

We expect to confirm several features of the VMC results using DMC estimators. The most important is the energy, which can be estimated directly (without a mixed estimator). We expect the DMC and VMC energy estimates to agree best in the weakly and in the strongly interacting regimes and to disagree significantly in the intermediate \( \zeta \sim \zeta_{c1} \) regime. The mixed estimator for all other quantities, like \( g_{\sigma\sigma'}(r) \) and \( n_\sigma(k) \), incurs error on the scale of \( O\left(|(\Psi^{2B} - \Phi_0)|^2\right) \). We expect our trial wave function to work well in the \( \zeta \rightarrow \pm \infty \) limits and to agree with the VMC results. We expect that the DMC mixed estimator will confirm the persistence of a condensate and add support for fermion-fermion-boson trimer states or correlations.

### 3.6 Conclusions and Outlook

We find two quantum phase transitions in a Bose-Fermi mixture with equal population within a VMC calculation. The first is associated with the destruction of the atomic Fermi surface at \( \zeta_{c1} \approx 2 \) and the second with the destruction of the BEC at \( \zeta_{c2} \approx 10 \). For \( \zeta_{c1} < \zeta < \)
$\zeta_{c2}$, the system exhibits strong trimer correlations even though there are no such correlations in the trial wave functions, reminiscent of results from few-body studies [146, 147]. A rough estimator for the molecular momentum distribution indicates that a molecular Fermi sea forms near $\zeta_{c1}$. Our results are directly applicable to $^{23}\text{Na}-^{40}\text{K}$ mixtures. The large magnitude of the boson-boson repulsion may be difficult to achieve in concert with $\zeta$, but a smaller boson-boson repulsion should be sufficient so long as the bosonic system retains mechanical stability. We also found that the potential’s range has little effect on the boson and fermion momentum distributions beyond changing $\zeta_{\text{eff}}$ and slightly moving $\zeta_{c1}$.

A few-body calculation with smaller mass ratio (in our case, around $m_F/m_B \approx 2$) should be useful for characterizing the intermediate phase and establishing any three-body correlations at the few body level. To distinguish these phases experimentally, it would be desirable to measure the condensate density $n_0$ as a function of $\zeta$ by performing time-of-flight imaging. $Z_A$ is much harder to measure, however, momentum resolved radio-frequency spectroscopy on the fermions could ascertain whether $n(k)$ is consistent with the Landau Fermi liquid behavior and would provide strong evidence for the first transition at $\zeta_{c1}$.

Future investigations should explore whether these emergent attractive interactions between fermions could destabilize the Fermi surface and generate a $p$-wave superfluid from the atomic fermions at intermediate coupling. An investigation over a broad range of mass ratios would also help to connect with limiting cases and other theoretical few- and many-body results. It would also be interesting to investigate polarized systems with more bosons than fermions, or vice versa, and observe the effect on $n_0$, $Z_A$ and on trimer correlations. From a numerical perspective, the crowning achievement would be finite-size scaling of DMC and mixed estimator results to precisely identify the nature of the quantum critical points $\zeta_{c1}$ and $\zeta_{c2}$ that we identified here.
Chapter 4

Numerical Methods

It is often the case that a system’s exact eigenstates, correlations or response functions cannot be analytically evaluated, so information must be sought through approximate and/or numerical means. Small-scale exact diagonalization, perturbative expansion and mean field theories are some approaches. This chapter outlines the primary numerical techniques employed in this thesis, which are all based on the Monte Carlo method of evaluating high-dimensional integrals. First we consider the zero temperature limit, where the variational and diffusion Monte Carlo methods are used to evaluate the energy and other observables of a trial ground state wave function. At finite temperatures, we turn to the world-line directed loop class of algorithms. Each algorithm is a type of quantum Monte Carlo (QMC) because each is based on the principles of quantum mechanics for zero and for finite temperatures, respectively.\(^6\)

The Monte Carlo methods employed here exemplify two paradigms in simulations of many-body quantum mechanics. The world-line type of QMC is formulated directly from the Hamiltonian at finite temperatures and is capable of simulating \(10^6\) atoms on \(64^3\) lattice sites – equivalent in size to many cold atom experiments. The results are exact aside from statistical variations and the zero temperature limit can be reached via extrapolation. World-line algorithm cannot be applied to the Bose-Fermi mixture, in general, because of the fermion sign problem that prevents formulation of an \textit{ab initio} positive definite probability distribution to sample in QMC. Instead, we resort to the approximate variational and

\(^6\)See Appendix D for a partial list of variables and their definitions used in this chapter.
diffusion QMC methods that are restricted to zero temperature. The purpose of the former
algorithm is to minimize the energy and evaluate the observables of a trial many-body wave
function, which serves as the probability distribution. Diffusion or projection QMC starts
with a sample set of configurations from variational QMC and projects to the ground state
by repeated application of a Green-function type propagator and guided by the variational
trial wave function.

4.1 Variational Monte Carlo

All the equilibrium properties of a system at zero temperature, such as the energy and the
momentum distribution, are entirely described by the ground state wave function. But the
ground state itself is usually unknown, so a physicist can only propose trial wave functions and
discriminate among them by each one’s energy (lowest is best). However, even extracting the
expectation value of an observable \( \langle \hat{O} \rangle \) from a correlated many-body state \( \Psi \) is extremely
difficult because it corresponds to evaluating the \( dN \)-dimensional integral

\[
\langle \hat{O} \rangle = \int \prod_{i=1}^{N} dr_i \Psi(r_1, \ldots, r_N) \hat{O} \Psi^\dagger(r_1, \ldots, r_N)
\]  

(4.1)

where \( N \) is the number of particles. The process whereby wave functions are optimized and
observables are estimated is known as variational Monte Carlo (VMC). The energy estimator
identifies the best trial wave function or trial wave function parameters because the energy
is bounded from below by the ground state energy. Strategies to optimize the parameters
of a trial wave function include energy variance minimization, steepest descent, conjugate
gradient and parallel tempering Monte Carlo. The formalism of VMC is outlined below
and details of its implementation for the Bose-Fermi mixture follow [Chapter 3 discusses
the results].

The modulus square of a trial wave function \( |\Psi|^2 \) defines a probability distribution over
the set of particle coordinates \( \{r_1, \ldots, r_N\} \). The goal of VMC is to efficiently and ergodically
sample the particle configurations \( \{r_1, \ldots, r_N\} \) from that probability distribution \( |\Psi|^2 \) and
thereby estimate an observable

\[
\left\langle \hat{O} \right\rangle = \int \prod_{i=1}^{N} dr_i |\Psi(r_1, \ldots, r_N)|^2 \frac{\hat{O}\Psi(r_1, \ldots, r_N)}{\Psi(r_1, \ldots, r_N)}.
\]

(4.2)

Equation 4.1 is rewritten here to emphasize that \( \left\langle \hat{O} \right\rangle \) is an expectation value with respect to \( |\Psi|^2 \). When \( \hat{O} = \hat{H} \), the resulting quantity

\[
E_L \equiv \frac{\hat{H}\Psi}{\Psi}
\]

(4.3)

is called the local energy.

There are many numerical methods to estimate the value of an integral but only Monte Carlo is capable of evaluating an integral like Equation 4.2. Methods like Simpson’s rule and Gaussian quadrature work very well in small dimensional systems but fail in the many-body, \( d^N \) dimensional space we consider. Part of the problem is that wave functions tend to be sharply peaked, which drives up the computational cost of such methods. The primary obstacle is the large number of dimensions; sampling the integrand in each volume element in large dimensional space is simply not feasible [149]. For example, if we are to sample just 10 points along each dimension in a 3D system with 20 particles, the number of points in the Simpson’s rule grid would be \( 10^6 \). A general rule of thumb is that Monte Carlo methods become more efficient when the integral encompasses more than 5-15 dimensions. Monte Carlo methods work better because they stochastically sample the integrand, or probability distribution, by choosing sample points according to the integrand’s weight and because the Monte Carlo error decreases as \( 1/\sqrt{\text{samplesize}} \) whereas the error associated with quadrature methods grows with the dimension.

Efficient Monte Carlo sampling of \( |\Psi|^2 \) relies on the Metropolis algorithm. This method requires that given the probability of the current configuration \( P(X) = |\Psi(X)|^2 \), the probability \( \mathcal{T}(Y|X) \) to transition to configuration \( Y \) is equal to the probability to transition to configuration \( X \) given the probability of configuration \( Y \). This condition is known as detailed balance and written as

\[
\mathcal{T}(Y|X)P(X) = \mathcal{T}(X|Y)P(Y).
\]

(4.4)
The two hardest parts of a VMC simulation are the choice of the wave function [see Section 3.3] and efficient ways to generate and accept new, relatively independent configurations, subject to detailed balance [see Section 4.1.1].

Observables are relatively simple to calculate. Those diagonal in the particle number space, like density $\hat{n}$ or density-density correlations $\hat{n}(0)\hat{n}(\mathbf{r})$ are simple because the wave function weights in Equation 4.2 cancel. Estimating the kinetic energy is more computationally intensive because the ratios $(\nabla_{\mathbf{r}_i}\Psi)/\Psi$ and $(\nabla_{\mathbf{r}_i}^2\Psi)/\Psi$ must be explicitly calculated.

The momentum distribution is the Fourier transform of the single particle density matrix

$$
\left\langle \hat{a}^\dagger(\mathbf{r}_j)\hat{a}(\mathbf{r}_j') \right\rangle = \int \prod_{i \neq j}^N d\mathbf{r}_i |\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_j, \ldots, \mathbf{r}_N)|^2 \frac{\hat{O}\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_j', \ldots, \mathbf{r}_N)}{\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_j, \ldots, \mathbf{r}_N)} 
$$

where $\hat{a}(\mathbf{r}_j)$ and $\hat{a}^\dagger(\mathbf{r}_j)$ are annihilation and creation operators at position $\mathbf{r}_j$. Many general methods have been developed to make this process more efficient for fermionic wave functions with determinants, such as the matrix determinant lemma and the Sherman-Morrison formula [150, 151]. In the remainder of this section, we discuss the schemes to generate new configurations and to optimize the wave functions in the context of the Bose-Fermi mixture.

### 4.1.1 VMC Update Moves

The trick to VMC is ensuring that all of configuration space is efficiently sampled. In particular: (1) new configurations should be generated according to their weight ($|\Psi|^2$); (2) the method for generating new configurations should be able to move from a configuration to any other configuration (the ability to sample every configuration is called ergodicity) and (3) successive configurations should be as uncorrelated as possible to speed the convergence of each estimator. To ensure that an algorithm meets the first condition, every update in VMC should obey the (extended) detailed balance formula

$$
T(Y|X)P(X)G(Y|X) = T(X|Y)P(Y)G(X|Y) 
$$

where $G(Y|X)$ is the a priori probability to generate $Y$ given $X$. This ensures the simulation is updated according to the correct probability distribution even if a second distribution is
guiding the generation of proposed update steps.

The most basic update step is to generate a new configuration entirely from scratch. This is sometimes called a global update, but it is usually extremely inefficient. It involves moving every particle to a new, random position in the simulation cell and accepting the proposed configuration $Y$ according to the ratio of the proposed configuration’s weight $P(Y)$ to the current configuration’s weight $P(X)$. Global updates can work well in a weakly interacting system, but when particles become strongly correlated, most proposed configurations will be exceedingly unlikely and they will result in very slow Monte Carlo convergence of observables. The following three local updates move only one or two particles in an attempt to make the simulation more likely to generate probable and relatively independent configurations.

**Basic Single Particle Move** One of the simplest possible update schemes is to randomly select a particle and then to propose a move to a uniform-randomly selected point within a box of size $\ell^3$ centered on its previous position. Clearly, in any configuration $X$ the probability to select particle $i$ at $r_i^X$ and propose a new position $r_i^Y$ is $1/N$ and $1/\ell^3$, respectively. Thus, $G(Y|X) = G(X|Y) = 1/N\ell^3$ and the detailed balance equation reduces to Equation 4.4

$$
\frac{T(Y|X)}{T(X|Y)} = \frac{P(Y)}{P(X)} \equiv R. \tag{4.7}
$$

This is trivially satisfied by the choice

$$
T(Y|X) = 1 \quad \text{and} \quad T(X|Y) = R^{-1} \quad \text{if} \ R \geq 1
$$

$$
T(Y|X) = R^{-1} \quad \text{and} \quad T(X|Y) = 1 \quad \text{if} \ R \leq 1. \tag{4.8}
$$

This basic update is obviously ergodic in a weakly interacting gas of particles and will generate an independent configuration after $O(N)$ update steps if $\ell^3$ is on the order of the system size $L^3$. In the strongly interacting limit of the Bose-Fermi mixture, however, this update scheme fails to be ergodic and to generate independent configurations. As boson-fermion molecules form, the probability for a fermion to be far from a boson is strongly suppressed by $\Psi$ and proposed configurations using this update step with $\ell \sim L$ are very
rarely accepted. On the other hand, if $\ell \ll L$ new configurations are often accepted but successive configurations are highly correlated. To resolve this difficulty we introduced several additional update schemes.

**Boson-Fermion Paired Move** Single particle moves are not efficient at significantly changing a molecule’s center of mass position so a boson-fermion paired movement is introduced. In this move, a new configuration is proposed in the following manner. First, a randomly chosen fermion and the nearest boson to it are identified as a “pair.” Then a new position is chosen from within a box of size $\ell_p^3$ centered on the pair center and both the boson and fermion are translated that distance, maintaining the same relative positions. If this new configuration results in a different boson nearest to the translated fermion then the step cannot be immediately reversed because the same boson-fermion pair cannot be chosen. In this case, detailed balance is violated and the proposed configuration is automatically rejected. Because the boson choice is determined by the fermion choice, the probability to create the new configuration is $G(Y|X) = G(X|Y) = 1/N\ell_p^3$ and the probability to accept and reject the proposed configuration is identical in form to the single particle move. This move helps the simulation to explore the possible boson-fermion pair positions and to prevent “sticking” where all the pairs are effectively frozen in place.

**Gaussian Boson Move** The motivating principle of this update step is to try to move bosons and fermions closer together. A boson $i$ is uniform-randomly chosen, and a nearby fermion $j$ is chosen with probability $\frac{|r_i^X - r_j^X|^p}{\sum_j |r_i^X - r_j^X|^p}$. The boson’s new position is drawn from a 3D normal distribution centered at $r_j$ with the width $\sigma$ as a simulation parameter. Note that to respect the periodic boundary conditions, a maximum range of $k\sigma < L/2$ is imposed on $|r_i - r_j|$. For this update the probability to generate configuration $Y$ from $X$ is

$$G(Y|X) = \frac{1}{N_B \sum_j |r_i^X - r_j^X|^p} \frac{e^{-|r_i^Y - r_j^Y|^2/2\sigma^2}}{(\sqrt{2\pi}\sigma \text{ Erf}(k/\sqrt{2}))^3} \quad (4.9)$$
where \( r_i^Y \) is the coordinate of the \( i \)th particle in configuration \( Y \) and \( p < 0 \). This leads to

\[
\frac{T(Y|X)}{T(X|Y)} = \frac{P(Y)}{P(X)} \frac{\left| r_i^Y - r_j^Y \right|^p}{\sum_j \left| r_i^Y - r_j^Y \right|^p} e^{-\frac{\left| r_i^X - r_j^X \right|^2}{2\sigma^2}} e^{-\frac{\left| r_i^Y - r_j^Y \right|^2}{2\sigma^2}} \equiv R
\] (4.10)

and the choice of \( R \) from Equation 4.8 satisfies detailed balance.

### 4.1.2 Variance Minimization

Often, a trial wave function \( \Psi(p) \) is formulated in terms of \( N_p \) variational parameters \( p \). Locating the optimal set of parameters at which the energy is minimized quickly becomes very challenging in large systems with many parameters. We describe the method used to optimize \( \Psi(p) \) and developed by Umrigar and Toulouse [144, 145]. Instead of minimizing the energy of \( \Psi(p) \), this method minimizes the energy variance. This is convenient because unlike the Monte Carlo energy estimates, every measurement of the energy variance must be bounded from below by zero. The variance is zero only if \( \Psi(p) \) is an eigenstate.

We begin by writing the normalized wave function

\[
|\bar{\Psi}(p)\rangle = \frac{|\Psi(p)\rangle}{\sqrt{\langle \Psi(p) | \Psi(p) \rangle}}.
\] (4.11)

Now we can meaningfully linearize \( \bar{\Psi} \) about a set of parameters \( p_0 \) by \( p = p_0 - \Delta p \):

\[
|\bar{\Psi}_{\text{lin}}(p)\rangle = |\Psi_0\rangle + \sum_i^{N_p} \Delta p_i |\bar{\Psi}_i\rangle
\] (4.12)

\[
|\bar{\Psi}_i\rangle = \left. \frac{\partial |\Psi(p)\rangle}{\partial p_i} \right|_{p=p_0} = |\Psi_i\rangle - S_{0i} |\Psi_0\rangle
\] (4.13)

where the contribution of \( |\Psi_i\rangle \) has been orthogonalized to \( |\bar{\Psi}_0\rangle = |\Psi_0\rangle = |\Psi(p_0)\rangle \) via the overlap \( S_{0i} = \langle \Psi_0 | \Psi_i \rangle \). We can formulate the energy of this linearized wave function

\[
E_{\text{lin}}(p) = \frac{\langle \bar{\Psi}_{\text{lin}}(p) | \hat{H} | \bar{\Psi}_{\text{lin}}(p) \rangle}{\langle \bar{\Psi}_{\text{lin}}(p) | \bar{\Psi}_{\text{lin}}(p) \rangle}
\] (4.14)

and minimize using by treating \( E_{\text{lin}} \) as Lagrange multiplier.
This minimization leads to the generalized eigenvalue problem

\[ \tilde{H} \cdot \Delta p = E_{\text{lin}} \tilde{S} \cdot \Delta p. \] (4.15)

The Hamiltonian \( \tilde{H}_{ij} = \langle \tilde{\Psi}_i | \hat{H} | \tilde{\Psi}_j \rangle \) and the overlap matrix \( \tilde{S}_{ij} = \langle \tilde{\Psi}_i | \tilde{\Psi}_j \rangle \) are evaluated within the subspace of the \{ \(| \Psi_0 \rangle \equiv | \tilde{\Psi}(p_0) \rangle , | \Psi_1 \rangle , \ldots , | \Psi_{N_p} \rangle \} \). The orthonormal condition on the \(| \tilde{\Psi}_i \rangle \) enforces \( \tilde{S}_{00} = 1 \) and \( \tilde{S}_{0i} = \tilde{S}_{i0} = 0 \). The eigenvector \( \Delta p \) associated with the lowest eigenvalue predicts a better set of parameters \( p = p_0 + \Delta p \). In practice, this procedure must be iterated several times (each time \( \langle \hat{H} \rangle \) and \( \langle \tilde{S} \rangle \) must be estimated within VMC at the parameter point \( p_0 \)) to ensure convergence to optimal parameters.

As is usual for numerical methods, there are tricks to improve convergence, especially if \(| \Psi(p) \rangle \) depends nonlinearly on \( p \). Perhaps the most important is to consider the situation given the different normalization \(| \tilde{\Psi}(p) \rangle = N(p) | \Psi(p) \rangle \) where \( N(p_0) = 1 \). This leads to a rescaling of the \( \Delta p \) eigenvector with a faster convergence. Note that it is essential to this procedure that \( \hat{H} \) is not symmetric, so every element must be individually evaluated within the VMC simulation.

### 4.2 Diffusion Monte Carlo

Variational Monte Carlo is extremely useful when optimizing a wave function with respect to a set of parameters or when estimating correlation functions. Diffusion Monte Carlo (DMC) goes beyond VMC by projecting the trial state onto the ground state, though it remains constrained by the nodal surface imposed by a trial or guiding wave function. Like VMC, DMC is a zero temperature technique whose energy estimator is an upper bound to the true ground state energy. The distance between the DMC and VMC energy hints at the accuracy of the trial wave function and the mixed estimator gives improved estimates for various correlation functions [152, 153]. In this section we derive a DMC algorithm and the mixed estimator formula, and briefly discuss the consequences of picking too large a time step.
4.2.1 The Algorithm

Diffusion Monte Carlo is a projective type of QMC. Roughly speaking, it projects an initial set of configurations onto the lowest overlapping energy eigenstate(s) and, after a burn-in period, estimates that eigenstate’s energy $E_0$. This projection is accomplished through repeated application of $e^{-dt(\hat{H}-E_t)}$ where $dt$ is the time step. We will see that the trial or offset energy $E_t$ approaches $E_0$ after the burn in period. Green Function and power Monte Carlo are formulated on the same principle but use a different projector [see Reference [154] for details]. Ideally, this algorithm would sample just the ground state $\Phi_0^2$, but such an \textit{ab initio} simulation is numerically costly and may be prone to instabilities. The standard solution is to introduce a trial wave function $\Psi_T$ and to use importance sampling during the Monte Carlo sampling of configuration space. Below, we derive the algorithm with no $\Psi_T$ and then modify it to sample from the probability distribution $\Phi_0\Psi_T$.

Projection onto the Ground State

First we describe a method to project onto the ground state of a Hamiltonian starting from a variational state that is assumed to have some overlap with the ground state. We begin with the imaginary time Schrödinger equation

$$ -\frac{\partial}{\partial t} \Phi(R, t) = (\hat{H} - E_t)\phi(R, t) \tag{4.16} $$

over all particle coordinates $R = \{r_1, \ldots, r_N\}$. This becomes the integral equation

$$ \Phi(R, t + dt) = \int G(R', R, dt)\Phi(R', t)dR' \tag{4.17} $$

with $\partial_t G(R', R, t) = -(\hat{H} - E_T)G(R', R, t)$ and the initial condition $G(R', R, 0) = \delta(R' - R)$. This integral equation can be solved by the Green function written in terms of the eigenstates $\hat{H}\Phi_\alpha = E_\alpha \Phi_\alpha$ as

$$ G(R', R, t) = \sum_\alpha e^{-t(E_\alpha - E_T)}\Phi_\alpha^*(R')\Phi_\alpha(R). \tag{4.18} $$
Then in the limit of $t \to \infty$, all excited states are exponentially suppressed relative to the ground state $\Phi_0$

$$\lim_{t \to \infty} e^{-t(\hat{H} - E_T)}\Psi = \lim_{t \to \infty} \int G(R', R, t)\Phi(R')dR' \lim_{t \to \infty} \langle \Psi | \Phi_0 \rangle e^{-t(E_0 - E_T)}\Phi_0(R). \quad (4.19)$$

**Diffusion and Branching**

For the Hamiltonian

$$H = -\frac{1}{2} \sum_i \nabla_i^2 + U(R), \quad (4.20)$$

a sum of kinetic and interaction energies, we derive a routine to step through configuration space from $R$ to $R'$ in terms of a diffusion and a branching process. By using the Suzuki-Trotter or the Zessenhaus formula $e^{-dt(\hat{A} + \hat{B})} = e^{-dt\hat{A}}e^{-dt\hat{B}} + O(dt^2)$ we rewrite the Green function as

$$G(R, R', dt) \approx e^{-(R-R')^2/(2dt)}e^{-dt(U(R)+U(R')-2E_T)/2} \quad (4.21)$$

where $G_d = e^{-(R-R')^2/(2dt)}$ is the solution of the diffusion equation, given by Equation 4.16 for only a kinetic term, i.e. $\partial_t\Phi(R, t) = -\frac{1}{2} \sum_i \nabla_i^2\Phi(R, t)$.

At this point, we can formulate a bare-bones DMC algorithm. We begin with an ensemble of walkers $R_i(t) = \{r_j\}_{j=1}^N$ at time $t$. Generate and accept a new configuration $R_i(t+dt)$ for each particle $j$ in each walker $i$ by $r_j(t+dt) = r_j(t) + \eta$ where $\eta$ is drawn from the 3D normal distribution $e^{-\eta^2/(2dt)}$ ($G_d$ is Hermitian so it automatically satisfies detailed balance). Now use the weight $W_i = e^{-dt(U(R_i(t))+U(R_i(t+dt))-2E_T)/2}$ to cull or branch the walkers:

1. If $W_i < 0$, the walker $i$ continues with probability $W_i$.

2. If $W_i > 1$, the walker $i$ is replicated floor($W_i$) times, and one extra with probability $W_i - \text{floor}(W_i)$.

The role of the trial energy $E_T$ here is clear: it is modified to maintain an approximately constant number of walkers.

This implementation has several drawbacks. The most important is that the potential energy can vary tremendously from one step to another, or a walker could drift into a
configuration with a divergent potential energy. In the latter case, that walker would branch and artificially dominate the simulation.

**Ψₜ and Importance Sampling**

Introducing a trial function Ψₜ to guide the diffusion process improves the performance of DMC in several respects. A good trial function can guide the walker diffusion through the 3N-dimensional space to the most likely configurations, and the ill-behaved potential energy \( U(\mathbf{R}) \) is replaced by the local energy \( E_L \) of \( \Psiₜ \), Equation 4.3. The \( \Psiₜ \) can also alleviate the sign problem imparted by fermion wave function antisymmetry. The ground state goes through a node and has no weight wherever it changes sign. A good \( \Psiₜ \) has a similar nodal surface to the ground state and helps the DMC avoid nodes by having vanishing weight in their vicinity.

As mentioned above, after importance sampling is implemented the DMC algorithm samples from \( f = \Phi₀Ψₜ \). This modifies the partial derivative and the integral Schrödinger equations (Equations 4.16 and 4.17) to

\[
-\frac{\partial}{\partial t} f(\mathbf{R}, t) = -\frac{1}{2} \sum_i \nabla_i^2 f - \nabla \cdot (f \nabla \log |\Psiₜ|) + (E_L(\mathbf{R}) - E_T) f
\]

\[
f(\mathbf{R}, t + dt) = \int G^*(\mathbf{R}', \mathbf{R}, dt) f(\mathbf{R}', t) d\mathbf{R}'
\]

with \( G^*(\mathbf{R}', \mathbf{R}, dt) = \frac{\Psiₜ(\mathbf{R})}{\Psiₜ(\mathbf{R})} G(\mathbf{R}', \mathbf{R}, dt) \). We again obtain the short time propagator by using the Trotter decomposition

\[
G^*(\mathbf{R}', \mathbf{R}, dt) \approx e^{-\left(\mathbf{R}' - \mathbf{R} - dt \nabla \log |\Psiₜ|\right)^2 / (2dt)} e^{-dt(E_L(\mathbf{R}) + E_L(\mathbf{R}') - 2E_T)/2}. \tag{4.24}
\]

Except for a few caveats, the simulation proceeds as before. The drift term \( \nabla \log |\Psiₜ| \) alters the update \( \mathbf{r}_j(t + dt) = \mathbf{r}_j(t) + \nabla \log |\Psiₜ| + \eta \) and makes \( G^* \) non-Hermitian, so the proposed configuration of each walker is accepted with probability \( P(\mathbf{R}'|\mathbf{R}) \) according to detailed balance

\[
\frac{P(\mathbf{R}'|\mathbf{R})}{P(\mathbf{R}|\mathbf{R})} = \frac{|\Psiₜ(\mathbf{R}')|}{|\Psiₜ(\mathbf{R})|} \frac{G^*(\mathbf{R}, \mathbf{R}', dt)}{G^*(\mathbf{R}', \mathbf{R}, dt)}. \tag{4.25}
\]

The branching weight now depends on \( E_L(\mathbf{R}) \) rather than \( U(\mathbf{R}) \), which has a smaller vari-
ance if $\Psi_T$ is a reasonably good approximation to the ground state. The drift term $\nabla \log |\Psi_T|$ biases the random walk toward more likely configurations and, with the detailed balance dependence on $|\Psi_T(R')|/|\Psi_T(R)|$, also prevents walkers from approaching or crossing nodal surfaces.

4.2.2 Mixed Estimators

With the above algorithm we can sample the distribution $\Phi_0\Psi_T$ but we really want to estimate $\langle \Phi_0 | \hat{A} | \Phi_0 \rangle$. To bridge the two distributions, we first assume that the difference between the trial wave function and the ground state is

$$\Phi_0(R) = \Psi_T(R) + \epsilon \phi(R) \quad (4.26)$$

where $\epsilon$ and $\phi(R)$ are small. Then the estimator for $\hat{A}$ within DMC becomes

$$\langle \hat{A} \rangle_{DMC} = \frac{\int dR \Phi_0 A(R) \Psi_T}{\int dR \Phi_0 \Psi_T} = \frac{\int dR \Psi_T A(R) \Psi_T}{\int dR \Psi_T^2} + \frac{\epsilon}{\int dR \Psi_T^2} \left[ \int dR \phi A(R) \Psi_T \right. \left. - \int dR \phi \Psi_T \int dR \Psi_T A(R) \Psi_T \right] + O \left( \int dR (\epsilon \phi(R))^2 \right)$$

$$= \langle \hat{A} \rangle_{VMC} + \epsilon A_1 + O \left( \int dR (\epsilon \phi(R))^2 \right). \quad (4.27)$$

A similar analysis for the ground state reveals

$$\langle \hat{A} \rangle_0 = \frac{\int dR \Phi_0 A(R) \Phi_0}{\int dR \Phi_0^2} = \langle \hat{A} \rangle_{VMC} + 2\epsilon A_1 + O \left( \int dR (\epsilon \phi(R))^2 \right) \quad (4.28)$$

and the combination yields the mixed estimator for the ground state

$$\langle A \rangle_{Mixed} = 2 \langle A \rangle_{DMC} - \langle A \rangle_{VMC} = \langle A \rangle_0 + O \left( \int dR (\epsilon \phi(R))^2 \right). \quad (4.29)$$

This mixed estimator is essential for observables that do not commute with the Hamiltonian, but the energy is significantly easier to estimate. The energy estimate has only time-step error, in principle, because $H$ commutes with the projection operator. Recall that $\Phi_0 \approx e^{-\tau H} \Psi_T$ so that after a sufficiently long time

$$\langle \hat{H} \rangle_{DMC} = \frac{\int dR \Phi_0 H(R) \Psi_T}{\int dR \Phi_0 \Psi_T} \approx \frac{\int dR \Phi_0 H(R) \Phi_0}{\int dR \Phi_0 \Phi_0} = \langle \hat{H} \rangle_0 \quad (4.30)$$
Figure 4.1: An illustration of persistent configurations. (a) One of the walkers discovers a very low energy configuration \( E_0 \approx -1 \) and is multiplied by the branching process with a moderately large \( dt \). Occasionally a new configuration is accepted, but it is quickly swamped. (b) The average \( \langle E_L \rangle_{DMC} \) over all walkers at each time for the same simulation as in (a). The stair step pattern indicates a jump in the walkers from one persistent configuration to a lower energy one. Note the “Time” is computation steps and the true “projected time” needs a factor of \( dt = 10^{-3} \).

4.2.3 Large Time-Step Errors and Persistent Configurations

Error can creep into DMC results from several places. The most catastrophic would be if the trial function \( \Psi_T \) has no overlap with the true ground state. Then the simulation would converge to the lowest energy eigenstate with \( \langle \Phi_{\alpha>0} | \Psi_T \rangle \neq 0 \). The fixed nodal surfaces of \( \Psi_T \) represent another, smaller source of error which is not extremely well understood but is generally minimized by optimizing \( \Psi_T \) in VMC simulations.

The most controllable source of error is associated with the time step \( dt \). In a continuum system, it is not obvious how large \( dt \) can be and still enable Monte Carlo estimators to converge. On the other hand, as \( dt \) decreases, the burn-in period lengthens and new configurations may be more correlated. Some care and experimentation is needed to find an appropriate \( dt \). One hallmark of choosing too large a time step are persistent configurations [152], illustrated in Figure 4.1. A large \( dt \) makes a walker more likely to reject a
proposed move, while simultaneously proliferating any walkers with energy $E_L(R) < E_T$ (even if $E_L(R) < E_0$!). In this way, an excessively low energy walker can overwhelm all other walkers, thereby artificially biasing the simulation and driving the energy estimator below the true ground state energy $E_0$. Based on observations, moves out of a low-energy persistent state are relatively likely to result in an even lower-energy persistent state.

4.3 World-line Quantum Monte Carlo

Over the last two decades, several algorithms of the “world-line” type have been developed. This class of algorithms efficiently samples the finite temperature partition function in imaginary time and is easily applied to the BHM and to Heisenberg-type lattice spin models. The simulation results are exact up to statistical error, for bosons, because the partition function weights are all positive and can be directly sampled. The best implementations of this algorithm for the BHM are capable of simulating BHM systems at the same scale as ultracold-atom experiments, with up to $10^6$ bosons and $64^3$ lattice sites.

These simulations can access a plethora of observables including density, compressibility, energy, susceptibility, single and pair correlations and even the superfluid density. On the other hand, a limitation of these algorithms is their lack of phase information; they are restricted to the boson-number basis because of their structure. This basis choice restricts world-line QMC investigations of phase structures and defects like vortices to indirect measurements because each boson’s phase is unknown. Nonetheless, world-line QMC simulations have played a very important role in confirming that ultracold bosons in optical lattices emulate the BHM and have aided interpretation of experiments like time-of-flight imaging. These algorithms have also played a key role in theoretical investigations of the accuracy of the local density approximation, in developing new methods with which to identify phases in experiments, in identification of universality classes and in studies of the disordered BHM.

All world-line QMC simulations take place in $d + 1$ dimensions; $d$ spatial dimensions and one imaginary time dimension whose extent is dictated by the inverse temperature
\( \beta = 1/T \). The algorithms employ an auxiliary field \( F \) that is updated in turn with a world-line configuration \( \Psi \) of local boson occupation numbers. The auxiliary field enables efficient estimators for several observables.

### 4.3.1 Approximating the Partition Function

Generally speaking, two choices classify world-line QMC algorithms: the method of expansion of the partition function, through either path integral or stochastic series expansion formalism, and the method for generating new configurations. In this work we will focus on the path-integral expansion in continuous imaginary time with directed loop updates [156, 157, 158]. More basic QMC routines emerge at several points during the development of the necessary formalism and those methods and their limitations will be briefly discussed. As in the mean field theory treatment, we constrain the maximum number of bosons on a site to be \( n_M \), although this requirement can be eliminated in advanced implementations of this algorithm.

It is convenient to break the Hamiltonian into its smallest constituent pieces. The Bose-Hubbard model’s Hamiltonian has single site terms and terms that operate on a link between neighboring sites \( i \) and \( j \), or

\[
\hat{H} = \hat{H}_{\text{onsite}} + \hat{H}_{\text{link}} \tag{4.31}
\]

\[
= \sum_i \left( \frac{U}{2} \tilde{n}_i \left( \hat{n}_i - 1 \right) - \mu \hat{n}_i \right) + \sum_{\langle i,j \rangle} \frac{t}{n_c} \left( \hat{a}_i^\dagger \hat{a}_j + \hat{a}_i \hat{a}_j^\dagger \right) \tag{4.32}
\]

\[
= \sum_i \hat{h}_{\text{onsite},i} + \sum_{\langle i,j \rangle} \hat{h}_{\text{link},ij} = \sum_{m=1}^{\mathcal{M}} \hat{h}_m \tag{4.33}
\]

There are \( \mathcal{M} = (d+1)L^d \) distinct terms in Equations 4.32 and 4.33. These basic constituents are denoted by \( \hat{h}_m \), where \( m \) is shorthand for both the local Hamiltonian term type and the site(s) it operates on. The lattice coordination number is denoted \( n_c \).
Expansion of $Z$ in Imaginary Time

World-line simulations expand the partition function $Z$ over imaginary time in the Foch basis $\{\Psi\} = \{n_1, n_2, \ldots, n_{L_d}\}$ with occupation number $n_i = 0, 1, \ldots, n_M$ on site $i$. The trace over states $Tr e^{-\beta \hat{H}}$ is replaced by a sum over all states $\{\Psi\}$. In the path-integral formulation, the Boltzmann weight is expanded as

$$Z = \sum_{\{\Psi\}} \langle \Psi | e^{-\beta \hat{H}} | \Psi \rangle = \sum_{\{\Psi\}} \left( \lim_{L_\tau \to \infty} \prod_{\ell=1}^{L_\tau} e^{-\Delta \tau \hat{H}} \right) \langle \Psi | e^{-\beta \hat{H}} | \Psi \rangle,$$

(4.34)

where imaginary time is discretized by $\Delta \tau = \beta / L_\tau$ and $L_\tau$ denotes the number of slices. The error incurred in this expansion is known as the Trotter error and scales with $\Delta \tau^2$.

Local Update QMC

The most basic type of QMC emerges immediately from the expansion in Equation 4.34 by inserting a complete set of states $\sum_{\{\Psi_\ell\}} |\Psi_\ell\rangle \langle \Psi_\ell|$ at every imaginary time slice $\ell$

$$Z = \lim_{L_\tau \to \infty} \sum_{\{\Psi\}} \langle \Psi_{L_\tau} | e^{-\Delta \tau \hat{H}} | \Psi_{L_\tau-1} \rangle \ldots \langle \Psi_2 | e^{-\Delta \tau \hat{H}} | \Psi_1 \rangle \langle \Psi_1 | e^{-\Delta \tau \hat{H}} | \Psi_0 \rangle \quad (4.35)$$

or

$$Z = \lim_{L_\tau \to \infty} \prod_{\ell=1}^{L_\tau} \langle \Psi_\ell | e^{-\Delta \tau \hat{H}} | \Psi_{\ell-1} \rangle \quad (4.36)$$

Now each state $\Psi_\ell$ represents the occupation at each site $i$ at imaginary time $\ell$, and the trace requires that $|\Psi_{L_\tau}\rangle = |\Psi_0\rangle$. A single configuration $\Psi = [\Psi_0 \ldots \Psi_{L_\tau-1}]$ of the bosons defines a worldline configuration [illustrated in Figure 4.2(a)]. A configuration $\Psi$ is valid only if $\langle \Psi_\ell | 1 | \Psi_{\ell-1} \rangle \neq 0$ and/or $\langle \Psi_\ell | \hat{H} | \Psi_{\ell-1} \rangle \neq 0$ for all time slices $\ell$, since otherwise the entire world-line configuration would have a total weight equal to zero. For example, a world-line with a total particle number that varies with $\ell$ is invalid.

This basic QMC algorithm attempts an update from $\Psi$ to $\Psi'$ in the following way. Each time slice has weight $w(\Psi_\ell) = \langle \psi_{\ell+1} | e^{-\Delta \tau \hat{H}} | \psi_{\ell} \rangle$ in the partition function, and the total weight of a configuration $\Psi$ is $w(\Psi) = \prod_\ell w(\Psi_\ell)$. First, a new and valid state $\Psi'_\ell$ is proposed to replace $\Psi_\ell$ [see Figure 4.2(b)]. The relative weights of the two configurations $w(\Psi')/w(\Psi) = w(\Psi'_\ell)/w(\Psi_\ell)$ is the probability to accept the proposed state, as is standard
Figure 4.2: For the partition function Equation 4.39, (a) an example worldline configuration $\Psi$ and (b) a proposed configuration $\Psi'$ under the local update scheme described in the text. To generate $\Psi'$, a single timeslice $\Psi_7$ from $\Psi$ has been selected and the boson number on sites 1-4 have been changed, indicated by the blue oval. There are 8 sites and $L_\tau = 10$ imaginary time slices, and the local boson occupation number is denoted graphically by a dotted line for $n(i, \tau) = 0$, a solid line for $n(i, \tau) = 1$ and a thick line for $n(i, \tau) = 2$. The occupation number can only change at integer multiples of the imaginary time discretization $\Delta \tau$.

for importance sampled Monte Carlo simulations where configurations are sampled directly from the probability distribution function $e^{-\beta H}/Z$. This process is straightforward and the systematic Trotter error can be reduced by taking $L_\tau$ large, but it takes $O(L_\tau)$ moves to update the entire configuration. Also, every update is local so the total particle number is fixed, the simulation slows dramatically near critical points.

**Expansion of Z into Local Terms**

The partition function must be expanded into the single site and link elements of the Hamiltonian to enable loop or global updates. Substituting the local Hamiltonian terms of Equation 4.33 into Equation 4.36 explicitly includes the action of every term in the
Hamiltonian within each time slice $\Delta \tau$

\[
Z = \lim_{L\tau \to \infty} \sum_{\{\Psi\}} \prod_{\ell=1}^{L\tau} \langle \Psi_\ell | e^{-\Delta \tau \sum_m \hat{h}_m} | \Psi_{\ell-1} \rangle \tag{4.37}
\]

\[
= \lim_{L\tau \to \infty} \sum_{\{\Psi\}} \prod_{\ell=1}^{L\tau} \langle \Psi_\ell | \prod_{m=1}^{M} e^{-\Delta \tau \hat{h}_m} | \Psi_{\ell-1} \rangle \tag{4.38}
\]

\[
= \lim_{L\tau \to \infty} \sum_{\{\Psi\}} \prod_{u}^{L\tau M} \langle \psi'_u | e^{-\Delta \tau \hat{h}_u} | \psi_u \rangle \tag{4.39}
\]

where we have inserted a complete set of states at every opportunity and wrapped the space $b$ and imaginary time $\ell$ indices into the single index $u$, which specifies the type of Hamiltonian term, the site or link it acts on and its imaginary time. We can treat these elements $\hat{h}_u$ as time ordered, illustrated in Figure 4.3(b). In Equation 4.39, the expectation value at time slice $\ell$ no longer depends on the full number configuration $\Psi_\ell$; instead it only depends on the state $\psi_u$ at the local site or link denoted by $u$, and on the configuration $\psi'_u$ after the action of $\hat{h}_u$. Several efficient local update algorithms based on Equation 4.39 are reviewed in Reference [159].

**Expansion of $Z$ into Auxiliary Field $F$**

The partition function must be further expanded into an auxiliary field to enable global or loop updates in QMC. The analogous procedure in classical Monte Carlo simulations are the Wolff and the Swendsen-Wang cluster update algorithms [160, 161]. For example, in a simulation of a classical Ising spin model, each bond $i$ between spins is probabilistically assigned an auxiliary field value $F_i$ either 0 or 1. A cluster of spins is constructed by identifying all spins connected by bonds with $F_u = 1$. A new configuration is proposed by assigning every spin in the cluster to be either +1 or -1, and this state is probabilistically accepted. A similar method can be realized in QMC by introducing an auxiliary field $F$ at
every \( u \) by further expanding the partition function in Equation 4.39 as

\[
Z = \lim_{L, \tau \to \infty} \sum_{\{\Psi\}} \prod_{u} \left\langle \psi'_u \left| 1 - \Delta \tau \hat{h}_u + O((\Delta \tau E^*)^2) \right| \psi_u \rightangle
\]  
(4.40)

\[
\approx \lim_{L, \tau \to \infty} \sum_{\{\Psi\}} \prod_{u} \sum_{F_u=0,1} \left\langle \psi'_u \left| (-\Delta \tau \hat{h}_u)^{F_u} \right| \psi_u \rightangle
\]  
(4.41)

\[
= \lim_{L, \tau \to \infty} \sum_{\{\Psi\}} \sum_{\{F\}} \prod_{u} w(\psi_u, F_u).
\]  
(4.42)

This expansion incurs error of order \((\Delta \tau E^*)^2\) where \( E^* \) is the leading order energy contribution in \( \hat{H} \). This error and the Trotter error vanish in the continuous time limit explicitly taken within the algorithm. The local weight for a configuration \((\Psi, F)\) at \( u \) is \( w(\Psi_u, F_u) = \left\langle \psi'_u \left| (-\Delta \tau \hat{h}_u)^{F_u} \right| \psi_u \right\rangle \) and the total weight of the entire world-line configuration is \( w(\Psi, F) = \prod_{u=1}^{L,\tau, M} w(\psi_u, F_u) \). Note that the term \( F_u = 0 \) corresponds to the identity operator, \( \left\langle \psi'_u \left| 1 \right| \psi_u \right\rangle = \delta_{\psi_u, \psi'_u} \). On the other hand, a boson can only hop from site \( i \) to a neighboring site \( j \) at imaginary time \( u \) if \( F_u = 1 \) and \( \hat{h}_u = \hat{h}_{\text{link},ij} \). We say there is a vertex at every \( u \) such that \( F_u = 1 \). An auxiliary field configuration is denoted by \( F \) and exemplified in Figure 4.3(b). Note that at every imaginary time slice \( u \), there is now a Hamiltonian \( h_u \) and two states slightly earlier \((\psi_{u-\delta u})\) and slightly later \((\psi_{u+\delta u})\) in imaginary time. For convenience, we denote \( \psi_{u-\delta u} \) by \( \psi_u \) and \( \psi_{u+\delta u} \) by \( \psi'_u \).

Several loop and worm update schemes are based on Equation 4.42 [156, 157, 158]. As in the Swendsen-Wang routine, they probabilistically assign \( F_u = 0,1 \) to each term \( \hat{h}_u \), generate a new configuration \( \Psi' \) by assembling a cluster from \( F_u \) and randomly choose to accept \( \Psi' \) based on the relative probability of \( w(\Psi')/w(\Psi) \). These updates are significantly better than local updates because they avoid the critical slowing down at low temperature and near critical points that is observed in the local update scheme, and because they ergodically sample configurations in a superfluid [see discussion below on the winding number].
Figure 4.3: Example worldline configurations drawn from the partition function expansions. (a) Equation 4.36 with the total Boltzmann weight $e^{-\Delta \tau \hat{H}}$ contributing at every time slice $\Delta \tau$. (b) Equation 4.39 with every single-site and link piece of the Hamiltonian contributing with weight $e^{-\Delta \tau \hat{h}_u}$ in a time ordered fashion. (c) Equation 4.41 with both the boson $\Psi$ and the auxiliary field $F$ configurations explicitly included as $\langle \psi'_u \mid (-\Delta \tau \hat{h}_u) F_u \mid \psi_u \rangle$. In each of these panels, $N_s = 6$, $N_b = 3$ and $L_\tau = 7$. In panel (c), the terms $\hat{h}_u$ are coded by black or grey depending on the auxiliary field $F_u = 0$ (identity operator) or $F_u = 1$ (vertex), as shown in (d).

**Stochastic Series Expansion**

Before describing the directed loop algorithm, we briefly outline the stochastic series expansion, an alternative way to expand the partition function into local terms $\hat{h}_u$. It leads to similar QMC algorithms as the path integral expansion, but the local weight $w(\psi_u, F_u)$ includes a combinatorial coefficient. Using a high-temperature series expansion, the partition function can be expanded into

$$Z = \lim_{L_\tau \rightarrow \infty} \sum_{\{\Psi\}} \sum_{k=0}^{L_\tau} \frac{\beta^k}{k!} \langle \Psi \mid (-\hat{H})^k \mid \Psi \rangle$$

(4.43)

Say the series is truncated at order $L_\tau$. There is exactly one term with $L_\tau$ powers of $\hat{H}$ but $L_\tau!/(n!(L_\tau - n)!)$ copies of the term with $n$ powers of $\hat{H}$. With local terms $\hat{h}_u$, the introduction of the auxiliary field $F_u = 0, 1$ and $n(F) = \sum_u F_u$ powers of $\hat{h}_u$, $Z$ becomes

$$Z = \lim_{L_\tau \rightarrow \infty} \sum_{\{\Psi\}} \sum_{\{F\}} \frac{\beta^{n(F)} (L_\tau - n(F))!}{L_\tau!} \prod_u \langle \psi'_u \mid (-\hat{h}_u)^{F_u} \mid \psi_u \rangle$$

(4.44)

with the insertion of complete sets of states $\sum_u |\psi_u\rangle \langle \psi_u|$. The series is stochastically sampled at all orders through the auxiliary field $F$. The local weights in Equations 4.41 and
4.44 can form the basis for most QMC algorithms, although we use Equation 4.41 below. In the \( L_\tau \to \infty \) limit, the prefactor \( \beta^n(F) (L_\tau - n(F))! / L_\tau! \) \( \to \) \( (\beta/L_\tau)^n(F) \) reduces to that of the path integral expansion.

### 4.3.2 Mechanics of the simulation

At this point the basic aspects of the simulation can be sketched out. There are five steps in this type of QMC simulation. 1) The auxiliary field \( F_u \) must be sampled as a function of \( \psi_u \) for each matrix element \( \hat{h}_u \) [see Figure 4.3]. The directed loop, called a worm, is initiated by inserting a single pair of annihilation and creation operators, one a head and one a tail, at a random point in the worldline configuration. 3) The head updates the bosons’ positions \( \psi_u \) by moving in the worldline configuration and changes direction only when it scatters at vertices. 4) The directed loop update ends when the head meets the tail and the loop closes. 5) After a specified number of worm updates under an identical \( F \) configuration, the auxiliary field is set to 0 at every \( u \) where a boson does not hop from one site to another.

We first discuss several necessary concepts and then describe the method to sample the auxiliary field \( F \). We introduce the twin processes of creating and destroying a worm and prescribe the rules governing the motion of the worm’s head or, in other words, the rules governing how to sample \( \{ \Psi \} \).

### Positive-Definite Weights

One caveat to this algorithm is that the local weight \( w(\psi_u, F_u = 1) = \langle \psi'_u | -\Delta \tau \hat{h}_u | \psi_u \rangle \) cannot be used as a probability when it is negative. For example, the onsite matrix element 
\[ -\Delta \tau \langle \psi'_u | \frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - \mu \hat{n}_i | \psi_u \rangle \]

is often negative, especially for large \( U \) or large \( n_i \). The solution is simple: subtract a positive constant \( C_{\text{onsite}} \) from \( \hat{H} \) larger than any possible \( \langle \psi'_u | \hat{h}_u | \psi_u \rangle \), i.e. \( C_{\text{onsite}} \geq \frac{U}{2} n_M (n_M - 1) - \mu n_M \). In addition, a constant \( C_{\text{link}} \geq t_n M \) must always be included with the link terms [see Sampling \( F_u \) below]. We redefine \( \hat{H} \to \hat{H} - L^d C_{\text{onsite}} - n_c L^d C_{\text{link}}, \hat{h}_{\text{onsite},i} \to \hat{h}_{\text{onsite},i} - C_{\text{onsite}} \) and \( \hat{h}_{\text{link},ij} \to \hat{h}_{\text{link},ij} - C_{\text{link},ij} \), and account for these offsets when estimating the energy.
**Detailed Balance**

Every step in a configuration update must be equally likely to happen in reverse; this is known as detailed balance and can be expressed as

\[
\mathcal{T}(Y|X)w(X) = \mathcal{T}(X|Y)w(Y)
\]  

(4.45)

where \(w(X)\) is the weight, or probability, of event \(X\) and \(\mathcal{T}(Y|X)\) is the probability to transition to event \(Y\) given that the current circumstance is \(X\). If detailed balance were not obeyed, the simulation would tend to sample certain parts of configuration space more often than others and thereby introduce an erroneous systematic bias.

**Time-Reversed Detailed Balance**

The processes of worm insertion and annihilation and of worm scattering are not well described by standard detailed balance because the worm’s head has an inherent directionality. In particular, the state \(Y\) resulting from a worm insertion or a scattering event cannot be directly reverted to the preceding state \(X\) \(\mathcal{T}(X|Y) = 0\) in Equation 4.45] because the worm head in \(Y\) points away from the vertex and therefore cannot immediately return. Time-reversed detailed balance resolves this conflict by postulating

\[
\mathcal{T}(Y|X)w(X) = \mathcal{T}(\bar{X}|\bar{Y})w(\bar{Y})
\]  

(4.46)

where \(\bar{X}\) indicates that the direction of the head in state \(X\) has been reversed. This process is illustrated below in *Creating and Destroying a Worm*, in *Building the Directed Loop* and in Figures 4.5, 4.6 and 4.7.

**1) Sampling \(F_u\)**

This step samples the expansion of \(Z\) into the auxiliary field \(F\). The entire step must obey detailed balance, but the structure of \(Z\) (i.e. the product over the local weight \(w(\psi_u, F_u)\)) allows the process to be reduced to the local detailed balance equation

\[
\mathcal{T}(F_u|\psi_u)w(\psi_u) = \mathcal{T}(\psi_u|F_u)w(F_u)
\]  

(4.47)
where \( w(F_u) = \sum_{\{\Psi\}} w(\psi_u, F_u) \) and \( w(\psi_u) = \sum_{F_u=0,1} w(\psi_u, F_u) \). If we let each side equal \( w(\psi_u, F_u) \), then for small \( \Delta \tau \) the transition probability to add and remove a vertex at space-imaginary time point \( u \) is

\[
T(F_u = 0 | \psi_u) = \begin{cases} 
0 & \text{if } |\psi_u'\rangle \neq |\psi_u\rangle \\
\frac{1}{1 - \Delta \tau \langle \psi_u' | \hat{h}_u | \psi_u \rangle} & \text{if } |\psi_u'\rangle = |\psi_u\rangle 
\end{cases}
\]

\[
T(F_u = 1 | \psi_u) \approx \begin{cases} 
1 & \text{if } |\psi_u'\rangle \neq |\psi_u\rangle \\
-\Delta \tau \langle \psi_u' | \hat{h}_u | \psi_u \rangle & \text{if } |\psi_u'\rangle = |\psi_u\rangle 
\end{cases}
\] (4.48)

In the continuous time limit, \( \Delta \tau \to 0 \) and \( T(F_u = 0 | \psi_u) = 1 \) for \( |\psi_u'\rangle = |\psi_u\rangle \). This is the step that requires the constant \( C_{link} \) to be added because otherwise a hopping-type vertex would never be placed in the ubiquitous case \( |\psi_u'\rangle = |\psi_u\rangle \).

The simulation runs in the continuous time \( \Delta \tau \to 0 \) limit, so we consider the circumstance that the state on any sites connected by the term \( \hat{h}_m \) does not change over the imaginary time interval \( I \gg \Delta \tau \). Since there is a binary choice for \( F_u \) at each \( u \), the probability to place \( k \) vertices in the interval \( I \) is

\[
\binom{I / \Delta \tau}{k} T(F_u = 1 | \psi_u)^k T(F_u = 0 | \psi_u)^{I / \Delta \tau - k}
\] (4.49)

which reduces to a Poissonian distribution in the continuous time limit

\[
\frac{1}{k!} (I \ T(F_u = 1 | \psi_u))^k e^{-I \ T(F_u = 1 | \psi_u)}. \quad (4.50)
\]

Thus, for a uniform interval \( I \) in imaginary time during which the occupation number of the site(s) connected by \( \hat{h}_m \) does not change, the number of vertices corresponding \( \hat{h}_m \) is randomly sampled from Equations 4.48 and 4.50 and those vertices are uniform randomly distributed along \( I \). To generate an auxiliary field configuration \( F \), each such uniform interval \( I \) for each term \( \hat{h}_m \) is sampled and the vertices placed. This process does not change the boson configuration \( \{\Psi\} \).
2) Creating and destroying a worm

Once the $F$ configuration is generated, the boson configuration $\Psi$ is updated via a directed loop or *worm*. The presence of the worm in the world-line configuration is included in the partition function by adding the source term $-\eta \hat{Q} = -\eta \sum_i \int d\tau \left( a_i(\tau) + a_i^\dagger(\tau) \right) / 2$ to the Hamiltonian. Exactly two sources occur within the world-line configuration during each directed loop update – one for the stationary *tail* and one for the mobile *head*. The space-time position of the head (tail) is denoted by $\odot$ ($\otimes$) (superseding the generic index $u$) and has weight $w_\odot = \langle \psi'_\odot | \Delta \tau \eta \hat{Q}_\odot | \psi_\odot \rangle \left( w_\otimes = \langle \psi'_\otimes | \Delta \tau \eta \hat{Q}_\otimes | \psi_\otimes \rangle \right)$, where $\eta$ is an adjustable factor. This modifies the partition function of Equation 4.41 with a worm to be

$$Z^W = \lim_{L_r \to \infty} \sum_{\{\Psi\}} \sum_{\{F\}} \langle \psi'_{u_{L_r,M-1}} \left( -\Delta \tau \hat{h}_{u_{L_r,M-1}} \right)^{F_{u_{L_r,M-1}}} | \psi_{u_{L_r,M-1}} \rangle \cdots$$

$$\langle \psi'_{u_{w+1}} \left( -\Delta \tau \hat{h}_{u_{w+1}} \right)^{F_{u_{w+1}}} | \psi_{u_{w+1}} \rangle \langle \psi'_\otimes \left| \Delta \tau \eta \hat{a}_\otimes \right\rangle | \psi_\otimes \rangle \langle \psi'_{u_w} \left( -\Delta \tau \hat{h}_{u_w} \right)^{F_{u_w}} | \psi_{u_w} \rangle \cdots$$

$$\langle \psi'_{u_v+1} \left( -\Delta \tau \hat{h}_{u_v+1} \right)^{F_{u_v+1}} | \psi_{u_{v+1}} \rangle \langle \psi'_\odot \left| \Delta \tau \eta \hat{a}_\odot \right\rangle | \psi_\odot \rangle \langle \psi'_{u_v} \left( -\Delta \tau \hat{h}_{u_v} \right)^{F_{u_v}} | \psi_{u_v} \rangle \cdots$$

$$\langle \psi'_{u_0} \left( -\Delta \tau \hat{h}_{u_0} \right)^{F_{u_0}} | \psi_{u_0} \rangle$$

(4.51)

for the imaginary time ordering $u_{L_r,M-1} > u_{w+1} > \otimes > u_w > u_{v+1} > \odot > u_v > u_0$ and the head and tail source terms $\hat{a}$ and $\hat{a}^\dagger$, respectively.
For the sake of minimal disruption to the worldline configuration, we choose to insert the head and tail source operators at a nearly identical time on the same site. Maintaining the same boson number above and below the two source terms requires that either the head is $\hat{a}$ and the tail is $\hat{a}^\dagger$ or vice versa. For a proposed worm insertion at space-time point $u$ in configuration $\Psi$, we can write the weight of the configuration with a worm, $\Psi^W$, as $w(\Psi^W) = w(\Psi)w_\otimes w_\odot$, where $w_\otimes$ and $w_\odot$ are the weights of the proposed tail and head, respectively. Note in this formulation that the head is equally likely to be slightly before or slightly after the tail in imaginary time and does not affect the weights $w_\odot$ and $w_\otimes$. This leads to the detailed balance equation

$$\mathcal{T}(\Psi^W|\Psi)w(\Psi) = \mathcal{T}(\Psi|\Psi^W)w(\Psi)w_\odot w_\otimes$$

(4.52)

where $\mathcal{T}(\Psi^W|\Psi)$ is the probability to insert a worm and $\mathcal{T}(\Psi|\Psi^W)$ is the probability to remove the worm. For a randomly chosen interval of length $\Delta \tau$ from any site in the worldline configuration, the chance to propose it as a worm creation site is $\Delta \tau/N_s \beta$. For a generic interval with $k$ bosons, any attempt to create or destroy a worm has five possible outcomes that, under time-reversal of the direction of the head, form a closed set of equations $\mathcal{T}_{ij}w_j = \mathcal{T}_{ji}w_i$. The weight of a uniform interval with no worm is just $\Delta \tau/N_s \beta \equiv P_I$ (i.e. the chance to randomly pick that $\Delta \tau$ interval on that site) and with a worm with $\hat{a}$ or $\hat{a}^\dagger$ first in imaginary time is $\Delta \tau^2 \eta^2(k$ or $k+1)/4$, respectively. A solution for this coupled set of 5 equations can be conveniently constructed by supposing the existence of a symmetric matrix $w_{ij} = w_{ji}$ of dimension $5 \times 5$ such that

$$w_i = \sum_{i} w_{ij}$$

(4.53)

and such that $\mathcal{T}_{ij} = w_{ij}/w_j$. One possible choice for this matrix and the parameter $\eta$ is shown in Figure 4.5. The time-reversal aspect of this process means that the creation and annihilation probabilities are inextricably linked and must be defined simultaneously.
Figure 4.5: Table showing worm creation, annihilation and pass-through probabilities for an interval with $k$ bosons and worm weight proportional to $\langle \hat{a} \rangle$ and $\langle \hat{a}^\dagger \rangle$. The top row are the symmetric weights $w_{ij}$ while the bottom row are the transition probabilities $T_{ij} = w_{ij}/w_{j}$ from state $j$ to state $i$. The probability of selecting this interval is $P_I = \Delta \tau/L^d \beta$. For the selection of $w_{ij}$ above, a worm is always created at the proposed site but the worm is not always destroyed when the head and tail meet. The parameter $\eta^2 = 4/L^d \beta \Delta \tau$ and the configuration weights with a worm $w_+ = \Delta \tau^2 \eta^2 (k+1)/4$ and $w_- = \Delta \tau^2 \eta^2 k/4$ are unaffected by the identification of $\hat{a}$ and $\hat{a}^\dagger$ with the worm head and tail, or vice versa.

### 3) Building the Directed Loop

The update step for the Foch space configuration $\Psi$ is a directed loop because the worm head has a directionality. The head source term travels in a single direction through imaginary time along a single site’s worldline and increments or decrements the boson number by one depending on its direction and source term. The head can change direction only at a vertex ($F_u = 1$), where it scatters to a different direction in imaginary time and/or onto a different site. This contrasts with a basic worm algorithm, where it is possible for the worm to inefficiently update the same interval many consecutive times.

This type of movement obeys time-reversed detailed balance just like the worm creation and removal process discussed above. The head is directional and always moves away from the vertex at which it just scattered, so there is no chance that a single scattering event...
can occur immediately in reverse. Instead, time-reversed detailed balance ensures that the worm is as likely to scatter from configuration and head state \( (\Psi_W^\alpha, \odot^\alpha) \) to \( (\Psi_W^\beta, \odot^\beta) \) as it is to scatter from \( (\Psi_W^\beta, \odot^\beta) \) to \( (\Psi_W^\alpha, \odot^\alpha) \), where the bar indicates that the head is directed away from the vertex and \( \alpha (\beta) \) denote two worm and \( \Psi \) configurations. Say the head is about to scatter off a vertex at \( u \). Then the time reversed detailed balance is

\[
T(\Psi_W^\beta, \odot^\beta | \Psi_W^\alpha, \odot^\alpha) w(\Psi_W^\alpha) = T(\Psi_W^\alpha, \odot^\alpha | \Psi_W^\beta, \odot^\beta) w(\Psi_W^\beta) \tag{4.54}
\]

\[
T(\psi_{u,\beta}, \odot^\beta | \psi_{u,\alpha}, \odot^\alpha) w(\psi_{u,\alpha}) w_{\odot^\alpha} = T(\psi_{u,\alpha}, \odot^\alpha | \psi_{u,\beta}, \odot^\beta) w(\psi_{u,\beta}) w_{\odot^\beta} \tag{4.55}
\]

In the second line we used the fact that a scattering event only changes the local state at \( \psi_u \) and that the tail is immobile. Reversing the direction of the head does not change the head weight so \( w_{\odot^\alpha} = w_{\odot^\alpha} \).

The vertex element \( \hat{h}_u \) can connect one or two sites so the head can scatter in two or four directions, respectively [see Figure 4.6]. Some reflection will show that Equation 4.55 decouples into closed sets of equations, each describing the chance to scatter from the initial state to each of the others. In other words, at a link vertex the state \( (\psi_u, \odot)_1 \) can scatter into any of \( (\psi_u, \odot)_{i=1}^4 \) states. But every one of those time-reversed states \( (\psi_u, \odot)_i \) can scatter into only the same set of states \( (\psi_u, \odot)_{i=1}^4 \). As above, this system of equations can be solved by constructing a symmetric matrix \( w_{ij} = w_{ji} \) of dimension \( 4 \times 4 \) (\( 2 \times 2 \) for single site vertices) such that

\[
w(\Psi_i) w_{hi} = \sum_j w_{ij}. \tag{4.56}
\]

Then the transition probability to state \( i \) from state \( j \) is \( T_{ij} = w_{ij} / w(\Psi_i) w_{hi} \). Possible choices for the single site and link vertices are shown in Figure 4.7. In general, the \( w_{ij} \) should be chosen to minimize the chance that the head backtracks and erases previous updates.

\^For the purposes of the loop construction, \( w_{\odot} \) is entirely arbitrary. The global detailed balance process requires that the probability of creating a given loop update equals the probability to then immediately make another loop that exactly undoes that loop update. The only restriction this requirement places on \( w_{\odot} \) is that it is Hermitian and independent of the head’s direction.
Figure 4.6: Standard scattering probabilities table where $w_a > w_b$. The structure of this diagram applies to the single site vertices $H_{\mu}$ and $H_U$ in the BHM, although the weights $w_{ij}$ (upper row) may need to be rearranged to ensure the transition probabilities are positive. The lower values in each row show the transition probabilities $T_{ij}$ from state $j$ to state $i$ for vertices of type $H_U$, with $w_A/\Delta \tau = C_{\text{onsite}} - \frac{U}{2} k(k-1)$, $w_B/\Delta \tau = C_{\text{onsite}} - \frac{U}{2} (k+1)k$ and $C_{\text{onsite}} = \frac{U}{2} n_M(n_M - 1)$. Note that in this case $k < n_M$ and $w_{\odot}$ is neglected because it is identical for each outcome.

Additional Comments

This algorithm is easily extended to boson models beyond the basic BHM. Any term that is diagonal in Foch space is permissible with an appropriate constant added to $\hat{H}$, including $\mu$- or $U$-disorder, inhomogeneous potentials and potentials of the form $\sum_i U_a \prod^K_{k=1} \hat{n}_{i+k}$. This algorithm’s basic requirement is that all hopping terms in the Hamiltonian have the form $-|t_{ij}| \left( \hat{a}_i \hat{a}^\dagger_j + \hat{a}^\dagger_i \hat{a}_j \right)$ so that each scattering state has a non-negative probability. Systems with exotic lattices and multiple species and bands are accessible while frustrated systems with $+|t_{ij}|$ for some $i$ and $j$, flux-threaded plaquettes and explicitly twisted boundary conditions are inaccessible.

There are several points where the algorithm has been improved. For example, consider the onsite vertices corresponding to the repulsion term $\hat{h}_{U,i} = C_{\text{onsite}} - \frac{U}{2} \hat{n}_i (\hat{n}_i - 1)$. For intervals with small boson number $n_i$, the density to place U-vertices is on the order of $\frac{U}{2} n_M(n_M - 1)$, so usually many are placed. Yet the probability for the worm head to pass through the vertex and continue in the original direction of travel is $\sim 1 - (n_i/n_M)^2$. Moving
Figure 4.7: A possible choice for the scattering probabilities table at a vertex corresponding to a hopping matrix element. The weights of each configuration are \( w_0 = \Delta \tau \Sigma \), \( w_A = \Delta \tau \eta \sqrt{k+1} \), and \( w_B = \Delta \tau \eta \sqrt{(k+1)(\ell+1)} \sqrt{\ell+1} \), with \( k, k+1, k+2, \ell, \ell+1 \) and \( \ell+2 \) indicate boson number on the corresponding worldline segment connecting to the vertex. The transition probability from the initial state \( i \) to the final state \( j \) is given by \( T_{ij} = w_{ij}/w_i \) and displayed in the lower row (\( w_{ij} \) are shown on the upper). The weight of the worm head \( w_\circ = \eta \langle \hat{a}^\dagger \rangle \) has been explicitly included.

the worm through these large number of vertices that contribute nothing to updating \( \Psi \) can become time- and memory-consuming. A solution is to generate vertices on the fly by creating a U-vertex only when the worm scatters from it, completely bypassing the vertex-placement step. This virtual placement of vertices can be done for all vertex types \([162]\). A second possible improvement is the elimination of the upper bound \( n_M \) on the number of bosons on an interval, which must be coupled with virtual generation of single site vertices and a judicious choice of \( \eta^2 \) that is independent of \( n_M \).

Now that the algorithm has been described in detail, we list the steps of the algorithm:

1. Sample the auxiliary field \( F \) by attempting to place each type of vertex (update \( F_u \)) at every possible imaginary time.

2. Randomly choose a space-time point and attempt to create a worm there. If successful, execute step 3, otherwise go to step 5.
3. Move worm head: advance it to the next vertex, update $\Psi$ along the uniform interval $I$ traveled, scatter according to the probabilities in Figures 4.6 and 4.7, and repeat until the next vertex is the tail.

4. Attempt to annihilate the worm. If unsuccessful, return to step 3.

5. Repeat the cycle of worm creation and annihilation (steps 2-4) until every interval in the worldline configuration has been updated, on average, and a new, independent $\Psi$ configuration generated.

6. Measure observables.

7. Delete vertices by setting $F_u = 0$ everywhere except where a boson hops from one site to another.

The above description of worm insertion and motion was naturally formulated in local, time-reversed detailed balance, but those components of this algorithm can be generalized. Rather than considering the local time-reversed detailed balance, the so-called worm-antiworm detailed balance for the entire loop update ensures that the loop update from
configuration $\Psi$ to $\Psi'$ and the reverse loop update from $\Psi'$ to $\Psi$ with identical scattering events are equally likely. This formulation enables the worm weight to be chosen with more freedom, which could lead to a more efficient algorithm. The detailed balance is

$$T(\Psi' | \Psi) w(\Psi) = T(\Psi | \Psi') w(\Psi')$$ (4.57)

where the probability to generate and accept $\Psi'$ from $\Psi$ using a loop update with $n$ scattering events labeled $\Psi'_n, \ldots, \Psi'_1, \Psi'_0, \Psi$, illustrated in Figure 4.8, is

$$T(\Psi' | \Psi) = P_{\text{Destroy}}(\Psi'_i | \Psi^W) T(\Psi^W | \Psi^W_{i-1}) \cdots T(\Psi^W | \Psi^W_0) P_{\text{Insert}}(\Psi^W_0 | \Psi).$$ (4.58)

The antiworm from $\Psi$ to $\Psi'$ consists of the intermediate states $\Psi, \tilde{\Psi}^W_0, \ldots, \tilde{\Psi}^W_n, \Psi'$.

Note that $w(\tilde{\Psi}^W_i)$ is the weight at scattering event $i$ in the antiworm update loop, in contrast to $w(\bar{\psi}_u)$ that includes only the reversal of the head’s direction and no change in $\bar{\psi}_u$. The previous two equations can be combined with the local, time-reversed detailed balance equation for $T(\Psi^W_i | \Psi^W_{i-1})$ at each scattering event $i$, Equation 4.55, to yield

$$\frac{w(\Psi)}{w(\Psi')} = \frac{P_{\text{Destroy}}(\Psi' | \Psi^W_n) P_{\text{Insert}}(\Psi^W_0 | \Psi)}{P_{\text{Destroy}}(\Psi | \tilde{\Psi}^W_0) P_{\text{Insert}}(\Psi^W_0 | \Psi')} \prod_{i=1}^{n} \frac{w(\Psi_i)}{w(\tilde{\Psi}_i)} w_{\ominus,i}$$ (4.59)

$$1 = \frac{P_{\text{Destroy}}(\Psi' | \Psi^W_n) P_{\text{Insert}}(\Psi^W_0 | \Psi)}{P_{\text{Destroy}}(\Psi | \tilde{\Psi}^W_0) P_{\text{Insert}}(\Psi^W_0 | \Psi')} \prod_{i=1}^{n} \frac{w_{\ominus,i}}{w_{\ominus,i}} w_{\ominus,i}.$$ (4.60)

The weights $w(\Psi^W_i) \neq w(\tilde{\Psi}^W_i)$ are evaluated before the worm updates the vertex. To obtain the second equation we note that $w(\Psi)/w(\Psi') = \prod_{i=1}^{n} w(\Psi_i)/w(\tilde{\Psi}_i)$. Surprisingly, this equation shows that the worm update will sample $Z$ as long as the worm weight $w_{\ominus,i}$ at scattering events is Hermitian and independent of the direction of travel, i.e. $w_{\ominus,i} = \bar{w}_{\ominus,i}$. For example, $w_{\ominus} = 1$ is a valid choice. With such a choice all measurements independent of the worm will be correct, although the the Green function estimator will fail unless properly modified. Similarly, the probabilities to insert and destroy a worm can be chosen independently of $w_{\ominus}$ and $w_{\ominus}$, although with the choices $P_{\text{Destroy}}(\tilde{\Psi} | \Psi^W_0) = T(\Psi | \Psi^W_0) w(\Psi) w_{\ominus} w_{\ominus}$ and $P_{\text{Insert}}(\Psi^W_0 | \Psi) = T(\Psi^W | \Psi) w(\Psi)$ reduces the latter equation to Equation 4.52.

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4.3.3 Efficient Measurements

Worldline algorithms admit several types of estimators including observables diagonal and off-diagonal in Foch space, susceptibility and the imaginary time Green function. Several types of observables can be calculated very efficiently by making use of either the auxiliary field or the worm motion.

To construct an estimator for the observable \( \hat{O} = \sum_b \hat{O}_b \), consider coupling it to the system by \( \hat{H} \rightarrow \hat{H} + \lambda \hat{O} \). Then the thermal expectation value is

\[
\langle \hat{O} \rangle_{\text{thermal}} = \frac{1}{\beta} \left. \frac{\partial}{\partial \lambda} Z(\lambda) \right|_{\lambda=0}
\]

\[
= \frac{1}{\beta} \sum_{u_0} \int d\tau \langle \psi'_{u_0} | \Delta \tau \hat{O}_{u_0} | \psi_{u_0} \rangle \prod_{u \neq u_0} \langle \psi'_u | (-\Delta \tau \hat{h}_u)^{F_u} | \psi_u \rangle
\]

\[
= \frac{1}{\beta} \sum_{u_0} \left( \frac{\langle \psi'_{u_0} | \Delta \tau \hat{O}_{u_0} | \psi_{u_0} \rangle}{\langle \psi'_{u_0} | (-\Delta \tau \hat{h}_u)^{F_{u_0}} | \psi_{u_0} \rangle} \right)_{\text{MC}}
\]

where \( \langle \ldots \rangle_{\text{MC}} \) denotes averaging with respect to the Monte Carlo weight of each configuration \( \prod_u \langle \psi'_u | (-\Delta \tau \hat{H})^{F_u} | \psi_u \rangle / Z \). There are two important cases for \( \hat{O} \).

\( \hat{O} \) Diagonal in Foch Space

If \( \hat{O} \) is diagonal in the Foch basis, then \( \langle \psi'_u | \hat{O}_u | \psi_u \rangle = 0 \) for \( |\psi'_u\rangle \neq |\psi_u\rangle \) and in Equation 4.63 we can neglect the \( \Delta \tau \hat{h}_u \) contributions to the denominator in the continuous time limit. Keeping in mind that \( u \) denotes a point in space-imaginary time, this leads to

\[
\langle \hat{O} \rangle = \frac{1}{\beta} \int d\tau \langle \psi'_u | \hat{O}_u | \psi_u \rangle_{\text{MC}}.
\]

If \( \hat{O} \) is independent of imaginary time, this generic prescription can be simplified rewritten in several forms. For example, the average particle number per site, \( n = \langle \hat{N} \rangle / L^d \), in the
BHM can be estimated as

\[ n = \frac{1}{\beta L^d} \int d\tau \langle \psi'_u | \hat{n}_u | \psi_u \rangle_{MC} \] (4.65)

\[ = \frac{1}{\beta} \int d\tau \langle \psi'_u | \hat{n}_{u,\text{site}=i} | \psi_u \rangle_{MC} \] (4.66)

\[ = \frac{1}{L^d} \langle \psi_{u=0} | \hat{n}_{u=0} | \psi_{u=0} \rangle_{MC} \] (4.67)

\[ = \langle \psi_{u=0} | \hat{n}_{u=0,\text{site}=i} | \psi_{u=0} \rangle_{MC} \] (4.68)

This method can be trivially extended to imaginary time correlations of the form

\[ \Pi_u \hat{n}(u = (i, \tau)) \text{ where } \langle \psi'_u | \hat{n}(u) | \psi_u \rangle = \langle \psi'_u | \hat{n}\delta_{u \mu} | \psi_u \rangle. \] The compressibility is one example of an observable that can be estimated through such a correlation function because

\[ \kappa = n^{-2} \partial n / \partial \mu = -(1/\beta N_s) \partial^2 F / \partial \mu^2. \] The estimator is

\[ \kappa = \frac{1}{\beta^2} \sum_{i,i'} \int d\tau \int d\tau' \langle \hat{n}_u \hat{n}_{u'} \rangle_{MC} - \langle \hat{n}_u \rangle_{MC} \langle \hat{n}_{u'} \rangle_{MC}, \] (4.69)

where the \( \langle \hat{n}_u \hat{n}_{u'} \rangle_{MC} \) is obtained via Equation 4.63.

\( \hat{O} \) not Diagonal in Foch Space

Observables \( \langle \hat{O}_{\text{off-diag}} \rangle \) that are not diagonal in Foch space are more difficult to estimate and include the kinetic energy, the Green function and the susceptibility. These off-diagonal operators yield zero when \( |\psi'_u\rangle = |\psi_u\rangle \), so all terms with \( F_u = 0 \) contribute nothing and the denominator of Equation 4.63 is now \( \langle \psi'_{u_0} | -\Delta \tau \hat{h}_{u_0} | \psi_{u_0} \rangle \) rather than one. Consider the special case of the kinetic energy \( KE + n_c C_{\text{link}} = \sum_{ij} \langle \hat{h}_{ij,\text{link}} \rangle \) that is composed of the off-diagonal terms in \( \hat{H} \). Then

\[ KE + n_c C_{\text{link}} = \frac{1}{\beta} \sum_u \left\langle \frac{\langle \psi'_u | \Delta \tau \hat{h}_{u,\text{link}} | \psi_u \rangle}{\langle \psi'_u | -\Delta \tau \hat{h} | \psi_u \rangle} \right\rangle_{MC} = -\frac{1}{\beta} \left\langle \sum_u F_{u}^{\text{link}} \right\rangle_{MC} \] (4.70)

where \( F_{u}^{\text{link}} \) are the auxiliary field variables associated with the \( \hat{h}_{\text{link}} \) terms of the Hamiltonian. The kinetic energy is estimated simply by counting vertices. It is important to note that this implies the \( KE \) cannot be estimated by evaluating \(-t \sum_{ij} \hat{a}_i^\dagger \hat{a}_j \) in the \( \Psi \) configuration! Indeed, the total energy \( E \) can be estimated by counting vertices: \( E = -\partial / \partial \beta (\ln Z) \)
so from Equation 4.41, and recalling that $\Delta \tau = \beta / L$, 

$$E - n_c L^d C_{\text{link}} - L^d C_{\text{onsite}} = -\frac{1}{Z} \frac{\partial}{\partial \beta} \lim_{L \tau \to \infty} T r \psi_{\tau, F} \left( \frac{\beta}{L \tau} \right) \sum_u F_u \prod_u \langle \psi'_u \left| (-\hat{h}_u) F_u \right| \psi_u \rangle$$

$$= \frac{\left[ \sum_u F_u \right]}{\beta} \text{MC}$$

(4.71)

where $\sum_u F_u$ is exactly the total number of all vertices. One tricky part of energy estimation is to remember that several constants, $C_{\text{link}}$ and $C_{\text{onsite}}$, were added to the Hamiltonian; the energy estimator must be adjusted to take these into account.

The imaginary time Green function can be written as the time-ordered product 

$$G(r_0, r_1, \tau, \tau') = \left\langle \hat{a}_{r_0}(\tau) a_{r_1}^\dagger(\tau') \right\rangle$$

(4.72)

For simplicity, we assume a translationally invariant system so that 

$$G(r, \tau) = \left\langle \hat{a}_0(0) a_r^\dagger(\tau) \right\rangle.$$ 

(4.73)

Within the worldline configuration and without a worm, $\left\langle \hat{a}_0(0) a_r^\dagger(\tau) \right\rangle_{\text{MC}}$ always evaluates to 0 except at a vertex of the kinetic term, where $r$ is a neighbor of site 0 and $\tau = 0$. However, the Green function weight naturally appears during the worm update step because the head is $\hat{a}_{r_0}(\tau_h) \ (\hat{a}_{r_0}^\dagger(\tau_h))$ and the tail is $\hat{a}_{r_1}(\tau_t) \ (\hat{a}_{r_1}^\dagger(\tau_t))$. In fact, the worm is explicitly sampling configurations based on the probability distribution $w_t w_h e^{-\beta \hat{H}}$ (the Green function). Then the Green function estimator is the almost-trivial estimator 

$$G(r_0, r_1, \tau) = \frac{1}{L^d \beta \Delta \tau \eta^2} \frac{1}{N_W} \left\langle \hat{N}^W(r_0, r_1, \tau) \right\rangle_{\text{MC}}$$

(4.74)

where $\hat{N}^W(r_0, r_1, \tau)$ is the number of times that the head and tail of the worm satisfy $r = r_0 - r_1$ and $\tau = \tau_h - \tau_l$ during the lifetime of a single worm and $N_W$ is the number attempts to insert a worm over the entire QMC simulation. Note that $\eta^{-2} \propto \Delta \tau$, as described in the caption of Figure 4.5. The factor of $\beta$ appears because we are counting all states of the worm when only the relative time between the head and the tail is $\tau$ and the $L^d$ appears because we have assumed the system is translationally invariant and averaged over the center of mass coordinate. This estimator is trivially extended to the full Green
Figure 4.9: Consider the winding number of this 1D configuration with 6 sites. Two bosons hop from site 1 to site 2 and only one hops from site 2 to site 1, giving a winding number of 1. This is true for every link in this configuration so the winding number is \( W_x = 1 \).

function \( G(r_0, r_1, \tau, \tau') \).

The superfluid susceptibility \( \chi \) is related to the imaginary time Green function in a uniform system by

\[
\chi = \int d\tau \sum_r G(r, \tau). \tag{4.75}
\]

Upon examination of the Green function in Equation 4.74, the estimator for the susceptibility is proportional to the length \( \hat{l}_W \) of each worm in imaginary time, or

\[
\chi = \frac{1}{\beta L^d} \langle \hat{l}_W \rangle_{MC} \tag{4.76}
\]

The final observable that we discuss is the superfluid density \( \rho_s \). There is no universally accepted definition of \( \rho_s \). The definition usually applied to world-line algorithm simulations measures the response

\[
\rho_s = \frac{1}{2(t/n_c)L^d} \left. \frac{\partial^2 F}{\partial \theta^2} \right|_{\theta=0} \tag{4.77}
\]

of the free energy \( F \) to a change in a gauge field \( \theta \) coupled to bosons, which manifests as a twisted boundary condition in a periodic system. However, at finite temperatures in 1D and 2D systems, this estimator differs from another common definition discussed.
in Section 2.1.1: the coefficient of the phase fluctuation term $|\nabla \theta|$ in the effective long-wavelength action Equation 2.7 or Equation 2.13. These two definitions are nearly equal in 3D, with a difference $\sim e^{-2\pi^2\rho_s L^2}$, but differ significantly in 1D. As usual, 2D is a marginal case and studies have observed in a square system of any size $L^2$, the value of $\rho_s(T_c)$ differs by $1 - 16\pi e^{-4\pi} < 2 \times 10^{-4}$.

Numerically applying a twist $\theta$ is unnecessary (and impossible) in a world-line simulation. Instead, $\rho_s$ is related to the number of boson paths that wind around the simulation cell, called the winding number as elucidated in the derivation below.

Recall that $F = -T \ln Z$ and write the partition function in boson Fock space as

$$Z[\theta] = Tr_{\Psi} \prod_u w_{\text{on-site},u} \prod_u w_{\text{link},u} \tag{4.78}$$

made up of onsite weights $w_{\text{on-site},u} = \langle \psi'_u \big| 1 - \Delta \tau \hat{h}_{\text{on-site},u} \big| \psi_u \rangle$ and bond or link weights $w_{\text{link},u} = \langle \psi'_u \big| 1 - \Delta \tau \hat{h}_{\text{link},u}[\theta] \big| \psi_u \rangle$, where $\hat{h}_{\text{link},u}[\theta] = \hat{a}_i^\dagger \hat{a}_j e^{i\theta \cdot (r_j - r_i)} + \hat{a}_j^\dagger \hat{a}_i e^{i\theta \cdot (r_i - r_j)}$. For simplicity we assume the field $\theta = |\theta| \hat{e}_x$ in the $x$ direction. Then

$$\frac{\partial^2 F}{\partial \theta^2} = -\frac{1}{\beta} \left( \sum_u Tr_{\Psi} W(\Psi) \frac{\partial^2 w_{\text{link},u}/\partial \theta^2}{w_{\text{link},u}} Z + \sum_{u \neq v} Tr_{\Psi} W(\Psi) \frac{\partial w_{\text{link},u}/\partial \theta}{w_{\text{link},u}} \times \frac{\partial w_{\text{link},v}/\partial \theta}{w_{\text{link},v}} Z \right)$$

$$- \left[ \sum_u Tr_{\Psi} W(\Psi) \frac{\partial w_{\text{link},u}/\partial \theta}{w_{\text{link},u}} Z \right]^2 \right) \tag{4.79}$$

where $W(\Psi)$ is the total weight of configuration $\Psi$. With the substitution of $\sum_{u \neq v}(\cdots) = [\sum_u (\cdots)]^2 - \sum_u (\cdots)^2$, the of the definition of each $w_{\text{link}}$ term, and recognizing that the
Monte Carlo weight is $W(\Psi)/Z$, we obtain

$$\frac{\partial^2 F}{\partial \theta^2}_{\theta=0} = -\frac{1}{\beta} \left( \sum_u \frac{\langle \psi^\prime_u | r_{ji}^2 (\hat{a}^\dagger_i \hat{a}_j + \hat{a}^\dagger_j \hat{a}_i) | \psi_u \rangle}{\langle \psi^\prime_u | \hat{a}^\dagger_i \hat{a}_j + \hat{a}^\dagger_j \hat{a}_i | \psi_u \rangle} \right)$$

$$+ \left\langle \left[ \sum_u \frac{\langle \psi^\prime_u | r_{ji} (\hat{a}^\dagger_i \hat{a}_j - \hat{a}^\dagger_j \hat{a}_i) | \psi_u \rangle}{\langle \psi^\prime_u | \hat{a}^\dagger_i \hat{a}_j + \hat{a}^\dagger_j \hat{a}_i | \psi_u \rangle} \right] - \left[ \sum_u \frac{\langle \psi^\prime_u | r_{ji} (\hat{a}^\dagger_i \hat{a}_j - \hat{a}^\dagger_j \hat{a}_i) | \psi_u \rangle}{\langle \psi^\prime_u | \hat{a}^\dagger_i \hat{a}_j + \hat{a}^\dagger_j \hat{a}_i | \psi_u \rangle} \right] \right\rangle^2$$

$$= -\frac{1}{\beta} \left[ \langle N_{\text{link}} \rangle + L^2 \langle W_x^2 \rangle - \langle N_{\text{link}} \rangle - L^2 \langle W_x \rangle^2 \right]$$

(4.81)

The first and third terms each count the number of vertices because $r_{ij} = r_j - r_i = \pm 1$ and because only one pair of operators from $\hat{a}^\dagger_i \hat{a}_j \pm \hat{a}^\dagger_j \hat{a}_i$ yields a nonzero expectation value for the pair of states $\psi^\prime_u, \psi_u$, which is equal to the denominator up to the sign. The winding number $W_x$ estimates the current of bosons across an arbitrary plane of the system (defined here by $\theta = |\theta| \hat{e}_x$ so it is the $yz$ plane) and $\langle W_x \rangle = 0$ because of mirror symmetry. Algorithmically, the system is divided by a plane at $r = (n + 0.5) a_{\text{Latt}} \hat{e}_x$ and $W_x$ counts the number of bosons that jump from site $i$ to site $j$ (from the left $n a_{\text{Latt}} \hat{e}_x$ to the right $(n+1) a_{\text{Latt}} \hat{e}_x$) less the number of bosons that jump from $j$ to $i$. The factor $L^2$ in Equation 4.81 results from restriction to a single plane across which $W_x$ is measured; note that $\rho_s$ is not so well-defined in a system where the number sites in the $x$ and the $y$ direction, say, are unequal. The final estimator for the superfluid density is

$$\rho_s = \frac{dL^{2-d}}{\beta t} \langle W_x^2 \rangle.$$  

(4.82)

### 4.4 Analytic Continuation

A drawback to most forms of quantum Monte Carlo is the restriction to imaginary time. All correlators may only be estimated as a function of space and imaginary time $\tau$ or Matsubara frequency $\omega_n$. This very real limitation prevents direct calculations of dynamic response functions that describe the response of experimental systems to real frequency.
or time-dependent probes. Fortunately, the inherent properties of the Green function and other correlators reveal that their values at all $\omega_n$ uniquely specify their value over the entire complex frequency domain. This enables an imaginary time Green function $G$ to be analytically continued from a discrete set of $\tau$ or $\omega_n$ points to the full range of real $t$ or $\omega$ in principle, although in practice this procedure is very nontrivial. It is extremely sensitive to numerical noise in the measured $G^{QMC}$ because the analytic continuation turns out to require inversion of a Laplace transform. In the following section, we describe analytic continuation in more detail and discuss two prescriptions for minimizing the influence of error in $G^{QMC}$ and for maximizing the likelihood of the real time Green function: singular value decomposition (SVD) and the maximum entropy method (MEM). The exposition below is restricted to the bosonic Green and spectral function because in this thesis it is only applied to the Bose-Hubbard model.

### 4.4.1 Analytic Continuation Derivation

The goal of analytic continuation is to analytically continue a Green function $G$ in imaginary time $\tau$ or in Matsubara frequency $\omega_n = \frac{2\pi n}{\beta}$ to a real time $t$ or a real frequency $\omega$ Green function $G$, where the integer $n$ is odd for fermions and even for bosons. Note that the imaginary correlation $G(\tau)$ must be periodic over the interval $[0, \beta]$ for bosons, i.e. $G(\tau) = G(\tau + \beta)$ where $\beta = \frac{1}{T}$ is the inverse temperature. The Green functions in imaginary or real variables are related by

$$G(i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} G(\tau)$$  \hspace{1cm} (4.83) \\
$$G(\omega) = \int_0^\infty dt e^{i\omega t} G(t).$$  \hspace{1cm} (4.84)

The real time Green function $G(z)$ is a Fourier/Laplace transform of a causal and decaying real time $G(t)$:

$$G(z) = \int_0^\infty dt e^{izt} G(t), \text{ Im}(z) > 0,$$  \hspace{1cm} (4.85)

where $z$ is a complex frequency. At first glance, this transform appears to be multi-valued be-
cause \( G(z) = G(z) + e^z + 1 \) at all \( z = i\omega_n \). However, Baym and Mermin showed that as long as \( G(z) \) is analytical in the upper half plane, \( G(i\omega_n) = G(i\omega_n) \) and \( \lim_{z \to \infty} zG(z) \to \text{constant} \), the analytical continuation from \( G(i\omega_n) \) to \( G \) is unique and is analytically continued by

\[
\lim_{i\omega_n \to \omega + i\eta} G(\omega_n) = \hat{G}(\omega) + iA(\omega).
\]

(4.86)

where \( \hat{G} \) and \( A \) are the real and imaginary parts of the retarded Green function, and \( A \) is commonly called the spectral function. If the Green function describes current correlations then \( A \) is the conductivity, while if the Green function is the single body density matrix \( G(r, r', \tau) = \langle [\hat{a}^\dagger(r, \tau)\hat{a}(r', 0)] \rangle \), the spectral function is denoted by \( A(k, \omega) \) and describes the single particle excitation spectrum.

The spectral representation for \( G(z) \) is given by integrating around the real line cut and yields the inverse transform

\[
G(z) = -\frac{1}{\pi} \int_{-\infty}^{\infty} d\omega A(\omega) \frac{1}{z - \omega}.
\]

(4.87)

When this relation is used to relate the real part to the imaginary part of \( G \), it is known as the Kramers-Kronig relation. With the choice \( z \to i\omega_n \), the imaginary and real frequency correlations are related by the exact relation

\[
G(i\omega_n) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \frac{\omega}{\omega^2_n + \omega^2} A(\omega)
\]

\[
= \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega K(\omega_n, \omega) A(\omega)
\]

(4.88)

with the kernel of the transformation

\[
K(\omega_n, \omega) = \frac{\omega}{\omega^2_n + \omega^2}
\]

(4.89)

With appropriate Fourier \((\int d\omega \exp(-i\omega t))\) and Laplace \((\sum_n \exp(-\omega_n \tau))\) transformations,
the kernel can be rewritten as

\begin{align}
K(\tau, \omega) &= \frac{e^{-\tau \omega}}{1 - e^{-\beta \omega}} \quad (4.90) \\
K(\tau, t) &= \sqrt{\frac{\pi}{2 \beta}} \left( \frac{\sinh (2\pi t/\beta)}{\cosh (2\pi t/\beta) - \cos (2\pi \tau/\beta)} - 1 \right) \quad (4.91) \\
K(\omega_n, t) &= \sqrt{\frac{\pi}{2}} e^{-\omega_n t} \quad (4.92)
\end{align}

Note that these kernels are written for bosons; the sign of the exponential in the denominator of the Equation 4.90 is positive for fermions. Sometimes modification of the kernel and the associated spectral function can be useful. For example, \( K(\tau, \omega) \) diverges as \( \omega \to 0 \) for bosons so it is convenient to rescale the transformation

\[ \mathcal{G}(\tau) = \int d\omega \frac{e^{-\tau \omega}}{1 + e^{-\beta \omega}} \left( \frac{1 + e^{-\beta \omega}}{1 - e^{-\beta \omega}} A = \int d\omega \frac{e^{-(\tau - \beta/2) \omega}}{2 \cosh (\omega \beta/2)} \tilde{A} \quad (4.93) \]

This transformation has the added benefit that \( \tilde{A}(\omega) = \coth (\omega \beta/2) A(\omega) \) is positive definite.

**Sum Rule for \( A(\omega) \)**

It is essential to check the spectral function that results from analytic continuation are consistent with constraints such as positive-definiteness and sum rules. Here we discuss the sum rules for \( A(\omega) \) for bosons, fermions and hard core boson lattice systems and their relation to the Green function.

As discussed above, the imaginary time Green function for a system described by the Hamiltonian \( \hat{H} \) is

\[ \mathcal{G}_q(\tau) \equiv \left\langle \hat{b}_q(\tau)\hat{b}_q^\dagger(0) \right\rangle = \left\langle e^{\tau \hat{H}}\hat{b}_q e^{-\tau \hat{H}}\hat{b}_q^\dagger \right\rangle = \frac{1}{\beta} \sum_{\omega_n} e^{-i\omega_n \tau} \mathcal{G}_q(\omega_n), \quad (4.94) \]

where \( \hat{b}_q (\hat{b}_q^\dagger) \) is the annihilation (creation) operator for \( q \)-momentum state and Matsubara
frequencies are denoted $\omega_n$. The spectral function is defined as

$$A_q(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} \rho(t)$$

$$= \int_{-\infty}^{\infty} dt e^{i\omega t} \langle [\hat{b}_q(t), \hat{b}^+_q(0)] \rangle$$

$$= \int_{-\infty}^{\infty} dt e^{i\omega t} \left( e^{i\hat{H}t} \hat{b}_q e^{-i\hat{H}t} \hat{b}_q^+ - \hat{b}_q^+ e^{i\hat{H}t} \hat{b}_q e^{-i\hat{H}t} \right)$$

$$= \int_{-\infty}^{\infty} dt \frac{e^{i\omega t}}{Tr e^{-\beta \hat{H}}} \sum_{\ell m} e^{-\beta \omega \ell} \left[ \langle \ell | \hat{b}_q^+ m \rangle \langle m | \hat{b}_q \ell \rangle e^{i\omega_{\ell m} t} - \langle \ell | \hat{b}_q^+ m \rangle \langle m | \hat{b}_q^+ \ell \rangle e^{-i\omega_{\ell m}} \right]$$

$$= \frac{2\pi}{Tr e^{-\beta \hat{H}}} \sum_{\ell m} e^{-\beta \omega \ell} \left[ \frac{1}{2} \delta(\omega + \omega_{\ell m}) - \frac{1}{2} \delta(\omega - \omega_{\ell m}) \right], \quad (4.95)$$

where $\omega_{\ell m} = \omega_\ell - \omega_m$ and $\hat{H} |\ell\rangle = \omega_\ell |\ell\rangle$.

Analytic continuation and a summation over bosonic (−) or fermionic (+) Matsubara frequencies ($\sum_{\omega_n \frac{e^{-i\omega_{\ell m} \tau}}{\omega_n + \omega} = \frac{e^{-\omega\tau}}{1 \pm e^{-\beta \omega}}$) links the Green and spectral functions by the formulae

$$G_q(\omega_n) = -\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{A_q(\omega)}{i\omega_n - \omega} \quad (4.96)$$

$$G_q(\tau) = \frac{1}{\beta} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_q(\omega) \sum_{\omega_n} \frac{e^{i\omega_{\ell m} \tau}}{i\omega_n + \omega}$$

$$= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_q(\omega) \frac{e^{-\omega \tau}}{1 \pm e^{-\beta \omega}} \quad (4.97)$$

where + corresponds to fermions and − to bosons. This allows us to identify the kernel of this transformation as $K(\omega, \tau) = \frac{e^{-\omega \tau}}{1 \pm e^{-\beta \omega}}$.

To link $G_q(\tau)$ to the sum rule for $A_q(\omega)$, consider the Green function at $\tau = 0, \beta$,

$$G_q(\tau = 0) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_q(\omega) \frac{1}{1 \pm e^{-\beta \omega}} \quad (4.98)$$

$$G_q(\tau = \beta) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_q(\omega) \frac{e^{-\beta \omega}}{1 \pm e^{-\beta \omega}} \quad (4.99)$$

$$G_q(0) \pm G_q(\beta) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_q(\omega) \frac{1 \pm e^{-\beta \omega}}{1 \pm e^{-\beta \omega}}$$

$$= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_q(\omega) \quad (4.100)$$

This yields a condition on both the normalization of $A_q(\omega)$ and on the relation of $G_q(0)$
and $G_q(\tau)$. Both conditions are useful in analytic continuation, and the latter is particularly useful for numerical analytic continuation because the world-line QMC estimator for $G_q(\tau)$ only includes information of either $G_q(0)$ or $G_q(\tau)$. The fermionic kernel is well behaved and Equation 4.100 is a good constraint. However, the bosonic kernel is singular at $\omega = 0$, so the integral equation is typically transformed into

\begin{align*}
G_q(\tau) & = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_q(\omega) \frac{1 + e^{-\beta\omega}}{1 - e^{-\beta\omega}} \frac{e^{-\omega\tau} - e^{-\beta\omega}}{1 + e^{-\beta\omega}} \\
G_q(\tau) & = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_q(\omega) \coth\left(\frac{\beta\omega}{2}\right) \frac{e^{-\omega\tau}}{1 + e^{-\beta\omega}},
\end{align*}

(4.101)
(4.102)

where the kernel is now $\frac{e^{-\omega\tau}}{1 + e^{-\beta\omega}}$ and analytic continuation now attempts to calculate $A_q^c(\omega) = A_q(\omega) \coth(\beta\omega/2)$. This leads to the sum rule for $A_q^c(\omega)$,

$$G_q(0) + G_q(\beta) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_q^c(\omega).$$

(4.103)

The preceding equations imply that the spectral function can be properly normalized using only the (measurable) Green function $G_q(\tau)$ at both $\tau = 0$ and $\tau = \beta$.

To derive the normalization of $A_q(\omega)$ for hard core boson systems, we need to expand
\[ A(\omega) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_q(\omega) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{2\pi}{\text{Tr} e^{-\beta H}} \sum_{\ell m} e^{-\beta \omega_{\ell}} \left[ \left| \langle m | \hat{b}^\dagger \ell \rangle \right|^2 \delta(\omega + \omega_{\ell m}) - \left| \langle m | \hat{b} \ell \rangle \right|^2 \delta(\omega - \omega_{\ell m}) \right] \]

\[ = \frac{1}{\text{Tr} e^{-\beta H}} \sum_{\ell m} e^{-\beta \omega_{\ell}} \left[ \left| \langle m | \hat{b}^\dagger \ell \rangle \right|^2 - \left| \langle m | \hat{b} \ell \rangle \right|^2 \right] \]

\[ = \frac{1}{\text{Tr} e^{-\beta H}} \sum_{\ell} e^{-\beta \omega_{\ell}} \left[ \sum_m \langle \ell | \hat{b}^\dagger_m \rangle \langle m | \hat{b}^\dagger \ell \rangle \langle m | \hat{b} \ell \rangle \right] - \sum_m \langle \ell | \hat{b}^\dagger_m \rangle \langle m | \hat{b} \ell \rangle \]

\[ = \frac{1}{\text{Tr} e^{-\beta H}} \sum_{\ell} e^{-\beta \omega_{\ell}} \left[ \langle \ell | \hat{b}^\dagger \hat{b} \ell \rangle - \langle \ell | \hat{b}^\dagger \hat{b} \ell \rangle \right] \]

\[ = \frac{1}{\text{Tr} e^{-\beta H}} \sum_{\ell} e^{-\beta \omega_{\ell}} \left[ \langle \ell | \hat{b} \hat{b}^\dagger \ell \rangle - \langle \ell | \hat{b}^\dagger \hat{b} \ell \rangle \right] \]

\[ = \frac{1}{\text{Tr} e^{-\beta H}} \sum_{\ell} e^{-\beta \omega_{\ell}} \left[ \langle \ell | \hat{b} \hat{b}^\dagger \ell \rangle - \langle \ell | \hat{b}^\dagger \hat{b} \ell \rangle \right] \]

\[ \text{The bosons are hard core in real space but not in momentum space so we must consider this commutator in real space. Say } \hat{b}_q (\hat{b}^\dagger_q) = \frac{1}{\sqrt{V}} \sum_r \hat{b}_r (\hat{b}^\dagger_r) e^{\pm qr}, \text{ where } V \text{ is the system volume. Then the commutator} \]

\[ [\hat{b}_q, \hat{b}^\dagger_q] = \frac{1}{V} \sum_{r,r'} e^{-iqr'} \left( \hat{b}_r \hat{b}^\dagger_{r'} - \hat{b}^\dagger_r \hat{b}_{r'} \right) \]

\[ = \frac{1}{V} \sum_{r,r'} e^{-iqr'} \delta_{r,r'} [\hat{b}_r, \hat{b}^\dagger_r] \]

\[ = \frac{1}{V} \sum_r [\hat{b}_r, \hat{b}^\dagger_r] . \]

Regular bosons commute, so \([\hat{b}_r, \hat{b}^\dagger_r] = 1\) and \(\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_q(\omega) = 1\). However, hard core bosons anticommute in real space \(\{\hat{b}_r, \hat{b}^\dagger_r\} = 1\), so the commutation relation is \([\hat{b}_r, \hat{b}^\dagger_r] = 1 - 2\hat{b}_r \hat{b}^\dagger_r\). Note that only fermions, and not hard core bosons, anticommute in momentum space. Then
the sum rule reduces to

\[
\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_q(\omega) = \frac{1}{V} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{Tr} e^{-\beta H} \sum_\ell e^{-\beta \omega_\ell} \left\langle \ell \left| V - 2 \sum_r b_r^\dagger b_r \right| \ell \right\rangle \quad (4.108)
\]

\[
= 1 - 2\bar{n},
\]

where \(\bar{n}\) is the average density per site.

Thus for hard core bosons, we can use the formula \(G_q(0) - G_q(\beta) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_q(\omega) = 1 - 2\bar{n}\) to calculate whichever of \(G_q(0)\) and \(G_q(\beta)\) was not estimated by QMC. Then the formula \(G_q(0) + G_q(\beta) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_q^c(\omega)\) is a check on the normalization of the weighted spectral function \(A_q^c(\omega)\) calculated via analytic continuation.

In quantum many body systems, the obstacle between numerical simulations and spectral functions is inversion of Equation 4.88. Analytic forms of \(G\) defined over all \(\omega_n\) can be exactly analytically continued to \(G\). However, \(G^{qmc}\) is only evaluated at a finite number of \(\omega_n\) and has, at the least, statistical error. The Lorentzian or exponential kernels tend to magnify any errors in unpredictable ways and so the inversion of Equation 4.88 requires careful treatment beyond a least-squares type of fit.

At this point we discretize and impose cutoffs so that all variables \(\omega_n, \tau, \omega, t\) are finite in number and the \(G\) and \(G\) are only evaluated at the included values of \(t\) and \(\omega\) or \(\tau\) and \(\omega_n\). From the perspective of numerical simulations, this is a natural course to take. Now \(G_\nu\) and \(G_\mu\) are vectors and \(K_{\mu\nu}\) is a matrix operator that takes a vector from the (real variable) \(\nu\) to the (imaginary variable) \(\mu\) Hilbert space. The kernel is not necessarily a square matrix.

### 4.4.2 Maximum Entropy Method

Briefly, the maximum entropy method (MEM) constructs the most likely spectral function given the data \(G^{qmc}\) and other information \(I\) such as a basic model for the spectral function \(A\) and sum rules. In other words, it maximizes the probability \(P(A^{image}|G^{qmc}, I)\) \cite{163, 164}. Note that it is trivial to generate the Green function \(G^{image}\) from a choice for \(A^{image}\) by

\[
G_\mu^{image} = \sum_\nu K_{\mu\nu} A_\nu^{image}.
\]
We begin by decomposing $P(A_{image}|G^{qmc}, I)$ into

$$P(A_{image}|G^{qmc}, I) \propto P(G^{qmc}|A_{image}, I) P(A_{image}|I),$$

the likelihood function $P(G^{qmc}|A_{image}, I)$ and the prior probability distribution $P(A_{image}|I)$. The former is the probability to measure $G^{qmc}$ if the spectral function was actually $A_{image}$ and given information $I$. In this and in following equations, $\propto$ simply represents a suppressed normalization factor.

Assuming that all errors are due to independent Gaussian noise,

$$P(G^{qmc}|A_{image}, I) \propto e^{-\chi^2/2} \quad \text{where} \quad \chi^2 = \sum_{\mu} \left( \frac{(g_{\mu}^{image} - g_{\mu}^{qmc})^2}{\sigma^2_{\mu}} \right).$$

If we have no further information, we cannot evaluate $P(A_{image}|I)$ and thus maximizing $P(A_{image}|G^{qmc}, I)$ is equivalent to minimizing $\chi^2$. This often yields quite poor results because there usually exists a large and diverse class of $A_{image}$ functions that minimize the $\chi^2$ of noisy $G^{qmc}$. Ringing or oscillations as a function of $\nu$ is a typical undesirable feature.

The image spectral function $A_{image}$ can be greatly improved through a few simple steps and assumptions. The spectral function is positive and additive, which implies that a reasonable prior probability distribution is \[ P(A_{image}|I, m_{\nu}, \alpha) \propto \exp(\alpha S[A_{image}, m_{\nu}]) \quad (4.113) \]

Here $\alpha$ and the “default” or minimal model $m_{\nu}$ are additional parameters, and $S$ represents an entropic cost for structure, like ringing, not built into $m_{\nu}$. The default model is hand picked and is effective even as a constant or a simple function like a Gaussian; its primary purpose is to constrain the information content of $A_{image}$.

Now we have a compact form for the probability of a spectral function $A_{image}$ as

$$P(A_{image}|G^{qmc}, I) \propto P(G^{qmc}|A_{image}, I) P(A_{image}|I) \propto \exp(-\chi^2/2 + \alpha S[A_{image}, m_{\nu}])$$

and we can maximize it by minimizing $-\chi^2/2 + \alpha S[A_{image}, m_{\nu}]$. $\alpha$ is still a mysterious
parameter but we can choose an optimal value $\hat{\alpha}$ for it as follows.

Begin by defining the probability distribution with $\alpha$ integrated out and then Bayes’ theorem applied

$$P(A^{image}|G^{qmc},m_\nu) = \int d\alpha P(A^{image},\alpha|G^{qmc},m_\nu)$$

$$= \int d\alpha P(A^{image}|G^{qmc},m_\nu,\alpha)P(\alpha|G^{qmc},m_\nu).$$

(4.116)

The probability $P(\alpha|G^{qmc},m_\nu)$ tends to be sharply peaked about $\hat{\alpha}$ for a large number of datapoints in $G^{qmc}$ because it is estimating a single parameter from all of them. Then the integral over $\alpha$ can be replaced with the single value of $\alpha = \hat{\alpha}$ or $P(A^{image}|G^{qmc},m_\nu) \propto P(A^{image}|G^{qmc},m_\nu,\hat{\alpha})$.

Now we calculate the probability distribution for $\alpha$ to find $\hat{\alpha}$. We expand

$$P(\alpha|G^{qmc},m_\nu) \propto \int DA P(A,\alpha|G^{qmc},m_\nu) = \int DA DG P(G,A,\alpha|m_\nu)$$

$$\propto \int DA P(G^{qmc}|A,\alpha|m_\nu) \int DG P \text{ is sharply peaked about } G^{qmc}$$

$$\propto \int DA P(G^{qmc}|A,\alpha,m_\nu)P(A,\alpha|m_\nu) \quad \text{By Bayes’ theorem}$$

$$\propto \int DA P(G^{qmc}|A,\alpha,m_\nu)P(A|\alpha,m_\nu)P(\alpha|A,m_\nu).$$

(4.118)

Presumably all values of $\alpha$ are equally likely so that $P(\alpha|A,m_\nu) = \text{constant}$. The forms for the other likelihood function and entropic prior have already been found in Equations 4.112 and 4.113. Then the $\hat{\alpha}$ that maximizes the probability of $\alpha$, $\frac{\delta}{\delta \alpha} P(\alpha|G^{qmc},m_\nu) = 0$, falls out of the Gaussian integral as

$$2\hat{\alpha} S[A^{image},m_\nu] = \sum_\nu \frac{\lambda_\nu}{\lambda_\nu + \hat{\alpha}}$$

(4.119)

where $\lambda_\nu$ are the eigenvalues of $M_{\nu\nu'} = \frac{\partial^2 S}{\partial A_\nu \partial A_{\nu'}}$.

There are many implementations of this MEM procedure throughout the scientific world. The distinguishing characteristic between them is the method used to sample the space of $A^{image}$. Some use the singular value decomposition of the kernel to define a function space. We prefer a tempered, importance-sampled Monte Carlo search of the probability
distribution in Equation 4.115 that proceeds as follows:

1. The MEM simulation begins with the data $G_{\mu}^{qmc}$, an initial guess $A_{\nu}^{image}$, a default model $m_{\nu}$ and large $\alpha$ and effective temperature $T^{MC}$.

2. Propose a new $A_{\nu}^{image*}$ where some weight has been moved from $A_{i}^{image}$ to $A_{j}^{image}$.

3. Accept $A_{\nu}^{image*}$ with probability $e^{-\Delta\chi^2/2+\alpha\Delta S}$, where $\Delta\chi^2$ and $\Delta S$ are the change in the $\chi^2$ and in the entropy. Reject the move if either $A_{i}^{image}$ or $A_{j}^{image}$ is negative.

4. Repeat steps 2 and 3 to achieve equilibrium, then lower the temperature and continue until the highest-probability $A^{image}$ has been found. Occasionally check the normalization of $A^{image}$.

5. Check to see if the condition for $\hat{\alpha}$, Equation 4.119 has been achieved. If not, update $\alpha$ and repeat steps 2, 3 and 4.

The maximum entropy method does require some amount of fine-tuning. For example, $A^{image}$ tends to be less smooth when the error in $G^{qmc}$ is small and requires manual smoothing or an average over $A^{image}$ from multiple MEM runs with the same $G^{qmc}$. Also, $A^{image}$ can be biased to obey sum rules through the entropic prior and must be positive definite [166].

### 4.4.3 The Singular Value Decomposition Approach

The singular value decomposition (SVD) of the kernel has the form

$$K_{\mu\nu} = U_{\mu\mu}W_{\mu\nu}V_{\nu\nu}^T$$

where $U$ and $V$ are orthonormal matrices consisting of eigenvectors $\{u_\alpha\}$ and $\{v_\alpha\}$ of $(KK^T)_{\mu\mu}$ and $(K^TK)_{\nu\nu}$, respectively. The diagonal $W$ matrix has elements $W_\alpha\delta_{\alpha\alpha}$ and $W_1 > W_2 > \ldots$.

The goal of numerical techniques for analytic continuation is to somehow control the appearance of spurious features caused by noise in the measured $G^{qmc}$ [167]. Explicitly split
\( G^{\text{mc}} \) into contributions due to signal \( G_{\text{sig}} \) and due to noise \( G_{\text{noise}} \):

\[
G_{\mu} = G_{\mu}^{\text{sig}} + G_{\mu}^{\text{noise}}.
\]  

(4.121)

Now define the projection

\[
F_{\alpha} = \langle u_{\alpha} | G \rangle
\]

(4.122)

\[
= \langle u_{\alpha} | G_{\text{sig}} \rangle + \langle u_{\alpha} | G_{\text{noise}} \rangle
\]

(4.123)

\[
= F_{\alpha}^{\text{sig}} + F_{\alpha}^{\text{noise}}.
\]

(4.124)

Then the inversion to \( G_{\nu} \) is accomplished through

\[
A_{\nu} = \min(\text{Dim}[\mu], \text{Dim}[\nu]) \sum_{\alpha=1}^{\text{Dim}[\nu]} \frac{F_{\alpha}}{w_{\alpha}v_{\alpha}}.
\]

(4.125)

This prescription is exact thus far but is essentially useless. Typically only 30 eigenvalues \( \omega_{\alpha} \) are greater than \( 10^{-10} \) [shown in Figure 4.10(left panel)], while the overlap between the noise and the eigenvectors \( F_{\alpha}^{\text{noise}} \) can only be expected to decrease to the scale of the noise, usually no smaller than \( 10^{-6} \). If we assume that \( v_{\alpha} \) is of order unity for all \( \alpha \), it is obvious that the noise from large \( \alpha \) eigenvectors will overwhelm the signal from small \( \alpha \) eigenvectors. A cutoff \( \alpha^* \) on the included eigenvectors is required.

Convergence requires that \( F_{\alpha} \) decays at least as fast as \( w_{\alpha} \). This must be the case for \( F_{\alpha}^{\text{sig}} \), but \( F_{\alpha}^{\text{noise}} \geq \sigma \) where \( \sigma \) is the noise or error in the measurement. A straightforward way to determine the cutoff is to only include \( \alpha \) such that \( F_{\alpha} > \sigma \). When plotted, \( |F_{\alpha}| \) typically decays rapidly with \( \alpha \) until the error level \( \sigma \) is reached and \( |F_{\alpha}| \) randomly jumps about \( \sigma \). The efficacy of this method can depend quite a bit on the choice of kernel; depending on the system, the overlap \( F_{\alpha} \) may be more favorable for certain choices of \( \mu \) and \( \nu \).

We conclude this section on analytic continuation via SVD of the kernel with an observation about its likely regime of applicability. It is clear in Figure 4.10(right panel) that the small-\( \alpha \) eigenvectors of \( K_{\mu\nu} \) have the most structure near zero frequency. Given numerical errors on the order of at least \( 10^{-6} \), we cannot expect to construct \( A \) from more than one
or two dozen eigenvectors. This restriction implies that SVD should be very effective when $A$ has a lot of weight at low $\omega$ or $t$, but should be less efficacious when $A$ is sharply peaked at relatively large $\omega$ or $t$. In addition, there is no guarantee that $\omega A$ is positive definite or that $A$ obeys any sum rules.

4.4.4 Comparing SVD and Max-Ent Methods

Both SVD and MEM have strengths and weaknesses that largely stem from the spectral function space. A general rule of thumb for SVD is: if the real frequency Green or spectral function is expected to have a large overlap with the low-lying eigenvectors of the kernel, SVD is likely to produce reasonable results. If there is very little overlap, however, the real frequency output is likely to be very noisy. On the other hand, MEM can operate over a general function space for the spectral function and can be counted on to accurately estimate features like a gap across zero energy or the $\omega$ positions of peaks in $A(\omega)$. Usually
okay but generically less reliable are the peak widths and the large-$\omega$ weight. We illustrate these observations with the following two examples.

**Spectral Function Heavily Weighted at $\omega = 0$**

We simultaneously illustrate the advantages of SVD and the shortcomings of MEM with the model spectral function

$$A_{\text{model}}(\omega) = \omega^3 e^{-\omega^2/2}.$$  

(4.126)

This is a relatively generic model for the conductivity. The imaginary time Green function $G_{\text{model}}(\tau)$ is obtained from Equation 4.93 and error is introduced from a normal distribution with standard deviation $10^{-3}$ [Figure 4.11(a)]. The spectral functions resulting from analytic continuation using MEM and SVD are shown in Figure 4.11(b).

The MEM result is an average over 20 MEM runs because when the error in $G_{\text{model}}(\tau)$ is very small, MEM tends to overfit with respect to $\chi^2$ and yields a jagged $A$. The peak position is well localized but the width estimate is less accurate. The sum rule $\int d\omega A(\omega)$ is correct to within 1%. To partially compensate for the emphasis on $\chi^2$ that results from
Figure 4.12: Model spectral function narrowly peaked far from the origin at $\beta = 20$. (a) The Green function $G_{\text{model}}$ with normally distributed error of order $10^{-5}$ and $G_{\text{image}}$ from MEM and SVD analytic continuation [see legend in (b)]. (b) The exact $A_{\text{model}}$ and $A_{\text{image}}$ from MEM and SVD analytic continuation. The MEM $A$ is from a single MEM run. (c) The eigenvalues $w_\alpha$ and the overlap $F_\alpha$ required to determine the SVD $\alpha$ cutoff; note that $F_\alpha$ asymptotes to the error $10^{-5}$.

Small error relative to $G$, the entropic prior can be tweaked by using a default model fixed at a larger, constant value.

The SVD $A$ is very close to $A_{\text{model}}$ with a cutoff $\alpha_c = 20$ [see Figure 4.11(c)]. Away from small and large $\omega$, $A$ is nearly perfect, while there is some noise near $\omega = 0$ and some ringing at large $\omega$. As discussed above, SVD works well here because a lot of the structure in $A_{\text{model}}$ is at small $\omega$ and there is no hard gap. The sum rule $\int d\omega A(\omega)$ is correct to within 0.1% even though $\omega A(\omega)$ is not positive-definite.

**Spectral Function Away from $\omega = 0$**

We contrast the spectral function of Equation 4.126 with

$$A_{\text{model}}(\omega) = -e^{-(\omega+1.5)^2/0.2^2} + e^{-(\omega-2.1)^2/0.3^2}. \quad (4.127)$$

This is a fair approximation of the spectral function of a Mott insulator. The imaginary time Green function $G_{\text{model}}(\tau)$ is obtained from Equation 4.93 and error is introduced from a normal distribution with standard deviation $10^{-5}$ [Figure 4.12(a)]. The spectral functions
resulting from analytic continuation using MEM and SVD are shown in Figure 4.11(b).

The MEM $A(\omega)$ plotted in Figure 4.12 comes from a single run because the significant error in $G^{\text{model}}(\tau)$ enables MEM to take the entropic prior into account. The peak position and the width estimate are quite accurate, as is the gap. The sum rule $\int d\omega A(\omega)$ is correct to within 1%.

It is difficult to even identify the two peaks in the SVD $A$ because of the overall ringing, even with the cutoff $\alpha_c = 20$ [see Figure 4.12(c)]. This uncertainty results from the fact that the low-$\alpha$ eigenvectors $v_\alpha$ have most of their structure at small $\omega$. Alternatively, a hard gap requires an exponentially decaying $G(\tau)$ and one can observe that is very hard to create from the appropriate low-$\alpha$ eigenvectors $u_\alpha$. The sum rule $\int d\omega A(\omega)$ is correct to within 1% and $\omega A(\omega)$ is not positive-definite. Even with significantly smaller error introduced into $G(\tau)$, in this case the SVD method is unsatisfactory because of the oscillations in the spectral function.

Both MEM and SVD methods for analytic continuation can be valuable. SVD does very well when the spectral function is known to be peaked near $\omega = 0$ and MEM can provide a useful check. On the other hand, characterizing a gap to excitations in a spectral function requires the MEM type of analytic continuation.


Appendix A

FROM THE OPTICAL Lattice

Potential to Hubbard Model

Parameters

Cold atom clouds can be diced into systems of reduced dimension by laser standing waves. For example, two counter-propagating laser beams create a stack of 2D potentials, 4 beams create an array of 1D tubes, and 6 beams create a 3D optical lattice of point-like potentials. Here, consider a 1D optical lattice formed by counterpropagating linearly polarized laser beams of wavelength \( \lambda = 2\pi/k \), which form a standing wave with nodes separated by a distance \( a_{\text{latt}} = \lambda/2 \). The laser’s electric field acts on atoms to produce a quasi-static potential according to the ac Stark effect. If the laser frequency is slightly lower than the transition frequency between two atomic levels (red-detuned), the atoms are attracted towards high intensities, i.e., the potential has minima at the intensity maxima; conversely, for a blue-detuned laser, the potential has minima at intensity minima. In either case one has a sinusoidal potential of spatial period \( a_{\text{latt}} = \lambda/2 \). It is conventional to work in units of the recoil energy \( E_R = \frac{\hbar^2 k^2}{2m} = \frac{2\pi^2 \hbar^2}{m\lambda^2} = \frac{\pi^2 \hbar^2}{2ma_{\text{latt}}^2} \), which is the change in kinetic energy of the atom associated with the emission or absorption of a photon with momentum \( k \). [6]

In the analysis below, for simplicity we consider a particle of mass \( m \) in a one-dimensional sinusoidal potential of depth \( V_0 \) and spacing \( a_{\text{latt}} \). The wavefunction satisfies the Schrödinger equation

\[
-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + \left( V_0 \sin^2 \frac{\pi x}{a_{\text{latt}}} \right) \psi(x) = E \psi(x).
\]
This is a form of Mathieu’s differential equation. The eigenenergies can be written in terms of Mathieu characteristic value functions as

\[ \frac{E_k}{E_R} = \alpha + \frac{V_0}{2E_R} \]  

(129)

where \( \alpha = \text{MathieuCharacteristicA} \left( \frac{k a_{\text{latt}}}{\pi}, -\frac{V_0}{4E_R} \right) \) (for concreteness we refer to the Mathieu functions as defined in Mathematica). This bandstructure is illustrated in Figure 13(a) and Figure 13(b) as a function of crystal momentum \( k \) (in the extended zone scheme) and lattice depth \( V_0 \). Eigenfunctions of crystal momentum (Bloch functions) can be written as linear combinations of even and odd Mathieu functions:

\[ \psi_k(x) = \text{MathieuC}[\alpha, -\frac{V_0}{4E_R}, \pi x a_{\text{latt}}] + (\text{sgn} k) \text{MathieuS}[\alpha, -\frac{V_0}{4E_R}, \pi x a_{\text{latt}}]. \]  

(130)

These Bloch functions are illustrated in Figure 13(e-g). It can be verified that they satisfy \( \psi_k(x + a_{\text{latt}}) = e^{ika_{\text{latt}}} \psi_k(x) \), and that they are normalized such that

\[ \int_0^1 dx \left| \psi_k(x) \right|^2 = 1. \]  

(131)

The Schrödinger equation can be approximated by a tight-binding model by representing the Hilbert space using a basis of localized Wannier functions. The lowest-band Wannier function \( W(x) \) can be constructed by taking a linear combination of Bloch functions, with phase factors chosen to give constructive interference near \( x = 0 \) and destructive interference elsewhere. As proved in Ref. [168], there is a unique form for the “correct” Wannier function; in this case it is

\[ W(x) = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \psi_k(x). \]  

(132)

The Wannier functions decay exponentially, and they are orthonormal such that

\[ \int_{-\infty}^{\infty} dx \ W(x - x_1) \ W(x - x_2) = \delta_{x_1 x_2} \]  

(133)

where \( x_1, x_2 = 0, \pm a_{\text{latt}}, \pm 2a_{\text{latt}}, \ldots \). See Figure 13(d). There is nevertheless a finite tun-
Figure 13: Quantum mechanical description of a particle moving in a 1D sinusoidal optical lattice potential. (a) Dispersion relation $E(k)$ in the extended zone scheme. (b) Development of energy bands and bandgaps with increasing lattice depth $V_0$. (c) Energies of the two lowest bands for $V_0 = 7E_R$. (d) Lowest Bloch function $\psi_0(x)$ (dashed) and two adjacent Wannier functions $W(x)$ and $W(x-a_{\text{latt}})$ for $V_0 = 7E_R$. Inset shows logarithmic plot. (e,f,g) Bloch functions $\psi_k(x)$ at crystal momenta $ka_{\text{latt}} = 0, \frac{\pi}{4}, \frac{\pi}{2}, \frac{3\pi}{4}, \pi$ for $V_0 = 7E_R$. 

neling matrix element between adjacent sites,

$$ t = \langle W_{x_1} | \hat{H} | W_{x_2} \rangle. $$

(134)
The value of $t$ can be computed by evaluating the matrix element as integrals over Wannier functions with the real-space Hamiltonian. However, it is easier to obtain $t$ by equating the bandwidth of the one-dimensional tight-binding model to the bandwidth in terms of Mathieu functions (see Figure A):

$$4t = E_{n,\pi} - E_{n,0}$$

$$\therefore \frac{4t}{E_R} = \text{MathieuCharacteristicB}[1, \frac{V_0}{\sqrt{E_R}}] - \text{MathieuCharacteristicA}[0, \frac{V_0}{\sqrt{E_R}}].$$

For a 3D cubic lattice formed by the sum of three sinusoidal potentials, the Schrödinger equation and the wavefunction are separable, and the tunneling amplitude between adjacent sites can be found from the depth of the sinusoidal potential in the relevant direction. The concepts can obviously be generalized to any lattice, although the eigenfunctions may have to be computed numerically for a general potential.

Wannier and Bloch states are summarized graphically in Figure 13. In contrast to the free particle ($V = 0$) dispersion, this simple crystal’s band structure becomes strongly gapped at the crystal momenta $ka_{\text{latt}} = 0, \pi, \ldots$ with increasing $V$, as shown in (a) and (b). In general, the deeper the band is relative to the optical lattice potential $V_0$ (c), the more like harmonic oscillator eigenstates $W(x)$ in (d) appear. However, the potential does not continue like $x^2$ between wells and instead rounds off. Therefore, $W(x)$ falls off more slowly between wells than the harmonic oscillator state would and enhances the amplitude for inter-well tunneling. Note that the Bloch functions are made up of a local state $u_{nk}(x - x_i)$ at each site $x_i$ convolved with an appropriate plane wave.

Now consider pairwise interactions. We will focus on cold atom systems dominated by $s$-wave scattering (between bosons or between different fermion species), so that we can ignore detailed features of the interatomic potential and work solely with the $s$-wave scattering length $a_s$. The interatomic potential can then be replaced by a pseudopotential $U(r) = g\delta(r)$ where $g = \frac{4\pi\hbar^2a_s}{2M_r}$ is a point interaction strength and $M_r$
Figure 14: Effective hopping amplitude $t$ and Hubbard interaction $U$ for particles in a 3D optical lattice with a sinusoidal potential of depth $V_0/E_R$. Upper curves show asymptotic forms. Lower curves are calculated from Mathieu functions and Wannier functions.

is the reduced mass. In the Wannier function basis one thus has an effective Hubbard interaction

$$U = g \int d^3r \ |W(r)|^4$$

(136)

$$U_{\text{as}} = \frac{8 a_{\text{latt}}}{\pi} \int d^3r \ |W(r)|^4 = \frac{8 a_{\text{latt}}}{\pi} \left[ \int dx \ |W(x)|^4 \right]^{3/4}. \quad (137)$$

**Asymptotic forms:** We will focus on optical lattices that are sufficiently deep ($V_0 \gtrsim 6E_R$) so that the system can be treated within a single-band Hubbard description. It is instructive to study the limit $V_0/E_R \gg 1$. To find the asymptotic form of $U$, it is sufficient to approximate the sinusoidal potential by a harmonic potential near $x = 0$, so that the Bloch functions and Wannier functions resemble a Gaussian near $x = 0$:

$$V(x) = V_0 \sin^2 \frac{\pi x}{a_{\text{latt}}} \approx \frac{V_0 \pi^2}{a_{\text{latt}}^2} x^2 \approx \frac{1}{2} m \Omega^2 x^2, \quad \Omega^2 = \frac{2 \pi^2 V_0}{ma_{\text{latt}}^2};$$

$$W(x) = \pi^{-1/4} x_0^{-1/2} \exp \left( -\frac{x^2}{2x_0} \right), \quad x_0 = \left( \frac{\hbar^2 a_{\text{latt}}^2}{2 \pi^2 m V} \right)^{1/4};$$

$$U_{\text{as}} = \sqrt{8 \pi} \frac{a_s}{a_{\text{latt}}} \left( \frac{V_0}{E_R} \right)^{3/4}. \quad (138)$$

The tunneling amplitude, however, is strongly influenced by the shape of the tails. Since the sinusoidal potential is lower than the approximating harmonic potential,
the actual wavefunction has more significant tails than a Gaussian (this can be seen from the JWKB approximation). The correct asymptotic form of $t$ can be obtained from the asymptotic behavior of Equation (135):

$$
\frac{t}{E_R} \approx \frac{4}{\sqrt{\pi}} \left( \frac{V_0}{E_R} \right)^{3/4} \exp \left( -2 \sqrt{\frac{V_0}{E_R}} \right).
$$

Equations (137), (138), (135), and (139) are plotted in Figure 14.

**Example:** Consider fermionic $^{40}\text{K}$ atoms ($m = 40m_p$), which have D1 and D2 transitions ($^{1}\text{S}_{1/2} \rightarrow ^{1}\text{P}_{1/2}$ and $^{1}\text{S}_{1/2} \rightarrow ^{1}\text{P}_{3/2}$) at 769 nm (390 THz). Consider a 3D optical lattice formed by six lasers at wavelength $\lambda = 830$nm, which is red-detuned from the D transitions. The lattice spacing is $a_{\text{latt}} = \lambda/2 = 415$nm, and the recoil energy is $E_R \approx 7240$ $h$ Hz, where $h$ is Planck’s constant.

For a laser intensity corresponding to a lattice depth $V_0 = 7E_R$, Equation (135) gives $t = 0.039E_R \approx 286$ $h$ Hz $\approx 14$ $k_B$ nK. This corresponds to hopping on the timescale of milliseconds.

In a magnetic field the two lowest hyperfine states are the state $|F = \frac{9}{2}, m_F = -\frac{9}{2}\rangle$ and the state $|F = \frac{9}{2}, m_F = -\frac{7}{2}\rangle$. For s-wave scattering between two $^{40}\text{K}$ atoms in these two states, there is a Feshbach resonance at 202.1 G (where 1 G = $10^{-4}$ T). At a field 220 G, the s-wave scattering length is $a_s \approx +110a_0$ where $a_0$ is the Bohr radius. Thus, if the two atoms are in the same well of the optical lattice described above, they experience a Hubbard repulsion given by $\frac{U_{\text{lat}}}{E_R a_s} \approx 15$, so $U \approx 0.21E_R$ $h$ Hz $\approx 74$ $k_B$ nK, corresponding to $U/t \approx 5.4$.

There are far more details and subtleties than we can address here; the reader is advised to consult References [6, 169] for more information.
Appendix B

THE FLUCTUATION-DISSIPATION
THEOREM

The quantum fluctuation-dissipation theorem (FDT) describes the response of a system defined by the Hamiltonian $\hat{H}$ to a perturbation coupled to an operator $\hat{A}$ within the system. It relates the imaginary part of the response function $\chi''(q,\omega)$ [dissipation] to the dynamic structure factor $S(q,\omega)$ [fluctuations] at inverse temperature $\beta = 1/T$, wavevector $q$ and frequency $\omega$. In the following, we derive the quantum FDT and discuss the limiting cases of high temperature and of $[\hat{A},\hat{H}] = 0$ before turning to its application to ultracold atom systems and the ratio $R(T)$ of the compressibility to the local number fluctuations.

Consider a quantum system of volume $V$ defined by $\hat{H}$ with many body states and energies $\hat{H} |\Psi_n\rangle = \epsilon_n |\Psi_n\rangle$ that is perturbed by a probe $\hat{H}'(t)$. We assume that the external perturbation $F_A(t)$ couples to $\hat{A}$ via $\hat{H}'(t) = -\hat{A}F_A(t)$. For a spatially varying probe $\hat{H}'(t) = -\int dr \hat{A}(r)F_A(r, t) = -\frac{1}{V} \sum_q \hat{A}_q F_q(t)$.

The response $\langle \hat{B} \rangle$ to linear order in the perturbation is $\langle \hat{B} \rangle(t) = \int_{-\infty}^{\infty} dt' \chi_{BA}(t - t') F_A(t')$ where $\chi_{BA}(t - t') = i\theta(t - t') \langle \left[ \hat{B}(t), \hat{A}(t') \right] \rangle$. By using a spectral representation in terms of the exact eigenstates of $\hat{H}$ and the Heisenberg representation of the time dependent operators, we obtain

$$\chi_{BA}(q, \omega) = \frac{1}{V} \sum_{m,n} e^{-\beta\epsilon_m} \frac{Z}{\omega + i\eta + \epsilon_{nm}} \left[ \frac{(A_{-q})_{mn}(B_q)_{nm}}{\omega + i\eta + \epsilon_{nm}} - \frac{(B_q)_{mn}(A_{-q})_{nm}}{\omega + i\eta - \epsilon_{nm}} \right]$$

(140)
where $\epsilon_{nm} = \epsilon_n - \epsilon_m$ and $\eta = 0^+$ is a small positive number to ensure convergence as $t \to \infty$. The well-known identity $\lim_{\eta \to 0^+} \frac{1}{x \pm i\eta} = P(\frac{1}{x}) \mp i\pi\delta(x)$ yields the imaginary part of the response function, 

$$
\chi''_{BA}(q, \omega) = \frac{\pi}{V} \sum_{m,n} \frac{e^{-\beta\omega_m}}{Z} [(A_{-q})_{mn}(B_q)_{nm}\delta(\omega - \epsilon_{nm}) - (B_{q})_{mn}(A_{-q})_{nm}\delta(\omega + \epsilon_{nm})]. \tag{141}
$$

Next we consider the corresponding correlation function defined as

$$
S_{BA}(r, t; r', t') = \langle \hat{B}(r, t) \hat{A}(r', t') \rangle \tag{142}
$$

$$
S_{BA}(q, t - t') = \frac{1}{V} \langle \hat{B}_{q}(t) \hat{A}_{-q}(t') \rangle \tag{143}
$$

for a translationally invariant system. Within the spectral representation we obtain

$$
S_{BA}(q, \omega) = \frac{2\pi}{V} \sum_{m,n} \frac{e^{-\beta\epsilon_m}}{Z}(B_{q})_{mn}(A_{-q})_{nm}\delta(\omega - \epsilon_{nm}). \tag{144}
$$

By exchanging the indices in the second term in Equation 141, we obtain the quantum FDT

$$
\chi''_{BA}(q, \omega) = \frac{\pi}{V} (1 - e^{-\beta\omega}) \sum_{m,n} \frac{e^{-\beta\omega_m}}{Z}(B_{q})_{mn}(A_{-q})_{nm}\delta(\omega - \omega_{nm})
$$

$$
= \frac{1 - e^{-\beta\omega}}{2} S_{BA}(q, \omega). \tag{145}
$$

**Static Structure Factor**

The definition of the static structure factor is

$$
S_{BA}(q) \equiv S_{BA}(q, t = 0) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S_{BA}(q, \omega) \tag{146}
$$

$$
= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{2}{1 - e^{-\beta\omega}} \chi''_{BA}(q, \omega). \tag{147}
$$
Using the oddness property $\chi''_{BA}(-\omega) = -\chi''_{BA}(\omega)$ yields

$$S_{BA}(q) = \frac{1}{V} \langle \hat{B}_q \hat{A}_{-q} \rangle = \int_0^\infty \frac{d\omega}{\pi} \coth \left( \frac{\beta \omega}{2} \right) \chi''_{BA}(q, \omega).$$ (147)

The High Temperature Limit of the Quantum FDT

At temperatures $k_B T \gg \hbar \omega$ larger than any characteristic frequencies of the system, $\coth \left( \frac{\beta \omega}{2} \right) \to 2/\beta \omega$ and the static structure factor reduces to

$$S_{BA}(q) = \frac{2}{\beta} \int_0^\infty \frac{d\omega}{\pi} \frac{\chi''_{BA}(q, \omega)}{\omega} = T\chi'_{BA}(q, \omega = 0) \quad (148)$$

where we have used the Kramers-Kröning relation $\chi'_BA(q, \omega) = P \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''_{BA}(q, \omega')}{\omega' - \omega}$ to relate the real and imaginary parts of the response function. Since $\chi'' = 0$ when $\omega = 0$, we can replace $\chi'$ by simply $\chi$.

The Quantum FDT for Conserved Quantities

We use (i) the definition of the correlation function for a conserved quantity, (ii) the quantum FDT, and (iii) the Kramers-Kröning relation to finally derive $\chi_{AA}(q \to 0, \omega = 0) = \beta S_{AA}(q \to 0, t = 0)$.

A conserved quantity $\hat{A}(q = 0) \equiv \hat{A}_0$ such as the total number of particles $\hat{n}(q = 0) = \sum_k \hat{a}_k^\dagger \hat{a}_k = \hat{N}$, must commute with the Hamiltonian $[\hat{A}_0, \hat{H}] = 0$. This implies that the matrix element $\langle \Psi_m | [\hat{A}_0, \hat{H}] | \Psi_n \rangle = 0$ or equivalently $(\epsilon_n - \epsilon_m)(A_0)_{mn} = 0$. If $m \neq n$, we must have $(A_0)_{mn} = 0$ which results in

$$\lim_{\omega \to 0} \lim_{q \to 0} \chi_{AA}(q, \omega) = \lim_{\omega \to 0} \frac{2}{V} \sum_{m,n} e^{-\beta \epsilon_m} \frac{\epsilon_{nm}}{(\omega + i\eta)^2 - \epsilon_{nm}^2}$$

$$= 0 \quad (149)$$

using Equation 140. Thus $\chi_{AA}(q = 0, \omega \to 0) = 0$ if $A_0$ is a conserved quantity.

However, reversing the order of the limits generally results in a finite result. For
the case of a density perturbation,

$$\lim_{q \to 0} \lim_{\omega \to 0} \chi_{AA}(q, \omega) = \lim_{q \to 0} \frac{2}{V} \sum_{m,n} \frac{e^{-\beta \epsilon_m}}{Z} \left[ \frac{\epsilon_{nm}}{(\omega + i \eta)^2 - \epsilon_{nm}^2} \right]$$

$$= n^2 \kappa_T. \quad (150)$$

The last equality in Equation 150 follows from the perturbation $\hat{H}' = -\int d\mathbf{r} \delta \hat{n}(\mathbf{r}) \delta \hat{\mu}(\mathbf{r}, t) = -\frac{1}{V} \sum_q \delta \hat{n}_q \delta \hat{\mu}_q(t)$ which produces the response

$$\chi_{nn}(q \to 0, \omega = 0) = \frac{\langle \delta \hat{n}_{-q \to 0} \rangle}{\delta \hat{\mu}_{q \to 0}}(\omega = 0) \quad (151)$$

$$= \left( \frac{\partial n}{\partial \mu} \right)_{T,V} = n^2 \kappa_T \quad (152)$$

where $\kappa_T$ is the isothermal compressibility and $n$ is the average density.

Another way to understand the behavior of the quantum FDT for a conserved quantity $\hat{A}(q = 0, t)$ is to note that both it and the correlation $\hat{A}(q = 0, t) \hat{A}(-q = 0, t')$ are independent of $t$ and $t'$ and hence its Fourier transform must be a delta function in frequency. Thus from Equation 143

$$S_{AA}(q = 0, \omega) = 2\pi \delta(\omega) S_{AA}(q = 0). \quad (153)$$

From the quantum FDT Equation 145 we obtain for a conserved quantity with the correlation function Equation 153,

$$\chi''_{AA}(q = 0, \omega) = (1 - e^{-\beta \omega}) \pi S_{AA}(q = 0) \delta(\omega). \quad (154)$$

By using the Kramers-Kröning relation we find

$$\chi_{AA}(q = 0, \omega \to 0) = S_{AA}(q = 0) \int_{-\infty}^{\infty} d\omega \frac{1 - e^{-\beta \omega}}{\omega} \delta(\omega)$$

$$= \beta S_{AA}(q = 0) = \frac{\beta}{V} \langle \hat{A}_0^2 \rangle \quad (155)$$

and for particle number perturbations $\delta \hat{N} = \hat{N} - \langle \hat{N} \rangle$

$$\chi_{\delta N \delta N}(q = 0) = \frac{\beta}{V} \langle \delta \hat{N}^2(q = 0) \rangle = n^2 \kappa_T. \quad (156)$$
We stress that while this result may look similar to the high temperature limit of Equation 148, because the particle number is a conserved quantity it is valid even in the quantum regime.

The Ideal Gas

We derive the high temperature behavior of the compressibility, $\partial n/\partial \mu$, and number fluctuations $\delta N^2 \equiv \langle N^2 \rangle - \langle N \rangle^2$ of the ideal gas. From the equation of state $PV = Nk_B T$, we get

$$\kappa_T \equiv -\frac{1}{V} \left( \frac{\partial V}{\partial P} \right)_{T,N} \equiv \frac{1}{n^2} \frac{\partial n}{\partial \mu} = \frac{\beta}{n}$$  \hspace{1cm} (157)

where $n = N/V$.

For an ideal gas, the chemical potential is related to the density by $\beta \mu = -\log \left( \frac{1}{n\lambda_T^d} \right)$, where the thermal deBroglie wavelength $\lambda_T = h/\sqrt{2\pi mk_B T}$. For a fixed $\mu$, the high temperature expansion of $n(\mu, T)$ is

$$n = \frac{e^{\beta \mu}}{\lambda_T^d} \sim T^{d/2} \left( 1 + \frac{\mu}{k_B T} + \frac{1}{2} \left( \frac{\mu}{k_B T} \right)^2 \right).$$  \hspace{1cm} (158)

which implies that the temperature dependence of the local compressibility is

$$n^2 \kappa = \frac{\partial n}{\partial \mu} \sim T^{d/2-1} \left( 1 + \mu T^{-1} \right).$$  \hspace{1cm} (159)

Using the local fluctuation-dissipation theorem at high temperatures, we find

$$\langle \delta n^2 \rangle \approx \frac{\partial n}{\partial \mu} T \sim T^{d/2} \left( 1 + \mu T^{-1} \right),$$  \hspace{1cm} (160)

as we might have guessed from a simple Brownian motion or diffusion model of the number fluctuations.

Thus, we find that in 2D, while the local compressibility $n^2 \kappa$ is independent of temperature and the number fluctuations $\langle \delta n^2 \rangle$ scale linearly with $T$.

In the presence of interactions, both number fluctuations and compressibility deviate from their classical values, however the ratio of the compressibility to the *total* number fluctuations continues to yield the inverse temperature $\beta$. On the other hand,
the ratio $R = n^2 \kappa / \langle \delta n^2 \rangle$ exhibits non-trivial behavior when quantum effects become important.
Appendix C

Lowest Order Constrained Variations

The lowest order constraint variation (LOCV) method is a standard starting point for treatment of strongly interacting quantum liquids. It was first introduced in the context of strongly interacting nuclear matter. More recently, it incorporated the correct short-range correlations in studies of the BEC-BCS crossover in Fermi gases and was later extended to strongly interacting boson systems. Although LOCV alone cannot account for many-body effects, it is very convenient for obtaining reasonable pair correlations at short distances where the many body system can be approximately treated as a two body system. LOCV reduces the many-body problem to a tractable two-body problem that can be easily solved.

In the explanation of LOCV below, we omit several tedious algebraic steps which can be found in [140]. In the Bose-Fermi mixture, we must include a boson-boson potential $v_{BB}(r)$ to stabilize the system and boson-fermion potential $v_{FB}(r)$ to tune the interspecies interaction. We develop the LOCV method in the more general boson-fermion context and comment on the boson-boson case at the end.

The assumption underlying LOCV is that the leading order contribution to the energy comes from short range correlations. The obvious trial wave function is of the Jastrow type

$$\left|\Psi^{JS}\right\rangle = \prod_{ij} f(r_{ij}) \left|\Phi^{AS}\right\rangle$$

where $f(r_{ij})$ is the boson-fermion Jastrow factor evaluated at $r_{ij} = r_i - r_j$ and $\left|\Phi^{AS}\right\rangle$
introduces the proper symmetrization for bosons (a trivial factor) and for fermions (a Slater determinant). LOCV makes a second assumption that the potential is short-ranged. Then the approximation $f(r > d) = 1$ and $f'(d) = 0$ with some healing length $d$ on the order of the range of the potential is reasonable.

Now consider the variational energy of $|\Psi^{JS}\rangle$ of a system $\hat{H}$ with $N_B$ and $N_F$ bosons and fermions, respectively,

$$\frac{2m_F}{\hbar^2} \langle \hat{H} \rangle = \frac{\langle \Phi^{AS} | \prod_{ij} f(r_{ij}) \left( -\sum_a \nabla_a^2 - \frac{1}{\lambda} \sum_b \nabla_b^2 + \sum_{ab} v(r_{ab}) \right) \prod_{ij} f(r_{ij}) | \Phi^{AS} \rangle}{\langle \Phi^{AS} | \prod_{ij} f(r_{ij}) \prod_{ij} f(r_{ij}) | \Phi^{AS} \rangle}$$

$$\frac{2m_F}{\hbar^2 \kappa_F^2 N_B + N_F} = \frac{N_F}{N_F + N_B} \left( \frac{3}{5} \right) + \frac{n}{2} \int f(r) \left( -\frac{m_F}{2m_r} \nabla_r^2 + v(r) \right) f(r) d\mathbf{r}$$

with $\lambda = m_B/m_F$, the reduced mass $m_r/m_F = \lambda/(1 + \lambda)$ and density $n$. The indices $a$ and $b$ indicate fermion and boson coordinates, respectively. The latter formula results from only consider the leading order contributions of the Jastrow factor to the kinetic and potential energies. By construction, these contain contributions only from single boson-fermion pairs so the average energy depends only on the energy of a single pair. Minimizing this variational energy with respect to $f(r)$ and $d$ leads to the LOCV equation

$$\left[ -\frac{\nabla^2}{2m_r} + v(r) \right] f_{BF}(r) = \Lambda f_{BF}(r)$$

(163)

where $\Lambda$ is an Euler-Lagrange multiplier that represents the pair energy. Under the assumption that $f$ depends only on the magnitude of $\mathbf{r}$, the substitution $u(r) = r f(r)$ in three dimensions recasts the previous formula into the simple equation

$$-u''(r) + v(r)u(r) = \Lambda u(r).$$

(164)

The healing length $d$ gives the boundary condition $f(r \geq d) = 1$ and $f'(d) = 0$, and is conventionally chosen such that, on average, only one boson is within a distance $d$
The typical $f_{FB}(r)$ has short range correlations very similar to the exact two body solution of $v_{FB}(r)$, $\phi^2B(r)$, but $f_{FB}$ decays to 1 (at $d$) rather than exponentially at large $r$. The LOCV solution for a hard-core interaction with range $a_{BB}$ (the boson-boson potential in the Bose-Fermi mixture) can be analytically derived as

$$f_{BB}(r) = \begin{cases} 
0 & r < a_{BB} \\
\frac{d \sin(k_F(r - a_{BB}))}{r \sin(k_F(d - a_{BB}))} & a_{BB} < r < d \\
1 & r > d 
\end{cases}$$

(166)
Appendix D

**Variable Definitions**

A handy guide to notation in chapter 4.

**Standard variable definitions**

- \langle \ldots \rangle: Indicates thermodynamic average.
- \beta: Inverse temperature equal to \(1/T\), which defines the duration of imaginary time in world-line simulations.
- \(d\): Spatial dimension.
- \(\tilde{H}\): The Hamiltonian.
- \(\mu\): Chemical potential.
- \(n_c\): Coordination number (4 in a square lattice).
- \(P(X)\): The probability of state \(X\).
- \(t\): Bose Hubbard model hopping parameter.
- \(T(Y|X)\): The probability to transition from state \(X\) to state \(Y\).
- \(U\): Bose Hubbard model onsite repulsion parameter.
- \(X,Y\): A generic state, event, configuration or sample of a probability distribution.
- \(Z\): Partition Function.

**VMC and DMC variable definitions**

- \(i\): Fermion particle index.
- \(j\): Boson particle index.
- \(\Psi\): A wave function.
- \(\Phi_\alpha\): Exact eigenstates, where \(\alpha = 0\) denotes the ground state.
Directed loop algorithm variable definitions

⊙ Space-imaginary time index symbolizing the worm head.
⊗ Space-imaginary time index symbolizing the worm tail.
$C_{\text{onsite}}$ Constants added to the Bose Hubbard model Hamiltonian for simulation purposes.
$\Delta \tau$ An imaginary time interval equal to $\beta/L_r$.
$F, F_u$ Auxilliary field configuration and value of auxilliary field $F$ at space-imaginary time $u$; takes on values $F_u = 0, 1$.
$\hat{a}_i, \hat{a}_i^\dagger$ Annihilation and creation operator on site $i$.
$\hat{h}_{\text{onsite},i}$ Single term of a Hamiltonian, where onsite and link indicate the term type and $i$ and $j$ indicate the sites acted on.
$\hat{h}_{\text{link},ij}$ Same as previous entry, but $m$ indicates both the type and the site(s).
$\hat{h}_u$ Same as previous entry, but $u$ indicates the type, the site(s) and the imaginary time.
$\mathcal{I}$ Imaginary time interval for which $n_i$ on the relevant site(s) is constant.
$i, j$ Site index.
$L_r$ Order of expansion in imaginary time of the partition function $Z$, i.e. number of time slices.
$\ell$ Imaginary time index.
$\mathcal{M}$ Number of terms $\hat{h}_m$ that $\hat{H}$ can be reduced to.
$\hat{n}_i$ Foch space operator on site $i$.
$N_s$ Number of sites in the lattice.
$n_i$ Number of particles on site $i$.
$n_M$ Maximum number of allowed particles.
$\Psi$ Full world-line configuration in Foch space.
$\Psi^W$ Full world-line configuration in Foch space plus two source terms from the worm head and tail.
$\psi_u$ Foch space configuration at the space-imaginary time point $u$.
$\hat{Q}$ Source term in the Bose Hubbard model that enables definition of the worm head and tail.
$u$ Denotes a small number of sites and a definite imaginary time.
w(...) Weight of the indicated global or local configuration.