SIMULATION OF HIGHER-ORDER QUANTUM FLUCTUATIONS IN THE DYNAMICS OF BOSE-EINSTEIN CONDENSATES

by

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ABSTRACT

Interatomic interactions in a Bose-Einstein condensate (BEC) may be tuned via a Feshbach resonance, as in experiments where a stable condensate is given attractive interactions and caused to collapse. The *Bosenova*, as this collapse is sometimes called, qualitatively resembles a supernova, with energetic bursts, jets of atoms, and formation of higher mass molecules from initially lower mass atomic constituents. Experiments performed in the seemingly opposite vein, with repulsive interactions, have similar features, including bursts and sometimes more than 50 percent of condensate atoms escaping detection.

Attempts to describe these experiments using mean field theory produce only qualitative agreement, suggesting that quantum fluctuations may play a signicant role in these experiments concerning BECs with order-unity diluteness parameters. Hartree-Fock-Bogoliubov (HFB) theories that incorporate lowest-order fluctuations have been proposed in the past to describe such situations. We present a rigorous derivation of dynamical HFB equations and use an established and successful model of the Feshbach resonance that is valid at the resonance, where the Gross-Pitaevskii equation is undefined. This model takes the form of four coupled nonlinear partial differential equations defined over time and six spatial independent variables. Assuming symmetries more general than those used in the past reduces the number of spatial independent variables to four, and simulations in cylindrical symmetry require five independent variables, in addition to time.

We approximate solutions to these equations by the method of lines, using an adaptive Runge-Kutta method for time propagation and pseudospectral approximations to spatial derivatives. Collapse simulations in spherical symmetry qualitatively resemble the experiments, and we are able to predict a rapid and oscillatory exchange of particles between condensed atomic and molecular fields. Such oscillations also exist in simulations with repulsive interactions and have been experimentally observed. Among our other predictions are an approximately quadratic time dependence of the time to collapse, and high molecular velocities, on the order of millimeters per second, when molecules dissociate. Simulations also suggest that initially contracted condensates have distinct regions of collapse and expansion, and that the total number of noncondensed atoms has a periodic modulation of a predictable frequency when the condensate is subjected to particular ramps in magnetic field. Though our goal is to reproduce the experiments in our simulations, our quantitative disagreement with experiments indicates that second order quantum fluctuations are not the primary mechanism for burst formation or condensate loss in experiments with either attractive or repulsive interactions. We have also written and tested parallel code that allows for simulation of experimental parameters in cylindrical geometry, which has previously been thought unfeasible.

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LIST OF ACRONYMS

- BEC Bose-Einstein condensate
- HFB Hartree-Fock-Bogoliubov
- GPE Gross-Pitaevskii equation
- TEBD Time evolving block decimation
- TWA Truncated Wigner approximation
- ZGN Zaremba-Griffin-Nikuni
- JILA Joint Institute for Laboratory Astrophysics
- PDE Partial differential equation
- ODE Ordinary differential equation
- SMP Symmetric multiprocessor
- MIMD Multiple instruction multiple data
- ODLRO Off-diagonal long range order
- BC Boundary condition
- ITR Imaginary time relaxation
- MPI Message Passing Interface

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Part of this D-minus belongs to God.

—Bartholemew J. Simpson

Chapter 1

INTRODUCTION

Bose-Einstein condensates (BECs) provide a medium in which to observe quantum mechanics on a macroscopic scale. BECs subject to external magnetic fields that influence the sign and strength of interatomic interactions within the condensate exhibit exotic behavior, as demonstrated by recent collapse experiments [1] that qualitatively resemble supernovas, with energetic bursts, jets, excited remnants with nonlinear dynamics, and formation of higher mass components from lower mass ones. Experiments [2, 3] performed in the seemingly opposite vein, using repulsive interatomic interactions, have some of the same mysterious features of the collapse experiments; namely, an energetic burst of atoms and a significant portion of atoms escaping detection. Experimental observations of collapsing Bose-Einstein condensates have eluded satisfactory quantitative explanation for years, with the mechanism for the formation of bursts in the case of collapse and that of repulsive interactions remaining particularly mysterious.

Mean field theory (namely, the Gross-Pitaevskii equation) appears able to explain neither the bursts' origin, nor a key element of the driving force towards collapse, as evidenced by consistent over-estimations of the time required for the condensate to collapse. This theory is essentially a classical field theory, and does not account for *quantum fluctuations*. These fluctuations are deviations from a measured average; manifestations of quantum fluctuations in other scenarios include the Casimir effect, in which nonzero fluctuations of an electric field that is zero on average cause two electrically neutral conducting plates to attract [4]; and some explanations of the Hawking radiation of a black hole, in which the fluctuations around the vacuum allow for the creation of particle-antiparticle pairs, with only one member of the pair falling into the black hole. In the quantum field theoretic description of BECs, quantum fluctuations correspond to particles that are not Bose-condensed, and the Gross-Pitaevskii equation, though it is computationally quite feasible, does not account for these. A full quantum treatment of BECs accounts exactly for all particles in the system, but is numerically and analytically impractical for the numbers of atoms and geometries encountered in experiments.

Besides providing insight into experimental quantum physics, the experiments concerning repulsive interactions may allow for the creation of a molecular BEC, which could provide a means by which to demonstrate the Einstein-Podolsky-Rosen paradox [5], and an explanation of the collapse may have implications for astrophysics. Indeed, the *Bosenova*, as the collapse is sometimes called, may be the only way to model a supernova-like process in a laboratory. Dimer, trimer, and tetramer formation from the consituent atoms of the BEC could be important to both processes, though our model will only account for dimers. The astrophysical connection may be more than qualitative, as superfluidity and possible condensation in the cores of neutron stars play an important role in neutron star evolution [6]. Neutron stars having kaon-condensed¹ cores may even be especially prone to later collapse into black holes [8, 9], making the laboratory study of collapsing BECs directly applicable to proposed astrophysical processes.

Our attempt to simulate the results of these experiments uses a Hartree-Fock-

¹A kaon is a strange meson with spin 0, composed of either an up quark and strange antiquark, a down quark and a strange antiquark, a down antiquark and a strange quark, or an up antiquark and a strange quark [7].

Bogoliubov (HFB) theory that accounts for low-order quantum fluctuations. HFB theories similar to our own have been applied successfully in explanations of certain repulsive-interaction experiments [10], and have been used with modest success in describing collapsing condensates [11, 12, 13]. We extend established theory by combining the proven Feshbach resonance model of Kokkelmans *et al.* [14] with more advanced numerical methods than have been used in past HFB simulations. Our model for spherical geometry is more general than that of Milstein *et al.* [11] and Wüster *et al.* [12, 13], in that we assume no symmetry in the relative momentum between two particles. We also provide a parallelization scheme and working implementation for a cylindrical geometry, which was previously thought to be impractical. As a consequence, this thesis is heavily computational in nature.

1.1 Bose-Einstein Condensation

Bose-Einstein condensation refers to a macroscopic occupation of a single quantum state by many bosons, first proposed by S. N. Bose in 1924 [15] for photons, and generalized to massive bosons by Einstein shortly thereafter [16, 17]. Though long suspected to play a key role in ⁴He superfluidity, Bose-Einstein condensation was unambiguously achieved experimentally for the first time in 1995 [18, 19, 20].

In the ideal gas approximation (see [21], for example), the excited states of a bosonic system can hold only a finite number of bosons, while the ground state has no such limitation below a critical temperature T_c . For a given number density n of noninteracting identical particles, condensation in an untrapped gas in three dimensions occurs at a temperature

$$T_c = \frac{h^2}{2\pi m k_B} \left[\frac{n}{\zeta\left(\frac{3}{2}\right)} \right]^{2/3},\tag{1.1}$$

where h is Planck's constant, m is a particle's mass, k_B is Boltzmann's contsant, and ζ is the Riemann zeta function. The presence of a harmonic trap changes the critical temperature to

$$T_c = \frac{h}{2\pi k_B} \left[\frac{N}{\zeta(3)} \right]^{1/3} \bar{\omega}, \qquad (1.2)$$

where N is the number of particles and $\bar{\omega} \equiv (\omega_x \omega_y \omega_z)^{1/3}$ is the geometric mean of the three dimensional trap's frequencies. Experimentally, it is most practical to work at very low densities and pressures (and thus very low temperatures, on the order of nanokelvin), though condensation, albeit far from the noninteracting limit, may occur in such dense systems as helium superfluids and neutron stars [22]. where N is the number of particles and $\bar{\omega} \equiv (\omega_x \omega_y \omega_z)^{1/3}$ is the geometric mean of the three dimensional trap's frequencies. Experimentally, it is most practical to work at very low densities and pressures (and thus very low temperatures, on the order of nanokelvin), though condensation, albeit far from the noninteracting limit, can occur in such dense systems as helium superfluids and neutron stars [22].

BECs are typically formed in magneto-optical traps, where atoms far from the origin of the trap are, due to a nonuniform magnetic field, more likely to transition to states that are subject to the radiation pressure of incident lasers, exerting a restoring force towards the trap center. Ever-present laser light can heat the condensate, so the atoms are then irradiated with a pump laser that forces them into a state where the atoms' electrons have particular orbital and spin magnetic moments (that is, a particular *hyperfine* state) so that they may be contained by a purely magnetic trap. This trap consists of a magnetic field that varies quadratically in space. The energy shift of an atom in a magnetic field due to the weak field Zeeman effect is approximately linear, making the magnetic trap effectively harmonic. The final stage of cooling usually consists of evaporative cooling, where the walls of the magnetic trap

are temporarily cut so that the faster-moving atoms can escape. The traps considered in some of the experiments below are somewhat unique in that evaporative cooling is accomplished with electromagnetic pulses to which the higher energy atoms respond by making transitions to hyperfine states that are not confined by the magnetic trap [22, 23, 24].

The dynamic properties of BECs in harmonic traps are usually well modeled by the Gross-Pitaevskii equation (GPE):

$$i\hbar \frac{\partial}{\partial t}\psi(\mathbf{x},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}} + g\left|\psi(\mathbf{x},t)\right|^2\right]\psi(\mathbf{x},t),\qquad(1.3)$$

where m is the mass of the constituent atom; V_{ext} is the possibly time- and positiondependent external potential; q controls the strength of the mean-field, or self interaction; and $\psi(\mathbf{x}, t)$, sometimes called the "wavefunction of the condensate," is the condensate's order parameter corresponding to a broken gauge symmetry (see [25], for example). The squared modulus of the condensate wavefunction gives the number density of atoms in the condensate at the position \mathbf{x} and time t, while the gradient of the condensate phase angle is proportional to the local velocity. Implicit in the GPE are many assumptions which the experiments described below challenge; we mention some of these assumptions (and corrections to them) throughout this thesis. The validity of the GPE in any particular situation may be most easily summarized by consideration of the diluteness parameter, $\sqrt{na^3}$, where n is the density of condensed particles and a is the s-wave scattering length, which characterizes the strength and sign of interatomic interactions. The diluteness parameter gives an order-of-magnitude estimate of the fraction of particles in the system that are not in the condensate [22]. As long as $\sqrt{na^3} \ll 1$, the GPE accounts for the majority of particles in the system [22, 23].

If the interactions between atoms are sufficiently attractive, the kinetic energy of the atoms (also called *quantum pressure*) may become overwhelmed by the potential energy of their interactions, and the condensate may collapse. A variational treatment of the GPE shows that a condensate with attractive interactions will be stable in a harmonic trap if [22, 23]

$$\kappa \equiv \frac{N|a|}{a_{\rm ho}} < 0.67, \tag{1.4}$$

where N is the number of particles in the condensate and $a_{\rm ho} = \sqrt{\hbar/m\omega}$ is the harmonic oscillator length. Numerical solutions [26] of the GPE replace the stability coefficient $k_{\rm stab}$ on the right hand side of (1.4) with the more accepted value of 0.574, which experiments [27, 28, 24] confirm.² The nearly ten percent disagreement between the variational treatment and the numerical results of Ruprecht *et al.* [26] is due to the Gaussian variational ansatz; the numerical studies show that the ground state of a stable, attractive condensate is narrower, closer to a double exponential.

1.1.0 Interatomic Interactions

The constituent atoms of a BEC are usually neutral alkali atoms, having a single valence electron outside of completely closed electronic shells. As described in Refs. [22] and [29], for example, the electron clouds of neutral atoms are not rigid in the presence of an external electric field and are subject to polarization. At long and moderate distances, two neutral atoms induce electric dipole moments in each other, resulting in an attractive potential proportional to r^{-6} , where r is the separation between the atoms' nuclei. This is the *van der Waals interaction*. The potential at long range varies as r^{-7} due to retardation effects, but characterizations of interactions

²Reference [27] has a measured stability coefficient substantially lower than 0.574, but Reference [24] states that the more accurate atomic parameters published in [28] make the measurements of

^[27] agree very well with the predicted value of 0.574.

are rarely concerned with these long distances. As two neutral atoms approach each other and their wavefunctions begin to overlap, the Pauli exclusion principle may have significant effects on their valence electrons. If the valence electrons of the two atoms have opposite spins, the valence electron clouds can spatially overlap without any increase in energy. If the electrons have the same spin, as the outer electrons of alkali atoms in magnetically trapped BECs do, the Pauli exclusion principle requires that one or both electrons make energetically expensive transitions to other states if they are to overlap, markedly reducing the attraction due to the electric dipole-dipole interaction. As the atoms grow nearer still, their closed-shell electrons must make prohibitively expensive transitions for the closed-shell clouds to overlap, resulting in an effectively hard-sphere repulsive potential. This hard-sphere potential is difficult to calculate from first principles, but computational convenience and agreement with empirical data suggest a r^{-12} model [30]. A linear combination of the r^{-6} and r^{-12} models is called the *Lennard-Jones* potential [29].

Alkali atoms have abundant hyperfine states, and magnetic and Coulombic interactions between atoms can cause the spin configurations of colliding atoms to change. Since most of the methods for trapping atoms (including those methods used in the experiments with which we are concerned) rely on the atoms having a particular spin configuration, such spin exchange processes can result in condensed atoms transitioning to untrapped states, and perhaps exiting the system entirely. Conversely, spin exchange processes between noncondensed atoms can contribute to the condensate, but usually the loss terms dominate. The rates of these losses are proportional to the square of the condensate's density. Other losses occur through three-body recombination, in which three atoms collide; two of the atoms form a bound pair, and the third absorbs the new molecule's binding energy. This loss rate is proportional to the cube of the condensate density, and so becomes especially important in regions of high density. Finally, some atoms are removed from the condensate by collisions with atoms or molecules not of the condensate's species, the presence of which is due to an imperfect vacuum in experiments. These loss rates are determined by the density of the impurities.

Following [22], for example, a *Feshbach resonance* is an elastic scattering phenomenon that is particularly susceptible to experimental control. Formally defined as a scattering process in which a bound state would result if some parameter of the governing Hamiltonian were slightly changed (see [31], for one), an example will best illustrate the application to BECs. Consider two atoms in unbound states having total energy E and subject to a potential $V_{in}(r)$ such that E is barely larger than $V_{\rm in}(r)$, where r is the separation of the nuclei. After some spin exchange process, the atoms may transition to other hyperfine states, making them now subject to a slightly different potential, $V_{out}(r)$. If the new potential is such that $E < V_{out}(r)$ for some r outside the hard-sphere radius, the atoms will form a bound pair. See Figure 1.1 for a conceptual illustration. It may happen that the colliding atoms have a poorly defined energy such that the uncertainty ΔE in that energy is much less than the characteristic width (in units of energy) of the resonance. In this case, a quasi-bound state may result, but will decay into unbound states after a sufficiently long time [32]. The large number of hyperfine states makes a realistic calculation difficult, and a coupled channels formalism is most convenient.

In practice, the offset of V_{out} relative to V_{in} is controlled by an external magnetic field, which interacts with atoms via the Zeeman effect. The effective scattering length is given by

$$a_{\rm eff} = a_{\rm bg} \left(1 - \frac{\Delta B}{B - B_{\rm res}} \right), \tag{1.5}$$



Figure 1.1: Conceptual illustration of Feshbach resonance. Two unbound particles with zero energy are initially in the open channel potential (solid curve). As they approach each other and interact, they may transition to other hyperfine states, in which they are subject to the closed channel potential (dashed curve). Since the closed channel potential is higher than the particles' energy, they now form a bound pair. The energy of the bound state in the closed channel potential nearest the continuum threshhold in the open channel is the detuning ν_0 (dotted curve).

where B is the external magnetic field, B_{res} is the value of the magnetic field for which a_{eff} diverges, $\Delta B = B_{\text{zero}} - B_{\text{res}}$, where B_{zero} is the value of the magnetic field for which $a_{\text{eff}} = 0$, and the background scattering length a_{bg} is particular to each atomic species and isotope.

1.2 Overview of Theory

Ideally, the physics of the N particles in a condensate would be calculated from the Schrödinger equation with at least binary interaction terms:

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) = \left[-\sum_{j=1}^N \frac{\hbar^2}{2m} \nabla_{\mathbf{x}_j}^2 + V_{\text{trap}}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) + \frac{1}{2} \sum_{j \neq k}^N V_{\text{int}}(\mathbf{x}_j - \mathbf{x}_k) \right] \Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N),$$
(1.6)

where $\Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$ is the many-body wavefunction, V_{trap} is the external trapping potential, and V_{int} is the potential of the binary interactions. This equation scales in a non-polynomial way with N, and so is impractical for the numbers of atoms we wish to consider. Quantum field theory formally allows for exact solution of many-body problems, but is often unfeasible for actual calculations. A mean field approach that deals only with averages is much simpler and has proven successful in many descriptions of BECs [23], but masks possibly important quantum fluctuations. Many theories, including ours, attempt to incorporate fluctuations in a practical way.

1.2.1 Quantum Field Theory

As a practical introduction to quantum field theory applied to bosons (somewhat in the spirit of [33]), consider a system of N indistinguishable particles. Each particle may occupy one of any number of single-particle states $|k\rangle$, where k is a discrete index, and the $\{|k\rangle\}$ form a complete basis. We could then describe the state of the entire system of particles by reporting the number of particles in each single-particle state; for example,

$$|\Phi\rangle = |n_1, \dots, n_k, \dots\rangle, \tag{1.7}$$

where n_k is the number of particles in the single-particle state $|k\rangle$. This representation is sometimes called the *occupation-number representation*, and the Hilbert space spanned by all vectors of the type (1.7) is called *Fock space*.

Now define the ladder operators \hat{a}_k and \hat{a}_k^{\dagger} such that

$$\hat{a}_k | n_1, \dots, n_k, \dots \rangle = \sqrt{n_k} | n_1, \dots, n_k - 1, \dots \rangle$$
(1.8)

$$\hat{a}_k^{\dagger}|n_1,\ldots,n_k,\ldots\rangle = \sqrt{n_k+1}|n_1,\ldots,n_k+1,\ldots\rangle$$
(1.9)

$$\left[\hat{a}_{k},\hat{a}_{l}^{\dagger}\right] = \delta_{k,l}, \quad \left[\hat{a}_{k},\hat{a}_{l}\right] = \left[\hat{a}_{k}^{\dagger},\hat{a}_{l}^{\dagger}\right] = 0.$$

$$(1.10)$$

 \hat{a}_k and \hat{a}_k^{\dagger} remove and add, respectively, a particle from the k^{th} single-particle state, and the constants on the right-hand sides in (1.8) and (1.9) are for normalization.

Consider a linear combination of the ladder operators above:

$$\hat{\Psi}(x) = \sum_{k} \zeta_k(x) \,\hat{a}_k,\tag{1.11}$$

$$\left[\hat{\Psi}(x), \hat{\Psi}^{\dagger}(y)\right] = \delta^{(3)}(x-y), \quad \left[\hat{\Psi}(x), \hat{\Psi}(y)\right] = \left[\hat{\Psi}^{\dagger}(x), \hat{\Psi}^{\dagger}(y)\right] = 0, \quad (1.12)$$

where $\zeta_k(x)$ is the position-space representation of the single-particle state $|k\rangle$. The field operators $\hat{\Psi}(x)$ and $\hat{\Psi}^{\dagger}(x)$ destroy and create a particle at the point x (time dependence is usually included in the Heisenberg or Interaction picture [4], which we neglect here for brevity). Note that, in this theory, x is not an operator, like momentum. It is a continuous parameter, along with time. We have effectively exchanged a discrete and large (possibly infinite) number of degrees of freedom (the k) for a single degree of freedom, defined over a single continuous independent variable (x). Many-body quantum mechanical systems can then be described entirely in terms of the ladder or field operators.

Following [34], the formal derivation of the results above begins with the Lagrangian formulation of classical mechanics. In the case of the non-relativistic Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{x}) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}) \right] \Psi(\mathbf{x}) , \qquad (1.13)$$

the Lagrangian is written using the wavefunction Ψ and its gradient as the generalized coordinates. Variational calculus leads to Poisson brackets for Ψ and Ψ^* ; the brackets are replaced by commutators, according to Dirac's quantization procedure

$$\{A, B\} \rightarrow \frac{1}{\mathrm{i}\hbar} \left[\hat{A}, \hat{B}\right],$$
 (1.14)

where A and B represent the two quantities that become quantized, and the braces denote Poisson brackets. Having performed this substitution, Ψ becomes $\hat{\Psi}$ and is now quantized and an operator, satisfying the commutation relations (1.12).

The expansion (1.11) of $\hat{\Psi}$ is always valid, assuming the $\zeta_k(x)$ form a basis of the Hilbert space (in position representation). One typically chooses a representation in which the number operator N_k is diagonal for all k. Then the treatment of the \hat{a}_k operators is identical to that for the harmonic oscillator in single-body quantum mechanics, but with the ladder operators indexed by k and having the interpretation of removing (or adding, in the case of \hat{a}_k^{\dagger}) particles from (to) the k^{th} single-particle state. Hence, the chosen representation is the occupation-number representation (1.7).

Note that the commutators cited above are valid for bosons; a quantum field theoretic treatment of a fermionic system has the commutators replaced with appropriate anti-commutators. Field theories other than that corresponding to the non-relativistic Schrödinger equation are quantized in similar ways.

1.2.2 Mean Field Theory

In describing a Bose-Einstein condensate, it will be convenient to decompose the field operator as

$$\hat{\Psi}(x) = \left\langle \hat{\Psi}(x) \right\rangle \hat{I} + \hat{\chi}(x) , \qquad (1.15)$$

where \hat{I} is the identity operator. By assuming that the vast majority of particles are Bose-condensed, we can interpret $\langle \hat{\Psi}(x) \rangle$ as a number density amplitude of condensed particles, where $|\langle \hat{\Psi}(x) \rangle|^2$ gives an actual number density. The condensate wavefunction also contains information on the local velocity [35]:

$$\frac{\hbar}{m}\nabla\operatorname{Arg}\left[\left\langle \hat{\Psi}\left(x\right)\right\rangle\right]\tag{1.16}$$

By the assumption that most particles are Bose-condensed, $\hat{\chi}(x)$, called the *depletion* of the condensate, is small.

Assuming that $\hat{\chi}(x)$ is small enough to completely neglect, one can find an equation of motion for the field operator, take its expectation value, assume particles interact only upon contact, and arrive at the Gross-Pitaevskii equation, (1.3). Recall that the fraction of noncondensed particles is approximately proportional to $\sqrt{na^3}$, where *n* is the density of particles and *a* is the scattering length. In harmonic traps, this parameter is usually less than 1 percent, so neglecting $\hat{\chi}(x)$ is acceptable [23]. During the experiments we will model, the diluteness parameter becomes unusually large (of order unity), indicating that the Gross-Pitaevskii equation may not adequately describe the processes. The derivation in Chapter 2 addresses this concern by including terms up to second order in $\hat{\chi}(x)$, a level of approximation called *Hartree-Fock-Bogoliubov*. This theory is a second-order correction to the Gross-Pitaevskii equation and is appropriate for BECs in which $\sqrt{na^3} \leq 1$. Both quantum field theory and the time evolution of averaged quantities are exact extensions of quantum mechanics—the formulation called "mean field theory" is an approximation due to the significant assumptions involved in the interpretation of (1.15), the form of interparticle potentials, and the neglect of the depletion.

1.2.3 Quantum Fluctuations

A quantum mechanical expectation value, like a mean field, may be understood as the average over many measurements. In the context of quantum field theory applied to Bose-Einstein condensation, an often-encountered expectation value is $\psi(\mathbf{x}, t) \equiv \langle \hat{\Psi}(\mathbf{x}, t) \rangle$, the condensate wavefunction. Though the condensate wavefunction is usually interpreted as the square root of the number of particles at that space-time point (up to a phase factor), any particular measurement of the number amplitude, that is, any single application of the field operator, may return a number other than the average. The difference between the measured number and the expectation value, an example of a quantum fluctuation, is related to the number density amplitude of particles *not* in the condensate. Mean field theories like the Gross-Pitaevskii equation that deal only with the condensate wavefunction neglect the fluctuations and therefore neglect all particles that are not a part of the condensate. This approximation can fail when there are already a significant percentage of noncondensed particles, or
in situations where noncondensed particles may be produced dynamically. Under these circumstances, quantum fluctuations may play an important role in condensate dynamics for which a simple mean field theory does not account.

Several authors have proposed techniques to account for quantum fluctuations in a tractable way. Gardiner and Zoller [36] developed a modification and quantum mechanical extension of the Boltzmann equation, which is an integro-differential equation governing the phase-space distribution function of particles in a classical gas [37]. Their "quantum kinetic master equation" (QKME) assumes that only a few of the noncondensed modes must be accounted for quantum mechanically and handles the rest classically. The theory is valid when the system is nearly in equilibrium, making it capable of treating nearly adiabatic processes but not the violent dynamics of a collapsing condensate.

Corney and Drummond [38] present a Monte Carlo method based on Gaussian quantum operators. Unlike typical Monte Carlo methods, this theory can determine both the static properties and the dynamics of a system. The method performs well in the simplistic situations in which it has been tested, with a low sampling error.

Most theories try to determine the time evolution of the N-body density operator, which describes the state of the entire system. Time evolving block decimation (TEBD) [39] does this numerically by concentrating only on the salient parts of the density matrix at each time step. The theory is restricted to one spatial dimension and nearest-neighbor interactions between atoms, but can handle limited amounts of entanglement. TEBD has proven effective at demonstrating beyond-mean field effects in systems of entangled solitons [40]. The P and positive-P approaches (summarized in [41]) derive quasi-probability distribution functionals from the N-body density matrix in terms of complex fields. Expectation values can be calculated from these functionals, so the task is then to determine the time evolution of the functionals. In practice, this approach is numerically unstable. Deuar and Drummond [42] describe a generalized positive-P method that correctly accounts for boundary terms that are often unjustly neglected in other positive-P theories. With a prudent choice of gauge, otherwise intractable problems become computationally feasible. The method outperforms typical positive-P methods in situations where exact results are known.

The truncated Wigner approximation (TWA) [41, 43] is similar to the P and positive-P methods in that a partial differential equation for a functional is derived from the density matrix. The complex fields upon which the functional depends are chosen to be a suitable basis for the problem at hand, and their time evolution is determined by an equation resembling the Gross-Pitaevskii equation with a spatial third derivative. This derivative is unfeasible to deal with in practice, and so is neglected. Wüster *et al.* [13] have used this method in the context of collapse, finding that the TWA requires an impractical number of complex fields to model the compact post-collapse condensate. Their simulations agree quite well with a Hartree-Fock-Bogoliubov method, but both overestimate by about 40 percent the time for the condensate to collapse.

Carusotto *et al.* [44] determine the evolution of the density matrix under the assumption that the system is in a Fock (definite particle number) or coherent (semiclassical) state. Fluctuations are included by adding noise with zero mean to the condensate wavefunction during time integration. The noise distribution has some dependence on the condensate itself, thus coupling the noncondensed component that the noise represents to the condensate's dynamics. Reliable numerical simulations using this scheme work best for small numbers of particles, on the order of ten. Zaremba, Griffin, and Nikuni [45] (ZGN) derive equations of motion for the field operator and a fluctuation operator, considering collisions between noncondensed atoms and between atoms in and out of the condensate. These authors simplify their equations and ensure consistency with their renormalization procedure by using the Popov approximation, in which a two-particle correlation function called the *anomalous fluctuations* is neglected. This approximation is strictly only valid when the condensate is nearly in static equilibrium. The ZGN equations take the form of hydrodynamic equations, but are difficult to solve; the authors recommend a variational technique. Fetter and Svidzinsky [46] summarize the more typical hydrodynamic approach to BEC, where the phase angle of the condensate wavefunction is used as a velocity potential.

Including the anomalous fluctuations can introduce an unphysical quasiparticle excitation gap, Hutchinson *et al.* [47] point out. They correct this problem by renormalizing and adjusting the strength of the two-particle contact interaction potential to depend on the condensate and anomalous densities. In simulations of a cylindrically-confined condensate near the critical temperature, a situation where the GPE performs poorly, Hutchinson *et al.*'s approach predicts condensate collective excitation frequencies only three percent different from those predicted by the Popov approximation.

Morgan [48] develops a gapless theory by requiring number conservation from a second-quantized Hamiltonian. The Hamiltonian is then predominantly quadratic in momentum-space ladder operators, with third and fourth order terms that are handled by perturbation theory. Our Hartree-Fock-Bogoliubov theory, similar to that used by Milstein *et al.* [11] and Wüster *et al.* [12], resembles Morgan's approach in that we exactly account for quadratic terms in the Hamiltonian, but approximate all third

and fourth order fluctuations. We find that this is usually a computationally feasible model of experiments concerning the dynamics of BECs with attractive or repulsive interactions.

1.3 Collapse Experiments

Lithium-7 atoms have inherently attractive interactions, so BECs of ⁷Li are supposed [49] to undergo a series of collapses whenever the number of atoms in the condensate, constantly fed by a nonequilibrium noncondensed cloud, approaches the critical number. Observations [50] at Rice University of a ⁷Li condensate indeed show large variations in condensate number, which is attributed to collapse and regrowth cycles. However, a given set of number-versus-time data is difficult to reproduce, as the particular collapse and regrowth sequence appears to depend sensitively on initial number and thermal and quantum fluctuations.

By exploiting a Feshbach resonance, the interactions between atoms can be tuned from repulsive to attractive values over only a few microseconds [3]. In an oftenexamined set of experiments [1, 27, 24] conducted at the Joint Institute for Laboratory Astrophysics (JILA), condensates of about 15,000 rubidium-85 atoms were formed at a temperature of 3 nK with slightly repulsive interactions. The repulsion was balanced by a magnetic trap that was well approximated by an axisymmetric harmonic potential, so that an initial condensate was stable and neither expanding nor collapsing. The interactions were then suddenly tuned to be attractive, so that the critical condition (1.4) was exceeded. A condensate appeared stable for a short time $t_{collapse}$ after this transition (the length of time decreasing as the magnitude of the interactions or the initial density increased), then suddenly lost atoms at an exponential rate, the decay constant τ_{decay} of which was only slightly influenced by the



Figure 1.2: *Schematic of a collapse.* Condensed atoms (blue) are suddenly given attractive interactions, causing the condensate to collapse and emit an anisotropic burst of noncondensed atoms (red). When interactions are shifted to slight repulsion, radial jets appear, and a core of colliding solitary waves remains after atom loss ends.

initial number of atoms and the magnitude of their interactions. Finally, a stable, excited, and highly anistotropic condensate remained, containing N_{remnant} atoms. See Figure 1.2 for a pictorial description of a collapse experiment and Figure 1.3 for a reproduction of experimental measurements [1] of condensate number versus time.

During the collapse, a surprising burst of energetic atoms was emitted from the condensate. Between experiments, the number of atoms in the bursts varied by as much as a factor of two, even for identical sets of controlled and observed experimental parameters. The energies of the burst atoms were usually higher for atoms emitted in the radial rather than axial direction, even though the trap was stronger in the radial direction.



Figure 1.3: Number loss during a collapse [1]. At $\tau_{\text{evolve}} = 0$, the interactions become attractive, but no appreciable loss is observed until t_{collapse} , when exponential loss occurs with decay constant τ_{decay} , until a nonzero number N_{remnant} of atoms remains. Used with permission [51].

A significant number of atoms lost from the condensate went undetected; for example, about 8500 atoms out of an initial condensate of 15,000 were missing after a collapse [24]. Atoms with energies greater than about 20 μ K,³ atoms in states that were not influenced by the trapping potential, and pairs of atoms bound to each other because of the Feshbach resonance (henceforth referred to as molecules) could not be detected by the imaging apparatus. Whatever the nature of these missing atoms, their fraction increased with the magnitude of the attractive interactions and was independent of the initial number of atoms.

 $^{^{3}}$ In this context, energy is often expressed in terms of temperature; multiplying by Boltzmann's constant restores the correct units.

If the atom loss was interrupted by changing the strength of the interactions a second time, now to a slightly repulsive value, atoms of a lower energy than the bursts were emitted, almost entirely in the radial direction. The sizes of such jets, which were sometimes asymmetrically distributed around the condensate, varied even when all noted experimental parameters were unchanged between experiments.

The fraction of atoms in the remnant decreased as the length of time for which the interactions were attractive increased, decreased as the magnitude of those interactions increased, and was independent of the initial number of atoms. The remnant itself entered a breathing mode, the dominant frequencies of which were approximately twice the radial and axial trap frequencies.

Subsequent experiments [52] showed that in nearly every case, the number of atoms in the remnant was above the critical value given by (1.4) at which collapse should occur. Equation (1.4) correctly predicted the initial collapse, yet no remnant collapsed; in fact, each persisted for about 3 s, the expected lifetime of a stable condensate in this experimental configuration. Remnants were observed to separate into distinct clouds, the number of which generally increased as either the magnitude of the interactions during collapse increased, or the initial number of atoms increased. These clouds collided tens of times during the life of the remnant. All these observations led the experimenters to infer that each cloud in the remnant was a solitary wave containing less than the critical number of atoms, and that all the solitary waves interacted repulsively with each other. Thus, the remnant condensate was thought to be composed of several small, colliding condensates that did not overlap.

In similar experiments [53] at Rice University, performed with lithium-7 atoms (this time exploiting a Feshbach resonance) in a long and narrow cylindrical trap, experimenters formed a stable condensate with an axial displacement and then altered the interactions to be slightly attractive or repulsive. In the case of slightly repulsive interactions, nothing more than a spreading of the condensate was observed. For small attractive interactions, a line of solitary waves formed, while a significant number of atoms escaped detection. If the trap was altered such that the axial displacement was no longer a stable arrangement (that is, the condensate was "released" from its initial position), the solitary waves oscillated in the trap without overlapping. The waves bunched up when concentrated in the ends of the trap, and spread out when concentrated in the center of the trap, implying that they interacted repulsively. The number of solitary waves seemed to depend not on the rate at which the magnetic field controlling the interactions was changed, but only on the time between the release of the initial condensate and the instant at which the interactions passed from repulsive to attractive. See Figure 1.4 for experimental images of the solitary wave dynamics [53].

We attempt to reproduce the JILA experiments in our simulations. The Rice experiments require careful consideration of a nonequilibrium thermal cloud, which would necessitate a more complicated model. The solitary wave experiment [53] is concerned primarily with the post-collapse dynamics rather than the collapse itself, which is our main concern. Finally, the trap used in the JILA experiments are better approximated by a spherical trap than those used in the Rice experiments, allowing more practical simulations in spherical symmetry.

1.4 Experiments with Repulsive Interactions

Collapsing BECs are not the only experiments to produce exotic results concerning condensates with order-unity diluteness parameters. One set of related experiments [2, 24] formed a stable, noninteracting or weakly repulsive BEC in the trap



Figure 1.4: *Post-collapse solitary wave dynamics* [53]. At 0 ms, interatomic interactions are made attractive, and a ⁷Li BEC forms a line of small clouds. The trap is then altered so that the condensate is "released," and the long-lived clouds are seen to oscillate in the trap as if they were solitary waves with repulsive interactions. Shown are time-slices of the density of the condensate, integrated along one radial direction. Used with permission [54].

used in the JILA collapse experiments, and then subjected it to a rapid magnetic field pulse (we henceforth refer to such experiments as *one-* or *single-pulse experiments*). The field was linearly ramped from its initial value to a value near the Feshbach resonance in tens to hundreds of microseconds, held at a constant value for one to hundreds of microseconds, called the *hold time*, and then quickly and linearly ramped back to the initial value. Likewise, the scattering length was ramped from zero or a small positive value, to a very large positive value, and finally back to its initial small value. Following a pulse, the experimenters observed that the number of atoms remaining in the condensate *increased* for longer ramp times, indicating that the loss mechanism is *not* the usual density-dependent loss responsible for the rethermalization of a stable condensate. Figure 1.5 is a plot from [2] showing the described trend. Varying the initial density of the BEC did not appreciably alter the rate of loss, further suggesting that the loss was not density-dependent. As expected, pulses which came closer to the resonance resulted in more loss from the condensate. If the magnetic field was held at 157.1 ± 0.1 G during the hold time,⁴ small, damped oscillations in atom number were apparent when the hold time was varied.

Surprisingly, a burst of atoms similar to that in the collapse experiments appeared in this experiment with repulsive interactions. The number of atoms in the burst increased with the hold time (saturating at about 4000 atoms out of a 16,600 atom condensate), yet the energy of the burst atoms decreased as the hold time increased. As in the collapse experiments, the bursts were markedly anisotropic, having larger velocities in the radial rather than axial direction. When the magnetic field was held above 160 G during the hold time, no burst atoms were observed. Varying the number of atoms in the surrounding thermal cloud did not appreciably affect the bursts, indicating that interactions with noncondensed atoms were not responsible. The burst atoms remained in the same spin state as the condensed atoms, indicating that spin-flip interactions were not involved.

These single-pulse experiments inspired experiments (henceforth referred to as *two-pulse experiments*) [3, 24] with two magnetic field pulses, separated by a "free precession" time, during which the magnetic field was held constant, below the initial value. As with the other experiments, an energetic burst of atoms emanated

 $^{^{4}}$ To put the number in context, consider that the effective scattering length is zero at 165.750 G and formally diverges at 155.041 G [28].



Figure 1.5: Condensate loss in one-pulse experiment [2]. Number of atoms remaining in an initially stable BEC after a single magnetic field pulse for various hold times. The horizontal axis has all values divided by 4, and the continuous lines are only meant to guide the eye. Note that loss *decreases* as time spent near the Feshbach resonance increases. Used with permission [51].

from the condensate. The most intriguing results of these experiments were damped oscillations in the number of condensed and burst atoms measured after the pulse sequence, when the free precession time was varied. The frequency of these oscillations increased when the magnetic field during the free precession time was held further from resonance, but had no obvious dependence on the duration or amplitude of the magnetic field pulses, the density of atoms, or the initial magnetic field. Again, between 8 and 50 percent of the atoms escaped detection, and this fraction increased as either the density or the length of the magnetic field pulses increased. The numbers



Figure 1.6: Oscillations in number for two-pulse experiments [3]. Observed oscillations in the number of burst atoms (open circles), condensed atoms (filled circles), and the total number of detected atoms (squares). The dashed horizontal line indicates the total number of atoms initially in the condensate. Since the total detected number oscillates, the number of missing atoms oscillates, as well. Used with permission [51].

of the three components—condensed, burst, and missing atoms—all oscillated with the same frequency, but out of phase. The oscillations were apparent for a wide range of magnetic fields, rather than the thin window in the single-pulse experiments. See Figure 1.6 [3] for an example of the experimental results.

1.5 Current Understanding

BEC collapse has been theoretically studied for several years. Kagan *et al.* [55] predicted that collapse occurs on a time scale $t_{\text{collapse}} \sim \omega^{-1}$, where ω is the trap frequency. The observations of [1] have shown this prediction to be incorrect. Kagan

and coworkers also supposed [56] that during a collapse, the condensate's density increases until density-dependent losses due to three-body recombination (see Section 1.1.0) take over, eventually causing expansion of the condensate. The cycle then repeats, as the trap pushes the remaining condensate back towards the trap center. The GPE simulations of Saito and Ueda and Bao [57, 58, 59, 60] clearly show such behavior, leading to significant atom loss and the prevention of the appearance of a singularity during collapse.

These and other [61, 62, 63, 64] simulations qualitatively reproduce the collapse process, the time to collapse t_{collapse} , the condensate number decay constant τ_{decay} , bursts, and jets, but have achieved no solid quantitative agreement with observation. Minor differences in these authors' results, as well as the lack of quantitative agreement with experiment, may be due to their different choices of density-dependent loss rates. These losses have been shown [65] to have a complicated dependence on magnetic field, especially near a Feshbach resonance, making them difficult to precisely characterize.

Recognizing the deficiency in atom loss models, Bao and coworkers [60] perform a GPE simulation with a loss rate chosen so that their simulations correctly reproduce the experimental values of t_{collapse} and condensate remnant number. The atom number decay constant τ_{decay} is reasonably well reproduced, but the simulated burst energies are much lower than what is experimentally observed. This failure suggests that a Gross-Pitaevskii model with simple density-dependent loss does not sufficiently describe the collapse. Savage *et al.* [66], surveying the literature and performing their own simulations with several different loss rate coefficients, arrive at the same conclusion, noting that theoretical values of t_{collapse} are consistently larger than the experimental values. The authors mention that this is especially odd, since the period before collapse begins should be the realm where the GPE applies.

Duine and Stoof [67] propose that two condensed atoms can collide, scattering one atom out of the condensate. They use a Gaussian variational technique to investigate this "quantum evaporation" as a possible player in the collapse, especially concerning remnant number and burst formation. Their simulations show a considerable loss from the condensate, but, disagreeing with observation, this loss begins immediately after the interatomic interactions become attractive.

Mackie and coworkers [68] suggest that pairs formed by the Feshbach resonance may dissociate into noncondensed atoms during the collapse, and the simulations of Milstein *et al.* [11], which neglect three-body losses but include quantum fluctuations and pair formation via the Feshbach resonance, show an energetic burst of noncondensed atoms, though using parameters not taken from experiments.

Calzetta and coworkers [69] downplay the importance of such a molecular component for the values of the scattering length a_{collapse} in the collapse experiments, which are far from resonance. Like Yurovsky [70], they attribute loss from the condensate to the growth of noncondensed modes. Calzetta *et al.* suggest that a theory accounting for fluctuations would have instabilities growing out of those fluctuations, which may account for earlier collapse times. The authors extract a scaling argument, $t_{\text{collapse}} = \alpha \left(a/a_{\text{critical}} - 1 \right)^{-1/2}$, where a_{critical} is the smallest scattering length that will allow collapse, according to Equation (1.4). A choice of $\alpha = 5$ ms creates good agreement with experimental data, but more recent work [71] finds no theoretical justification for that particular choice of α . Calzetta now attributes condensate loss to a loss of coherence between atoms, though no significant investigations of this proposal have yet been performed.

Wüster and coworkers [12] use the same theory of fluctuations as Milstein *et al.*,

but also regard the molecular component as unimportant to collapse. Their simulations still find a t_{collapse} exceeding the observed value. Using an alternate, truncated Wigner, formulation and including initial and dynamical noise, a background thermal component, and cylindrical geometry with experimental parameters, Wüster *et al.* [13] still overestimate the experimentally measured t_{collapse} by about 40 percent.

All these models have at least some qualitative agreement with observation, and some provide insight into other aspects of the collapse experiments. Saito and Ueda [59] show that the collapse in a cylindrical trap forms several density spikes, rather than a single, spherical clump. The authors allege that interference among these spikes' matter waves is responsible for the observed jets. Bao *et al.* [60] find that slight disturbances in initial conditions can be responsible for the significant anisotropy of the jets and the wide variation in the number of atoms in the jets. Adhikari [62] agrees with the experimenters' interpretation [1] of the jets as expanding density spikes, but his simulations clarify that those spikes are a consequence of the collapse dynamics in a non-spherical trap, and not of a "lumpy" initial condition.

Saito and Ueda [57] suggest the bursts are atoms originally near the center of the collapse that acquire kinetic energy when three-body losses suddenly remove a large number of atoms from the center of the collapse. In these simulations and others [59, 61, 62, 63, 64, 60], the burst atoms are distinguished from the condensate purely by their location. In the simulations of Milstein *et al.* and Wüster *et al.* the burst is assumed to be a distinct noncondensed field, which can occupy the same space as the condensate.

Finally, Parker and coworkers [72] have used a GPE without loss terms to model the remnant observed in [52]. Without making specific quantitative comparisons, they find that two solitary waves governed by the GPE in a cylidrical trap can, under certain circumstances that probably [52] occured in the experiments, survive more than 40 collisions. Both the waves' velocities and their relative phase are found to be important to the waves' stability. Carr and Brand [73] show that solition trains like those observed in the Rice experiment [53] may be the result of a modulational instability that is seeded by the initial condensate's self-interference and manifests itself when the interatomic interactions are made attractive.

The magnetic field pulse experiments on repulsive condensates have stimulated fewer simulations than the collapse experiments. Duine and Stoof [74] use coupled mean fields allowing for molecule formation, quantum evaporation, and three-body losses in modeling the one-pulse experiments. These simulations had only general qualitative agreement with the experiments, but with the interesting observation that the inclusion of three-body losses supressed oscillations in numbers of atoms and molecules, despite the fact that these density-dependent losses should be unimportant under the experimental circumstances [24]. Mackie and coworkers [68] use a coupled mean field model that allows for dissociation of molecules into noncondensed atom pairs, but find only about five percent loss to the noncondensed component, with very few molecules being retained. The authors observe a larger loss in simulations of the two-pulse experiments, but the oscillation envelopes have a behavior markedly different from the slight damping observed in the experiments. Kokkelmans and Holland [10] use the same model as the Milstein *et al.* collapse simulation [11], but use a Gaussian average over a homogeneous gas to simulate the behavior of a trapped gas. These simulations agreed well both qualitatively and quantitatively with the two-pulse experiments, showing that the majority of atoms lost from the condensate go into noncondensed modes, and the missing atoms are identified as molecules. Köhler and coworkers [75] model the two-pulse experiments with a theory that includes molecule formation and quantum fluctuations, and find good qualitative agreement with the experiments. They also find that the presence of the trap moves the means of the condensate and burst numbers' oscillations closer together in a way not captured by a Gaussian average of a homogeneous gas. They attribute this difference to the presence of a length scale not found in the homogeneous gas simulations.

1.6 Overview of Numerical Methods

Our model for the experiments leads to four coupled, nonlinear, partial differential equations defined over continuous domains. Useful analytical solutions of these equations are presently unknown and may not exist, so we must properly discretize the equations using prudent numerical methods and implement the resulting algorithms on a computer. Assuming spherical or cylindrical symmetry and coordinates reduces the number of independent variables, but parallel computation is still necessary for simulations to run in a reasonable amount of time, especially in the cylindrical case.

1.6.1 Analytical Treatment of Nonlinear Partial Differential Equations

As described in [76], a nonlinear partial differential equation (PDE) contains terms which are not linear in the dependent variable or its derivatives (in out case, a quantum average, itself a function of space and time). A quasilinear PDE is linear in the dependent variable's derivatives, but may contain any function of the dependent variable itself, or multiply any derivative of the dependent variable by the dependent variable. In either case, analytical solutions are often very difficult to obtain, since most of the methods used on linear equations do not apply. Especially noteworthy is the fact that superposition is not valid for nonlinear equations—the sum of two solutions is not, in general, also a solution, thus making separation of variables, one of the most powerful methods of solving PDE's, unavailable. Some nonlinear equations can be solved analytically, and quasilinear equations are particularly susceptible to the method of characteristics, which is effectively a change of independent variables that leads to simpler, often coupled linear, equations. Many nonlinear equations that have wave-like solutions balance the dispersion of the waves with a focusing or defocusing nonlinearity, leading to solitary waves and, sometimes, solitons. However, the vast majority of nonlinear equations are analytically intractable.

Important exceptions, one of which is the one-dimensional Gross-Pitaevskii equation, are integrable equations (see [77], for example). According to one of many definitions, an integrable PDE has a Lax pair formulation, which is based on an operator equation closely resembling a Heisenberg equation of motion in quantum mechanics. A Lax pair implies that the PDE has infinitely many conserved quantities and may be formally solved by the inverse scattering transform (see [78], for example), a generalized Fourier transform method requiring the solution of a linear integral equation.

1.6.2 Approximate Numerical Solutions

We approximate the solutions to our equations by numerical methods. Finite difference schemes are perhaps the most popular method of solving partial differential equations, but past research with nonlinear Schrödinger equations [79] and a Hartree-Fock-Bogoliubov simulation [11] of the collapse suggests that finite differences are inaccurate and inefficient in this situation.

We seek a method of lines solution. Our particular approach discretizes in space using pseudospectral approximations to derivatives, which may be viewed as the discrete Fourier transform analogy of the Fourier transform method of solving continuous PDE's, or analytical derivatives of truncated basis function expansions. Time propagation is performed using an adaptive Runge-Kutta method, which estimates by a truncated Taylor series the solution to the system of ODE's which results from spatial discretization. Thus, our initially continuous model remains continuous in time but is discretized in space.

1.6.3 Implementation

The simulation is written in C++. The code consists of several libraries mostly containing easily extended and reusable functions, such as a Runge-Kutta integrator and numerical derivatives. Most code is custom-written, with the notable exception of the Fourier transform routines, which are taken from [80] and modified.

The several independent variables in the cylindrical model of Chapter 3 necessitate parallel computing. As described in [81], choice and implementation of parallel algorithms is highly machine-dependent—given our resources, we will only consider parallelization on a cluster. Such a computer consists of several connected nodes, each of which is a symmetric multiprocessor (SMP), or a unique computer having multiple processors that all address a common memory space. Machines of this type lend themselves well to multiple-instruction, multiple-data (MIMD) programming paradigms, since different nodes see different memory spaces (hence multiple data streams), and multiple processors on a single node see the same memory space (hence multiple instructions).

While there is no consensus on parallel programming implementations, two general approaches dominate: threading and message passing. In threading, a single process, or instance of a program, spawns several threads, all of which see the same memory space and may each run on a different processor in an SMP. Unique threads spawned from a single process require less overhead and startup time than an equal number of individual processes.

In message passing, each process sees a unique memory space and is able to send data to and receive data from the other processes. The physical communication channel usually consists of Ethernet connections or a specially-made high-speed switch. The most advanced parallelization schemes on the computer we consider use threading on each node and message passing to move data between nodes.

Not all algorithms benefit from parallelization. Amdahl's law [82] says that the time t_M for M processors to perform a task is

$$t_M = t_S + \frac{t_P}{M},\tag{1.17}$$

where t_P and t_S are the times to sequentially execute the portions of the code that can and cannot be parallelized, respectively. For example, a Runge-Kutta method applied to a one-dimensional ODE has little or no opportunity for parallelization, since each calculation in the method depends on at least one of the calculations that preceeded it. However, a system of ODE's could be solved by running several Runge-Kutta integrators in parallel, with the ratio t_S/t_P declining as the number and complexity of the ODE's increase.

Our simulations in spherical symmetry use threading to share work among different processing cores in an SMP. This parallelization scheme can better than halve such a simulation's wallclock runtime when using four cores. Simulations in cylindrical symmetry have four spatial independent variables; this code is written for a cluster, with message passing between nodes and on-node threading. Communication time could be kept to a minimum by using every core on a node to simultaneously send and receive data from other nodes during the communication phases of the parallel algorithm.

Chapter 2

PHYSICAL MODEL

Our theory to describes the dynamics of trapped condensates with order-unity diluteness parameters by a mean field approach with two-point equal-time correlations, or lowest-order quantum fluctuations. The general equations of this model have been written, in some form, in [14] and [83], for example; we present an unusually thorough derivation. Motivated by the success of Kokkelmans and Holland [10] in explaining the two-pulse experiments, our model includes pairing of atoms due to the Feshbach resonance. Despite controversy [12, 69], some work [11, 10, 68] suggests that this molecular component is important to both collapse and pulse experiments.

We derive equations of motion for field operators and two pairs of fluctuation operators, average these equations, factorize consistently, and apply the renormalized theory of [14] to model the Feshbach resonance. The result is four, coupled, nonlinear PDE's that include quantum fluctuations up to second order.

2.1 Field Operators

Define $\hat{\Psi}_a(\mathbf{x}, t)$ as the atomic field operator, which destroys a bosonic atom at the position \mathbf{x} and time t. Its Hermitian conjugate, $\hat{\Psi}_a^{\dagger}(\mathbf{x}, t)$, creates a bosonic atom at position \mathbf{x} and time t. The molecular field operator $\hat{\Psi}_m(\mathbf{x}, t)$ and its Hermitian conjugate $\hat{\Psi}_m^{\dagger}(\mathbf{x}, t)$ are the corresponding operators for bosonic molecules. A *molecule* is defined as a pair atoms bound because of the Feshbach resonance. The same instant in time is used in everything that follows, so we usually omit the t for brevity; for example, the atomic field operator is written $\hat{\Psi}_a(\mathbf{x})$. All four operators are taken to be in the Heisenberg picture.

The field operators obey the following commutation relations:

$$\left[\hat{\Psi}_{a}(\mathbf{x}),\hat{\Psi}_{a}(\mathbf{x}')\right] = \left[\hat{\Psi}_{m}(\mathbf{x}),\hat{\Psi}_{m}(\mathbf{x}')\right] = \left[\hat{\Psi}_{a}^{\dagger}(\mathbf{x}),\hat{\Psi}_{a}^{\dagger}(\mathbf{x}')\right] = \left[\hat{\Psi}_{m}^{\dagger}(\mathbf{x}),\hat{\Psi}_{m}^{\dagger}(\mathbf{x}')\right] = 0$$
(2.1)

$$\left[\hat{\Psi}_{a}(\mathbf{x}),\hat{\Psi}_{a}^{\dagger}(\mathbf{x}')\right] = \left[\hat{\Psi}_{m}(\mathbf{x}),\hat{\Psi}_{m}^{\dagger}(\mathbf{x}')\right] = \delta^{(3)}(\mathbf{x}-\mathbf{x}'), \qquad (2.2)$$

where $\delta^{(3)}(\mathbf{x})$ is the three-dimensional Dirac delta function. Other useful commutators are

$$\begin{bmatrix} \hat{\Psi}_a(\mathbf{x}), \hat{\Psi}_m(\mathbf{x}') \end{bmatrix} = \begin{bmatrix} \hat{\Psi}_a^{\dagger}(\mathbf{x}), \hat{\Psi}_m(\mathbf{x}') \end{bmatrix} = \begin{bmatrix} \hat{\Psi}_a(\mathbf{x}), \hat{\Psi}_m^{\dagger}(\mathbf{x}') \end{bmatrix} = \begin{bmatrix} \hat{\Psi}_a^{\dagger}(\mathbf{x}), \hat{\Psi}_m^{\dagger}(\mathbf{x}') \end{bmatrix} = 0,$$
(2.3)

which are true because the atomic and molecular field operators act in different subspaces of the full Hilbert space. Conceptually, this means that an operator acting on an atom has no effect on a molecule. It is an approximation in that by writing, for example, $\left\langle \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \, \hat{\Psi}_{m}(\mathbf{x}) \right\rangle = \left\langle \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \right\rangle \left\langle \hat{\Psi}_{m}(\mathbf{x}) \right\rangle$, we are assuming that $\hat{\Psi}_{m}(\mathbf{x}) |\lambda\rangle$ is completely uncorrelated with $\hat{\Psi}_{a}(\mathbf{x}') |\lambda\rangle$, where $|\lambda\rangle$ is the state of the system.

We decompose the atomic field operator as its average plus a fluctuation around that average; that is,

$$\hat{\Psi}_a(\mathbf{x}) = \left\langle \hat{\Psi}_a(\mathbf{x}) \right\rangle \hat{I} + \hat{\chi}_a(\mathbf{x}) , \qquad (2.4)$$

where the identity operator I will usually be omitted for brevity. We should in principle decompose the molecular field operator in the same fashion, but this would lead to computationally and presently theoretically intractable four-particle fluctuations. Thus we have our second approximation:

$$\hat{\Psi}_m(\mathbf{x}) = \left\langle \hat{\Psi}_m(\mathbf{x}) \right\rangle I. \tag{2.5}$$

2.2 Hamiltonian

We are interested in the kinetic and potential energies of the atoms, that of the molecules, the energy associated with collisions between atoms, and the energy associated with collisions between atoms in which a molecule is formed due to the Feshbach resonance. The corresponding Hamiltonian is

$$\hat{H} = \hat{H}_a + \hat{H}_m + \hat{H}_{aa} + \hat{H}_{am},$$
 (2.6)

where

$$\hat{H}_{a} = \int \mathrm{d}^{3}y \; \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \left[-\frac{\hbar^{2}}{2m} \nabla_{y}^{2} + V_{a}\left(\mathbf{y}\right) - \mu_{a} \right] \hat{\Psi}_{a}(\mathbf{y}) \tag{2.7}$$

$$\hat{H}_m = \int \mathrm{d}^3 y \; \hat{\Psi}_m^{\dagger}(\mathbf{y}) \left[-\frac{\hbar^2}{4m} \nabla_y^2 + V_m(\mathbf{y}) - \mu_m \right] \hat{\Psi}_a(\mathbf{y}) \tag{2.8}$$

$$\hat{H}_{aa} = \frac{U}{2} \int \mathrm{d}^3 y \, \hat{\Psi}_a^{\dagger}(\mathbf{y}) \, \hat{\Psi}_a^{\dagger}(\mathbf{y}) \, \hat{\Psi}_a(\mathbf{y}) \, \hat{\Psi}_a(\mathbf{y}) \tag{2.9}$$

$$\hat{H}_{am} = \frac{g}{2} \int \mathrm{d}^3 y \, \hat{\Psi}_m^{\dagger}(\mathbf{y}) \, \hat{\Psi}_a(\mathbf{y}) \, \hat{\Psi}_a(\mathbf{y}) + \frac{g}{2} \int \mathrm{d}^3 y \, \hat{\Psi}_a^{\dagger}(\mathbf{y}) \, \hat{\Psi}_a^{\dagger}(\mathbf{y}) \, \hat{\Psi}_m(\mathbf{y}) \,. \tag{2.10}$$

In these four equations, \mathbf{y} is a position variable used for integration, and the integrals run over the entire domain. The mass m is that of a single atom; ∇_y^2 is the Laplacian acting on functions defined over \mathbf{y} coordinates; $V_a(\mathbf{y})$ is the external potential felt by an atom at position \mathbf{y} , and $V_m(\mathbf{y})$ is that felt by a molecule; μ_a and μ_m are the atomic and molecular chemical potentials, respectively; U relates to the energy of interactions between atoms; and g relates to the energy of atom-atom interactions in which a molecule is formed or dissociated. The form of the interaction terms (2.9) and (2.10) assume a contact interaction between atoms; specifically, $V_{aa}(\mathbf{y} - \mathbf{y}') = U \,\delta^{(3)} (\mathbf{y} - \mathbf{y}')$ and $V_{am}(\mathbf{y} - \mathbf{y}') = g \,\delta^{(3)} (\mathbf{y} - \mathbf{y}')$, where V_{aa} is the interatomic potential between two atoms which scatter off of each other, and V_{am} is the interatomic potential between two colliding atoms that form a molecule. We shall see later that this approximation does well for the ultracold systems we consider.

While the Hamiltonian (2.6) is a reasonable model of boson fields in which pair formation and fluctuations are important, it is also approximate in that we have neglected the energy associated with collisions between molecules and the energy associated with collisions between molecules and atoms in which pair formation or dissociation is not involved. To be completely inclusive of all events, the Hamiltonian should really account for collisions between all possible particles and involving all possible numbers of such particles, but we neglect all interactions not mentioned in (2.7) through (2.10) for simplicity. We also neglect density dependent losses to establish the importance of the molecular component and quantum fluctuations, as well as to understand our numerics in a situation where number is conserved.

2.3 Quantities of Interest

In modeling a collapsing Bose-Einstein condensate, we are interested in the average number density amplitude of Bose-condensed atoms as a function of position,

$$\phi_a(\mathbf{x}) \equiv \left\langle \hat{\Psi}_a(\mathbf{x}) \right\rangle, \qquad (2.11)$$

and the average number density amplitude of Bose-condensed molecules as a function of position,

$$\phi_m(\mathbf{x}) \equiv \left\langle \hat{\Psi}_m(\mathbf{x}) \right\rangle. \tag{2.12}$$

Again, time dependence is implied, but not explicitly written. The term "number density amplitude" is an analogy to the probability amplitudes of single- or fewparticle quantum mechanics, which are complex valued functions, the square moduli of which are probability densities. Recall that the number density amplitude is the order parameter of the condensate, and also contains information about velocity in its phase angle.

We also desire quantities related to the fluctations about the atomic mean field,

$$G_N(\mathbf{x}, \mathbf{x}') \equiv \left\langle \hat{\chi}_a^{\dagger}(\mathbf{x}') \, \hat{\chi}_a(\mathbf{x}) \right\rangle \tag{2.13}$$

and

$$G_A(\mathbf{x}, \mathbf{x}') \equiv \langle \hat{\chi}_a(\mathbf{x}') \, \hat{\chi}_a(\mathbf{x}) \rangle \,, \tag{2.14}$$

called the *normal* and *anomalous fluctuations*, respectively.¹ Recalling Equation (2.4), we see that the normal and anomalous fluctuations satisfy the definition of correlation functions (see, for example, [84]). In interpreting (2.13) and (2.14), we must be careful to note that same-time correlations alone imply nothing about causality. Expanding the correlation functions in terms of field operators, we have

$$G_N(\mathbf{x}, \mathbf{x}') = \left\langle \hat{\Psi}_a^{\dagger}(\mathbf{x}') \, \hat{\Psi}_a(\mathbf{x}) \right\rangle - \left\langle \hat{\Psi}_a^{\dagger}(\mathbf{x}') \right\rangle \left\langle \hat{\Psi}_a(\mathbf{x}) \right\rangle \tag{2.15}$$

$$G_A(\mathbf{x}, \mathbf{x}') = \left\langle \hat{\Psi}_a(\mathbf{x}') \, \hat{\Psi}_a(\mathbf{x}) \right\rangle - \left\langle \hat{\Psi}_a(\mathbf{x}') \right\rangle \left\langle \hat{\Psi}_a(\mathbf{x}) \right\rangle.$$
(2.16)

Let us concentrate on the first terms on the right-hand sides of (2.15) and (2.16). Naming the system's state $|\lambda\rangle$, $\langle \hat{\Psi}_a^{\dagger}(\mathbf{x}') \hat{\Psi}_a(\mathbf{x}) \rangle$ gives the overlap between states $\hat{\Psi}_a(\mathbf{x}) |\lambda\rangle$ and $\hat{\Psi}_a(\mathbf{x}') |\lambda\rangle$. That is, if we remove a condensed atom from point \mathbf{x} , $\langle \hat{\Psi}_a^{\dagger}(\mathbf{x}') \hat{\Psi}_a(\mathbf{x}) \rangle$

¹The anomalous fluctuations are sometimes referred to in the literature as the "anomalous density" or a "pairing field," not to be confused with our $\phi_m(\mathbf{x})$.

is the amplitude of how likely we are to find the system in a state with a condensed atom removed from \mathbf{x}' ; $\langle \hat{\Psi}_a^{\dagger}(\mathbf{x}') \hat{\Psi}_a(\mathbf{x}) \rangle$ contains information about how the system at the points \mathbf{x} and \mathbf{x}' is correlated. Now recall that if two quantities are uncorrelated, the average of their product factorizes: $\langle \hat{\Psi}_a^{\dagger}(\mathbf{x}') \hat{\Psi}_a(\mathbf{x}) \rangle = \langle \hat{\Psi}_a^{\dagger}(\mathbf{x}') \rangle \langle \hat{\Psi}_a(\mathbf{x}) \rangle$. The subtraction of the product of expectation values [the final terms in Equations (2.15) and (2.16)] sets the zeros of the correlation functions to be states that are completely uncorrelated. In a classical system, these correlation functions should be approximately zero for large $|\mathbf{x} - \mathbf{x}'|$. If the correlation functions are significant over such distances, we have off-diagonal long range order (ODLRO), one of the hallmarks of a system where many-body quantum mechanical effects are important [21]. The definition (2.16) also illustrates that $G_A(\mathbf{x}, \mathbf{x})$ is equivalent to the variance in the expectation value of the atomic field operator.

Finally, note that by Equation (2.4) and our definition of $\left|\left\langle \hat{\Psi}_{a}(\mathbf{x})\right\rangle\right|^{2}$ as the number density of *condensed* atoms, $\hat{\chi}_{a}(\mathbf{x})$ is the field operator for all of the atoms that are *not* condensed. Thus we may interpret $\left\langle \hat{\chi}_{a}^{\dagger}(\mathbf{x}) \hat{\chi}_{a}(\mathbf{x}) \right\rangle$ as the number density of noncondensed atoms.

We will find these four quantities, $\phi_a(\mathbf{x})$, $\phi_m(\mathbf{x})$, $G_N(\mathbf{x}, \mathbf{x}')$, and $G_A(\mathbf{x}, \mathbf{x}')$, by first computing the Heisenberg equations of motion for each of $\hat{\Psi}_a(\mathbf{x})$, $\hat{\Psi}_m(\mathbf{x})$, $\hat{\chi}_a^{\dagger}(\mathbf{x}') \hat{\chi}_a(\mathbf{x})$, and $\hat{\chi}_a(\mathbf{x}') \hat{\chi}_a(\mathbf{x})$, and then taking the expectation value of each side of the resulting equations. We must consistently factorize some of the resulting expectation values so that the desired partial differential equations depend only on the four fields they govern.

2.4 Equations of Motion

The time evolution of any operator \hat{A} in the Heisenberg picture is determined by

$$i\hbar \frac{\partial}{\partial t} \hat{A} = \left[\hat{A}, \hat{H} \right], \qquad (2.17)$$

where \hat{H} is the system's Hamiltonian. This equation is the Heisenberg equation of motion for \hat{A} , for \hat{A} time independent in the Schrödinger picture.

2.4.1 Atomic Field Operator

In order to find an equation for $\phi_a(\mathbf{x})$, we must first calculate

$$i\hbar \frac{\partial}{\partial t} \hat{\Psi}_{a}(\mathbf{x}) = \left[\hat{\Psi}_{a}(\mathbf{x}), \hat{H}\right]$$
$$= \left[\hat{\Psi}_{a}(\mathbf{x}), \hat{H}_{a}\right] + \left[\hat{\Psi}_{a}(\mathbf{x}), \hat{H}_{m}\right] + \left[\hat{\Psi}_{a}(\mathbf{x}), \hat{H}_{aa}\right] + \left[\hat{\Psi}_{a}(\mathbf{x}), \hat{H}_{am}\right]. \quad (2.18)$$

We proceed term-by-term using the commutation relations given in Equations (2.1) through (2.3).

$$\begin{bmatrix} \hat{\Psi}_{a}(\mathbf{x}), \hat{H}_{a} \end{bmatrix} = \int d^{3}y \ \hat{\Psi}_{a}(\mathbf{x}) \ \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \begin{bmatrix} -\frac{\hbar^{2}}{2m} \nabla_{y}^{2} + V_{a}(\mathbf{y}) - \mu_{a} \end{bmatrix} \hat{\Psi}_{a}(\mathbf{y})$$
$$- \int d^{3}y \ \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \begin{bmatrix} -\frac{\hbar^{2}}{2m} \nabla_{y}^{2} + V_{a}(\mathbf{y}) - \mu_{a} \end{bmatrix} \hat{\Psi}_{a}(\mathbf{y}) \ \hat{\Psi}_{a}(\mathbf{x})$$
$$= \int d^{3}y \ \left[\hat{\Psi}_{a}(\mathbf{x}), \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \right] \begin{bmatrix} -\frac{\hbar^{2}}{2m} \nabla_{y}^{2} + V_{a}(\mathbf{y}) - \mu_{a} \end{bmatrix} \hat{\Psi}_{a}(\mathbf{y})$$
$$= \begin{bmatrix} -\frac{\hbar^{2}}{2m} \nabla_{x}^{2} + V_{a}(\mathbf{y}) - \mu_{a} \end{bmatrix} \hat{\Psi}_{a}(\mathbf{x}), \qquad (2.19)$$

where we have used the fact that $\hat{\Psi}_a(\mathbf{x})$ commutes with ∇_y^2 (since the Laplacian is only acting on **y** coordinates) and the evenness of the Dirac delta function.

Since $\hat{\Psi}_a(\mathbf{x})$ commutes with every factor appearing in H_m , we may immediately write

$$\left[\hat{\Psi}_a(\mathbf{x}), \hat{H}_m\right] = 0. \tag{2.20}$$

Then

$$\begin{aligned} \frac{2}{U} \left[\hat{\Psi}_{a}(\mathbf{x}), \hat{H}_{aa} \right] &= \int \mathrm{d}^{3}y \; \hat{\Psi}_{a}(\mathbf{x}) \, \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \; \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \; \hat{\Psi}_{a}(\mathbf{y}) \; \hat{\Psi}_{a}(\mathbf{y}) \\ &- \int \mathrm{d}^{3}y \; \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \; \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \; \hat{\Psi}_{a}(\mathbf{y}) \; \hat{\Psi}_{a}(\mathbf{y}) \; \hat{\Psi}_{a}(\mathbf{x}) \\ &= \int \mathrm{d}^{3}y \; \hat{\Psi}_{a}(\mathbf{x}) \; \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \; \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \; \hat{\Psi}_{a}(\mathbf{y}) \; \hat{\Psi}_{a}(\mathbf{y}) \\ &- \int \mathrm{d}^{3}y \; \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \; \hat{\Psi}_{a}(\mathbf{x}) \; \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \; \hat{\Psi}_{a}(\mathbf{y}) \; \hat{\Psi}_{a}(\mathbf{y}) \\ &+ \int \mathrm{d}^{3}y \; \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \; \hat{\Psi}_{a}(\mathbf{x}) \; \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \; \hat{\Psi}_{a}(\mathbf{y}) \; \hat{\Psi}_{a}(\mathbf{y}) \\ &- \int \mathrm{d}^{3}y \; \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \; \hat{\Psi}_{a}(\mathbf{y}) \; \hat{\Psi}_{a}(\mathbf{y}) \; \hat{\Psi}_{a}(\mathbf{y}) \\ &= 2 \int \mathrm{d}^{3}y \; \delta^{(3)}(\mathbf{y} - \mathbf{x}) \; \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \; \hat{\Psi}_{a}(\mathbf{y}) \; \hat{\Psi}_{a}(\mathbf{y}) \\ &= 2 \; \hat{\Psi}_{a}^{\dagger}(\mathbf{x}) \; \hat{\Psi}_{a}(\mathbf{x}) \; \hat{\Psi}_{a}(\mathbf{x}), \end{aligned}$$
(2.21)

where we have employed the common trick of adding and subtracting a term of our choice in order to form a commutator.

For the pair formation/dissociation term,

$$\frac{2}{g} \left[\hat{\Psi}_{a}(\mathbf{x}), \hat{H}_{am} \right] = \int d^{3}y \, \hat{\Psi}_{a}(\mathbf{x}) \, \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \, \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \, \hat{\Psi}_{m}(\mathbf{y}) \\
- \int d^{3}y \, \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \, \hat{\Psi}_{a}^{\dagger}(\mathbf{y}) \, \hat{\Psi}_{m}(\mathbf{y}) \, \hat{\Psi}_{a}(\mathbf{x}) \\
= 2 \int d^{3}y \, \delta^{(3)}(\mathbf{y} - \mathbf{x}) \, \hat{\Psi}_{m}(\mathbf{y}) \, \hat{\Psi}_{a}^{\dagger}(\mathbf{x}) \\
= 2 \, \hat{\Psi}_{m}(\mathbf{x}) \, \hat{\Psi}_{a}^{\dagger}(\mathbf{x}) \,.$$
(2.22)

Equation (2.18), the equation of motion for the atomic field operator, is then

$$i\hbar \frac{\partial}{\partial t} \hat{\Psi}_{a}(\mathbf{x}) = \left[-\frac{\hbar^{2}}{2m} \nabla_{x}^{2} + V_{a}(\mathbf{x}) - \mu_{a} \right] \hat{\Psi}_{a}(\mathbf{x}) + U \hat{\Psi}_{a}^{\dagger}(\mathbf{x}) \hat{\Psi}_{a}(\mathbf{x}) \hat{\Psi}_{a}(\mathbf{x}) + g \hat{\Psi}_{m}(\mathbf{x}) \hat{\Psi}_{a}^{\dagger}(\mathbf{x}) . \quad (2.23)$$

2.4.2 Molecular Field Operator

The techniques used above for calculating an equation of motion are the same for every operator; having established those techniques, we will dispense with much of the detail in finding the equation of motion for the molecular field operator,

$$i\hbar \frac{\partial}{\partial t} \hat{\Psi}_{m}(\mathbf{x}) = \left[\hat{\Psi}_{m}(\mathbf{x}), \hat{H}\right]$$
$$= \left[\hat{\Psi}_{m}(\mathbf{x}), \hat{H}_{a}\right] + \left[\hat{\Psi}_{m}(\mathbf{x}), \hat{H}_{m}\right] + \left[\hat{\Psi}_{m}(\mathbf{x}), \hat{H}_{aa}\right] + \left[\hat{\Psi}_{m}(\mathbf{x}), \hat{H}_{am}\right].$$
(2.24)

In this case, only two of the above commutators are non-zero. They are

$$\left[\hat{\Psi}_{m}(\mathbf{x}), \hat{H}_{m}\right] = \left[-\frac{\hbar^{2}}{4m}\nabla_{x}^{2} + V_{m}\left(\mathbf{x}\right) - \mu_{m}\right]\hat{\Psi}_{m}(\mathbf{x}), \qquad (2.25)$$

which was derived in the same manner as Equation (2.19), and

$$\begin{bmatrix} \hat{\Psi}_m(\mathbf{x}), \hat{H}_{am} \end{bmatrix} = \frac{g}{2} \int d^3 y \, \left[\hat{\Psi}_m(\mathbf{x}), \hat{\Psi}_m^{\dagger}(\mathbf{y}) \right] \hat{\Psi}_a(\mathbf{y}) \, \hat{\Psi}_a(\mathbf{y}) = \frac{g}{2} \hat{\Psi}_a(\mathbf{x}) \, \hat{\Psi}_a(\mathbf{x}) \,.$$
(2.26)

The equation of motion is then

$$i\hbar\frac{\partial}{\partial t}\hat{\Psi}_{m}(\mathbf{x}) = \left[-\frac{\hbar^{2}}{4m}\nabla_{x}^{2} + V_{m}(\mathbf{x}) - \mu_{m}\right]\hat{\Psi}_{m}(\mathbf{x}) + \frac{g}{2}\hat{\Psi}_{a}(\mathbf{x})\hat{\Psi}_{a}(\mathbf{x}).$$
(2.27)

2.4.3 Normal Fluctuations Operator

To simplify some of the math and enable us to use results we have already found, we will use the product rule in computing the Heisenberg equation for $\hat{\chi}_a^{\dagger}(\mathbf{x}') \hat{\chi}_a(\mathbf{x})$:

$$i\hbar\frac{\partial}{\partial t}\left[\hat{\chi}_{a}^{\dagger}(\mathbf{x}')\,\hat{\chi}_{a}(\mathbf{x})\right] = \left[i\hbar\frac{\partial}{\partial t}\hat{\chi}_{a}^{\dagger}(\mathbf{x}')\right]\hat{\chi}_{a}(\mathbf{x}) + \hat{\chi}_{a}^{\dagger}(\mathbf{x}')\left[i\hbar\frac{\partial}{\partial t}\hat{\chi}_{a}(\mathbf{x})\right]$$
$$= \left[\hat{\chi}_{a}^{\dagger}(\mathbf{x}')\,,\hat{H}\right]\hat{\chi}_{a}(\mathbf{x}) + \hat{\chi}_{a}^{\dagger}(\mathbf{x}')\left[\hat{\chi}_{a}(\mathbf{x})\,,\hat{H}\right].$$
(2.28)

Solving Equation (2.4) for $\hat{\chi}_a(\mathbf{x})$ and finding the Hermitian conjugate of the result provides further simplification:

$$\left[\hat{\chi}_{a}^{\dagger}(\mathbf{x}'),\hat{H}\right] = \left[\hat{\Psi}_{a}^{\dagger}(\mathbf{x}'),\hat{H}\right] - \left\langle\hat{\Psi}_{a}(\mathbf{x}')\right\rangle^{*}\left[I,\hat{H}\right] = \left[\hat{\Psi}_{a}^{\dagger}(\mathbf{x}'),\hat{H}\right]$$
(2.29)

and

$$\left[\hat{\chi}_{a}(\mathbf{x}),\hat{H}\right] = \left[\hat{\Psi}_{a}(\mathbf{x}),\hat{H}\right] - \left\langle\hat{\Psi}_{a}(\mathbf{x})\right\rangle\left[\hat{I},\hat{H}\right] = \left[\hat{\Psi}_{a}(\mathbf{x}),\hat{H}\right],\qquad(2.30)$$

 \mathbf{SO}

$$i\hbar \frac{\partial}{\partial t} \left[\hat{\chi}_{a}^{\dagger}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}) \right] = \left[\hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \,, \hat{H} \right] \left[\hat{\Psi}_{a}(\mathbf{x}) - \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \right] \\ + \left[\hat{\Psi}_{a}^{\dagger}(\mathbf{x}') - \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle^{*} \right] \left[\hat{\Psi}_{a}(\mathbf{x}) \,, \hat{H} \right]. \quad (2.31)$$

We have already found $\left[\hat{\Psi}_{a}(\mathbf{x}), \hat{H}\right]$ as the right-hand side of Equation (2.23), so we must compute $\left[\hat{\Psi}_{a}^{\dagger}(\mathbf{x}'), \hat{H}\right]$. But observe that

$$\begin{bmatrix} \hat{\Psi}_{a}^{\dagger}(\mathbf{x}'), \hat{H} \end{bmatrix} = \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \hat{H} - \hat{H} \hat{\Psi}_{a}^{\dagger}(\mathbf{x}')$$
$$= \begin{bmatrix} \hat{H} \hat{\Psi}_{a}(\mathbf{x}') - \hat{\Psi}_{a}(\mathbf{x}') \hat{H} \end{bmatrix}^{\dagger}$$
$$= -\begin{bmatrix} \hat{\Psi}_{a}(\mathbf{x}'), \hat{H} \end{bmatrix}^{\dagger}.$$
(2.32)

This expression gives

$$\begin{bmatrix} \hat{\Psi}_{a}^{\dagger}(\mathbf{x}'), \hat{H} \end{bmatrix} = -\hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \begin{bmatrix} -\frac{\hbar^{2}}{2m} \nabla_{x'}^{2} + V_{a}(\mathbf{x}') - \mu_{a} \end{bmatrix} - U\hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \hat{\Psi}_{a}(\mathbf{x}') - g\hat{\Psi}_{m}^{\dagger}(\mathbf{x}') \hat{\Psi}_{a}(\mathbf{x}'), \quad (2.33)$$

where we have assumed that the external potential felt by atoms is Hermitian.

2.4.4 Anomalous Fluctuations Operator

The methods used to obtain Equation (2.31) give for the Heisenberg equation for $\hat{\chi}_a(\mathbf{x}') \hat{\chi}_a(\mathbf{x})$

$$i\hbar \frac{\partial}{\partial t} \left[\hat{\chi}_a(\mathbf{x}') \, \hat{\chi}_a(\mathbf{x}) \right] \\= \left[\hat{\Psi}_a(\mathbf{x}') \, , \hat{H} \right] \left[\hat{\Psi}_a(\mathbf{x}) - \left\langle \hat{\Psi}_a(\mathbf{x}) \right\rangle \right] + \left[\hat{\Psi}_a(\mathbf{x}') - \left\langle \hat{\Psi}_a(\mathbf{x}') \right\rangle \right] \left[\hat{\Psi}_a(\mathbf{x}) \, , \hat{H} \right]. \quad (2.34)$$

Again, we have aleady computed the necessary commutator.

2.5 Partial Differential Equations for Scalar Quantities

We obtain partial differential equations for the desired quantities from the Heisenberg equations of motion derived above by averaging and then factorizing those averages of products of operators in a consistent way.

2.5.1 Expectation Values

Though lengthy, let us explicitly write the expectation values of each of the four equations of motion. The following four equations are a landmark in the derivation because some of the factorizations required for further simplification involve a significant assumption about the system.

$$i\hbar\frac{\partial}{\partial t}\left\langle\hat{\Psi}_{a}(\mathbf{x})\right\rangle = \left[-\frac{\hbar^{2}}{2m}\nabla_{x}^{2} + V_{a}\left(\mathbf{x}\right) - \mu_{a}\right]\left\langle\hat{\Psi}_{a}(\mathbf{x})\right\rangle + U\left\langle\hat{\Psi}_{a}^{\dagger}(\mathbf{x})\,\hat{\Psi}_{a}(\mathbf{x})\,\hat{\Psi}_{a}(\mathbf{x})\right\rangle + g\left\langle\hat{\Psi}_{m}(\mathbf{x})\,\hat{\Psi}_{a}^{\dagger}(\mathbf{x})\right\rangle \tag{2.35}$$

$$i\hbar\frac{\partial}{\partial t}\left\langle\hat{\Psi}_{m}(\mathbf{x})\right\rangle = \left[-\frac{\hbar^{2}}{4m}\nabla_{x}^{2} + V_{m}\left(\mathbf{x}\right) - \mu_{m}\right]\left\langle\hat{\Psi}_{m}(\mathbf{x})\right\rangle + \frac{g}{2}\left\langle\hat{\Psi}_{a}(\mathbf{x})\,\hat{\Psi}_{a}(\mathbf{x})\right\rangle \quad (2.36)$$

$$\begin{split} \mathrm{i}\hbar\frac{\partial}{\partial t}\left\langle\hat{\chi}_{a}^{\dagger}(\mathbf{x}')\,\hat{\chi}_{a}(\mathbf{x})\right\rangle &= -\left[-\frac{\hbar^{2}}{2m}\nabla_{x'}^{2}+V_{a}\left(\mathbf{x}'\right)-\mu_{a}\right]\left\langle\hat{\Psi}_{a}^{\dagger}(\mathbf{x})\,\hat{\Psi}_{a}(\mathbf{x}')\right\rangle^{*} \\ &\quad -U\left\langle\hat{\Psi}_{a}^{\dagger}(\mathbf{x}')\,\hat{\Psi}_{a}^{\dagger}(\mathbf{x}')\,\hat{\Psi}_{a}(\mathbf{x}')\,\hat{\Psi}_{a}(\mathbf{x})\right\rangle - g\left\langle\hat{\Psi}_{m}^{\dagger}(\mathbf{x}')\,\hat{\Psi}_{a}(\mathbf{x}')\,\hat{\Psi}_{a}(\mathbf{x})\right\rangle \\ &\quad +\left[-\frac{\hbar^{2}}{2m}\nabla_{x'}^{2}+V_{a}\left(\mathbf{x}'\right)-\mu_{a}\right]\left\langle\hat{\Psi}_{a}(\mathbf{x}')\right\rangle^{*}\left\langle\hat{\Psi}_{a}(\mathbf{x})\right\rangle \\ &\quad +U\left\langle\hat{\Psi}_{a}^{\dagger}(\mathbf{x}')\,\hat{\Psi}_{a}^{\dagger}(\mathbf{x}')\,\hat{\Psi}_{a}(\mathbf{x}')\right\rangle\left\langle\hat{\Psi}_{a}(\mathbf{x})\right\rangle \\ &\quad +g\left\langle\hat{\Psi}_{m}^{\dagger}(\mathbf{x}')\,\hat{\Psi}_{a}(\mathbf{x}')\right\rangle\left\langle\hat{\Psi}_{a}(\mathbf{x})\right\rangle \\ &\quad +\left[-\frac{\hbar^{2}}{2m}\nabla_{x}^{2}+V_{a}\left(\mathbf{x}\right)-\mu_{a}\right]\left\langle\hat{\Psi}_{a}^{\dagger}(\mathbf{x}')\,\hat{\Psi}_{a}(\mathbf{x})\right\rangle \\ &\quad +U\left\langle\hat{\Psi}_{a}^{\dagger}(\mathbf{x}')\,\hat{\Psi}_{a}^{\dagger}(\mathbf{x})\,\hat{\Psi}_{a}(\mathbf{x})\right\rangle + g\left\langle\hat{\Psi}_{m}(\mathbf{x})\,\hat{\Psi}_{a}^{\dagger}(\mathbf{x}')\,\hat{\Psi}_{a}^{\dagger}(\mathbf{x})\right\rangle \\ &\quad -\left[-\frac{\hbar^{2}}{2m}\nabla_{x}^{2}+V_{a}\left(\mathbf{x}\right)-\mu_{a}\right]\left\langle\hat{\Psi}_{a}(\mathbf{x}')\right\rangle^{*}\left\langle\hat{\Psi}_{a}(\mathbf{x})\right\rangle \\ &\quad -U\left\langle\hat{\Psi}_{a}^{\dagger}(\mathbf{x})\,\hat{\Psi}_{a}(\mathbf{x})\,\hat{\Psi}_{a}(\mathbf{x})\right\rangle\left\langle\hat{\Psi}_{a}(\mathbf{x}')\right\rangle^{*} \\ &\quad -U\left\langle\hat{\Psi}_{a}^{\dagger}(\mathbf{x})\,\hat{\Psi}_{a}(\mathbf{x})\,\hat{\Psi}_{a}(\mathbf{x})\right\rangle\left\langle\hat{\Psi}_{a}(\mathbf{x}')\right\rangle^{*} \end{aligned}$$

$$\begin{split} \mathrm{i}\hbar\frac{\partial}{\partial t} \langle \hat{\chi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}) \rangle &= \left[-\frac{\hbar^{2}}{2m} \nabla_{x'}^{2} + V_{a}\left(\mathbf{x}'\right) - \mu_{a} \right] \left\langle \hat{\Psi}_{a}(\mathbf{x}') \, \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \\ &+ U \left\langle \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \, \hat{\Psi}_{a}(\mathbf{x}') \, \hat{\Psi}_{a}(\mathbf{x}') \, \hat{\Psi}_{a}(\mathbf{x}) \right\rangle + g \left\langle \hat{\Psi}_{m}(\mathbf{x}') \, \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \, \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \\ &- \left[-\frac{\hbar^{2}}{2m} \nabla_{x'}^{2} + V_{a}\left(\mathbf{x}'\right) - \mu_{a} \right] \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \\ &- U \left\langle \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \, \hat{\Psi}_{a}(\mathbf{x}') \, \hat{\Psi}_{a}(\mathbf{x}') \right\rangle \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \\ &- U \left\langle \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \, \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \right\rangle \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \\ &+ \left[-\frac{\hbar^{2}}{2m} \nabla_{x}^{2} + V_{a}\left(\mathbf{x}\right) - \mu_{a} \right] \left\langle \hat{\Psi}_{a}(\mathbf{x}') \, \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \\ &+ U \left\langle \hat{\Psi}_{a}(\mathbf{x}') \, \hat{\Psi}_{a}^{\dagger}(\mathbf{x}) \, \hat{\Psi}_{a}(\mathbf{x}) \, \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \\ &- \left[-\frac{\hbar^{2}}{2m} \nabla_{x}^{2} + V_{a}\left(\mathbf{x}\right) - \mu_{a} \right] \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \left\langle \hat{\Psi}_{a}(\mathbf{x}') \, \hat{\Psi}_{a}^{\dagger}(\mathbf{x}) \right\rangle \\ &- \left[-\frac{\hbar^{2}}{2m} \nabla_{x}^{2} + V_{a}\left(\mathbf{x}\right) - \mu_{a} \right] \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \left\langle \hat{\Psi}_{a}(\mathbf{x}') \, \hat{\Psi}_{a}^{\dagger}(\mathbf{x}) \right\rangle \\ &- U \left\langle \hat{\Psi}_{a}^{\dagger}(\mathbf{x}) \, \hat{\Psi}_{a}(\mathbf{x}) \, \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle \\ &- U \left\langle \hat{\Psi}_{a}^{\dagger}(\mathbf{x}) \, \hat{\Psi}_{a}(\mathbf{x}) \, \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle \\ &- g \left\langle \hat{\Psi}_{m}(\mathbf{x}) \, \hat{\Psi}_{a}^{\dagger}(\mathbf{x}) \right\rangle \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle \end{split}$$
(2.38)

We have made some use of Equation (2.3).

2.5.2 Factorizations

In the equations above, many terms are expectation values of products of more than two operators, or are expectation values of a product of two operators for which we do not have an equation of motion (for example, $\langle \hat{\Psi}_a^{\dagger}(\mathbf{x}') \hat{\Psi}_a(\mathbf{x}) \rangle$). We would like to express Equations (2.35) through (2.38) entirely in terms of expectation values of operators for which we have derived equations of motion. Many of these products can be exactly factorized, but others will require the use of Wick's theorem.

Exact Factorizations By applying Equation (2.5), and so making no further approximations beyond those we have already made, we can replace expectation values

involving a molecular field operator or its Hermitian conjugate by the expectation value of that molecular field operator or conjugate times the expectation value of the remaining product of operators. For example,

$$\left\langle \hat{\Psi}_{m}(\mathbf{x}) \, \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \right\rangle = \left\langle \hat{\Psi}_{m}(\mathbf{x}) \right\rangle \left\langle \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \right\rangle$$
(2.39)

and

$$\left\langle \hat{\Psi}_{m}(\mathbf{x}) \, \hat{\Psi}_{a}(\mathbf{x}') \, \hat{\Psi}_{a}^{\dagger}(\mathbf{x}) \right\rangle = \left\langle \hat{\Psi}_{m}(\mathbf{x}) \right\rangle \left\langle \hat{\Psi}_{a}(\mathbf{x}') \, \hat{\Psi}_{a}^{\dagger}(\mathbf{x}) \right\rangle.$$
 (2.40)

We can also apply Equation (2.4) to write products of two atomic field operators in terms of operators mostly for which we have equations. Noting $\langle \hat{\chi}_a(\mathbf{x}) \rangle = \langle \hat{\chi}_a^{\dagger}(\mathbf{x}) \rangle = 0$, we have

$$\left\langle \hat{\Psi}_{a}^{\dagger}(\mathbf{x}')\,\hat{\Psi}_{a}(\mathbf{x})\right\rangle = \left\langle \hat{\Psi}_{a}(\mathbf{x}')\right\rangle^{*}\left\langle \hat{\Psi}_{a}(\mathbf{x})\right\rangle + \left\langle \hat{\chi}_{a}^{\dagger}(\mathbf{x}')\,\hat{\chi}_{a}(\mathbf{x})\right\rangle,$$
 (2.41)

$$\left\langle \hat{\Psi}_{a}(\mathbf{x}')\,\hat{\Psi}_{a}^{\dagger}(\mathbf{x}) \right\rangle = \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle^{*} + \left\langle \hat{\chi}_{a}(\mathbf{x}')\,\hat{\chi}_{a}^{\dagger}(\mathbf{x}) \right\rangle,$$
(2.42)

$$\left\langle \hat{\Psi}_{a}(\mathbf{x}') \, \hat{\Psi}_{a}(\mathbf{x}) \right\rangle = \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle + \left\langle \hat{\chi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle,$$
(2.43)

$$\left\langle \hat{\Psi}_{a}^{\dagger}(\mathbf{x}')\,\hat{\Psi}_{a}^{\dagger}(\mathbf{x})\right\rangle = \left\langle \hat{\Psi}_{a}(\mathbf{x})\,\hat{\Psi}_{a}(\mathbf{x}')\right\rangle^{\dagger} = \left\langle \hat{\Psi}_{a}(\mathbf{x})\right\rangle^{*} \left\langle \hat{\Psi}_{a}(\mathbf{x}')\right\rangle^{*} + \left\langle \hat{\chi}_{a}(\mathbf{x})\,\hat{\chi}_{a}(\mathbf{x}')\right\rangle^{*} (2.44)$$

Approximate Factorizations—Wick's Theorem After making the substitutions described above, expectation values of products of more than two atomic field operators remain. Applying Equation (2.4) to these products will only result in more complicated terms, many of which are also expectation values of products of more than two operators. To factorize such expectation values, we will use Wick's theorem (described in Appendix A). This factorization is exact if the state of the system is an eigenstate of every Bogoliubov quasiparticle annihilation operator, which is an
operator that is a linear superposition of the momentum-space creation and annihilation operators (the a_k^{\dagger} and a_k of Section 1.2.1). This state is a squeezed state, and it saturates the number-phase Heisenberg uncertainty relation $\Delta N \Delta \phi \geq 1/2$, where ΔN and $\Delta \phi$ are the variances in the number and phase, respectively [4].² Though the system is likely not always in such a state, we must make such an approximation in order for our equations to be numerically tractable. The fact that our simulations resemble known results for simple scenarios suggests the approximation is reasonable.

Note that a quasiparticle coherent state (a squeezed state) is not generally the same as a coherent state of the field operator, which would be

$$\left\langle \hat{\Psi}_{a}(\mathbf{x}) \, \hat{\Psi}_{a}(\mathbf{x}') \right\rangle = \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle.$$
 (2.45)

If the state is such that Equation (2.45) would be true, one obtains the Gross-Pitaevskii equation, lacking (effectively assuming negligible) the fluctuations in which we are interested.

Using Wick's theorem, the high-order expectation values factorize as

$$\left\langle \hat{\Psi}_{a}^{\dagger}(\mathbf{x}) \, \hat{\Psi}_{a}(\mathbf{x}) \, \hat{\Psi}_{a}(\mathbf{x}) \right\rangle = \left| \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \right|^{2} \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle + \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle^{*} \left\langle \hat{\chi}_{a}(\mathbf{x}) \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle + 2 \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \left\langle \hat{\chi}_{a}^{\dagger}(\mathbf{x}) \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle$$

$$\left. + 2 \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \left\langle \hat{\chi}_{a}^{\dagger}(\mathbf{x}) \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle$$

$$(2.46)$$

$$\left\langle \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \, \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \, \hat{\Psi}_{a}(\mathbf{x}') \right\rangle = \left| \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle \right|^{2} \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle^{*} + \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle \left\langle \hat{\chi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}') \right\rangle^{*} \\ + 2 \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle^{*} \left\langle \hat{\chi}_{a}^{\dagger}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}') \right\rangle$$
(2.47)

 $^{^{2}}$ The discussion of the phase operator is a subtle one; we refer the reader to Pegg and Barnett [85, 86].

$$\begin{split} \left\langle \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \, \hat{\Psi}_{a}(\mathbf{x}') \, \hat{\Psi}_{a}(\mathbf{x}') \, \hat{\Psi}_{a}(\mathbf{x}) \right\rangle &= \left| \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle^{2} \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle^{*} \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \\ &+ \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle^{*2} \left\langle \hat{\chi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle \\ &+ 2 \left| \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle^{*} \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \left\langle \hat{\chi}_{a}^{\dagger}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}') \right\rangle \\ &+ 2 \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle^{*} \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \left\langle \hat{\chi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}') \right\rangle \\ &+ \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle^{*} \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \left\langle \hat{\chi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}') \right\rangle^{*} \\ &+ \left\langle \hat{\chi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}') \right\rangle^{*} \left\langle \hat{\chi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle \\ &+ 2 \left\langle \hat{\chi}_{a}^{\dagger}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle \\ &+ 2 \left\langle \hat{\chi}_{a}^{\dagger}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle \left\langle \hat{\psi}_{a}(\mathbf{x}) \right\rangle \\ &+ 2 \left\langle \hat{\chi}_{a}^{\dagger}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle \left\langle \hat{\chi}_{a}(\mathbf{x}) \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle \\ &+ 2 \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle^{*} \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \left\langle \hat{\psi}_{a}(\mathbf{x}) \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle \\ &+ 2 \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle^{*} \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \left\langle \hat{\chi}_{a}^{\dagger}(\mathbf{x}) \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle \\ &+ 2 \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle^{*} \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \left\langle \hat{\chi}_{a}^{\dagger}(\mathbf{x}) \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle \\ &+ 2 \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle^{2} \left\langle \hat{\chi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle \\ &+ 2 \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle^{2} \left\langle \hat{\chi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle \\ &+ 2 \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle^{2} \left\langle \hat{\chi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle \\ &+ 2 \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle^{2} \left\langle \hat{\chi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle \\ &+ 2 \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle^{2} \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \\ &+ 2 \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle^{2} \left\langle \hat{\Psi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}') \right\rangle \\ &+ 2 \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle \left\langle \hat{\Psi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}') \right\rangle \\ &+ 2 \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle \left\langle \hat{\chi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}') \right\rangle \\ &+ 2 \left\langle \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}') \right\rangle \langle \hat{\chi}_{a}(\mathbf{x}') \right\rangle \\ &+ 2 \left\langle \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}') \right\rangle \langle \hat{\chi}_{a}(\mathbf{x}') \right\rangle \\ &+ 2 \left\langle \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}') \right\rangle \langle \hat{\chi}_{a}(\mathbf{x}') \right\rangle \\ &+ 2 \left\langle \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}') \right\rangle \langle \hat{\chi}_{a}(\mathbf{x}') \right\rangle \\ &+ 2 \left\langle \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}') \right\rangle \langle \hat{\chi}_{a}$$

$$\left\langle \hat{\Psi}_{a}(\mathbf{x}') \, \hat{\Psi}_{a}^{\dagger}(\mathbf{x}) \, \hat{\Psi}_{a}(\mathbf{x}) \, \hat{\Psi}_{a}(\mathbf{x}) \right\rangle = \left| \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \right|^{2} \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle + \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle^{*} \left\langle \hat{\chi}_{a}(\mathbf{x}) \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle + 2 \left\langle \hat{\Psi}_{a}(\mathbf{x}') \right\rangle \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \left\langle \hat{\chi}_{a}^{\dagger}(\mathbf{x}) \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle + 2 \left| \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle \right|^{2} \left\langle \hat{\chi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle + \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle^{2} \left\langle \hat{\chi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}^{\dagger}(\mathbf{x}) \right\rangle + \left\langle \hat{\chi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}^{\dagger}(\mathbf{x}) \right\rangle \left\langle \hat{\chi}_{a}(\mathbf{x}) \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle + 2 \left\langle \hat{\chi}_{a}(\mathbf{x}') \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle \left\langle \hat{\chi}_{a}^{\dagger}(\mathbf{x}) \, \hat{\chi}_{a}(\mathbf{x}) \right\rangle$$
(2.51)

2.5.3 General Six-Dimensional Equations

After factorizing according to Wick's theorem, we arrive at four coupled, nonlinear, second order partial differential equations for the quantities in which we are interested. By the definitions of Section 1.6.1, these equations are actually *quasilinear* in that they are linear in the dependent variables' partial derivatives.

$$i\hbar \frac{\partial}{\partial t} \phi_a \left(\mathbf{x} \right) = \left\{ -\frac{\hbar^2}{2m} \nabla_x^2 + V_a \left(\mathbf{x} \right) - \mu_a + U \left[|\phi_a \left(\mathbf{x} \right)|^2 + 2G_N \left(\mathbf{x}, \mathbf{x} \right) \right] \right\} \phi_a \left(\mathbf{x} \right) + \left[UG_A \left(\mathbf{x}, \mathbf{x} \right) + g\phi_m \left(\mathbf{x} \right) \right] \phi_a^* \left(\mathbf{x} \right)$$
(2.52)

$$i\hbar\frac{\partial}{\partial t}\phi_m\left(\mathbf{x}\right) = \left[-\frac{\hbar^2}{4m}\nabla_x^2 + V_m\left(\mathbf{x}\right) - \mu_m\right]\phi_m\left(\mathbf{x}\right) + \frac{g}{2}\left[\phi_a^2\left(\mathbf{x}\right) + G_A\left(\mathbf{x},\mathbf{x}\right)\right]$$
(2.53)

$$i\hbar \frac{\partial}{\partial t} G_N(\mathbf{x}, \mathbf{x}') = \left[-\frac{\hbar^2}{2m} \left(\nabla_x^2 - \nabla_{x'}^2 \right) + V_a(\mathbf{x}) - V_a(\mathbf{x}') \right] G_N(\mathbf{x}, \mathbf{x}') + 2U \left[|\phi_a(\mathbf{x})|^2 - |\phi_a(\mathbf{x}')|^2 + G_N(\mathbf{x}, \mathbf{x}) - G_N(\mathbf{x}', \mathbf{x}') \right] G_N(\mathbf{x}, \mathbf{x}') + \left\{ g\phi_m(\mathbf{x}) + U \left[\phi_a^2(\mathbf{x}) + G_A(\mathbf{x}, \mathbf{x}) \right] \right\} G_A^*(\mathbf{x}, \mathbf{x}') - \left\{ g\phi_m^*(\mathbf{x}') + U \left[\phi_a^{*2}(\mathbf{x}') + G_A^*(\mathbf{x}', \mathbf{x}') \right] \right\} G_A(\mathbf{x}, \mathbf{x}')$$
(2.54)

$$i\hbar \frac{\partial}{\partial t} G_A \left(\mathbf{x}, \mathbf{x}' \right) = \left\{ -\frac{\hbar^2}{2m} \left(\nabla_x^2 + \nabla_{x'}^2 \right) + V_a \left(\mathbf{x} \right) + V_a \left(\mathbf{x}' \right) - 2\mu_a \right\} G_A \left(\mathbf{x}, \mathbf{x}' \right) + 2U \left[|\phi_a \left(\mathbf{x} \right)|^2 + |\phi_a \left(\mathbf{x}' \right)|^2 + G_N \left(\mathbf{x}, \mathbf{x} \right) + G_N \left(\mathbf{x}', \mathbf{x}' \right) \right] G_A \left(\mathbf{x}, \mathbf{x}' \right) + \left\{ g\phi_m \left(\mathbf{x} \right) + U \left[\phi_a^2 \left(\mathbf{x} \right) + G_A \left(\mathbf{x}, \mathbf{x} \right) \right] \right\} G_N^* \left(\mathbf{x}, \mathbf{x}' \right) + \left\{ g\phi_m \left(\mathbf{x}' \right) + U \left[\phi_a^2 \left(\mathbf{x}' \right) + G_A \left(\mathbf{x}', \mathbf{x}' \right) \right] \right\} G_N \left(\mathbf{x}, \mathbf{x}' \right) + \left\{ g\phi_m \left(\mathbf{x} \right) + U \left[\phi_a^2 \left(\mathbf{x} \right) + G_A \left(\mathbf{x}, \mathbf{x} \right) \right] \right\} \delta^{(3)} \left(\mathbf{x} - \mathbf{x}' \right)$$
(2.55)

Similarities between equations are apparent when presented in this slightly unconcise form. Note that we have used $G_N(\mathbf{x}', \mathbf{x}) = \langle \hat{\chi}_a^{\dagger}(\mathbf{x}) \hat{\chi}_a(\mathbf{x}') \rangle = \langle \hat{\chi}_a^{\dagger}(\mathbf{x}') \hat{\chi}_a(\mathbf{x}) \rangle^{\dagger} = G_N^*(\mathbf{x}, \mathbf{x}').$

For convenience, we summarize the unknowns in Equations (2.52) through (2.55).

- The independent variables **x** and **x**' are two generally distinct three-dimensional coordinates.
- The independent variable t is the time.
- The dependent variable $\phi_a(\mathbf{x})$ is the generally complex wavefunction of the atomic condensate, which contains information about the number density of condensed atoms at the point \mathbf{x} and time t and about the local flow velocity at that point and time.
- The dependent variable $\phi_m(\mathbf{x})$ contains the same information as $\phi_a(\mathbf{x})$, but about the molecular condensate.
- The dependent variable $G_N(\mathbf{x}, \mathbf{x}')$ is the generally complex normal fluctuations field and contains information about second-order quantum fluctuations. Its diagonal elements $G_N(\mathbf{x}, \mathbf{x})$ give a number density of noncondensed atoms at the points \mathbf{x} and time t.

The dependent variable G_A(**x**, **x**') is the generally complex anomalous fluctuations field and contains information about second-order quantum fluctuations. Its diagonal elements G_A(**x**, **x**) give the variance in the atomic mean field φ_a(**x**). The normal and anomalous fluctuations are both correlations functions and Green's functions [83].

Chapter 3 simplifies these equations, mainly with symmetry arguments, so that they are computationally feasible.

2.6 Physical Parameters

Having the mathematical form of our model, let us explore and refine some of the physical quantities appearing so far.

2.6.1 Renormalization

The parameters appearing in Equations (2.52) through (2.55)—namely, U, g, μ_a , and μ_m —must be properly renormalized to avoid an unphysical divergence of the ground-state energy. Kokkelmans *et al.* [14] model pair formation via a Feshbach resonance as scattering in coupled square wells (see Appendix B for an example solution to such a system). The good agreement of the square well model with the more rigorous Feshbach formalism (described in [87], for example) demonstrates that only a few parameters are needed to accurately model the resonance, despite the divergence of the effective scattering length (1.5), which is the *only* parameter needed to describe non-resonant scattering in ultracold systems with short-range interactions. Next, by introducing a wavenumber cutoff and taking the limiting case of the square wells' radii going to zero, Kokkelmans *et al.* derive a contact interaction model of the resonance in which the ground state energy does not diverge. Comparison with a

detailed coupled channels calculation that incorporates realistic interatomic potentials and hyperfine structure shows that the contact interaction [which was assumed in the form of the terms (2.9) and (2.10) of the Hamiltonian] accurately models pair formation via a Feshbach resonance in ultracold systems.

In applying the above renormalization procedure, we follow Kokkelmans and Holland [10]. By defining $\nu = 2\mu_a - \mu_m$ and taking $\mu_a = 0$, we identify in our own Hamiltonian (2.6) the same parameters that appear in the Hamiltonian considered in [10].³ Then

$$U = \Gamma U_0 \tag{2.56}$$

$$g = \Gamma g_0 \tag{2.57}$$

$$\nu = \nu_0 + \frac{1}{2}\alpha gg_0, \tag{2.58}$$

where

$$\Gamma \equiv \frac{1}{1 - \alpha U_0} \tag{2.59}$$

$$\alpha \equiv \frac{mK}{2\pi^2\hbar^2} \tag{2.60}$$

with K the wavenumber cutoff, which in practice is determined by the range of a relative coordinate and the number of relative grid points.

Parameters with a subscript 0 are unrenormalized parameters; they are

$$U_0 = \frac{4\pi\hbar^2 a_{\rm bg}}{m},$$
 (2.61)

³Our Hamiltonian (2.6) includes external trapping potentials which [10] lacks, but these do not affect the definitions of the parameters.

$$g_0 = \sqrt{U_0 \,\Delta B \,\Delta \mu^{\rm mag}},\tag{2.62}$$

$$\nu_0 = (B - B_{\rm res}) \,\Delta\mu^{\rm mag},\tag{2.63}$$

where a_{bg} is the background scattering length of the atom; ΔB is the width of the Feshbach resonance, defined as the distance from the resonance position to the point where the effective scattering length, Equation (1.5), is zero; $\Delta \mu^{mag}$ is the difference in magnetic moments of a bound and unbound pair of atoms; B is the external magnetic field; and B_{res} is the position of the resonance, defined as the value of the magnetic field for which the effective scattering length diverges.

The above definitions are taken from [10], except for g_0 , which can be calculated from Equations (1) and (14) in [14]; that reference's Equation (1) is the same as our Equation (1.5) from Chapter 1, while [14]'s (14) is

$$a_{\rm eff} = a_{\rm bg} - \frac{m}{4\pi\hbar^2} \frac{|g_0|^2}{\nu_0},$$
(2.64)

where a_{eff} is the effective scattering length, and we have neglected the possible second resonance mentioned in [14]. Equating these two expressions for the effective scattering length gives Equation (2.62) above.

Table 2.1 has values of the relevant physical parameters of ⁸⁵Rb, and Figures 2.1 through 2.5 show how the renormalized parameters depend on the magnetic field and wavenumber cutoff.

Parameter	Value
$a_{ m bg}$	$-443 a_0$
ΔB	10.71 G
$\Delta \mu^{\rm mag}$	$-2.23 \ \mu_B$
$B_{\rm res}$	155.041 G
m	84.91174 amu
U_0	$-2.32 \times 10^{-50} \text{ J m}^3$
g_0	$2.27 \times 10^{-38} \text{ J m}^{3/2}$

Table 2.1: *Physical parameters of* ⁸⁵*Rb*. These values are intrinsic properties of ⁸⁵Rb. The given values for $a_{\rm bg}$, ΔB , and $B_{\rm res}$ are from Claussen *et al.* [28], the given value of $\Delta \mu^{\rm mag}$ is mentioned in [10], and U_0 and g_0 are calculated from the other parameters.



Figure 2.1: Effective scattering length $a_{eff}(B)$ for ⁸⁵Rb. The effective scattering length is given by Equation (1.5). The vertical line indicates the position B_{res} of the Feshbach resonance. Note that the scattering length passes through zero only for $B > B_{res}$. Inset: effective scattering length near $B = B_{zero}$ where $a_{eff} = 0$.



Figure 2.2: Renormalized detuning $\nu(B)$ for ⁸⁵Rb. The detuning is given by Equation (2.58), here for a wavenumber cutoff of $K = 5 \times 10^7 \text{ m}^{-1}$. The vertical dotted line on the left indicates the position $B_{\rm res}$ of the Feshbach resonance. The thick dashed line on the right is the value of ν where the effective scattering length is zero. The effective scattering length $a_{\rm eff}$ is positive only between the vertical lines.



Figure 2.3: K-dependence of renormalized detuning ν for ⁸⁵Rb. The detuning is given by Equation (2.58) as a function of wavenumber cutoff K, here for $B = B_{\text{res}}$ (solid curve) and $B = B_{\text{zero}}$ (dotted curve).



Figure 2.4: K-dependence of renormalized self-interaction U for ^{85}Rb . The parameter U is given by Equation (2.56) as a function of wavenumber cutoff K. Notice that U depends only on K and the intrinsic properties of ^{85}Rb given in Table 2.1, and is independent of B.



Figure 2.5: K-dependence of renormalized molecular coupling g for ${}^{85}Rb$. The parameter g is given by Equation (2.57) as a function of wavenumber cutoff K. Notice that g depends only on K and the intrinsic properties of ${}^{85}Rb$ given in Table 2.1, and is independent of B.

2.6.2 Length and Time Scales

By nondimensionalizing Equations (2.52) through (2.55), we can discover the natural length and time scales of the problem. We explicitly include the dimensions by letting

$$t \to t_0 t, \quad \mathbf{x} \to x_0 \mathbf{x}$$

$$\phi_a(\mathbf{x}) \to \frac{1}{x_0^{3/2}} \phi_a(\mathbf{x}), \quad \phi_m(\mathbf{x}) \to \frac{1}{x_0^{3/2}} \phi_m(\mathbf{x})$$

$$G_N(\mathbf{x}, \mathbf{x}') \to \frac{1}{x_0^3} G_N(\mathbf{x}, \mathbf{x}'), \quad G_A(\mathbf{x}, \mathbf{x}') \to \frac{1}{x_0^3} G_A(\mathbf{x}, \mathbf{x}'),$$

where now t_0 and x_0 carry the dimensions, and t, \mathbf{x} , and all four fields are dimensionless. We substitute these into (2.52) through (2.55) (recall that $\nu = 2\mu_a - \mu_m$ and $\mu_a \to 0$) and form dimensionless quantities. From any of the four equations, we could recover the natural scales of the harmonic oscillator,

$$t_0 = \frac{1}{\omega}, \ x_0 = \sqrt{\frac{\hbar}{m\omega}}.$$

We are most interested in the physics intrinsic to the interatomic interactions and independent of the trap, so we only concentrate on scales independent of ω .

In the equation for ϕ_a , the dimensionless factors⁴

$$\frac{Ut_0}{\hbar x_0^3},$$
(2.65)
$$gt_0$$
(2.66)

$$\frac{3^{20}}{\hbar x_0^{3/2}},$$
 (2.66)

⁴Such factors are typically called *dimensionless groups*, and can convey basic information about a complicated process; the Reynolds number in fluid mechanics is another example.

and

$$\frac{\hbar t_0}{m x_0^2}.$$
(2.67)

appear (after some algebraic manipulation). Since the nondimensionalization procedure only introduces two new degrees of freedom (t_0 and x_0), we must choose two of the three groups above and set them equal to 1 when solving for t_0 and x_0 . Combining (2.65) with (2.67), (2.66) with (2.67), and (2.65) with (2.66), we get, respectively,

$$t_0 = \frac{m^3}{\hbar^5} U^2, \quad x_0 = \frac{m}{\hbar^2} U;$$
 (2.68)

$$t_0 = \frac{\hbar^7}{m^3} \frac{1}{g^4}, \quad x_0 = \frac{\hbar^4}{m^2} \frac{1}{g^2}; \tag{2.69}$$

$$t_0 = \hbar \frac{U}{g^2}, \ x_0 = \left(\frac{U}{g}\right)^{2/3},$$
 (2.70)

where the last pair is just a combination of the first two.

Using the same procedure on the equation for ϕ_m , we get the pair (2.69) in addition to

$$t_0 = \frac{\hbar}{\nu}, \ x_0 = \sqrt{\frac{\hbar^2 1}{m \nu}};$$
 (2.71)

$$t_0 = \frac{\hbar}{\nu}, \ x_0 = \left(\frac{g}{\nu}\right)^{2/3}.$$
 (2.72)

Nondimensionalizing the equations for G_N and G_A reveals no new scales.

To summarize, each parameter that appears in the Hamiltonian and characterizes interactions has a time and length scale that is independent of the trap:

$$t_U = \frac{m^3}{\hbar^5} U^2, \quad x_U = \frac{m}{\hbar^2} U;$$
 (2.73)

$$t_g = \frac{\hbar^7}{m^3} \frac{1}{g^4}, \quad x_g = \frac{\hbar^4}{m^2} \frac{1}{g^2}; \tag{2.74}$$

$$t_{\nu} = \hbar \frac{1}{\nu}, \ x_{\nu} = \sqrt{\frac{\hbar^2}{m} \frac{1}{\nu}}.$$
 (2.75)

These scales are unique in that there no other scales involving each parameter $(U, g, \text{ or } \nu)$ by itself. Using U_0 , g_0 , and m for ⁸⁵Rb from Table 2.1, observe that $t_{U_0} = 1.16 \times 10^{-4}$ s and $t_{g_0} = 1.95 \times 10^{-13}$ s, indicating that a numerical solution may encounter stiff sets of equations.

2.7 Energy and Momentum

Whenever the magnetic field is constant, no energy enters or leaves the system, and so average total energy must be conserved. The total energy in the system is calculated from the expectation value of the Hamiltonian, Equation (2.6). With the aid of the field operator's expansion (2.4) in terms of an average plus a fluctuation and Wick's theorem, Equation (2.48) specifically, the total energy neglecting kinetic terms is

$$E - T = \int d^{3}x \ V_{a}(\mathbf{x}) \left[G_{N}(\mathbf{x}, \mathbf{x}) + |\phi_{a}(\mathbf{x})|^{2} \right] + \int d^{3}x \ \left[V_{m}(\mathbf{x}) + \nu \right] |\phi_{m}(\mathbf{x})|^{2} + \frac{U}{2} \int d^{3}x \left\{ \left| \phi_{a}(\mathbf{x}) \right|^{4} + 2 \operatorname{Re} \left[\phi_{a}^{*2}(\mathbf{x}) \ G_{A}(\mathbf{x}, \mathbf{x}) \right] + 4 \left| \phi_{a}(\mathbf{x}) \right|^{2} G_{N}(\mathbf{x}, \mathbf{x}) + \left| G_{A}(\mathbf{x}, \mathbf{x}) \right|^{2} + 2G_{N}^{2}(\mathbf{x}, \mathbf{x}) \right\} + g \int d^{3}x \operatorname{Re} \left\{ \phi_{m}^{*}(\mathbf{x}) \left[G_{A}(\mathbf{x}, \mathbf{x}) + \phi_{a}^{2}(\mathbf{x}) \right] \right\}.$$
(2.76)

Equation (2.76) only involves quantities for which we have derived equations; that is, all parts of the energy except for the kinetic contribution can be computed from the atomic and molecular mean fields and the normal and anomalous fluctuations. The kinetic contribution requires a more involved treatment.

If the system were in a coherent state $|\lambda\rangle$ such that

$$\hat{\Psi}_a(\mathbf{x}) |\lambda\rangle = \phi_a(\mathbf{x}) |\lambda\rangle,$$
(2.77)

which would make the GPE exact to within the approximations of the contact potential, the kinetic energy could be calculated as

$$\left\langle \hat{T} \right\rangle = -\frac{\hbar^2}{2m} \int \mathrm{d}^3 x \,\left\langle \lambda \right| \hat{\Psi}_a^{\dagger}(\mathbf{x}) \,\nabla^2 \hat{\Psi}_a(\mathbf{x}) \left| \lambda \right\rangle = \frac{\hbar^2}{2m} \int \mathrm{d}^3 x \,\left| \nabla \phi_a(\mathbf{x}) \right|^2, \qquad (2.78)$$

where we have integrated by parts and assumed normalized states and box boundary conditions. Since we neglect fluctuations around the molecular mean field, Equation (2.78) may be immediately adapted to the molecules' contributions T_m to the kinetic energy:

$$T_m = -\frac{\hbar^2}{4m} \int \mathrm{d}^3 x \, \left| \nabla \phi_m(\mathbf{x}) \right|^2.$$
(2.79)

If Equation (2.77) is not true, as in the case of the atomic part of our model, we may apply the decomposition (2.4) and arrive at Equation (2.78) for the condensate's contribution to the kinetic energy. The noncondensed fluid's contribution remains; it is

$$-\frac{\hbar^2}{2m} \int \mathrm{d}^3 x \,\left\langle \hat{\chi}_a^{\dagger}(\mathbf{x}) \,\nabla^2 \hat{\chi}_a(\mathbf{x}) \right\rangle, \qquad (2.80)$$

which cannot immediately be expressed in terms of the four quantities that our model includes. Integration by parts is available to transfer the Laplacian from the fluctuation operator to its Hermitian conjugate, but does not result solely in a derivative applied to a product of the operators (namely, the normal fluctuations). Thus, it appears we are unable to calculate the kinetic energy of the noncondensed fraction using only the atomic and molecular mean fields and the normal and anomalous fluctuations.

The calculation of total momentum is hindered by similar concerns. The calculation starts with

$$\left\langle \hat{\mathbf{P}}_{\text{tot}} \right\rangle = -\mathrm{i}\hbar \int \mathrm{d}^3 x \, \left\langle \hat{\Psi}_a^{\dagger}(\mathbf{x}) \, \nabla \hat{\Psi}_a(\mathbf{x}) \right\rangle - \mathrm{i}\hbar \int \mathrm{d}^3 x \, \left\langle \hat{\Psi}_m^{\dagger}(\mathbf{x}) \, \nabla \hat{\Psi}_m(\mathbf{x}) \right\rangle. \tag{2.81}$$

Applying Equation (2.4) and recalling that we neglect molecular fluctuations, the total momentum reduces in a similar fashion as the kinetic energy did:

$$\left\langle \hat{\mathbf{P}}_{\text{tot}} \right\rangle = -\mathrm{i}\hbar \int \mathrm{d}^3 x \; \phi_a^*(\mathbf{x}) \, \nabla \phi_a(\mathbf{x}) - \mathrm{i}\hbar \int \mathrm{d}^3 x \; \phi_m^*(\mathbf{x}) \, \nabla \phi_m(\mathbf{x}) \\ - \mathrm{i}\hbar \int \mathrm{d}^3 x \; \left\langle \hat{\chi}_a^{\dagger}(\mathbf{x}) \, \nabla \hat{\chi}_a(\mathbf{x}) \right\rangle. \quad (2.82)$$

All but the last term, the momentum of noncondensed atoms, may be calculated in terms of the four fields accounted for by our model. Again, integration by parts does not result in a useful expression.

Chapter 3

SIMPLIFICATIONS AND MODIFICATIONS

Equations (2.52) through (2.55) are capable of handling a completely general geometry, but their seven independent variables, six in space and one in time, present a formidable computational challege. We proceed to make some assumptions about the geometry and symmetry of the problem in order to simplify the equations.

3.1 Change of Coordinates

Since the experimental results with which we will compare primarily concern the atomic and molecular condensed and atomic uncondensed number densities, we seek to retain as much information as possible about these quantities. Looking at Equations (2.52) through (2.55), we lose absolutely no information about number densities by placing some restrictions on the relative values of \mathbf{x} and \mathbf{x}' . Specifically, the evolutions of the atomic and molecular fields and the diagonal (that is, $\mathbf{x} = \mathbf{x}'$) elements of the correlation functions are determined only by single-coordinate fields. One could go so far as to require $\mathbf{x} = \mathbf{x}'$ in Equations (2.54) and (2.55) without affecting the evolution of number densities or the diagonal elements of G_A . The system of equations (2.52) through (2.55) would be reduced from six to three spatial independent variables, even in the absence of any symmetries, and the derivatives in the correlation functions would greatly simplify. (A delta function evaluated at zero appears in the G_A equation, but may be replaced by a commutator.) While important observable quantities (that is, number densities) would be unaffected, we lose all knowledge of off-diagonal correlations. Seeking to retain as much of this potentially useful information as possible, we back off from the $\mathbf{x} = \mathbf{x}'$ restriction, and employ symmetry assumptions to simplify (2.52) through (2.55). Again, looking at Equations (2.54) and (2.55), the evolutions of the off-diagonal correlations that we do retain are completely unaffected by those correlations of which we would have no knowledge.

In the case of spherical geometry, we assume that all external potentials $V_a(\mathbf{x})$ and $V_m(\mathbf{x})$ are rotationally invariant, as are the initial conditions on fields which are functions of a single coordinate, namely, $\phi_a(\mathbf{x})$, $\phi_m(\mathbf{x})$, $G_A(\mathbf{x}, \mathbf{x})$, and $G_N(\mathbf{x}, \mathbf{x})$. The combination of these two sets of assumptions ensures that those single-coordinate fields will always be rotationally invariant. We wish to write Equations (2.52) through (2.55) in terms of center of mass and relative coordinates (which will facilitate a Fourier transform later—see [88] for substantial theory surrounding this procedure in the context of quantum mechanical correlation functions), but without knowing the forms of the single-coordinate fields, terms such as $|\phi_a(\mathbf{x})|^2 - |\phi_a(\mathbf{x}')|^2$ cannot immediately be written in terms of a function $\bar{\phi}_a$ that is a function only of a single center of mass coordinate \mathbf{R} . However, if we restrict our attention to \mathbf{x} and $\mathbf{x'}$ such that x = x', where $x \equiv |\mathbf{x}|$, that is, we restrict our knowledge of correlations only to those between points on the surface of a spherical shell (see Figure 3.1), all the terms requiring knowledge of unknown fields' forms vanish, and several terms combine in (2.54) and (2.55).

With similar assumptions and restrictions, Equations (2.52) through (2.55) for a cylindrical geometry reduce in the same way as for the spherical case. Specifically, we must assume that the external potentials and single-coordinates fields' initial conditions (and therefore their later values) are invariant with respect to rotations only



Figure 3.1: Coordinate restrictions for spherical symmetry. In a spherically symmetric trap (the blue outer circle, cut in half for visibility), rotationally invariant single-coordinate fields have the same value all over the surface of a spherical shell (inner, sharp-edged, green circle). The two vectors (bold red), \mathbf{x} and \mathbf{x}' , are not equal, but both point to the shell; we can then write, for example, $\phi_a(\mathbf{x}) = \phi_a(\mathbf{x}')$, facilitating a change to center of mass and relative coordinates. With this restriction x = x', the only two-point correlations we will know about for a given center of mass coordinate R are those between points on a single shell. This is physically motivated by bursts produced by collapsing condensates.

about a particular vertical axis (let it be the z-axis), and invariant about reflections over a particular plane, normal to the axis of rotational symmetry (let this be the xy-plane passing through the origin). Then, if we restrict our attention to \mathbf{x} and \mathbf{x}' such that their z-components x_z and x'_z are equal in magnitude, and the components of \mathbf{x} and \mathbf{x}' lying in the xy-plane, \mathbf{x}_{ρ} and \mathbf{x}'_{ρ} , are equal in magnitude, the same terms that canceled and combined in the spherical case cancel and combine here, too. In this case, our knowledge of correlations is restricted to those between a point lying on a ring x_z above the xy-plane and another point on a ring of the same radius as the first, but lying x_z below the xy-plane, or between two points on the same ring (see Figure 3.2).



Figure 3.2: Coordinate restrictions for cylindrical symmetry. In a cylindrically symmetric trap (blue rectangle, and cut in half for visibility), single-coordinate fields are invariant with respect to rotations about the z-axis and to reflections over the xy-plane. Such fields will have a single value at all points on two rings (curved green lines) of equal radii, equidistant from and parallel to the xy-plane, and centered on the z-axis. The two vectors \mathbf{x} and \mathbf{x}' (bold red), are not equal, but each may point to a different ring; we can then write, for example, $\phi_a(\mathbf{x}) = \phi_a(\mathbf{x}')$, facilitating a change to center of mass and relative coordinates. With the restrictions $x_z = x'_z$ and $x_\rho = x'_\rho$, the only two-point correlations we will know about for a given center of mass coordinate R are those between points lying on the same or different rings. Physically, this allows us to study correlations between bursts running along the axial direction of a collapsing condensate in a cylindrically symmetric trap, or on a ring moving outwards radially.

To put these assumptions and restrictions in a concise mathematical form, define the center of mass and relative coordinates, respectively, as

$$\mathbf{R} = \frac{\mathbf{x} + \mathbf{x}'}{2},\tag{3.1}$$

$$\mathbf{r} = \mathbf{x} - \mathbf{x}'. \tag{3.2}$$

Then the functions in Equations (2.52) through (2.55) transform as

$$\phi_a(\mathbf{x}) = \phi_a(\mathbf{x}') \equiv \bar{\phi}_a(\mathbf{R}) ,$$

$$\phi_m(\mathbf{x}) = \phi_m(\mathbf{x}') \equiv \bar{\phi}_m(\mathbf{R}) ,$$

$$G_N(\mathbf{x}, \mathbf{x}) = G_N(\mathbf{x}', \mathbf{x}') \equiv \bar{G}_N(\mathbf{R}, \mathbf{0}) ,$$

$$G_A(\mathbf{x}, \mathbf{x}) = G_A(\mathbf{x}', \mathbf{x}') \equiv \bar{G}_A(\mathbf{R}, \mathbf{0}) ,$$

$$G_N(\mathbf{x}, \mathbf{x}') \equiv \bar{G}_N(\mathbf{R}, \mathbf{r}) ,$$

$$G_A(\mathbf{x}, \mathbf{x}') \equiv \bar{G}_A(\mathbf{R}, \mathbf{r}) ,$$

$$V_a(\mathbf{x}) = V_a(\mathbf{x}') \equiv \bar{V}_a(\mathbf{R}) ,$$

$$V_m(\mathbf{x}) = V_m(\mathbf{x}') \equiv \bar{V}_m(\mathbf{R}) ,$$

a notation general enough to handle either the spherical or cylindrical geometries and their corresponding assumptions and restrictions. For consistency with the assumptions that single-coordinate fields have no angular dependence for the spherical case and no azimuthal dependence for the cylindrical case, we make the same assumptions for the dependence of the correlation functions on \mathbf{R} , so that only the magnitude Ris important in all the fields in the spherical case, and only R_z and R_ρ (the magnitudes of \mathbf{R} 's components lying along the z-axis and in the xy-plane, respectively) are important in the cylindrical case. **Transformation of Laplacians** In order to explicitly re-write the collapse equations in center of mass and relative coordinates, we must transform the Laplacians in Equations (2.54) and (2.55), all of which act on quantities that are defined over two distinct variables. We first calculate the most general case.

Consider two Cartesian vectors, \mathbf{x} and \mathbf{y} , and the transformations $\mathbf{R} \equiv (\mathbf{x} + \mathbf{y})/2$ and $\mathbf{r} \equiv \mathbf{x} - \mathbf{y}$. In terms of the new vectors, \mathbf{x} and \mathbf{y} are $\mathbf{x} = \mathbf{R} + \mathbf{r}/2$ and $\mathbf{y} = \mathbf{R} - \mathbf{r}/2$.¹ Then we have

$$\mathbf{R} = \frac{1}{2} \left(x^{1} + y^{1} \right) \hat{\mathbf{i}} + \frac{1}{2} \left(x^{2} + y^{2} \right) \hat{\mathbf{j}} + \frac{1}{2} \left(x^{3} + y^{3} \right) \hat{\mathbf{k}} = R^{1} \hat{\mathbf{i}} + R^{2} \hat{\mathbf{j}} + R^{3} \hat{\mathbf{k}}$$
(3.3)

$$\mathbf{r} = (x^{1} - y^{1})\,\hat{\mathbf{i}} + (x^{2} - y^{2})\,\hat{\mathbf{j}} + (x^{3} - y^{3})\,\hat{\mathbf{k}} = r^{1}\hat{\mathbf{i}} + r^{2}\hat{\mathbf{j}} + r^{3}\hat{\mathbf{k}}$$
(3.4)

$$\mathbf{x} = \left(R^1 + \frac{r^1}{2}\right)\hat{\mathbf{i}} + \left(R^2 + \frac{r^2}{2}\right)\hat{\mathbf{j}} + \left(R^3 + \frac{r^3}{2}\right)\hat{\mathbf{k}} = x^1\hat{\mathbf{i}} + x^2\hat{\mathbf{j}} + x^3\hat{\mathbf{k}}$$
(3.5)

$$\mathbf{y} = \left(R^{1} - \frac{r^{1}}{2}\right)\hat{\mathbf{i}} + \left(R^{2} - \frac{r^{2}}{2}\right)\hat{\mathbf{j}} + \left(R^{3} - \frac{r^{3}}{2}\right)\hat{\mathbf{k}} = y^{1}\hat{\mathbf{i}} + y^{2}\hat{\mathbf{j}} + y^{3}\hat{\mathbf{k}}, \quad (3.6)$$

where $\hat{\mathbf{i}}$, $\hat{\mathbf{j}}$, and $\hat{\mathbf{k}}$ are Cartesian unit vectors.

Now consider a scalar function of \mathbf{x} and \mathbf{y} , $f(\mathbf{x}, \mathbf{y})$. Denoting partial differentiation with a subscript, the chain rule gives

$$f_{x^1} = f_{R^1} R_{x^1}^1 + f_{R^2} R_{x^1}^2 + f_{R^3} R_{x^1}^3 + f_{r^1} r_{x^1}^1 + f_{r^2} r_{x_1}^2 + f_{r^3} r_{x^1}^3, \qquad (3.7)$$

which reduces to

$$f_{x^1} = f_{R^1} R_{x^1}^1 + f_{r^1} r_{x^1}^1 \tag{3.8}$$

given our chosen forms of \mathbf{R} and \mathbf{r} .

 $^{^{1}}$ For the duration of the derivation of the Laplacians' transformation, a superscript denotes a particular component of a vector, not a power.

Another careful application of the chain rule gives

$$f_{x^{1}x^{1}} = \frac{\partial}{\partial (x^{1})} \left(f_{R^{1}} R_{x^{1}}^{1} + f_{r^{1}} r_{x^{1}}^{1} \right) = f_{R^{1}x^{1}} R_{x^{1}}^{1} + f_{R^{1}} R_{x^{1}x^{1}}^{1} + f_{r^{1}x^{1}} r_{x^{1}}^{1} + f_{r^{1}} r_{x^{1}x^{1}}^{1}$$
$$= f_{R^{1}x^{1}} R_{x^{1}}^{1} + f_{r^{1}x^{1}} r_{x^{1}}^{1}, \quad (3.9)$$

where we have again used our choices for **R** and **r** in making simplifications. We are still not done, since the above equation mixes partial derivatives with respect to R^1 , x^1 , and r^1 . Another pass with the chain rule finally results in

$$f_{x^{1}x^{1}} = \left(f_{R^{1}R^{1}}R_{x^{1}}^{1} + f_{R_{1}r_{1}}r_{x^{1}}^{1}\right)R_{x^{1}}^{1} + \left(f_{r^{1}R^{1}}R_{x^{1}}^{1} + f_{r^{1}r^{1}}r_{x^{1}}^{1}\right)r_{x^{1}}^{1}.$$
 (3.10)

The derivatives with respect to the other components of \mathbf{x} can be found by letting $1 \to 2$ and $1 \to 3$, and the derivatives with respect to the components of \mathbf{y} can be found by letting $x \to y$. Now we can write the Laplacian with respect to \mathbf{x} , ∇_x^2 , as

$$\nabla_x^2 f = \left[\frac{\partial^2}{\partial (x^1)^2} + \frac{\partial^2}{\partial (x^2)^2} + \frac{\partial^2}{\partial (x^3)^2} \right] f
= \left(f_{R^1 R^1} R_{x^1}^1 + f_{R^1 r^1} r_{x^1}^1 \right) R_{x^1}^1 + \left(f_{r^1 R^1} R_{x^1}^1 + f_{r^1 r^1} r_{x^1}^1 \right) r_{x^1}^1
+ \left(f_{R^2 R^2} R_{x^2}^2 + f_{R^2 r^2} r_{x^2}^2 \right) R_{x^2}^2 + \left(f_{r^2 R^2} R_{x^2}^2 + f_{r^2 r^2} r_{x^2}^2 \right) r_{x^2}^2
+ \left(f_{R^3 R^3} R_{x^3}^3 + f_{R^3 r^3} r_{x^3}^3 \right) R_{x^3}^3 + \left(f_{r^3 R^3} R_{x^3}^3 + f_{r^3 r^3} r_{x^3}^3 \right) r_{x^3}^3, \quad (3.11)$$

where $\frac{\partial^2}{\partial (x^1)^2}$ means the second partial derivative with respect to the component of **x** called x^1 . The analogy of Equation (3.11) for ∇_y^2 is found by letting $x \to y$. Referring to the definitions of **R** and **r**, we find

$$R_{x^1}^1 = R_{x^2}^2 = R_{x^3}^3 = R_{y^1}^1 = R_{y^2}^2 = R_{y^3}^3 = \frac{1}{2}$$

$$r_{x^1}^1 = r_{x^2}^2 = r_{x^3}^3 = -r_{y^1}^1 = -r_{y^2}^2 = -r_{y^3}^3 = 1,$$
(3.12)

so Equation (3.11) reduces to

$$\nabla_x^2 f = \frac{1}{4} \left(f_{R^1 R^1} + f_{R^2 R^2} + f_{R^3 R^3} \right) + f_{R^1 r^1} + f_{R^2 r^2} + f_{R^3 r^3} + f_{r^1 r^1} + f_{r^2 r^2} + f_{r^3 r^3}$$
(3.13)

$$\nabla_y^2 f = \frac{1}{4} \left(f_{R^1 R^1} + f_{R^2 R^2} + f_{R^3 R^3} \right) - f_{R^1 r^1} - f_{R^2 r^2} - f_{R^3 r^3} + f_{r^1 r^1} + f_{r^2 r^2} + f_{r^3 r^3}.$$
(3.14)

In finding the preceeding two equations, we assumed $f_{R^ir^i} = f_{r^iR^i}$, $i \in \{1, 2, 3\}$, which is true if $f_{R^ir^i}$ and $f_{r^iR^i}$, $i \in \{1, 2, 3\}$, are all continuous on the domain containing every point in which we are interested, a reasonable assumption for a physical system.

Taking the gradients with respect to \mathbf{R} and \mathbf{r} , ∇_R and ∇_r , respectively, to mean

$$\nabla_{R} = \frac{\partial}{\partial (R^{1})} \hat{\mathbf{i}} + \frac{\partial}{\partial (R^{2})} \hat{\mathbf{j}} + \frac{\partial}{\partial (R^{3})} \hat{\mathbf{k}}, \qquad (3.15)$$

$$\nabla_{r} = \frac{\partial}{\partial (r^{1})} \hat{\mathbf{i}} + \frac{\partial}{\partial (r^{2})} \hat{\mathbf{j}} + \frac{\partial}{\partial (r^{3})} \hat{\mathbf{k}}, \qquad (3.16)$$

we have four useful results:

$$\nabla_x^2 f = \left(\frac{1}{4}\nabla_R^2 + \nabla_R \cdot \nabla_r + \nabla_r^2\right) f \tag{3.17}$$

$$\nabla_y^2 f = \left(\frac{1}{4}\nabla_R^2 - \nabla_R \cdot \nabla_r + \nabla_r^2\right) f \tag{3.18}$$

$$\left(\nabla_x^2 + \nabla_y^2\right) f = \left(\frac{1}{2}\nabla_R^2 + 2\nabla_r^2\right) f \tag{3.19}$$

$$\left(\nabla_x^2 - \nabla_y^2\right) f = 2\nabla_R \cdot \nabla_r f. \tag{3.20}$$

The position-space representation of the equations (2.52) through (2.55) in center

of mass and relative coordinates, given the appropriate assumptions and restrictions described above, is now, in the most general notation,

$$i\hbar \frac{\partial}{\partial t} \bar{\phi}_a(\mathbf{R}) = \left\{ -\frac{\hbar^2}{2m} \nabla_R^2 + \bar{V}_a(\mathbf{R}) + U \left[\left| \bar{\phi}_a(\mathbf{R}) \right|^2 + 2\bar{G}_N(\mathbf{R}, \mathbf{0}) \right] \right\} \bar{\phi}_a(\mathbf{R}) + \left[U\bar{G}_A(\mathbf{R}, \mathbf{0}) + g\bar{\phi}_m(\mathbf{R}) \right] \bar{\phi}_a^*(\mathbf{R})$$
(3.21)

$$i\hbar\frac{\partial}{\partial t}\bar{\phi}_m(\mathbf{R}) = \left[-\frac{\hbar^2}{4m}\nabla_R^2 + \bar{V}_m(\mathbf{R}) + \nu\right]\bar{\phi}_m(\mathbf{R}) + \frac{g}{2}\left[\bar{\phi}_a^2(\mathbf{R}) + \bar{G}_A(\mathbf{R},\mathbf{0})\right]$$
(3.22)

$$i\hbar \frac{\partial}{\partial t} \bar{G}_N(\mathbf{R}, \mathbf{r}) = -\frac{\hbar^2}{m} \nabla_R \cdot \nabla_r \bar{G}_N(\mathbf{R}, \mathbf{r}) + \left\{ g \bar{\phi}_m(\mathbf{R}) + U \left[\bar{\phi}_a^2(\mathbf{R}) + \bar{G}_A(\mathbf{R}, \mathbf{0}) \right] \right\} \bar{G}_A^*(\mathbf{R}, \mathbf{r}) - \left\{ g \bar{\phi}_m^*(\mathbf{R}) + U \left[\bar{\phi}_a^{*2}(\mathbf{R}) + \bar{G}_A^*(\mathbf{R}, \mathbf{0}) \right] \right\} \bar{G}_A(\mathbf{R}, \mathbf{r})$$
(3.23)

$$i\hbar \frac{\partial}{\partial t} \bar{G}_A(\mathbf{R}, \mathbf{r}) = \left\{ -\frac{\hbar^2}{2m} \left(\frac{1}{2} \nabla_R^2 + 2 \nabla_r^2 \right) + 2 \bar{V}_a(\mathbf{R}) + 4 U \left[\left| \bar{\phi}_a(\mathbf{R}) \right|^2 + \bar{G}_N(\mathbf{R}, \mathbf{0}) \right] \right\} \bar{G}_A(\mathbf{R}, \mathbf{r}) + \left\{ g \bar{\phi}_m(\mathbf{R}) + U \left[\bar{\phi}_a^2(\mathbf{R}) + \bar{G}_A(\mathbf{R}, \mathbf{0}) \right] \right\} \times \left[\bar{G}_N^*(\mathbf{R}, \mathbf{r}) + \bar{G}_N(\mathbf{R}, \mathbf{r}) + \delta^{(3)}(\mathbf{r}) \right],$$
(3.24)

where we have made the $\nu = 2\mu_a - \mu_m$, $\mu_a \rightarrow 0$ substitution described in Section 2.6.1.

3.2 Fourier Transform

Equations (3.23) and (3.24) may equivalently be given in a relative momentum representation, obtained by a Fourier transform over the **r** variable. This transform will replace some of the derivatives, which are often a source of numerical error in simulation, with simple multiplication. The transform also serves to remove the Dirac delta function appearing in the \bar{G}_A equation, which may also be a source of computational inaccuracy (though rigorously discretized delta functions, catered to computation, do exist—see [89], for example).

We adopt the conventions

$$\tilde{f}(\mathbf{k}) = \int_{\text{all }\mathbf{r}} d^3 r \ \bar{f}(\mathbf{r}) \, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}}$$
(3.25)

$$\bar{f}(\mathbf{r}) = \int_{\text{all }\mathbf{k}} \frac{\mathrm{d}^3 k}{(2\pi)^3} \tilde{f}(\mathbf{k}) \,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}},\tag{3.26}$$

where $\bar{f}(\mathbf{r})$ is an arbitrary function. In Equations (3.23) and (3.24), we multiply each side of the equations by $e^{-i\mathbf{k}\cdot\mathbf{r}}$ and integrate over all \mathbf{r} -space.

The transform of the Dirac delta function in Equation (3.24) becomes unity. The diagonal parts of the normal fluctuations $\bar{G}_N(\mathbf{R}, \mathbf{0})$ can be expressed in terms of the momentum representation as

$$\bar{G}_{N}^{I}(\mathbf{R}) \equiv \bar{G}_{N}(\mathbf{R}, \mathbf{0}) = \int_{\text{all }\mathbf{k}} \frac{\mathrm{d}^{3}k}{(2\pi)^{3}} \tilde{G}_{N}(\mathbf{R}, \mathbf{k}) \,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} = \int_{\text{all }\mathbf{k}} \frac{\mathrm{d}^{3}k}{(2\pi)^{3}} \tilde{G}_{N}(\mathbf{R}, \mathbf{k}) \,. \tag{3.27}$$

The same is true for $N \to A$.

3.2.0 Transforms of Derivatives

We first consider a term appearing in the transformed Equation (3.23):

$$\nabla_R \cdot \int \mathrm{d}^3 r \, \nabla_r \left[\bar{G}_N(\mathbf{R}, \mathbf{r}) \right] \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}},\tag{3.28}$$

where henceforth the range of integration is understood to be all **r**-space in all threedimensional integrals, unless otherwise noted. Looking only at the v^{th} Cartesian component of the integral above,

$$I_v \equiv \int_{-\infty}^{\infty} \mathrm{d}r_v \; \frac{\partial \bar{G}_N}{\partial r_v} \mathrm{e}^{-\mathrm{i}(k_u r_u + k_v r_v + k_w r_w)},\tag{3.29}$$

we may integrate by parts. Assuming that

$$\lim_{r_v \to \infty} \bar{G}_N(\mathbf{R}, \mathbf{r}) = \lim_{r_v \to -\infty} \bar{G}_N(\mathbf{R}, \mathbf{r}) = 0$$
(3.30)

and recognizing that this procedure applies as well to the u^{th} and w^{th} Cartesian components of Equation (3.28), we have

$$\nabla_R \cdot \int \mathrm{d}^3 r \, \nabla_r \left[\bar{G}_N(\mathbf{R}, \mathbf{r}) \right] \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}} = \mathrm{i}\nabla_R \cdot \mathbf{k} \int \mathrm{d}^3 r \, \bar{G}_N(\mathbf{R}, \mathbf{r}) \, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}}$$
$$= \mathrm{i}\nabla_R \cdot \mathbf{k} \tilde{G}_N(\mathbf{R}, \mathbf{r}) \,. \quad (3.31)$$

In Equation (3.29), we replace the partial derivative with a second partial derivative. Then I_v becomes

$$I_v = \frac{\partial \bar{G}_N}{\partial r_v} e^{-i\mathbf{k}\cdot\mathbf{r}} \bigg|_{-\infty}^{\infty} + ik_v \int_{-\infty}^{\infty} dr_v \ \frac{\partial \bar{G}_N}{\partial r_v} e^{i(k_u r_u + k_v r_v + k_w r_w)}.$$
 (3.32)

Assuming that the first partial derivatives of $\bar{G}_N(\mathbf{R}, \mathbf{r})$ are also bounded as $r_v \to \pm \infty$, we recognize Equation (3.29) in Equation (3.32). Using the result from Equation (3.31), we have

$$\int \mathrm{d}^3 r \,\nabla_r^2 \left[\bar{G}_N(\mathbf{R}, \mathbf{r}) \right] \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}} = -k^2 \int \mathrm{d}^3 r \,\bar{G}_N(\mathbf{R}, \mathbf{r}) \,\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}} = -k^2 \tilde{G}_N(\mathbf{R}, \mathbf{k}) \,. \quad (3.33)$$

The equations in momentum space (for the relative coordinate) are then

$$i\hbar \frac{\partial}{\partial t} \bar{\phi}_a(\mathbf{R}) = \left\{ -\frac{\hbar^2}{2m} \nabla_R^2 + \bar{V}_a(\mathbf{R}) + U \left[\left| \bar{\phi}_a(\mathbf{R}) \right|^2 + 2\bar{G}_N^I(\mathbf{R}) \right] \right\} \bar{\phi}_a(\mathbf{R}) \\ + \left[U \bar{G}_A^I(\mathbf{R}) + g \bar{\phi}_m(\mathbf{R}) \right] \bar{\phi}_a^*(\mathbf{R})$$
(3.34)

$$i\hbar\frac{\partial}{\partial t}\bar{\phi}_m(\mathbf{R}) = \left[-\frac{\hbar^2}{4m}\nabla_R^2 + \bar{V}_m(\mathbf{R}) + \nu\right]\bar{\phi}_m(\mathbf{R}) + \frac{g}{2}\left[\bar{\phi}_a^2(\mathbf{R}) + \bar{G}_A^I(\mathbf{R})\right]$$
(3.35)

$$i\hbar \frac{\partial}{\partial t} \tilde{G}_N(\mathbf{R}, \mathbf{k}) = -i \frac{\hbar^2}{m} \mathbf{k} \cdot \nabla_R \tilde{G}_N(\mathbf{R}, \mathbf{k}) + \left\{ g \bar{\phi}_m(\mathbf{R}) + U \left[\bar{\phi}_a^2(\mathbf{R}) + \bar{G}_A^I(\mathbf{R}) \right] \right\} \tilde{G}_A^*(\mathbf{R}, \mathbf{k}) - \left\{ g \bar{\phi}_m^*(\mathbf{R}) + U \left[\bar{\phi}_a^{*2}(\mathbf{R}) + \bar{G}_A^{*I}(\mathbf{R}) \right] \right\} \tilde{G}_A(\mathbf{R}, \mathbf{k})$$
(3.36)

$$i\hbar \frac{\partial}{\partial t} \tilde{G}_{A}(\mathbf{R}, \mathbf{k}) = \left\{ -\frac{\hbar^{2}}{2m} \left(\frac{1}{2} \nabla_{R}^{2} - 2k^{2} \right) + 2\bar{V}_{a}(\mathbf{R}) + 4U \left[\left| \bar{\phi}_{a}(\mathbf{R}) \right|^{2} + \bar{G}_{N}^{I}(\mathbf{R}) \right] \right\} \tilde{G}_{A}(\mathbf{R}, \mathbf{k}) + \left\{ g\bar{\phi}_{m}(\mathbf{R}) + U \left[\bar{\phi}_{a}^{2}(\mathbf{R}) + \bar{G}_{A}^{I}(\mathbf{R}) \right] \right\} \times \left[\tilde{G}_{N}(\mathbf{R}, \mathbf{k}) + \tilde{G}_{N}^{*}(\mathbf{R}, \mathbf{k}) + 1 \right], \qquad (3.37)$$

where $\bar{G}_N^I(\mathbf{R})$ and $\bar{G}_A^I(\mathbf{R})$ are defined by Equation (3.27). We emphasize that the vec-

tor notation is for generality; these equations will not actually be taken to have seven independent variables, but a lesser number, depending on the particular symmetry.

3.3 Equations for Spherical Symmetry

We now concentrate on the spherically symmetric case, and acknowledge that all the dependence on \mathbf{R} is encoded entirely in R, the magnitude of \mathbf{R} , by replacing \mathbf{R} with R everywhere. Strictly speaking, we should then use different symbols to name the functions when changing the arguments from vectors to scalars, but we forego this formality to simplify notation. As explained in Ref. [11], we may evaluate the gradients in any coordinate system we choose, and given the spherical symmetry and geometry, we use spherical coordinates with the z-axis aligned with \mathbf{k} . Then

$$\mathbf{k} \cdot \hat{e}_{\phi} = 0$$
$$\mathbf{k} \cdot \hat{e}_{\rho} = k \cos \theta$$
$$\mathbf{k} \cdot \hat{e}_{\theta} = k \cos \left(\theta + \frac{\pi}{2}\right) = -k \sin \theta,$$

where \hat{e}_{ϕ} , \hat{e}_{ρ} , and \hat{e}_{θ} are the spherical unit vectors of some arbitrary vector (see Figure 3.3). Now ∇_R^2 becomes the spherical Laplacian, and $\nabla_R \cdot \mathbf{k}$ becomes

$$\nabla_R \cdot \mathbf{k} = k \left(\cos \theta \frac{\partial}{\partial R} - \frac{\sin \theta}{R} \frac{\partial}{\partial \theta} \right), \qquad (3.38)$$

where we are careful to note the distinction between the gradient and Laplacian operators themselves, and those operators acting on particular fields.²

 $^{^{2}}$ Hence, the disappearance of angular derivatives when a Laplacian acts on a single-coordinate field and the persistence of those derivatives when acting on a two-coordinate field.



Figure 3.3: Coordinate axes for spherical symmetry. Since all fields are independent of the orientation of \mathbf{R} , we are free to rotate the axes (keeping the origin fixed), and so we align the z-axis with \mathbf{k} . Then the dependence of the correlation functions' values on the relative orientations of \mathbf{k} and \mathbf{R} (thin arrows) can be expressed in spherical coordinates. The spherical unit vectors (bold arrows) of some particular vector (\mathbf{R} , in this case) depend on the orientation of that vector.

To simplify the radial derivatives, we define

$$\varphi_{a}(R) = R\bar{\phi}_{a}(R) = \left|\frac{\mathbf{x} + \mathbf{x}'}{2}\right| \phi_{a}(\mathbf{x}) = \left|\frac{\mathbf{x} + \mathbf{x}'}{2}\right| \phi_{a}(\mathbf{x}'),$$
$$\varphi_{m}(R) = R\bar{\phi}_{m}(R) = \left|\frac{\mathbf{x} + \mathbf{x}'}{2}\right| \phi_{m}(\mathbf{x}) = \left|\frac{\mathbf{x} + \mathbf{x}'}{2}\right| \phi_{m}(\mathbf{x}'),$$
$$\mathcal{G}_{N}(R, k, \theta, \phi) = R\tilde{G}_{N}(R, k, \theta, \phi) = R\mathcal{F}_{\mathbf{r}}\left[\bar{G}_{N}(R, \mathbf{r})\right] = \left|\frac{\mathbf{x} + \mathbf{x}'}{2}\right| \mathcal{F}_{\mathbf{x} - \mathbf{x}'}\left[G_{N}(\mathbf{x}, \mathbf{x}')\right],$$
$$\mathcal{G}_{A}(R, k, \theta, \phi) = R\tilde{G}_{A}(R, k, \theta, \phi) = R\mathcal{F}_{\mathbf{r}}\left[\bar{G}_{A}(R, \mathbf{r})\right] = \left|\frac{\mathbf{x} + \mathbf{x}'}{2}\right| \mathcal{F}_{\mathbf{x} - \mathbf{x}'}\left[G_{A}(\mathbf{x}, \mathbf{x}')\right],$$
$$(3.39)$$

where $\mathcal{F}_{\mathbf{y}}$ denotes a Fourier transform over the variable \mathbf{y} , and for notational consis-

tency,

$$\mathcal{G}_{N}^{I}(R) = R\bar{G}_{N}^{I}(R) = \left|\frac{\mathbf{x} + \mathbf{x}'}{2}\right| G_{N}(\mathbf{x}, \mathbf{x}) = \left|\frac{\mathbf{x} + \mathbf{x}'}{2}\right| G_{N}(\mathbf{x}', \mathbf{x}')$$
$$\mathcal{G}_{A}^{I}(R) = R\bar{G}_{A}^{I}(R) = \left|\frac{\mathbf{x} + \mathbf{x}'}{2}\right| G_{A}(\mathbf{x}, \mathbf{x}) = \left|\frac{\mathbf{x} + \mathbf{x}'}{2}\right| G_{A}(\mathbf{x}', \mathbf{x}').$$

The HFB equations become, for the spherically symmetric case expressed in spherical coordinates,

$$i\hbar\frac{\partial}{\partial t}\varphi_{a}(R) = \left\{-\frac{\hbar^{2}}{2m}\frac{\partial^{2}}{\partial R^{2}} + \bar{V}_{a}(R) + U\left[\frac{|\varphi_{a}(R)|^{2}}{R^{2}} + 2\frac{\mathcal{G}_{N}^{I}(R)}{R}\right]\right\}\varphi_{a}(R) + \left[U\frac{\mathcal{G}_{A}^{I}(R)}{R} + g\frac{\varphi_{m}(R)}{R}\right]\varphi_{a}^{*}(R), \qquad (3.40)$$

$$i\hbar\frac{\partial}{\partial t}\varphi_m(R) = \left[-\frac{\hbar^2}{4m}\frac{\partial^2}{\partial R^2} + \bar{V}_m(R) + \nu\right]\varphi_m(R) + \frac{g}{2}\left[\frac{\varphi_a^2(R)}{R} + \mathcal{G}_A^I(R)\right], \quad (3.41)$$

$$i\hbar\frac{\partial}{\partial t}\mathcal{G}_{N}(R,k,\theta,\phi) = -i\frac{\hbar^{2}k}{m} \left[\cos\theta \left(\frac{\partial}{\partial R} - \frac{1}{R}\right) - \frac{\sin\theta}{R}\frac{\partial}{\partial \theta}\right]\mathcal{G}_{N}(R,k,\theta,\phi) \\ + \left\{g\frac{\varphi_{m}(R)}{R} + U\left[\frac{\varphi_{a}^{2}(R)}{R^{2}} + \frac{\mathcal{G}_{A}^{I}(R)}{R}\right]\right\}\mathcal{G}_{A}^{*}(R,k,\theta,\phi) \\ - \left\{g\frac{\varphi_{m}^{*}(R)}{R} + U\left[\frac{\varphi_{a}^{*2}(R)}{R^{2}} + \frac{\mathcal{G}_{A}^{I}(R)}{R}\right]\right\}\mathcal{G}_{A}(R,k,\theta,\phi), \quad (3.42)$$

$$i\hbar \frac{\partial}{\partial t} \mathcal{G}_A(R,k,\theta,\phi) = \left\{ -\frac{\hbar^2}{4m} \left[\frac{\partial^2}{\partial R^2} + \frac{1}{R^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{R^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} - 4k^2 \right] \\ + 2\bar{V}_a(R) + 4U \left[\frac{|\varphi_a(R)|^2}{R^2} + \frac{\mathcal{G}_N^I(R)}{R} \right] \right\} \mathcal{G}_A(R,k,\theta,\phi) \\ + \left\{ g \frac{\varphi_m(R)}{R} + U \left[\frac{\varphi_a^2(R)}{R^2} + \frac{\mathcal{G}_A^I(R)}{R} \right] \right\} \\ \times \left\{ \mathcal{G}_N(R,k,\theta,\phi) + \mathcal{G}_N^*(R,k,\theta,\phi) + R \right\}.$$
(3.43)

Note that ϕ (with no subscript) indicates the azimuthal angle in spherical coordinates.

3.3.0 Partial Wave Expansion

We begin removing the angular derivatives in Equations (3.42) and (3.43) by expanding the correlation functions in partial waves; that is,

$$\mathcal{G}_N(R,k,\theta,\phi) = \sum_{l=0}^{\infty} \sum_{q=-l}^{l} \mathcal{G}_N^{l,q}(R,k) Y_l^q(\theta,\phi) , \qquad (3.44)$$

and similarly for the anomalous fluctuations. Being Laplace series, these expansions are uniformly convergent, allowing us to differentiate each series term by term. Appendix C develops recurrence relations for the derivatives and trigonometric factors appearing in Equations (3.42) and (3.43). Since the spherical harmonics are linearly independent, we can equate expansion coefficients term by term in (3.42) and (3.43), as long as the sums on both sides of each equation cover an identical range and have no coupling between spherical harmonics with different indices. To this end, we expand the lone R appearing in (3.43) as

$$R = \sqrt{4\pi} R \sum_{l=0}^{\infty} \sum_{q=-l}^{l} \delta_{0,l} \,\delta_{0,q} Y_l^q(\theta,\phi) \,, \tag{3.45}$$

where $\delta_{i,j}$ is the Kroenecker delta symbol. Also note that

$$\mathcal{G}_{N}^{*}(R,k,\theta,\phi) = \sum_{l=0}^{\infty} \sum_{q=-l}^{l} \mathcal{G}_{N}^{*l,q}(R,k) Y_{l}^{*q}(\theta,\phi),$$

$$= \sum_{l=0}^{\infty} \sum_{q=l}^{-l} \mathcal{G}_{N}^{*l,-q}(R,k) (-1)^{q} Y_{l}^{q}(\theta,\phi), \qquad (3.46)$$

where we have allowed $q \rightarrow -q$ in the last step. The order of summation is unimpor-

tant, though, and we may write

$$\mathcal{G}_{N}^{*}(R,k,\theta,\phi) = \sum_{l=0}^{\infty} \sum_{q=-l}^{l} \mathcal{G}_{N}^{*l,-q}(R,k) (-1)^{q} Y_{l}^{q}(\theta,\phi) , \qquad (3.47)$$

with the same holding true for $N \to A$. Finally, employing the results derived in Appendix C, both sides of Equations (3.42) and (3.43) are summed over the same spherical harmonics, and we can equate the expansion coefficients:

$$\begin{split} \mathrm{i}\hbar\frac{\partial}{\partial t}\mathcal{G}_{N}^{l,q}(R,k) &= -\mathrm{i}\frac{\hbar^{2}k}{m} \Bigg[\sqrt{\frac{(l-q+1)(l+q+1)}{(2l+1)(2l+3)}} \left(\frac{\partial}{\partial R} + \frac{l+1}{R}\right) \mathcal{G}_{N}^{l+1,q}(R,k) \\ &+ u_{-l+1}^{q} \sqrt{\frac{(l+q)(l-q)}{(2l+1)(2l-1)}} \left(\frac{\partial}{\partial R} - \frac{l}{R}\right) \mathcal{G}_{N}^{l-1,q}(R,k) \Bigg] \\ &+ (-1)^{q} \left\{ g \frac{\varphi_{m}(R)}{R} + U \left[\frac{\varphi_{a}^{2}(R)}{R^{2}} + \frac{\mathcal{G}_{A}^{I}(R)}{R} \right] \right\} \mathcal{G}_{A}^{*l,-q}(R,k) \\ &- \left\{ g \frac{\varphi_{m}^{*}(R)}{R} + U \left[\frac{\varphi_{a}^{*2}(R)}{R^{2}} + \frac{\mathcal{G}_{A}^{*I}(R)}{R} \right] \right\} \mathcal{G}_{A}^{l,q}(R,k) , \end{split}$$
(3.48)

$$i\hbar \frac{\partial}{\partial t} \mathcal{G}_{A}^{l,q}(R,k) = \left\{ -\frac{\hbar^{2}}{4m} \left[\frac{\partial^{2}}{\partial R^{2}} - \frac{l\left(l+1\right)}{R^{2}} - 4k^{2} \right] \right. \\ \left. + 2\bar{V}_{a}(R) + 4U \left[\frac{|\varphi_{a}(R)|^{2}}{R^{2}} + \frac{\mathcal{G}_{N}^{I}(R)}{R} \right] \right\} \mathcal{G}_{A}^{l,q}(R,k) \\ \left. + \left\{ g \frac{\varphi_{m}(R)}{R} + U \left[\frac{\varphi_{a}^{2}(R)}{R^{2}} + \frac{\mathcal{G}_{A}^{I}(R)}{R} \right] \right\} \\ \left. \times \left[\mathcal{G}_{N}^{l,q}(R,k) + (-1)^{q} \mathcal{G}_{N}^{*l,-q}(R,k) + \sqrt{4\pi}\delta_{0,l} \,\delta_{0,q}R \right].$$
(3.49)

Equations (3.48) and (3.49) hold true for integers $l \ge 0$ and $|q| \le l$, with

$$u_{-l+1}^{q} \equiv \begin{cases} 1, & q \ge -l+1 \\ 0, & q < -l+1. \end{cases}$$
(3.50)

An entire Laplace series need not be summed to find $\mathcal{G}_N^I(R)$; only the l = q = 0 term survives, due to the periodicity of the $e^{iq\phi}$ appearing in the definition of the spherical harmonic and the recurrence relations and even- and oddness of the associated Legendre polynomials. Thus

$$\mathcal{G}_{N}^{I}(R) = \frac{1}{4\pi^{5/2}} \int_{0}^{\infty} \mathrm{d}k \; k^{2} \, \mathcal{G}_{N}^{0,0}(R,k) \,, \qquad (3.51)$$

which is also true for $N \to A$.

Equations (3.40), (3.41), (3.48), and (3.49) are the final computational form of the equations for spherical symmetry in the center of mass coordinate. This represents the first publication of a spherical harmonic expansion of the equations, rather than a regular Legendre polynomial expansion in which the azimuthal angle ϕ is assumed to be unimportant, making these equations more general than those used by Milstein *et al.* [11].

3.4 Equations for Cylindrical Geometry

We now specialize Equations (3.34) through (3.37) to the cylindrically symmetric case, acknowledging that all the **R** dependence is encoded entirely in R_z , the component of **R** along the z-axis, and R_ρ , the magnitude of the component lying in the *xy*-plane.

It would be most expedient to re-use the spherical coordinates and Laplace series of the preceeding section, but the alignment of the z-axis with \mathbf{k} violates our
assumption of rotational invariance about the z-axis and invariance with respect to reflections over the x-y plane. Instead, we rotate the coordinate axes about the zaxis so that **k** has only x- and z-components. Single-coordinate fields maintain their invariances with respect to rotations about the z-axis, since the z-axis remains fixed, and maintain their invariances about reflections over the x-y-plane, since this plane has not changed orientation. Then

$$\mathbf{k} \cdot \hat{e}_{\rho} = k_{\rho} \cos \phi, \qquad (3.52)$$

$$\mathbf{k} \cdot \hat{e}_{\phi} = k_{\rho} \cos\left(\phi + \frac{\pi}{2}\right) = -k_{\rho} \sin\phi, \qquad (3.53)$$

$$\mathbf{k} \cdot \hat{e}_z = k_z \tag{3.54}$$

where \hat{e}_{ρ} , \hat{e}_{ϕ} , and \hat{e}_z are the cylindrical unit vectors of some arbitrary vector (see Figure 3.4). The Laplacian ∇_R^2 becomes the cylindrical Laplacian, and $\mathbf{k} \cdot \nabla_R$ becomes

$$\mathbf{k} \cdot \nabla_R = k_\rho \cos \phi \frac{\partial}{\partial R_\rho} - \frac{k_\rho}{R_\rho} \sin \phi \frac{\partial}{\partial \phi} + k_z \frac{\partial}{\partial R_z}.$$
 (3.55)

To simplify the radial derivatives, define

$$\begin{split} \varphi_a(R_\rho,R_z) &\equiv R_\rho^{1/2} \bar{\phi}_a(R_\rho,R_z) \,, \\ \varphi_m(R_\rho,R_z) &\equiv R_\rho^{1/2} \bar{\phi}_m(R_\rho,R_z) \,, \\ \mathcal{G}_N(R_\rho,R_z,k_\rho,k_z,\phi) &\equiv R_\rho^{1/2} \tilde{G}_N(R_\rho,R_z,k_\rho,k_z,\phi) \,, \\ \mathcal{G}_A(R_\rho,R_z,k_\rho,k_z,\phi) &\equiv R_\rho^{1/2} \tilde{G}_A(R_\rho,R_z,k_\rho,k_z,\phi) \,, \end{split}$$



Figure 3.4: Coordinate axes for cylindrical symmetry. Since all fields are independent of the azimuthal angle of \mathbf{R} , we are free to rotate the axes so long as the z-axis and origin remain fixed. We align the x-axis with the component of \mathbf{k} lying in the x-y plane. Then the dependence of the correlation functions' values on the relative orientations of \mathbf{k} and \mathbf{R} (thin arrows) can be expressed in cylindrical coordinates. The cylindrical unit vectors (bold arrows) of some particular vector (\mathbf{R} , in this case) depend on the orientation of that vector.

and

$$\mathcal{G}_N^I(R_\rho, R_z) \equiv R_\rho^{1/2} \bar{G}_N^I(R_\rho, R_z) ,$$
$$\mathcal{G}_A^I(R_\rho, R_z) \equiv R_\rho^{1/2} \bar{G}_A^I(R_\rho, R_z)$$

for consistency.

The HFB equations become, for the cylindrically symmetric case expressed in

cylindrical coordinates,

$$i\hbar \frac{\partial}{\partial t} \varphi_{a}(R_{\rho}, R_{z}) = \left\{ -\frac{\hbar^{2}}{2m} \left(\frac{1}{4R_{\rho}^{2}} + \frac{\partial^{2}}{\partial R_{\rho}^{2}} + \frac{\partial^{2}}{\partial R_{z}^{2}} \right) + \bar{V}_{a}(R_{\rho}, R_{z}) + U \left[\frac{|\varphi_{a}(R_{\rho}, R_{z})|^{2}}{R_{\rho}} + 2 \frac{\mathcal{G}_{N}^{I}(R_{\rho}, R_{z})}{R_{\rho}^{1/2}} \right] \right\} \varphi_{a}(R_{\rho}, R_{z}) + \left[U \frac{\mathcal{G}_{A}^{I}(R_{\rho}, R_{z})}{R_{\rho}^{1/2}} + g \frac{\varphi_{m}(R_{\rho}, R_{z})}{R_{\rho}^{1/2}} \right] \varphi_{a}^{*}(R_{\rho}, R_{z}), \quad (3.56)$$

$$i\hbar\frac{\partial}{\partial t}\varphi_m(R_\rho, R_z) = \left[-\frac{\hbar^2}{4m}\left(\frac{1}{4R_\rho^2} + \frac{\partial^2}{\partial R_\rho^2} + \frac{\partial^2}{\partial R_z^2}\right) + \bar{V}_m(R_\rho, R_z) + \nu\right]\varphi_m(R_\rho, R_z) + \frac{g}{2}\left[\frac{\varphi_a^2(R_\rho, R_z)}{R_\rho^{1/2}} + \mathcal{G}_A^I(R_\rho, R_z)\right],$$
(3.57)

$$i\hbar \frac{\partial}{\partial t} \mathcal{G}_{N}(R_{\rho}, R_{z}, k_{\rho}, k_{z}, \phi) = -i\frac{\hbar^{2}}{m} \left[k_{\rho} \cos \phi \left(\frac{\partial}{\partial R_{\rho}} - \frac{1}{2R_{\rho}} \right) - \frac{k_{\rho}}{R_{\rho}} \sin \phi \frac{\partial}{\partial \phi} + k_{z} \frac{\partial}{\partial R_{z}} \right] \\ \times \mathcal{G}_{N}(R_{\rho}, R_{z}, k_{\rho}, k_{z}, \phi) \\ + \left\{ g \frac{\varphi_{m}(R_{\rho}, R_{z})}{R_{\rho}^{1/2}} + U \left[\frac{\varphi_{a}^{2}(R_{\rho}, R_{z})}{R_{\rho}} + \frac{\mathcal{G}_{A}^{I}(R_{\rho}, R_{z})}{R_{\rho}^{1/2}} \right] \right\} \\ \times \mathcal{G}_{A}^{*}(R_{\rho}, R_{z}, k_{\rho}, k_{z}, \phi) \\ - \left\{ g \frac{\varphi_{m}^{*}(R_{\rho}, R_{z})}{R_{\rho}^{1/2}} + U \left[\frac{\varphi_{a}^{*2}(R_{\rho}, R_{z})}{R_{\rho}} + \frac{\mathcal{G}_{A}^{*I}(R_{\rho}, R_{z})}{R_{\rho}^{1/2}} \right] \right\} \\ \times \mathcal{G}_{A}(R_{\rho}, R_{z}, k_{\rho}, k_{z}, \phi) , \qquad (3.58)$$

$$i\hbar \frac{\partial}{\partial t} \mathcal{G}_{A}(R_{\rho}, R_{z}, k_{\rho}, k_{z}, \phi) = \left\{ -\frac{\hbar^{2}}{4m} \left[\frac{1}{4R_{\rho}^{2}} + \frac{\partial^{2}}{\partial R_{\rho}^{2}} + \frac{1}{R_{\rho}^{2}} \frac{\partial^{2}}{\partial \phi^{2}} + \frac{\partial^{2}}{\partial R_{z}^{2}} - 4\left(k_{\rho}^{2} + k_{z}^{2}\right) \right] \right. \\ \left. + 4U \left[\frac{|\varphi_{a}(R_{\rho}, R_{z})|^{2}}{R_{\rho}} + \frac{\mathcal{G}_{N}^{I}(R_{\rho}, R_{z})}{R_{\rho}^{1/2}} \right] \right. \\ \left. + 2\bar{V}_{a}(R_{\rho}, R_{z}) \right\} \times \mathcal{G}_{A}(R_{\rho}, R_{z}, k_{\rho}, k_{z}, \phi) \\ \left. + \left\{ g \frac{\varphi_{m}(R_{\rho}, R_{z})}{R_{\rho}^{1/2}} + U \left[\frac{\varphi_{a}^{2}(R_{\rho}, R_{z})}{R_{\rho}} + \frac{\mathcal{G}_{A}^{I}(R_{\rho}, R_{z})}{R_{\rho}^{1/2}} \right] \right\} \\ \left. \times \left[\mathcal{G}_{N}(R_{\rho}, R_{z}, k_{\rho}, k_{z}, \phi) + \mathcal{G}_{N}^{*}(R_{\rho}, R_{z}, k_{\rho}, k_{z}, \phi) + R_{\rho}^{1/2} \right].$$

$$(3.59)$$

3.4.0 Cosine Series Expansion

We expand the angular dependence of Equations (3.58) and (3.59) in a set of basis functions, with the foresight that we will need to severely truncate the expansion to make the problem computationally feasible. Legendre polynomials are a popular basis, but lead to complicated expressions in Equations (3.58) and (3.59), especially in the case of the second angular derivative in (3.59). Trigonometric functions lead to simpler expressions, and such expansions are common in the angular part of spectral solutions to PDE's in cylindrical or spherical coordinates [90].

We expand the correlation functions as

$$\mathcal{G}_N(R_\rho, R_z, k_\rho, k_z, \phi) \equiv \sum_{n=0}^{\infty} \mathcal{G}_N^n(R_\rho, R_z, k_\rho, k_z) \cos\left(n\phi\right)$$
(3.60)

$$\mathcal{G}_A(R_\rho, R_z, k_\rho, k_z, \phi) \equiv \sum_{n=0}^{\infty} \mathcal{G}_A^n(R_\rho, R_z, k_\rho, k_z) \cos(n\phi) , \qquad (3.61)$$

where a superscript n is an index, not a power. These series can be differentiated term by term if $\frac{\partial}{\partial \phi} \mathcal{G}_N$ and $\frac{\partial}{\partial \phi} \mathcal{G}_A$ are piecewise smooth [76], or if we truncate the series and accept them as approximations.³ Appendix C develops the recurrence relations to handle the angular derivatives and sine and cosine factors appearing in (3.58) and (3.59). Using the definition of the step function in Equation (3.50) and

$$R_{\rho}^{1/2} = \sum_{n=0}^{\infty} R_{\rho}^{1/2} \delta_{n,0} \cos\left(n\phi\right), \qquad (3.62)$$

each side of Equations (3.58) and (3.59) is summed over the same linearly independent basis functions, allowing us to equate each expansion coefficient. Then

$$\begin{split} \mathrm{i}\hbar\frac{\partial}{\partial t}\mathcal{G}_{N}^{n}(R_{\rho},R_{z},k_{\rho},k_{z}) &= -\mathrm{i}\frac{\hbar^{2}}{2m}\bigg[k_{\rho}\left(\frac{\partial}{\partial R_{\rho}}+\frac{2n+1}{2R_{\rho}}\right)\mathcal{G}_{N}^{n+1}(R_{\rho},R_{z},k_{\rho},k_{z}) \\ &+k_{\rho}\left(\frac{\partial}{\partial R_{\rho}}-\frac{2n-1}{2R_{\rho}}\right)u_{1}^{n}\mathcal{G}_{N}^{n-1}(R_{\rho},R_{z},k_{\rho},k_{z}) \\ &+k_{\rho}\left(\frac{\partial}{\partial R_{\rho}}-\frac{1}{2R_{\rho}}\right)\delta_{n,1}\mathcal{G}_{N}^{0}(R_{\rho},R_{z},k_{\rho},k_{z}) \\ &+2k_{z}\frac{\partial}{\partial R_{z}}\mathcal{G}_{N}^{n}(R_{\rho},R_{z},k_{\rho},k_{z})\bigg] \\ &+\bigg\{g\frac{\varphi_{m}(R_{\rho},R_{z})}{R_{\rho}^{1/2}}+U\bigg[\frac{\varphi_{a}^{2}(R_{\rho},R_{z})}{R_{\rho}}+\frac{\mathcal{G}_{A}^{I}(R_{\rho},R_{z})}{R_{\rho}^{1/2}}\bigg]\bigg\} \\ &\times\mathcal{G}_{A}^{n*}(R_{\rho},R_{z},k_{\rho},k_{z}) \\ &-\bigg\{g\frac{\varphi_{m}^{*}(R_{\rho},R_{z})}{R_{\rho}^{1/2}}+U\bigg[\frac{\varphi_{a}^{*2}(R_{\rho},R_{z})}{R_{\rho}}+\frac{\mathcal{G}_{A}^{*I}(R_{\rho},R_{z})}{R_{\rho}^{1/2}}\bigg]\bigg\} \\ &\times\mathcal{G}_{A}^{n}(R_{\rho},R_{z},k_{\rho},k_{z}), \end{split}$$
(3.63)

³We have chosen cosines instead of sines because sine series are slightly more stringent in their criteria for uniform convergence [76].

$$\begin{split} \mathrm{i}\hbar\frac{\partial}{\partial t}\mathcal{G}_{A}^{n}(R_{\rho},R_{z},k_{\rho},k_{z}) = & \left\{ -\frac{\hbar^{2}}{4m} \left[\frac{1-4n^{2}}{4R_{\rho}^{2}} + \frac{\partial^{2}}{\partial R_{\rho}^{2}} + \frac{\partial^{2}}{\partial R_{z}^{2}} - 4\left(k_{\rho}^{2}+k_{z}^{2}\right) \right] \\ & + 2\bar{V}_{a}(R_{\rho},R_{z}) + 4U \left[\frac{|\varphi_{a}(R_{\rho},R_{z})|^{2}}{R_{\rho}} + \frac{\mathcal{G}_{N}^{I}(R_{\rho},R_{z})}{R_{\rho}^{1/2}} \right] \right\} \\ & \times \mathcal{G}_{A}^{n}(R_{\rho},R_{z},k_{\rho},k_{z}) \\ & + \left\{ g \frac{\varphi_{m}(R_{\rho},R_{z})}{R_{\rho}^{1/2}} + U \left[\frac{\varphi_{a}^{2}(R_{\rho},R_{z})}{R_{\rho}} + \frac{\mathcal{G}_{A}^{I}(R_{\rho},R_{z})}{R_{\rho}^{1/2}} \right] \right\} \\ & \times \left[\mathcal{G}_{N}^{n}(R_{\rho},R_{z},k_{\rho},k_{z}) + \mathcal{G}_{N}^{n*}(R_{\rho},R_{z},k_{\rho},k_{z}) + R_{\rho}^{1/2}\delta_{n,0} \right], \end{split}$$
(3.64)

with

$$\mathcal{G}_{N}^{I}(R_{\rho}, R_{z}) = \frac{1}{(2\pi)^{2}} \int_{-\infty}^{\infty} \mathrm{d}k_{z} \int_{0}^{\infty} k_{\rho} \,\mathrm{d}k_{\rho} \,\mathcal{G}_{N}^{0}(R_{\rho}, R_{z}, k_{\rho}, k_{z}) \,, \qquad (3.65)$$

with the same holding for $N \to A$. Note that only the n = 0 coefficients appear in the integral, due to the periodicity of the basis functions for n > 0.

3.5 Boundary Conditions

Boundary and initial conditions are required to solve these partial differential equations in space and time. The initial condition is determined by an imaginary time relaxation method, and is described in detail in Section 4.3. To determine the boundary conditions (BC's), we first assume that far from the origin the trap is strong enough that the probability for a particle to be found beyond a certain distance from the origin is negligible, this distance depending on direction in the cylindrical case.⁴ Then, for spherical symmetry, we have

⁴The outer boundary conditions are really for computational convenience; physically, we can only claim that all fields are bounded as $|\mathbf{R}| \to \infty$.

$$\varphi_a(R_{\max}) = 0,$$

$$\varphi_m(R_{\max}) = 0,$$

$$\mathcal{G}_N^{l,q}(R_{\max}, k) = 0,$$

$$\mathcal{G}_A^{l,q}(R_{\max}, k) = 0,$$

(3.66)

where R_{max} is the outermost center of mass grid point in a simulation, that distance beyond which no particle is likely to be found. In the cylindrical case, we have

$$\varphi_{a}(R_{\rho,\max}, R_{z}) = \varphi_{a}(R_{\rho}, |R_{z}| = R_{z,\max}) = 0,$$

$$\varphi_{m}(R_{\rho,\max}, R_{z}) = \varphi_{m}(R_{\rho}, |R_{z}| = R_{z,\max}) = 0,$$

$$\mathcal{G}_{N}^{n}(R_{\rho,\max}, R_{z}, k_{\rho}, k_{z}) = \mathcal{G}_{N}^{n}(R_{\rho}, |R_{z}| = R_{z,\max}, k_{\rho}, k_{z}) = 0,$$

$$\mathcal{G}_{A}^{n}(R_{\rho,\max}, R_{z}, k_{\rho}, k_{z}) = \mathcal{G}_{A}^{n}(R_{\rho}, |R_{z}| = R_{z,\max}, k_{\rho}, k_{z}) = 0,$$

(3.67)

where $R_{\rho,\text{max}}$ is the distance from the origin of the radial center-of-mass grid point that is furthest from the origin and in the *x-y* plane, and $R_{z,\text{max}}$ is the distance from the origin of the axial center-of-mass grid point furthest from the origin and lying along the *z*-axis.

To determine the boundary conditions at the origin in the spherical case, recall that we have assumed spherical symmetry in R and consider that negative values of R are equivalent to positive values of R with $\phi \to \phi + \pi$ and $\theta \to \theta + \pi$; that is, any field that is a function of R is even in R. Now require that each of the four fields are bounded at the origin, and assume that their R dependence may be expressed in terms of power series. Then each field will be proportional to either 1 or R^2 , to lowest order. From Equation (3.39), each of these fields is multiplied by R, so that $\varphi_a(R)$, $\varphi_m(R)$, $\mathcal{G}_N^{l,q}(R,k)$, and $\mathcal{G}_A^{l,m}(R,k)$, which are the dependent variables we are simulating, are proportional to either R or R^3 , to lowest order. Thus, at the origin, the variables for which we numerically approximate solutions are identically zero:

$$\varphi_{a}(0) = 0,
\varphi_{m}(0) = 0,
\mathcal{G}_{N}^{l,q}(0,k) = 0,
\mathcal{G}_{A}^{l,q}(0,k) = 0.$$
(3.68)

The argument for the cylindrical case along the z-axis is very similar to that for the spherically symmetric model at the origin. A negative value of R_{ρ} is equivalent to a positive value of R_{ρ} with $\phi \rightarrow \phi + \pi$, and since we assume that all four fields are invariant with respect to rotations about the z-axis, the four fields must be even with respect to R_{ρ} . If they are bounded at the origin and their R_{ρ} dependence can be expanded in power series, they go as either 1 or R_{ρ}^2 , to lowest order. We do not numerically approximate solutions to these four fields, but to these fields each multiplied by $\sqrt{R_{\rho}}$, so that $\varphi_a(R_{\rho}, R_z)$, $\varphi_m(R_{\rho}, R_z)$, $\mathcal{G}_N^0(R_{\rho}, R_z, k_{\rho}, k_z)$, and $\mathcal{G}_A^0(R_{\rho}, R_z, k_{\rho}, k_z)$ all scale as either $R_{\rho}^{1/2}$ or $R_{\rho}^{5/2}$ to lowest order, and so vanish at $R_{\rho} = 0$. That is,

$$\varphi_{a}(0, R_{z}) = 0,
\varphi_{m}(0, R_{z}) = 0,
\mathcal{G}_{N}^{n}(0, R_{z}, k_{\rho}, k_{z}) = 0,
\mathcal{G}_{A}^{n}(0, R_{z}, k_{\rho}, k_{z}) = 0$$
(3.69)

for the cylindrically symmetric case.

3.6 Summary of Model and Approximations

For the spherical case, the HFB model consists of Equations (3.40), (3.41), (3.48), and (3.49), along with (3.51), which is needed to compute the diagonal parts of the normal and anomalous fluctuations. The equations corresponding to the atomic, molecular, and anomalous fields are second order in the radial center of mass variable R, and the equations corresponding to the normal fluctuations are first order in R. Derivatives with respect to the relative coordinate \mathbf{r} have been replaced by multiplication by the relative momentum magnitude k and recurrence relations among spherical harmonics. Because of the partial wave expansions, there are infinitely many equations (3.48) and (3.49) for a given (R, k) point. All equations are quasilinear and first order in time.

The model for the cylindrical case consists of Equations (3.56), (3.57), (3.63), and (3.64), along with (3.65) for computing the diagonal parts of the normal and anomalous densities. The equations corresponding to the atomic, molecular, and anomalous fields are second order in the radial and axial center of mass variables R_{ρ} and R_z , respectively, and the equations corresponding to the normal fluctuations are first order in R_{ρ} and R_z . Derivatives with respect to the relative coordinate **r** are replaced by multiplication by radial and axial relative momentum variables k_{ρ} and k_z , respectively, and by recurrence relations among cosines. Because of the cosine series expansions, there are infinitely many equations (3.63) and (3.64) for a given $(R_{\rho}, R_z, k_{\rho}, k_z)$ point. All equations are quasilinear and first order in time.

In both geometries, all center of mass variables are subject to homogeneous Dirichlet boundary conditions, which we often refer to as *box boundary conditions*. As a practical note, observe that as long as every part of the normal fluctuations field is initially real, Equations (3.48) and (3.63) ensure that the normal fluctuations remains purely real.

Several approximations were used in deriving the equations of our models. We enumerate the approximations common to both geometries.

- 1. The states $\hat{\Psi}_m(\mathbf{x}) |\lambda\rangle$ and $\hat{\Psi}_a(\mathbf{x}') |\lambda\rangle$ are completely uncorrelated, where $|\lambda\rangle$ is the state of the system.
- 2. Quantum fluctuations of the molecular mean field are negligible.
- 3. Atoms interact only on contact.
- 4. We neglect all collisions except those between two atoms.
- 5. We neglect all density-dependent losses from the condensate, such as three-body recombination.
- 6. The trapping potential is Hermitian.
- 7. The system is in a squeezed state $|\lambda\rangle$ that is an eigenstate of a Bogoliubov quasiparticle operator \hat{b}_k , such that $\hat{a}_k = \sum_j \left(U_{jk} \hat{b}_j + V_{jk}^* \hat{b}_j^\dagger \right)$ for all k, where \hat{a}_k removes a particle with wavenumber k.
- We only account for a single Feshbach resonance, while many real atoms, including ⁸⁵Rb, have at least two that are relevant to experiments.
- 9. Any practical calculation with our models is subject to the experimental inaccuracies in the measured intrinsic atomic properties that are used.

We make several more approximations when we specialize the equations to the spherical case.

1. The external potentials are rotationally invariant.

- 2. The initial conditions on every function of a single coordinate are rotationally invariant.
- 3. We only consider coordinates x and x' such that their moduli are equal: x = x'. This is not truly an approximation, since it does not alter the values of any of the fields we do consider, but rather is a restriction on our knowledge of the system.
- 4. The dependence of the off-diagonal parts of the normal and anomalous fluctuations on the center of mass coordinate **R** is entirely encoded in the magnitude *R* of that coordinate.
- 5. All fields are such that $\frac{\partial}{\partial R_i} \frac{\partial}{\partial r_j} = \frac{\partial}{\partial r_j} \frac{\partial}{\partial R_i}$, where $\frac{\partial}{\partial R_i}$ represents partial differentiation with respect to the *i*th component of the **R** coordinate and likewise for $\frac{\partial}{\partial r_j}$, for all *i* and *j*. This assumption will be true if these partial derivatives are continuous.
- 6. The integrals $\int d^3r \ \bar{G}_N(R, \mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}$ and $\int d^3r \ \bar{G}_N(R, \mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}$ converge when integrated over all *r*-space.
- 7. The correlation functions $\bar{G}_N(R, \mathbf{r})$ and $\bar{G}_A(R, \mathbf{r})$ and their derivatives with respect to any component of \mathbf{r} both go zero as that component of \mathbf{r} goes to plus or minus infinity. Physically, this means that two points infinitely far apart are completely uncorrelated.
- 8. The correlation functions $\tilde{G}_N(R, k, \theta, \phi)$ and $\tilde{G}_A(R, k, \theta, \phi)$ are continuous in θ and ϕ .

The specialization to the cylindrical case requires very similar assumptions.

- 1. The external potentials are invariant with respect to rotations about the z-axis and invariant with respect to reflections over the x-y plane.
- 2. The initial conditions on every function of a single coordinate are invariant with respect to rotations about the z-axis and invariant with respect to reflections over the x-y plane.
- 3. We only consider coordinates \mathbf{x} and \mathbf{x}' such that their radial (in the sense of cylindrical coordinates) components are equal, and the absolute values of their axial components are equal: $x_{\rho} = x'_{\rho}$ and $|x_z| = |x'_z|$. Again, this does not alter the values of quantities we do consider, but merely restricts our knowledge of the system.
- 4. All dependence of the off diagonal parts of the normal and anomalous densities on the center of mass coordinate \mathbf{R} is entirely encoded in the magnitude of the radial and axial components R_{ρ} and R_z of that coordinate.
- 5. All fields are such that $\frac{\partial}{\partial R_i} \frac{\partial}{\partial r_j} = \frac{\partial}{\partial r_j} \frac{\partial}{\partial R_i}$, where $\frac{\partial}{\partial R_i}$ represents partial differentiation with respect to the *i*th component of the **R** coordinate and likewise for $\frac{\partial}{\partial r_i}$, for all *i* and *j*.
- 6. The integrals $\int d^3r \ \bar{G}_N(R_{\rho}, R_z, \mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}$ and $\int d^3r \ \bar{G}_N(R_{\rho}, R_z, \mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}$ converge when integrated over all *r*-space.
- 7. The correlation functions $\bar{G}_N(R_\rho, R_z, \mathbf{r})$ and $\bar{G}_A(R_\rho, R_z, \mathbf{r})$ and their derivatives with respect to any component of \mathbf{r} both go zero as that component of \mathbf{r} goes to plus or minus infinity.
- 8. The derivatives of the correlation functions with respect to the azimuthal angle ϕ are piecewise smooth.

Numerical solutions to either of the two models introduces still more approximations.

- 1. A quantum mechanical particle is never truly excluded from any region where the potential is finite; our box boundary conditions are an approximation at the outer edge of the trap. This is a finite domain approximation.
- 2. We truncate the eigenfunction expansions of the correlation functions.
- 3. The dependence of any function on its center of mass variable or variables is represented by a truncated eigenfunction expansion (a defining characteristic of pseudospectral approximations to derivatives).
- 4. We use a set of discrete momenta k in the spherical case and k_{ρ} and k_z in the cylindrical case appropriate for box confinement, rather than the momenta appropriate for interacting particles in a harmonic trap.
- 5. The time dependence of every function is represented by a Taylor series, truncated after fifth order.

Chapter 4

NUMERICAL METHODS

Even with our mathematical modifications and assumptions about symmetry, an analytical solution to our model appears unfeasible, and we turn to numerical methods for approximate solutions.

Perez-Garcia and Liu find that a finite difference approximation to the solution of nonlinear Schrödinger equations requires a very small time step and produces inaccurate results for long simulations [79]. Past simulations [11] of the collapse used a Crank-Nicholson scheme to solve the equations for spherical symmetry, but the negative experiences cited in [79] motivate the choice of a different method of solving these nonlinear partial differential equations; therefore, we use the method of lines, in which a system of PDE's is approximated by a larger, coupled system of ODE's. A numerical integrator is used on the resulting ODE's, and the other derivatives that appeared in the PDE must be represented by some algebraic means.

Our method of lines approach amounts to a discretization of the spatial domain while retaining the continuous time domain, which is plausible when comparing the resolutions in the experiments. In the widely-studied JILA experiments [1], the imaging apparatus had a spatial resolution of 7 μ m, while a typical image was 60 μ m in the radial direction and 310 μ m in the axial direction, giving about 9 × 43 spatial samples. In the Rice experiments [53], the apparatus had a resolution of about 10 μ m, while the cross-sectional area in which the solitary waves oscillated was about 1.5 μ m in the radial direction and 1280 μ m in the axial direction, giving about 1 × 128 spatial samples. Neither experiment cites a temporal resolution, but Leggett [91] asserts that this resolution is affected mostly by the time required to turn on the imaging laser, so that temporal measurements are effectively instantaneous. If a mechanical shutter is placed between a laser and its target, the turn-on time can effectively be on the order of 10^{-9} seconds [92], while experimental time scales are $\gtrsim 10^{-6}$ s for the Feshbach resonance and $\gtrsim 10^{-4}$ for the nonlinearities.

4.1 Time Propagation

Wüster *et al.* [12] use a fixed-step Runge-Kutta method for time propagation of equations similar to ours, and, unlike Milstein *et al.* [11] are able to examine the experimental parameter regime (albeit with multiple processors). The important ability to simulate a real atom, as well as our own positive experiences in other contexts, motivates the use of a Runge-Kutta method. We opt for adaptive step size selection, which allows for more efficient computation and acts as a real-time convergence check on the temporal solution. See Appendix D for a derivation of a typical Runge-Kutta method; it effectively estimates the solution to an ordinary differential equation by a truncated Taylor series evaluated at particular points of a continuous domain.

We use Cash and Karp's [93, 80] fifth-order method with an embedded fourthorder formula. This method approximates the solution y(x + h) to the first-order ordinary differential equation

$$\frac{\mathrm{d}y}{\mathrm{d}x} = f(x,y)\,,\tag{4.1}$$

given a known value y(x), by

$$y(x+h) = y(x) + \frac{37}{378}K_1 + \frac{250}{621}K_3 + \frac{125}{594}K_4 + \frac{512}{1771}K_6 + \mathcal{O}(h^6), \qquad (4.2)$$

where

$$K_{1} = hf[x, y(x)],$$

$$K_{2} = hf\left[x + \frac{1}{5}h, y(x) + \frac{1}{5}K_{1}\right],$$

$$K_{3} = hf\left[x + \frac{3}{10}h, y(x) + \frac{3}{40}K_{1} + \frac{9}{40}K_{2}\right],$$

$$K_{4} = hf\left[x + \frac{3}{5}h, y(x) + \frac{3}{10}K_{1} - \frac{9}{10}K_{2} + \frac{6}{5}K_{3}\right],$$

$$K_{5} = hf\left[x + h, y(x) - \frac{11}{54}K_{1} + \frac{5}{2}K_{2} - \frac{70}{27}K_{3} + \frac{35}{27}K_{4}\right],$$

$$K_{6} = hf\left[x + \frac{7}{8}h, y(x) + \frac{1631}{55296}K_{1} + \frac{175}{512}K_{2} + \frac{575}{13824}K_{3} + \frac{44275}{110592}K_{4} + \frac{253}{4096}K_{5}\right].$$

$$(4.3)$$

The difference between the fifth-order formula (4.2) and the embedded fourth-order formula is

$$\Delta = \left(\frac{37}{378} - \frac{2825}{27648}\right) K_1 + \left(\frac{250}{621} - \frac{18575}{48384}\right) K_3 + \left(\frac{125}{594} - \frac{13525}{55296}\right) K_4 - \frac{277}{14336} K_5 + \left(\frac{512}{1771} - \frac{1}{4}\right) K_6, \quad (4.4)$$

which provides an estimate of the truncation error in the fourth-order formula. This error estimate provides the basis for the step size adjustment, which follows *Numerical Recipes*'s [80] approach: if that error is below some tolerance Δ_0 , the fifth-order stepped solution is accepted, and the step size h_{next} to try during the next iteration is

$$h_{\text{next}} = \frac{9}{10} h_{\text{now}} \left| \frac{\Delta_0}{\Delta} \right|^{1/5}, \qquad (4.5)$$

where h_{now} is the current step size. If the estimated error Δ is larger than the



Figure 4.1: Illustration of adaptive Runge-Kutta algorithm. All the pieces necessary for computing a stepped solution are calculated, and then those pieces are combined to estimate the truncation error in the solution. If the error is too high, the step size is reduced, and the pieces necessary for computing a stepped solution are re-calculated using the new step size. If the error is acceptable, the stepped solution is accepted (either recorded or used as the next step's initial condition), and a step size to use when computing the *next* stepped solution is computed. The process then repeats for the next stepped solution.

tolerance, the step size is re-scaled as

$$h_{\rm now} \to \frac{9}{10} h_{\rm now} \left| \frac{\Delta_0}{\Delta} \right|^{1/4},$$
(4.6)

and the current step is repeated using the re-scaled step size. Figure 4.1 illustrates the algorithm.

4.2 Spatial Derivatives

While the time domain remains continuous in the numerical solution of our model, we discretize the spatial domain. This discretization allows us to represent the model's spatial derivatives with algebraic expressions, as required by the method of lines. Since a derivative is defined as a limit in which a step size goes to zero, derivatives in the continuum sense are not defined for functions on a discrete domain. However, we may discretize a derivative by finding formulas that approximate the derivative of a function using that function evaluated at a finite number of points. Two options are finite differences and pseudospectral derivatives.

Given a continuous function f(x), Taylor series expansions of f(x+h) and f(x-h) may be combined to form an approximation to a second derivative, as described in [94]:

$$\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} = \frac{1}{h^2} \left[f(x+h) - 2f(x) + f(x-h) \right] + \mathcal{O}(h^2) \,, \tag{4.7}$$

called the *three-point formula*. Including expansions of $f(x \pm 2h)$ produces a more accurate formula:

$$\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} = \frac{1}{12h^2} \Big[-f(x+2h) + 16f(x+h) - 30f(x) + 16f(x-h) - f(x-2h) \Big] + \mathcal{O}(h^4) \,, \quad (4.8)$$

called the *five-point formula*.

Pseudospectral derivatives (derived in Appendix E) offer an alternative to finite differences. The pseudospectral derivatives we consider can be computed using fast transform algorithms.

We can approximate a function f(x) by a truncated sine series

$$f(x) \approx \sum_{k=1}^{N} \tilde{f}_k \sin(kx) \,. \tag{4.9}$$

The expansion coefficients \tilde{f}_k are computed by the discrete sine transform:

$$\tilde{f}_k = \frac{2}{N} \mathcal{S}_k[f(x_j)], \ k \in \{1, \dots, N-1\},$$
(4.10)

where $S_k[f(x_j)]$ denotes the k^{th} value of the discrete sine transform of the set of values $f(x_j)$. Taking derivatives of the series (4.9) gives pseudospectral first and second derivatives at the grid points $x_j = \frac{j}{N} (b-a) + a, j \in \{1, \ldots, N-1\},$

$$\frac{\mathrm{d}f(x_j)}{\mathrm{d}x} \approx \frac{\pi}{b-a} \mathcal{C}_j\left(k\tilde{f}_k\right), \ j \in \{1,\dots,N-1\}$$
(4.11)

$$\frac{\mathrm{d}^2 f(x_j)}{\mathrm{d}x^2} \approx \frac{\pi^2}{(b-a)^2} \mathcal{S}_j\left(-k^2 \tilde{f}_k\right), \ j \in \{1, \dots, N-1\},$$
(4.12)

where C_j denotes a discrete cosine transform. Each of these derivatives assumes box boundary conditions.

Similarly, we may take finite differences of the series (4.9), giving

$$\frac{f(x_{j+1}-x_{j-1})}{2h} = \frac{N}{b-a} \mathcal{C}_j \left[\tilde{f}_k \sin\left(\frac{\pi k}{N}\right) \right], \qquad (4.13)$$

$$\frac{f(x_{j+1}) - 2f(x_j) + f(x_{j-1})}{h^2} = \frac{2}{h^2} S_j \left\{ \tilde{f}_k \left[\cos\left(\frac{\pi k}{N}\right) - 1 \right] \right\}, \quad (4.14)$$

where h is the grid spacing.¹ Relatively little theory surrounds these pseudospectral derivatives based on finite differences [95]. Kosloff [96] shows that in the context of the linear Schrödinger equation, approximation of a kinetic energy operator by means of a finite difference applied to an interpolating trigonometic polynomial in the Fourier basis inaccurately accounts for higher-momentum modes, while analytical

¹Note that we are not equating a finite difference to a pseudospectral derivative, but rather simplifying a finite difference formula applied to Equation (4.9). The right hand side of Equation (4.14) is sometimes called a pseudospectral derivative, though this is a slight misnomer; we see here that it is only second-order accurate, as is the finite difference.

derivatives of interpolants like (4.11) and (4.12) handle these modes more accurately. Such pseudospectral derivatives are the subject of extensive study [97, 98, 99, 100, 101], and may be shown to converge faster than any power of 1/N. Fornberg [90] derives such pseudospectral derivatives as limiting cases of finite differences in which every available grid point is used. For these reasons, and to use methods as far removed from finite differences as possible in this context, we shall concentrate on pseudospectral derivatives which are analytical derivatives of interpolants. In the numerical solution of the spherical model, Equations (3.40), (3.41), (3.48), and (3.49), we employ Equations (4.11) and (4.12).

Recall that for the cylindrical model, we multiplied the four functions to be solved for by $\sqrt{R_{\rho}}$. If $\bar{\phi}_a(R_{\rho}, R_z)$, for example, has a power series expansion, as many functions encountered in the modeling of nature do, this division results in a function that scales as $R_{\rho}^{1/2}$ or $R_{\rho}^{5/2}$ to lowest order. The sinusoidal basis assumed in Equation (4.9), upon which (4.11) and (4.12) are based, then requires a large number N of basis functions to converge. (The derivatives in the R_z direction have no such issue, so we continue to use sinusoidal pseudospectral derivatives for these.) As an alternative, we use a set of N + 1 first-kind Chebyshev polynomials $T_k(x)$:

$$f(x) \approx \sum_{k=0}^{N} \tilde{f}_k T_k(x) , \qquad (4.15)$$

where $x \in [-1,1]^2$ Table 4.1 lists the first five Chebyshev polynomials. Using $x_j = \cos\left(\frac{\pi j}{N}\right), j \in \{0, \ldots, N-1\}$ as the grid points, the expansion coefficients are found from

$$\tilde{f}_k = \frac{1}{N} \mathcal{C}_k[f(x_j)], \qquad (4.16)$$

²The physical grid runs from a to b, so we must multiply the first and second pseudospectral derivatives by 2/(b-a) and $4/(b-a)^2$, respectively, according to the chain rule.

and the back transform is given by

$$f(x_j) = \mathcal{C}_j\left(2b_k \tilde{f}_k\right), \qquad (4.17)$$

where $b_k = 1/2$ for 0 < k < N, and $b_0 = b_N = 1$. Now write the derivative of Equation (4.15) as its own Chebyshev series with expansion coefficients \tilde{f}'_k :

$$f'(x) \approx \sum_{k=0}^{N} \tilde{f}'_k T_k(x)$$
 (4.18)

From recurrence relations among Chebyshev polynomials, the \tilde{f}'_k are calculated by

$$\tilde{f}_{k-1}' = \frac{1}{c_{k-1}} \left(2k\tilde{f}_k + \tilde{f}_{k+1}' \right), \ k \ge 1.$$
(4.19)

The recurrence begins at k = N, with $\tilde{f}'_{N+1} = \tilde{f}'_N = 0$, and the second derivative is found by applying the recurrence twice, then with $\tilde{f}'_{N-1} = 0$. Having the expansion coefficients \tilde{f}'_k , one applies the back transform (4.17) to obtain the pseudospectral derivative. Chebyshev interpolants on this nonuniform grid have the advantage that they do not exhibit a Gibbs phenomenon, or rapid oscillations near a discontinuity, at the ends of the grid (though a discontinuity on the interior will have an overshoot), and resolves the Runge phenomenon, in which interpolation on a uniform grid does not converge as the number of interpolation nodes increases [100]. Figure 4.2 is an example of a grid for the cylindrical model, and Figure 4.3 is an example for the spherical model.

Order k	$T_k(x)$
0	1
1	x
2	$2x^2 - 1$
3	$4x^3 - 3x$
4	$8x^4 - 8x^2 + 1$

Table 4.1: First five Chebyshev polynomials of the first kind.



Figure 4.2: Example of center of mass grid in cylindrical model. The grid is uniformly spaced in the R_z direction, but nonuniformly spaced in R_{ρ} . There are $N_{R_{\rho}} + 1$ grid points, indexed from zero and including the boundaries, in the R_{ρ} direction, and $N_{R_z} + 1$ grid points in the R_z direction.



Figure 4.3: Example of center of mass grid in spherical model. At any given time, the center of mass grid points are evenly spaced. There are N + 1 grid points, indexed from 0, including the boundaries.

4.3 Imaginary Time Relaxation

Since most of the collapse experiments start out with a condensate in a stable, steady state, we should use the lowest energy eigenstate as the initial condition for any collapse simulation. For a noninteracting condensate the ground state is that of the Schrödinger equation in a harmonic potential, and so is analytically solvable. However, in most experiments the initial condensate is weakly interacting, or perhaps we want to include a non-harmonic potential. In these cases, most of which are analytically unsolvable, we must resort to numerical means of calculating the ground state. Even in the noninteracting case, the analytical ground state may be significantly different from zero at the end of the grid, causing undesired reflections due to the box boundary conditions. Imaginary time relaxation resolves both of these issues, achieving the true ground state in the simulation geometry.

A Hamiltonian must be Hermitian in order for it to correspond to some observable quantity, and ours is no exception, as inspection of Equation (2.6) reveals. Being Hermitian, its eigenkets $|n\rangle$ span the Hilbert space in which it acts, and the operator also has a spectral decomposition such that

$$e^{-iHt/\hbar} = \sum_{n=0}^{\infty} e^{-iE_n t/\hbar} |n\rangle \langle n|, \qquad (4.20)$$

where E_n is the n^{th} eigenvalue of the Hamiltonian H, and t is some scalar. This statement is true even for Hilbert spaces of infinite dimension. Note that we have assumed that the Hilbert space consists only of bound states. Recalling that the Hamiltonian is the generator of time translations, Equation (4.20) is the (unitary) time evolution operator [4], where t is the time. Applying this operator to some arbitrary state $|\psi(t=0)\rangle$, a vector in the Hilbert space in which H acts, and noting that $H \neq H(t)$,

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle = \sum_{n=0}^{\infty} e^{-iE_nt/\hbar} \langle n|\psi(0)\rangle |n\rangle.$$
(4.21)

Making the substitution $\tau = it$, Equation (4.21) becomes

$$|\psi(-i\tau)\rangle = \sum_{n=0}^{\infty} e^{-E_n\tau/\hbar} \langle n|\psi(0)\rangle |n\rangle.$$
(4.22)

For large τ , higher energy eigenkets will be exponentially supressed. This same evolution can be achieved through the Schrödinger equation with the substitution $\tau = it$. Hence, imaginary-time propagation of the Schrödinger equation will eventually result in only the lowest energy eigenket in the sum (4.22) having any appreciable weight. If the initial state $|\psi(0)\rangle$ has any non-zero component $\langle n|\psi(0)\rangle$, then the solution of the imaginary-time Schrödinger equation for large τ will effectively be the lowest energy eigenstate. A position-space representation is obtained by left-multiplying Equation (4.22) by some state of definite position $\langle \mathbf{x}|$. As a practical note, if the ground state energy eigenvalue is non-zero, then even the ground state will become exponentially supressed for large τ (albeit less so than all other eigenstates), so the state should be normalized at every step to ensure computationally feasible values.

4.4 Postprocessing Methods

After a simulation completes, we may calculate total number, which should be conserved, as a gauge of the stability and physical relevance of the simulation. We also wish to extract the dominant frequencies of oscillation in particle number for a given field, and to examine kinematics by calculating flow velocities.

4.4.1 Monitoring Total Number

Summing all the number densities and integrating over all space gives the total number of particles,

$$N_{\text{tot}} = \int d^3x \, \left[|\phi_a(\mathbf{x})|^2 + 2 \, |\phi_m(\mathbf{x})|^2 + G_N(\mathbf{x}, \mathbf{x}) \right], \qquad (4.23)$$

which should be constant in time, since our model has no imaginary loss terms. A deviation in any conserved quantity is usually expressed in terms of average error, or

$$\epsilon_{\text{avg}} \equiv 2 \frac{N_{\text{tot}}(t) - N_{\text{tot}}(0)}{N_{\text{tot}}(t) + N_{\text{tot}}(0)}$$

$$(4.24)$$

for the case of total number. Allowing for roundoff error, ϵ_{avg} may vary randomly (or seemingly so) from time step to time step, by about machine precision. We interpret a monotonic trend in the change in N_{tot} versus time as an indicator of instability or a lack of convergence.

In the spherical model, the total number may be calculated as

$$N_{\text{tot}} = 4\pi \int_0^\infty \mathrm{d}R \, |\varphi_a(R)|^2 + 8\pi \int_0^\infty \mathrm{d}R \, |\varphi_m(R)|^2 + \frac{1}{\pi^{3/2}} \int_0^\infty \mathrm{d}R \, R \int_0^\infty \mathrm{d}k \, k^2 \mathcal{G}_N^{0,0}(R,k) \,. \quad (4.25)$$

We calculate this during postprocessing using the trapezoid rule:

$$N_{\text{tot}} \approx 4\pi \sum_{j=1}^{N_R-1} \delta R |\varphi_a(R_j)|^2 + 8\pi \sum_{j=1}^{N_R-1} \delta R |\varphi_m(R_j)|^2 + \frac{1}{\pi^{3/2}} \sum_{j=1}^{N_R-1} \delta R (j \,\delta R) \sum_{i=0}^{N_r-1} \delta k (i \,\delta k)^2 \mathcal{G}_N^{0,0}(R_j, k_i), \quad (4.26)$$

where $N_R + 1$ is the number of center of mass grid points, including the boundaries; R_j is the *j*th center of mass grid point, where R_0 is the origin and $R_N = R_{\text{max}}$ is the outer boundary; $\delta R = R_{\text{max}}/N_R$ is the center of mass grid spacing; N_r is the number of relative grid points (in practice, the relative grid only serves to determine the largest momentum and number of distinct momenta accounted for); $\delta k = \pi/r_{\text{max}}$ is the smallest nonzero momentum and momentum grid spacing, where r_{max} is the extent of the relative coordinate; and k_i is the *i*th momentum grid point, such that $k_i = i\delta k$. Note that we have left off the ends of the center of mass grid, since all dependent variables are zero there. The trapezoid rule has an error on the order of the square of the grid spacing, which in most simulations is about 10^{-7} , giving an error of about 10^{-14} , very near machine precision.

The total number in the cylindrical model is

$$N_{\text{tot}} = 2\pi \int_{0}^{\infty} \mathrm{d}R_{\rho} \int_{-\infty}^{\infty} \mathrm{d}R_{z} |\varphi_{a}(R_{\rho}, R_{z})|^{2} + 4\pi \int_{0}^{\infty} \mathrm{d}R_{\rho} \int_{-\infty}^{\infty} \mathrm{d}R_{z} |\varphi_{m}(R_{\rho}, R_{z})|^{2} + \frac{1}{2\pi} \int_{0}^{\infty} \mathrm{d}R_{\rho} R_{\rho}^{1/2} \int_{-\infty}^{\infty} \mathrm{d}R_{z} \int_{-\infty}^{\infty} \mathrm{d}k_{z} \int_{0}^{\infty} \mathrm{d}k_{\rho} k_{\rho} \mathcal{G}_{N}^{0}(R_{\rho}, R_{z}, k_{\rho}, k_{z}).$$
(4.27)

The grids in the R_z , k_z , and k_ρ directions are uniform, so we use the trapezoid rule, as above. Using Chebyshev pseudospectral derivatives for the R_ρ direction derivatives requires an integration scheme appropriate for the grid $R_{\rho,j} = \frac{R_{\rho,\max}}{2} \left[\cos\left(\frac{\pi j}{N_{R_\rho}}\right) + 1 \right]$, where $R_{\rho,\text{max}}$ is the outer extent of the radial center of mass grid. The grid points $x_j = \cos\left(\frac{\pi j}{N_{R_{\rho}}}\right)$ (where $N_{R_{\rho}} + 1$ is the number of radial grid points in the center of mass coordinate, including the boundaries) are the nodes of Chebyshev-Gauss-Lobatto quadrature, which we use to calculate the R_{ρ} parts of the integrals. The weights of this Gaussian quadrature scheme are $w_j = \pi/N_{R_{\rho}}$ for $0 < j < N_{R_{\rho}}$ and $w_0 = w_N = \pi/2N_{R_{\rho}}$. Then, noting that $\sqrt{1-x_j^2} = \sin\left(\frac{\pi j}{N_{R_{\rho}}}\right)$, the total number from a given time step in a cylindrical simulation is calculated in postprocessing using

$$N_{\text{tot}} \approx \pi R_{\rho,\max} \sum_{j=-\frac{N_{R_z}-1}{2}}^{\frac{N_{R_z}-1}{2}} \delta R_z \sum_{l=0}^{N_{R_\rho}} w_l \sin\left(\frac{\pi l}{N_{R_\rho}}\right) \left[|\varphi_a(R_{\rho,l}, R_{z,j})|^2 + 2 |\varphi_m(R_{\rho,l}, R_{z,j})|^2 \right] + \frac{R_{\rho,\max}}{4\pi} \sum_{j=-\frac{N_{R_z}-1}{2}}^{\frac{N_{R_z}-1}{2}} \delta R_z \sum_{q=\frac{N_{k_z}-1}{2}}^{\frac{N_{k_z}-1}{2}} \delta k_z \sum_{n=0}^{N_{k_\rho}} (n \, \delta k_\rho) \, \delta k_\rho \sum_{l=0}^{N_{R_\rho}} \sqrt{l \, \delta R_\rho} \times w_l \sin\left(\frac{\pi l}{N_{R_\rho}}\right) \mathcal{G}_N^0(R_{\rho,l}, R_{z,j}, k_{\rho,n}, k_{z,q}), \qquad (4.28)$$

where δR_z , δk_z , and δk_ρ are the axial center of mass, axial relative momentum, and radial relative momentum grid spacings, respectively; $R_{\rho,l}$ and $R_{z,j}$ are the l^{th} radial and j^{th} axial center of mass grid points; $k_{\rho,n}$ and $k_{z,q}$ are the n^{th} radial and q^{th} axial relative momentum grid points; and a double-prime on a sum indicates that the first and last terms of the sum are halved, though the first and last terms of the sum over j do not strictly need to be halved, since the box boundary conditions ensure that these terms are zero, anyway.

4.4.2 Estimating Power Spectra

The total number of particles in a particular field is given by one of the sums above; for example, the number of condensed atoms in a spherically symmetric simulation is

$$N_a \approx 4\pi \sum_{j=1}^{N_R-1} \delta R \left| \varphi_a(R_j) \right|^2.$$
(4.29)

As a function of time, this or any total number of particles may exhibit oscillations, the frequency of which we wish to determine. If the number data were taken at equally-spaced intervals, we would use the discrete Fourier transform to estimate the power spectrum, but the adaptive nature of our time integration method results in nonuniform sampling intervals. Experience suggests that uniformly sampling an interpolant of the data produces specious results. Reference [80] summarizes a method for calculating a *Lomb normalized periodogram*, which is a method for more reliably estimating the prominence of periodic signals in a set of nonuniformly sampled data.

Consider a set of data points $f_i = f(t_i), i \in \{0, ..., N-1\}$, where now N represents the total number of samples. The times t_i of the samples are not necessarily evenly spaced. Lomb [102] shows that the function

$$P(\omega) = \frac{1}{2\sigma^2} \left\{ \frac{\left[\sum_i \left(f_i - \bar{f}\right)\cos\left(\omega t_i - \omega\tau\right)\right]^2}{\sum_i \cos^2\left(\omega t_i - \omega\tau\right)} + \frac{\left[\sum_i \left(f_i - \bar{f}\right)\sin\left(\omega t_i - \omega\tau\right)\right]^2}{\sum_i \sin^2\left(\omega t_i - \omega\tau\right)} \right\},\tag{4.30}$$

where \bar{f} is the arithmetic mean of the $\{f_i\}$, σ^2 is their variance, and

$$\tau = \frac{1}{2\omega} \tan^{-1} \left[\frac{\sum_{i} \sin\left(2\omega t_{i}\right)}{\sum_{i} \cos\left(2\omega t_{i}\right)} \right], \qquad (4.31)$$

is the least-squares fit of the data to the function $f(t) = a \cos(\omega t) + b \sin(\omega t)$, where ω is an angular frequency. Scargle [103] extends this result by showing that, for F independent frequencies,

$$p = 1 - \{1 - \exp\left[-P(\omega)\right]\}^F$$
(4.32)

is the probability that a value of $P(\omega)$ or larger is due to random noise. Thus, a spike in $P(\omega)$ indicates a prominent periodic signal of angular frequency ω in the data. The number F of independent frequencies can be roughly estimated as F = N when the data are almost evenly spaced and the highest frequency considered is the average Nyquist frequency $N/2(t_{N-1} - t_0)$ [80].

When comparing two peaks in a Lomb periodogram, we must recall that the frequency of the larger peak is exponentially more prominent in the actual signal than the smaller peak. Figure 4.4 shows a normalized Lomb periodogram of the function $\sin (7.5t)$, sampled at 10,000 points between 0 and 10π . The most prominent peak occurs at 1.1938 Hz, which is the frequency $7.5/2\pi$ of the sampled signal; thus, the algorithm correctly estimates the dominant frequency. However, the periodogram contains frequency spikes adjacent to the largest peak that may be misinterpreted as harmonics, which are not actually present in the sampled signal. Therefore, we will only accept the largest frequency component in a Lomb periodogram; all smaller peaks may or may not actually exist in the signal.

4.4.3 Calculating Velocities

As mentioned in the Introduction, a hydrodynamic treatment [46, 23, 22] of BEC uses the condensate wavefunction's phase angle to find a velocity potential Φ such that

$$\Phi(\mathbf{x}) = \frac{\hbar}{m} S(\mathbf{x}), \qquad (4.33)$$

where $S(\mathbf{x}) = \arg [\phi_a(\mathbf{x})]$ for the atomic condensate, for example. Then an irrotational (since the curl of a gradient is zero) flow velocity is

$$\mathbf{v} = \nabla \Phi(\mathbf{x}) \,. \tag{4.34}$$



Figure 4.4: Example of Lomb normalized periodogram. The periodogram has been computed from a 10,000 point sampling of the function $\sin(7.5t)$. Only the largest peak represents a frequency component actually present in the signal. Adjacent points are connected by a line, to guide the eye.

This procedure could be applied to the atomic or molecular field in our model. Since we do not have a complex amplitude whose squared modulus is the noncondensed density, we cannot apply this hydrodynamic formulation to the noncondensed field. Using finite differences in time and space would fail to capture events in which atoms enter or leave the noncondensed field for the condensed or molecular fields. Lacking a truthful and straightforward method of calculation, we ignore velocities of noncondensed atoms.

By convention, the phase angle of a complex number lies between plus and minus π . Therefore, if the phase angle at one location is π and at a neighboring location

is $\pi + \delta$, where δ is positive and arbitrarily small, a naive calculation of the phase angle would result in approximately $-\pi$, introducing an unphysical discontinuity in the velocity potential. When calculating phase angles, we are careful to remain at all times on the same Riemann sheet; in practice, given a sequence of angles, we add to or subtract from each angle whatever integer multiple of 2π gives the value that differs the least from the neighboring angles in the sequence. As this process often results in phases that are not zero on the domain boundaries, we must use finite differences to approximate the gradients, as sinusoidal pseudospectral derivatives applied to data with nonhomogeneous boundary values would result in a substantial Gibbs phenomenon, corrupting the velocity data with unphysical, spatially-periodic values.

Chapter 5

SIMULATIONS AND ANALYSES

We present the results of simulations that are intended to quantitatively mimic experiments, and of simulations that could inspire new experiments. Besides qualitatively reproducing collapses and bursts, our simulations predict shorter collapse times for stronger traps, and rapid pre-collapse atom-molecule oscillations. We find that molecules move extremely rapidly before or during dissociation, and form in a relatively static state. Simulations with single and double magnetic field pulses, though quantitatively inaccurate, qualitatively resemble most aspects of the corresponding experiments, with the notable exception that we observe condensate remnant number increasing with hold time instead of decreasing. All simulations are done in spherical symmetry, so that only days or weeks of CPU time are needed for an insightful simulation.

5.1 Collapse Simulations

Collapse may be the most interesting experimental scenario, but it requires the most computation, since these are the longest experiments we consider. Still, we may extract physically meaningful data from even the initial stages of such simulations.

5.1.1 Experimental Parameters

Anticipating the simulations to be time-consuming, we attempt to model the experimental situation that resulted in the shortest collapse time. From Donley et

al.'s [1] Figure 2, we see that an effective scattering length of $-55a_0$ gave a time to collapse of about 1 ms for an initial condensate number of 6000.

Using the geometric mean of these experiments' trap frequencies, $2\pi \times 12.77$ Hz, we find a noninteracting initial state using imaginary time relaxation and immediately set the external magnetic field to B = 167.2691701 G.¹ All other fields are initialized to zero, though the experiments [1] actually begin with a small thermal cloud. The results below are for 33 center of mass points ranging from R = 0 to $R = 10.0 \ \mu\text{m}$, 16 noncondensed modes ranging from k = 0 to $k = 3\pi/2 \ \mu\text{m}^{-1}$, four spherical harmonics with q = 0 only (that is, no azimuthal dependence) in the correlation function expansions, and a maximum allowed truncation error limit of 10^{-16} in the adaptive Runge-Kutta integrator. This limit resulted in time step sizes on the order of 7×10^{-12} s for the duration of the simulation, making simulations with finer spatial resolutions prohibitively time-consuming.

Figures 5.1 and 5.2 each show the time evolution of the density and number of condensed atoms and molecules. The atomic and molecular fields oscillate rapidly and 180° out of phase. The oscillations, which have never before been simulated in the context of collapse, have very small amplitudes, such that not even an entire particle is lost from the atomic field. The size and frequency of these oscillations would make them extremely hard to detect and measure.

Figure 5.3 is a normalized Lomb periodogram for the molecule number during the time t = 0.4046465526444529 to 0.4048009943305098 ms. This periodogram is calculated from every computed time step in the interval, and so is not subject to aliasing due to sampling the computed data. The frequency of the number oscillations is 40

 $^{^{1}}$ Values such at the magnetic field that are used in a simulations may cited to 16 significant figures, since they are computational parameters and not results of a simulation.



Figure 5.1: Condensed particle densities in a realistic collapse simulation. Densities (a) $|\bar{\phi}_a(R)|^2$ of atoms and (b) $|\bar{\phi}_m(R)|^2$ of molecules.

MHz.² The time scales (2.73) through (2.75) may be inverted to give characteristic frequencies of the system; these are $f_{U_0} = 8.62$ kHz, $f_{g_0} = 5120$ GHz, and $f_{\nu_0} = 240$ MHz when using unrenormalized parameters, or $f_U = 9.96$ kHz, $f_g = 3830$ GHz, and $f_{\nu} = 232$ MHz when using renormalized parameters. Note that $2\pi \times 40$ MHz = 300 MHz.

The time evolution of the density and number of noncondensed atoms is shown in Figure 5.4. At about t = 0.4 ms the noncondensed density starts to form a cloud near the origin; as time progresses, the cloud moves outward and increases in density, resembling a burst. This burst contains only a small fraction of a single atom, and cannot account for any significant loss from the condensate. The condensate still retains nearly all of its atoms at this time. If the next burst of noncondensed atoms,

 $^{^{2}}$ We write all frequencies taken from simulations with a single significant figure. See Appendix F for discussion. The characteristic frequencies for our model depend on the accuracy of the experimental measurements of the resonance parameters; we choose to include three significant figures for these values.



Figure 5.2: Condensed particle numbers in a realistic collapse simulation. Numbers (a) N_a of condensed atoms and (b) N_m of those molecules, exhibiting rapid, small-amplitude oscillations. The upper figures cover the entire duration of the simulation, while the lower figures are for a short interval in the middle of the simulation. The lower figures use every computed time step, and so are not subject to aliasing the computed solution.


Figure 5.3: *Pre-collapse molecule number power spectrum*. Lomb periodogram of molecule number during that time.

visibly forming at the origin at about t = 0.8 ms grows as did its predecessor, the condensate could lose a large number of atoms to the noncondensed component.

For computational reasons, the simulation stops just short of the experimental collapse time. By t = 0.8 ms, the noncondensed density already has several points which have large negative values. Beyond the times shown in the plots, the noncondensed density, which should be positive-definite, consists mostly of very negative values, and the total noncondensed number also becomes negative. These unphysical developments could indicate a lack of convergence or the growth of an instability. Preliminary simulations at higher resolution, though terminated well before t = 0.8 ms, also had grid points with increasingly negative noncondensed densities. The poor number conservation shown in Figure 5.5, with its smooth and clearly defined trends, is another indicator of poor convergence or growing instability.

Figure 5.6 shows the magnitude of the anomalous fluctuations. This complex field with units of density may or may not indicate computational inaccuracies.

The velocities of condensed atoms and molecules are shown for the entire simula-



Figure 5.4: Noncondensed atoms in a realistic collapse simulation. (a) Density $\bar{G}_N(R,0)$ and (b) number N_{non} of those noncondensed atoms. Something resembling a burst has emanated from the origin and gained substantial density when far from the origin, near the end of the simulation.

tion in Figure 5.7, and the velocities and density of molecules for the interval of Figure 5.3 are shown in Figure 5.8. As expected for attractive interactions, inward radial velocities dominate the atomic and molecular fields. The velocities of the molecules over very short time scales (Figure 5.8a) exhibit an interesting behavior in which the molecules about 6 μ m from the origin acquire a large outward velocity; then the molecules remaining in this region resume their inward velocities while molecules slightly nearer the origin assume large outward velocities. The trend continues until the outgoing molecules appear at $R = 3 \mu$ m; then, suddenly, the molecules remaining in this region resume their for dramatic kinetics appear whenever the molecular density decreases. It seems that molecules form in a nearly static state, but just before dissociation, their binding energies are converted to kinetic energy, until the molecules are destroyed and their constituent atoms reenter



Figure 5.5: Average error in number during a realistic collapse simulation. A smooth curve, like the one above, as opposed to a jagged, seemingly random curve, indicates a lack of convergence or an instability. The divergent error near the end signals that the simulation's results have become unphysical.



Figure 5.6: Diagonal parts of anomalous fluctuations in a realistic collapse simulation. Shown is the magnitude $|\bar{G}_A(R,0)|$.



Figure 5.7: *Condensed particle velocities in a realistic collapse simulation*. Radial velocities for (a) condensed atoms and (b) molecules. Consistent with attractive interactions, the dominant velocities are inwards. Notice the "noise" in the molecular velocities.

the condensate. The process occurs in about 4 ns; the comparable time scale in the problem is $t_{\nu} = 1/f_{\nu} = 4.31$ ns. Note the "noise" in the molecular velocity plot in Figure 5.7b, which uses every 10,000th computed time step; this noise does not appear in Figure 5.8a, which uses every single computed time step. We conclude that noise such as that in Figure 5.7b and many of the other molecular velocity plots in this chapter are a result of an undersampling of the kinetic phenomenon exhibited in Figure 5.8a. We provide Figure 5.9, which is a plot of a single episode of high molecular velocities, to show that this phenomenon is not a numerical anomaly occuring on a single time step.



Figure 5.8: *Pre-collapse molecule (a) velocities and (b) density.* Extremely high velocities appear when the density decreases. Notice the absence of noise in the molecular velocities.



Figure 5.9: *Single episode of molecular velocities on dissociation*. The high molecular velocities at a given radius are spread over several time steps, indicating that these velocities are not a numerical anomaly.

5.1.2 Influence of Trapping Potential

No experiments to date have investigated any dependence of the collapse on the strength of the trapping potential. To this end, we simulate condensates having stability coefficients [the stability coefficient κ was defined in Equation (1.4)] $\kappa = 0.26$, 0.52, and 0.60 in trapping potentials of strength $\omega = 2\pi \times 12.77$ and $8\pi \times 12.77$ Hz. Preliminary explorations of the parameter space suggested that using a mass one quarter that of ⁸⁵Rb's resulted in faster simulations, though now it appears that this may be true only for initial conditions that are more compact than the ground state. For a given κ , the trap frequency and initial number of particles are both changed; $a_{\rm eff} = -400a_0$ in all cases, so that collapse occurs as soon as possible. The extent of the 33-point center of mass grid is altered between 50 μ m in the $\omega = 2\pi \times 12.77$ and 12 μ m in the $8\pi \times 12.77$ Hz simulations so that the condensate is spread over several grid points, but a pair of simulations for a given κ uses the same 16-point relative momentum grid, ranging from 0 to $3\pi/10 \ \mu m^{-1}$, so that the dynamics of one simulation does not show effects of momenta not included in the other simulation. All simulations use four q = 0 spherical harmonics. As with all the simulations we present, all fields but the atomic field are initialized to zero. The atomic field is initialized to unity everywhere, and imaginary time relaxation runs for 100,000 iterations.

As seen in Figures 5.10, 5.11, and 5.12, every condensate contracts, including the stable ($\kappa = 0.26$ and 0.52) ones. For the $\kappa = 0.60$ case, we also conduct simulations that neglect normal and anomalous fluctuations but are otherwise identical to the simulations including quantum fluctuations. A plot of condensate contraction appears indistinguishable from Figure 5.12, and the values differ in no reliable significant figures between the mean-field-only and HFB simulation. This suggests that second-

order quantum fluctuations are unimportant at this very early stage of collapse. For the $\kappa = 0.60$ HFB simulation, Figure 5.13 shows the same information as Figure 5.12 along with bounds on numerical error.

Returning to the simulations including fluctuations, the contraction is more dramatic for larger (that is, less stable) stability coefficients, though the contractions for the $\kappa = 0.52$ and 0.60 simulations are very similar. In every case, the stronger trapping potential results in a faster contraction. This difference suggests that t_{collapse} , defined as the time at which the condensate width reaches a given fraction of its initial width, does depend on the trap frequency. Recall that we did not scale space and time to harmonic oscillator units. It is possible that for κ very near the critical value, collapse may or may not occur, depending on the trap strength; Figure 5.14 shows that the stronger trap results in condensate atoms away from the origin rushing inward with a velocity an order of magnitude larger than in the case of the weaker trap.

For a sufficiently strong trap, the quantum pressure of the condensate may not be able to balance both the attractive interaction *and* the kinetic energy of this contraction. Based on the Gaussian variational treatment of the GPE mentioned in Section 1.1, any stable condensate is only metastable; as the width of the condensate decreases, macroscopic quantum tunneling becomes increasing likely, and a stable condensate may collapse (see Figure 5.15). An initially stable condensate in a very strong trap, then, may be especially prone to collapse, as Figure 5.10 shows that the initially quite compact condensate does indeed contract further.

As expected from consideration of the stability coefficients, only in the $\kappa = 0.60$ case does a visible contraction of the condensate occur for the simulated times, as shown in Figure 5.16, and even then only for the stronger trap.

An interesting manipulation of trapping potentials results if one forms a noninteracting condensate in a strong trap, and then suddenly weakens the trap at the same time attractive interactions are introduced. The result is a condensate that is already contracted but lacks the kinetic energy of contraction. Since the initial state is not the ground state of the trap, the estimate of 0.574 for the critical value of the stability coefficient does not apply; Figures 5.17, 5.18, and 5.19 show that even for $\kappa = 0.26$, the condensate quickly collapses and a burst of noncondensed density, though small in magnitude, emanates from the origin. The velocities of the atoms and molecules, shown in Figure 5.20, during this collapse are towards the origin for R smaller than about 3 μ m, and away from the origin for R larger. Spatially distinct regions of a single condensate are then governed by drastically different dynamics, the beyond mean field effects of the order-unity diluteness parameter in the inner region, and simple harmonic oscillator dynamics in the sparse outer region.

Finally, Figure 5.21 shows that t_{collapse} decreases as initial density increases, which is consistent with experimental observation. If t_{collapse} is defined as the time it takes for the condensate to contract to 88 percent of its initial width, our simulations indicate that doubling the density doubles the time to collapse. It is important to note that both simulations represented in Figure 5.21 have developed large, unphysical, negative noncondensed densities by the time they ended, signally a lack of stability, convergence, or both. All these simulations have an erratic average error in total number less than or on the order of 10^{-12} over their durations, with the exception of the initially contracted simulations, both of which develop monotonic trends in error after about t = 0.14 ms.

Finally, we attempt to more precisely characterize the behavior of the widths of the condensates described above. For each trap and stability coefficient examined above, we fit the ratio of the width to its initial width, σ/σ_{ini} , to a power law of the form

$$\frac{\sigma}{\sigma_{\rm ini}} = \alpha t^{\beta} + 1, \tag{5.1}$$

where α and β are parameters to be found from a least-squares procedure. The parameters for each fit are summarized in Table 5.1, which also includes solutions to the power law (5.1) for t such that $\sigma/\sigma_{\rm ini} = 1/e$. We see that the condensate width in each simulation is well described by such a fit, with the exception of the $\kappa = 0.26$ simulation. In this case, the fit's r^2 value is about 10^{-10} (recall that a value very close to 1 is ideal). The discrepancy could be due to the fact that this simulation ran longer than the others, into a regime where the Gaussian fit from which the width is found is a poor approximation, and where concentration of the dynamics on a few grid points results in very poor convergence. Alternatively, the failure of the power law fit could be due to physical reasons, as the situation of a highly contracted but nominally quite stable condensate could be very different from every other situation we present.

For the condensates that are initially in the trap's ground state, we observe that both the power and coefficient of the fit depend more sensitively on the trap potential than the stability coefficient. Whenever $\omega = 2\pi \times 12.77$ Hz, the power β is 1.6 and the coefficient α is on the order of -10. Whenever $\omega = 8\pi \times 12.77$ Hz, the power β increases to 1.8 or 1.9, and the coefficient α increases in magnitude such that it is on the order of -1000. As is clear from Figures 5.10 through 5.12 and 5.21, the stronger traps result in much faster condensate contraction, but note that Table 5.1 assumes that every condensate continues contracting and that such contraction obeys the same power law; it is quite possible that these condensates, especially for $\kappa = 0.26$, enter breathing modes well before their widths have reached 1/e of their initial values.



Figure 5.10: Condensate contraction for different trap strengths: $\kappa = 0.26$. The width σ of a condensate, initially in the ground state, is found from a Gaussian fit to the density $|\bar{\phi}_a(R)|^2$ and compared to its initial value. Even in this configuration for which κ is well below the critical value, the trap frequency influences the rate of contraction. The solid curve is the width for a trap frequency four times that of the dashed curve.



Figure 5.11: Condensate contraction for different trap strengths: $\kappa = 0.52$. Same as Figure 5.10, but for a less stable configuration. For this κ slightly below the critical value, the trap frequency influences the rate of contraction; both condensates contract faster than did the $\kappa = 0.26$ condensates.



Figure 5.12: Condensate contraction for different trap strengths: $\kappa = 0.60$. Same as Figures 5.10 and 5.11, but for an unstable configuration. For this κ slightly above the critical value, the trap frequency influences the rate of contraction; both condensates contract faster than did the $\kappa = 0.26$ and 0.52 condensates.



Figure 5.13: Condensate contration for $\kappa = 0.60$, with error bounds. The solid curves give the same information as Figure 5.12, where now panel (a) represents the $\omega = 2\pi \times 12.77$ Hz simulation and (b) is for the stronger trap. The dotted lines place upper and lower bounds on the possible numerical error. This error analysis is discussed in Appendix F.



Figure 5.14: Atom velocities for different trap strengths. At a given time, the radial velocities of condensate atoms for (a) $\omega = 2\pi \times 12.77$ Hz is an order of magnitude less than those for (b) $\omega = 8\pi \times 12.77$ Hz. Both panels are for $\kappa = 0.52$.



Figure 5.15: Width dependence of BEC stability [104]. For a stability coefficient $\kappa < 0.574$, there exists a width at which the condensate will be in metastable equilibrium. There always exists a nonzero probability of macroscopic quantum tunneling, by which a nominally stable condensate could collapse. As the condensate's width decreases, the likelihood of tunneling to collapse increases. Used with permission.



Figure 5.16: Condensate density for different trap strengths. For $\kappa = 0.60$, an unstable value, the condensate (a) in the weaker trap has not visibly contracted, while the condensate (b) in the stronger trap is beginning to (barely) visibly contract.

κ	$\omega \; (\times 2\pi \times 12.77 \; \mathrm{Hz})$	α	β	r^2	$t_{\rm collapse} \ ({\rm ms})$
0.26	1	-40	1.6	0.9823	80
0.26	4	-2000	1.8	0.9998	10
0.52	1	-70	1.6	0.9822	50
0.52	4	-6000	1.9	0.9999	8
0.60	1	-90	2	0.9822	50
0.60	4	-8000	1.93	0.9999	8
0.26*	1	~ 0	-1.7	-2.020	1×10^{-7}
0.52*	1	-2×10^6	2.0	1.000	0.5

Table 5.1: Power laws and collapse times for hypothetical experiments. For various values of the stability coefficient κ and trap strength ω , α and β are determined by a least squares fit to $\sigma/\sigma_{\text{ini}} = \alpha t^{\beta} + 1$. An r^2 value very near one indicates a good fit. The time to collapse t_{collapse} is the time, according to the fit, for the width of the condensate to reach 1/e of its initial value. The starred (*) values of κ are for condensates that are initially one-fourth the width of the trap's ground state. The analysis of Appendix F suggests that three significant figures are reliable in the power β for the $\kappa = 0.6$, $\omega = 4 \times 2\pi \times 12.77$ Hz case.



Figure 5.17: Condensed atoms for an initially contracted condensate. (a) Density $|\bar{\phi}_a(R)|^2$ and (b) change in number $N_a(t) - N_a(0)$ of those atoms. Dramatic contraction of the condensate and a downturn in condensate number are visible even for this case of $\kappa = 0.26$, when the initial condensate has a width one quarter that of the trap's ground state. By the end of the simulation, nearly all of the dynamics occurs on the innermost two grid points, even though the initial state was spread over 33 grid points. Note that the number plot gives a general trend and oscillation amplitude only; every 10,000th computed time step is recorded, so frequencies cannot be reliably measured.



Figure 5.18: Molecules for an initially contracted condensate. (a) Density $|\bar{\phi}_m(R)|^2$ and (b) number N_m of those molecules, for $\kappa = 0.26$, where the initial state has one quarter the width of the trap's ground state. As the collapse progresses, the molecular oscillations become larger in amplitude and more concentrated near the origin. Again, every 10,000th computed time step is recorded.



Figure 5.19: Noncondensed atoms for an initially contracted condensate. (a) Density $\bar{G}_N(R,0)$ and (b) number N_{non} of those atoms, for $\kappa = 0.26$, where the initial state has one quarter the width of the trap's ground state. Burst-like behavior is apparent, though only a fraction of a noncondensed atom is produced.



Figure 5.20: Condensed particle velocities for an initially contracted state. Radial velocities for (a) condensed atoms and (b) molecules, for $\kappa = 0.26$, where the initial state has one quarter the width of the trap's ground state. Note the distinct regions of inward and outward velocities.



Figure 5.21: Condensate width for initially contracted states. Both condensates start with an initial width one quarter that of the trap ground state. The width at any later time is the width of a Gaussian fit to the density $|\bar{\phi}_a(R)|^2$. The condensate having a stability coefficient $\kappa = 0.52$ (the dashed curve) differs from the $\kappa = 0.26$ condensate (solid curve) only in that it initially has twice as many atoms.

5.2 Single Pulse Simulations

In the spirit of Claussen *et al.* [2], we perform simulations of a condensate subjected to a magnetic field pulse of the shape shown in Figure 5.22. Figure 5.23 shows the corresponding behavior of the effective scattering length. The weakly interacting initial state is found by imaginary time relaxation, with all other fields initialized to zero. The magnetic field then linearly ramps to the hold value, which is closer to resonance, thus increasing the effective scattering length. After an amount of time t_{hold} , the field is ramped to its final value, which in practice is the same as the initial value, and the field is held at that value for a time t_{tail} .

All of the single-pulse simulations start with 16,600 atoms at $a_{\rm ini} = 7a_0$ and use $\omega = 2\pi \times 12.77$ rad/s, which is the geometric mean of the trap frequencies cited in [2]. The center of mass coordinate has 65 grid points and ranges from R = 0 to $R = 10 \ \mu {\rm m}$, there are 30 noncondensed modes with wavenumbers ranging from k = 0 to $29\pi/10 \ \mu {\rm m}^{-1}$, and seven q = 0 spherical harmonics in the correlation function expansions. Comparison with lower resolution simulations in a few cases suggests that these results are spatially converged. By setting the maximum allowable truncation error to 10^{-16} in the Runge-Kutta integrator, the simulations are temporally converged. In all simulations, the average error in total number never exceeds 1.3×10^{-13} and behaves erratically (see Figure 5.24), suggesting that the solutions are stable and converged.

In each case, we present plots of number density and total number of condensed atoms, molecules, and noncondensed atoms, along with normalized Lomb periodograms. The characteristic frequencies taken from the time scales (2.73) and (2.74) are $f_{U_0} = 8.62$ kHz and $f_{g_0} = 5120$ GHz for unrenormalized parameters and $f_U = 11.2$ kHz and $f_g = 3020$ GHz for renormalized parameters, while the frequencies



Figure 5.22: Computational model of magnetic field pulse. The magnetic field starts at B_{ini} at t = 0 and linearly ramps to B_{hold} in an amount of time $t_{\text{ramp 1}}$. The field remains at this value for t_{hold} , then ramps to the final value B_{fin} in $t_{\text{ramp 2}}$, at which it remains for t_{tail} .

corresponding to the detuning depend on the magnetic field. Oscillations have only been measured in these experiments for very particular values of magnetic field; we predict that rapid oscillations in condensate number occur for every set of parameters.

5.2.1 Varying Magnetic Field Pulse Strength

For times $t_{\text{ramp 1}} = t_{\text{ramp 2}} = 12.5 \ \mu\text{s}$, $t_{\text{hold}} = 1 \ \mu\text{s}$, and $t_{\text{tail}} = 1 \ \mu\text{s}$, we consider three different magnetic field strengths during the hold time: $B_{\text{hold}} = 158 \text{ G}$, 156 G, and $B_{\text{res}} = 155.041 \text{ G}$. When using the first two fields, we are simulating the



Figure 5.23: Behavior of effective scattering length during magnetic field pulse. The condensate is initially weakly interacting, strongly repulsive during a time interval t_{hold} , and again weakly interacting at the end of the simulation.

parameters that experimentally produced the top and bottom left-most points in Claussen *et al.*'s [2] Figure 4, which shows that the stronger magnetic field results in a smaller number of atoms remaining in the condensate at the end of the experiment. The field $B_{\text{hold}} = B_{\text{res}}$ is beyond the realm of typical (that is, Gross-Pitaevskii) mean field theory, since the effective scattering length formally diverges here, though our model, using the resonance theory of Reference [14], remains valid. This value of magnetic field has not been investigated experimentally, though it is possible to do so.

Figures 5.25, 5.26, and 5.27 show the time evolution of the density and number



Figure 5.24: *Example of number conservation during a single-pulse simulation*. Average error in total number for one of the cases considered below, as calculated by Equation (4.24). The erratic behavior and nearly machine level magnitude of the error suggests stability and convergence. These error data are representative of those for each of the single-pulse simulations we present.

of condensed atoms, molecules, and noncondensed atoms, respectively, for the case of $B_{\text{hold}} = 158$ G. As the magnetic field and effective scattering length increase, the atomic and molecular fields pass particles back and forth in rapid oscillations. The noncondensed number shows generally smooth trends, but small amplitude, high frequency oscillations are present.

The frequencies of the number oscillations during the time intervals $t_{\text{ramp 1}}$, t_{hold} , and $t_{\text{ramp 2}}$ are shown in Figure 5.28. During both ramps, the condensate number is dominated by low frequency components, corresponding to the overall decline (during the first ramp) and rise (during the second ramp) in number seen in Figure 5.25b. During the hold time, a frequency of 7 MHz dominates, while the characteristic frequencies taken from the time scale (2.75) are $f_{\nu_0} = 58.0$ MHz and $f_{\nu} = 45.1$



Figure 5.25: Condensed atoms in a simulation of a single weak magnetic field pulse. (a) Density $|\bar{\phi}_a(R)|^2$ and (b) number N_a of those atoms, about eight of which are lost to the molecular field during the peaks of the oscillations.

MHz for unrenormalized and renormalized parameters, respectively. Note that $2\pi \times 7$ MHz = 40 MHz (angular frequency). The lowest frequency component dominates the noncondensed number during the hold time, but frequencies of 60 kHz and 80 kHz are prevalent during $t_{\text{ramp 1}}$ and $t_{\text{ramp 2}}$, respectively. These are within an order of magnitude of $f_U = 11.2$ kHz.

Next, we consider a magnetic field $B_{\text{hold}} = 156$ G. Figures 5.29, 5.30, and 5.31 show the time evolution of the density and number of condensed atoms, molecules, and noncondensed atoms, and Figure 5.32 shows normalized Lomb periodograms of the condensed and noncondensed number during the ramp and hold times. In this simulation, it is apparent that a molecular component persists even after the magnetic field pulse has ended, and the higher frequency oscillations in noncondensed number are larger in amplitude than for the $B_{\text{hold}} = 158$ G case, though they are still small. As in the previous case, low frequency components dominate the condensate number



Figure 5.26: Molecules in a simulation of a single weak magnetic field pulse. (a) Density $|\bar{\phi}_m(R)|^2$ and (b) number N_m of those molecules. As many as four molecules are formed from the atoms lost from the atomic field during the peaks of the oscillations.



Figure 5.27: Noncondensed atoms in a simulation of a single weak magnetic field pulse. (a) Density $\bar{G}_N(R,0)$ and (b) number N_{non} of those noncondensed atoms. Only a fraction of a single noncondensed atom is formed.



Figure 5.28: Frequency components of atom numbers during a simulation of a single weak magnetic field pulse. Normalized Lomb periodogram of (a) condensed atom number data and (b) noncondensed atom number data. A periodogram of the molecule number data looks the same as that for the condensed atom number. A solid curve represents data during $t_{\text{ramp 1}}$, the dashed curve is for t_{hold} , and the dotted curve is for $t_{\text{ramp 2}}$.

during the ramp times, while a frequency of 1 MHz dominates during the hold time. Compare this to characteristic frequencies of $f_{\nu_0} = 18.8$ MHz and $f_{\nu} = 5.86$ MHz and note that $2\pi \times 1$ MHz = 6 MHz. The noncondensed number has a distinct frequency component only during the second ramp, where again 80 kHz dominates, within an order of magnitude of f_U . Figure 5.33 shows the time evolution of the diagonal parts of the anomalous fluctuations, which exhibit nontrivial behavior reminiscent of the diagonal parts of the normal fluctuations.

Now we consider $B_{\text{hold}} = B_{\text{res}}$, where the Gross-Pitaevskii equation is undefined due to a divergent effective scattering length. Figures 5.34, 5.35, and 5.36 show the time evolution of the condensed atoms, molecules, and noncondensed atoms. After prounounced oscillations, a molecular component persists after the pulse has ended, and now the noncondensed density and number qualitatively resemble the



Figure 5.29: Condensed atoms in a simulation of a single magnetic field pulse. (a) Density $|\bar{\phi}_a(R)|^2$ and (b) number N_a of those atoms, about 400 of which are lost to the molecular field during the peak of the oscillations.



Figure 5.30: Molecules in a simulation of a single magnetic field pulse. (a) Density $|\bar{\phi}_m(R)|^2$ and (b) number N_m of those molecules. As many as 200 molecules are formed from the atoms lost from the atomic field during the peak of the oscillations.



Figure 5.31: Noncondensed atoms in a simulation of a single magnetic field pulse. (a) Density $\bar{G}_N(R,0)$ and (b) number N_{non} of those noncondensed atoms. Only a fraction of a single noncondensed atom is formed.



Figure 5.32: Frequency components of atom numbers during a simulation of a single magnetic field pulse. Same as Figure 5.28, but for a stronger pulse.



Figure 5.33: Anomalous fluctuations for a single magnetic field pulse. Shown are the magnitudes of the diagonal parts, $|\bar{G}_A(R,0)|$.

molecular evolution. Figure 5.37 shows the dominant frequencies during the three time intervals. Only during the hold time is a single high frequency pronounced in the condensed number, which is 2 MHz. Compare this to $f_{\nu} = 12.9$ MHz, and note that $2\pi \times 2$ MHz = 13 MHz. The frequency corresponding to the unrenormalized detuning is formally zero for this value of magnetic field. The prevalent frequency in the noncondensed number is nearly the same as that in the condensed number, indicating that atom-molecule oscillations completely dominate the dynamics of the system on resonance.

Figure 5.38 shows the diagonal parts of the anomalous fluctuations, which qualitatively mimics the other fields.

In this case, we conduct another simulation that is identical in set-up, but neglects quantum fluctuations.³ Plots of condensate and molecule number from this mean-field-only simulation are indistinguishable from Figures 5.34b and 5.35b, and

 $^{^3\}mathrm{While}$ the GPE is undefined at resonance, recall that the resonance theory of Ref. [14], which we use, is not.



Figure 5.34: Condensed atoms in a simulation of a single strong magnetic field pulse. (a) Density $|\bar{\phi}_a(R)|^2$ and (b) number N_a of those atoms, nearly 4000 of which are lost to the molecular field during the peak of the oscillations.

the numbers and dominant frequencies of oscillation differ in no reliable significant figures between the simulations. We conclude that second order quantum fluctuations are unimportant to the experiment in this brief but strong magnetic field pulse.

We compare the number of atoms remaining in the consendate after the pulse is over, for the three values of B_{hold} . This comparison is reminiscent of the left-most data points of Claussen *et al.*'s [2] Figure 4. About 14,000 atoms remain in the condensate at the end of the experiment when $B_{\text{hold}} = 158$ G, and slightly more than 10,000 remain when $B_{\text{hold}} = 156$ G. Our simulations greatly overestimate these numbers, with nearly 16,600 atoms (the initial number) remaining when $B_{\text{hold}} = 158$ G and 16,550 remaining when $B_{\text{hold}} = 156$ G. Still, the simulations qualitatively reproduce the experimentally observed trend of remnant number decreasing as B_{hold} approaches the resonance. Figure 5.39 shows the time evolution of the number of atoms in the condensate for the three values of B_{hold} we studied during t_{tail} .



Figure 5.35: Molecules in a simulation of a single strong magnetic field pulse. (a) Density $|\bar{\phi}_m(R)|^2$ and (b) number N_m of those molecules. Nearly 2000 molecules are formed from the atoms lost from the atomic field during the peak of the oscillations.



Figure 5.36: Noncondensed atoms in a simulation of a single strong magnetic field pulse. (a) Density $\bar{G}_N(R, 0)$ and (b) number N_{non} of those noncondensed atoms. Only a fraction of a single noncondensed atom is formed. A nearly constant noncondensed component persists after the pulse has ended.



Figure 5.37: Frequency components of atom numbers during a simulation of a single strong magnetic field pulse. Same as Figure 5.28, but for the strongest pulse.



Figure 5.38: *Diagonal parts of anomalous fluctuations for a single strong magnetic field pulse*. Same as Figure 5.33, but for a pulse to resonance.



Figure 5.39: Pulse strength dependence of condensate number in single-pulse simulations. Number of condensed atoms N_a during t_{tail} , when the magnetic field is constant, after the pulse is over. The solid curve is for $B_{\text{hold}} = 158$ G, the dashed curve is for $B_{\text{hold}} = 156$ G, and the dotted curve is for $B_{\text{hold}} = B_{\text{res}}$.

Lastly, we compare the velocities of atoms and molecules for the different pulse strengths. Figures 5.40, 5.41, and 5.42 show the velocities of condensed atoms and molecules when $B_{\text{hold}} = 158$ G, 156 G, and B_{res} , respectively. When the field is far from resonance during the hold time, both fields have a small *inward* velocity during the first ramp, even though the interatomic interactions are becoming more repulsive. This slight contraction could be a novel physical effect, or it could be the result of an initial state that is not perfectly relaxed. In all three cases, the atoms acquire a large outward velocity during the second ramp, which increases as the magnetic field approaches resonance. This velocity saturates at about $140 \,\mu\text{m/s}$, even when B_{hold} is not on resonance. We may estimate the speed of sound for these atoms as [23]

$$c_s = \sqrt{\frac{4\pi\hbar^2 \left|\bar{\phi}_a(R)\right| a_{\text{eff}}}{m^2}},\tag{5.2}$$

where we take $R \approx 2 \ \mu m$ so that $|\bar{\phi}_a(R)| \approx 6 \times 10^{13} \ cm^{-3}$ and $B_{hold} = 158 \ G$. Then $c_s \approx 10,000 \ \mu m/s$, which greatly exceeds the maximum velocity of 140 $\mu m/s$ we observe in these simulations. Excitations of the superfluid such as vortices are therefore unlikely, though excitations of the normal (noncondensed) fraction are possible.

During the second ramp, the molecules acquire mostly inward velocities that are about half the magnitude of the atoms' velocities. When $B_{\text{hold}} = B_{\text{res}}$, the second ramp is marked by a region, about 3 μ m from the origin and 0.5 μ m in width, where molecules take on large inward and outward velocities. In Figure 5.42b this region has a noisy appearance, leading us to believe this region has dynamics similar to those of Figure 5.8a in the case of collapse, where molecules dissociate with high outward and then inward velocities in a very short period of time. The region of high velocities does not correspond to a region of significant density in Figure 5.35a, though, suggesting that these are small-amplitude oscillations. In all cases (but most easily seen for the moderate-strength pulse), molecules produced during the hold time, when most molecules are produced, move rapidly outwards.

5.2.2 Varying Pulse Shape

We now compare the effects of changing $t_{\text{ramp 1}}$, t_{hold} , and $t_{\text{ramp 2}}$ for a magnetic field $B_{\text{hold}} = 156$ G. Again, we use realistic ⁸⁵Rb parameters.

First, consider the case of a longer first ramp, where $t_{\text{ramp 1}} = 16.5 \ \mu\text{s}$, $t_{\text{hold}} = 1.00 \ \mu\text{s}$, and $t_{\text{ramp 2}} = 12.5 \ \mu\text{s}$. Figures 5.43, 5.44, and 5.45, the densities and numbers



Figure 5.40: Condensed particle velocities for a weak magnetic field pulse. Radial velocities for (a) atoms and (b) molecules for a simulation where $B_{\text{hold}} = 158$ G. Notice the atoms' small but increasing inward velocities during the first ramp.



Figure 5.41: Condensed particle velocities for a moderate magnetic field pulse. Radial velocities for (a) atoms and (b) molecules for a simulation where $B_{\text{hold}} = 156$ G. Particles' inward velocities are especially pronounced during the second ramp.



Figure 5.42: Condensed particle velocities for a strong magnetic field pulse. Radial velocities for (a) atoms and (b) molecules for a simulation where $B_{\text{hold}} = B_{\text{res}}$ G. The atoms' inward velocities are no larger than in the $B_{\text{hold}} = 156$ G case, while the molecules' velocities rapidly alter between large inward and outward values in a region about 3 μ m from the origin.

of condensed atoms, molecules, and noncondensed atoms, are all qualitatively very similar to Figures 5.29, 5.30, and 5.31, which are the corresponding plots for the same parameters, but with $t_{\text{ramp 1}} = 12.5 \ \mu\text{s}$. The atomic and molecular fields' oscillations have the same structure and amplitude, but the noncondensed number reaches a 20 percent larger value than in the $t_{\text{ramp 1}}$ case, suggesting that very long first ramp times may result in depletion of the condensate. The frequencies of oscillation extracted from the data (see Figure 5.46) look very similar to those from the $t_{\text{ramp 1}} = 12.5 \ \mu\text{s}$ case, with a frequency of condensate number oscillations of 1 MHz during t_{hold} and a frequency of noncondensed number oscillations of 80 kHz during $t_{\text{ramp 2}}$. Recall that for this value of B_{hold} , the characteristic frequency corresponding to the renormalized detuning is $f_{\nu} = 5.86$ MHz.

Next, consider a longer second ramp, where $t_{\text{ramp 1}} = 12.5 \ \mu\text{s}$, $t_{\text{hold}} = 1.00 \ \mu\text{s}$,


Figure 5.43: Condensed atoms in a simulation of a single magnetic field pulse: long first ramp. (a) Density $|\bar{\phi}_a(R)|^2$ and (b) number N_a of those atoms, about 400 of which are lost to the molecular field during the peak of the oscillations.



Figure 5.44: Molecules in a simulation of a single magnetic field pulse: long first ramp. (a) Density $|\bar{\phi}_m(R)|^2$ and (b) number N_m of those atoms, about 200 of which formed from condensed atoms during the peak of the oscillations.



Figure 5.45: Noncondensed atoms in a simulation of a single magnetic field pulse: long first ramp. (a) Density $\bar{G}_N(R, 0)$ and (b) number N_{non} of those noncondensed atoms. Only a fraction of a single noncondensed atom is formed.



Figure 5.46: Frequency components of atom numbers during a simulation of a single magnetic field pulse: long first ramp. Same as Figure 5.32, but for a long first ramp.



Figure 5.47: Condensed atoms in a simulation of a single magnetic field pulse: long second ramp. (a) Density $|\bar{\phi}_a(R)|^2$ and (b) number N_a of those atoms, about 400 of which are lost to the molecular field during the peak of the oscillations.

and $t_{\text{ramp 2}} = 16.5 \ \mu\text{s}$. The number and number density results, shown in Figures 5.47, 5.48, and 5.49, are nearly identical with the results for the longer first ramp, only shifted towards earlier times. One notable feature is the slight decrease in the number of remaining condensed atoms compared to the previous case (this is examined in more detail later). Figure 5.50 shows the frequencies extracted from the number data, which is effectively identical to the $t_{\text{ramp 1}} = 16.5 \ \mu\text{s}$ case.

Now consider the case where both ramps are long: $t_{\text{ramp 1}} = t_{\text{ramp 2}} = 12.5 \,\mu\text{s}$ and $t_{\text{hold}} = 1.00 \,\mu\text{s}$. Once more, the density and number data in Figure 5.51, 5.52, and 5.53 and the frequency data in Figure 5.54 is nearly identical to that from the case of $t_{\text{ramp 1}} = t_{\text{ramp 2}} = 12.5 \,\mu\text{s}$. A notable exception is the nearly 60 percent increase in peak noncondensed number; since the noncondensed number typically grows as time with significant interactions increases, this long simulation has a higher noncondensed number than others.



Figure 5.48: Molecules in a simulation of a single magnetic field pulse: long second ramp. (a) Density $|\bar{\phi}_m(R)|^2$ and (b) number N_m of those atoms, about 200 of which formed from condensed atoms during the peak of the oscillations.



Figure 5.49: Noncondensed atoms in a simulation of a single magnetic field pulse: long second ramp. (a) Density $\bar{G}_N(R, 0)$ and (b) number N_{non} of those noncondensed atoms. Only a fraction of a single noncondensed atom is formed.



Figure 5.50: Frequency components of atom numbers during a simulation of a single magnetic field pulse: long second ramp. Same as Figure 5.32, but for a long second ramp.



Figure 5.51: Condensed atoms in a simulation of a single magnetic field pulse: long ramps. (a) Density $|\bar{\phi}_a(R)|^2$ and (b) number N_a of those atoms, about 400 of which are lost to the molecular field during the peak of the oscillations.



Figure 5.52: Molecules in a simulation of a single magnetic field pulse: long ramps. (a) Density $|\bar{\phi}_m(R)|^2$ and (b) number N_m of those atoms, about 200 of which formed from condensed atoms during the peak of the oscillations.



Figure 5.53: Noncondensed atoms in a simulation of a single magnetic field pulse: long ramps. (a) Density $\bar{G}_N(R, 0)$ and (b) number N_{non} of those noncondensed atoms. Only a fraction of a single noncondensed atom is formed.



Figure 5.54: Frequency components of atom numbers during a simulation of a single magnetic field pulse: long ramps. Same as Figure 5.32, but for two long ramps.

Having explored the effects of varying the ramp times, we now consider a longer hold time of $t_{\text{hold}} = 4.00 \ \mu\text{s}$, with $t_{\text{ramp 1}} = t_{\text{ramp 2}} = 12.5 \ \mu\text{s}$. Figures 5.55, 5.56, and 5.57 show the density and number of the condensed atoms, molecules, and noncondensed atoms. All these are very similar to the $t_{\text{hold}} = 1.00 \ \mu\text{s}$ case, except that the oscillations during the hold time are visibly damped, and the peak in the noncondensed number is increased about 400 percent over the short hold time case. As in the case of the long ramps, increased time with significant interaction strength increases the noncondensed number; in this simulation, the condensate spends more time having the strongest interactions, and so sees the highest loss to the noncondensed number of any simulation presented so far. Again, Figure 5.58 shows that the oscillation frequencies are unchanged compared to previous simulations with $B_{\text{hold}} = 156$ G. In this case, we also present the diagonal parts of the anomalous fluctuations in Figure 5.59.

The last pulse shape we consider is one with a hold time of $t_{\text{hold}} = 12.0 \ \mu\text{s}$, with $t_{\text{ramp 1}} = t_{\text{ramp 2}} = 12.5 \ \mu\text{s}$. The density and number data in Figures 5.60,



Figure 5.55: Condensed atoms in a simulation of a single magnetic field pulse: long hold. (a) Density $|\bar{\phi}_a(R)|^2$ and (b) number N_a of those atoms, about 400 of which are lost to the molecular field during the peak of the oscillations.



Figure 5.56: Molecules in a simulation of a single magnetic field pulse: long hold. (a) Density $|\bar{\phi}_m(R)|^2$ and (b) number N_m of those atoms, about 200 of which formed from condensed atoms during the peak of the oscillations.



Figure 5.57: Noncondensed atoms in a simulation of a single magnetic field pulse: long hold. (a) Density $\bar{G}_N(R,0)$ and (b) number N_{non} of those noncondensed atoms. Only a fraction of a single noncondensed atom is formed.



Figure 5.58: Frequency components of atom numbers during a simulation of a single magnetic field pulse: long hold. Same as Figure 5.32, but for a long hold time.



Figure 5.59: Diagonal parts of the anomalous densisty during a simulation of a single magnetic field pulse: long hold. Same as Figure 5.33, but a long hold time.

5.61, and 5.62 are still mostly similar to the $t_{\text{hold}} = 4.00 \ \mu\text{s}$ and $t_{\text{hold}} = 1.00 \ \mu\text{s}$ cases, with the noncondensed number peaking around 2500 percent of its largest value when $t_{\text{hold}} = 1.00 \ \mu\text{s}$. This simulation has the condensate spending more time with strong interactions than any other simulation we present; hence, this simulation has a higher number of noncondensed atoms than any other. Table 5.2 summarizes the noncondensed number at the end of the $t_{\text{hold}} = 1.0$, 4.0, and 12.0 μ s simulations. Figures 5.64, 5.65, and 5.66 are the same plots of number as in Figures 5.60, 5.61, and 5.62, but include estimates of numerical error.⁴

For this pulse shape, which is the longest hold time we consider, we fit a curve of the form

$$N_{\rm non}(t) = \alpha t^{\beta} \tag{5.3}$$

to the noncondensed number $N_{\rm non}$ during the hold time. A least squares procedure estimates $\alpha = 1.85 \times 10^{20} \, {\rm s}^{-\beta}$ and $\beta = 4.73$ with an r^2 goodness-of-fit parameter of

⁴The plots including error bounds are kept separate for clarity.

0.9906. If this power law remains in effect until the condensate is entirely depleted, we can estimate that a hold time of $t_{\rm th} = t_{\rm hold} = 400 \pm 150 \ \mu s$ would completely rethermalize the condensate, entirely by means of second order quantum fluctuations and pairing via the Feshbach resonance.⁵ Over this time scale, density-dependent losses are quite likely to play an effect.

The molecular density now exhibits some behavior distinct from previous cases. The rapid oscillations in density form long, narrow, straight, radial spikes early on during t_{hold} . Later on during the hold time, the small regions of high molecular density far from the origin lag the regions of high molecular density near the origin (the spikes start to "bend"). Also, during the second ramp and after the pulse ends, the molecule density forms two distinct and nearly constant bands, one centered on the origin and extending about 1 μ m outward, and the other, smaller band centered at about $R = 3 \mu$ m. Development of a technique for imaging the molecular condensate, preferably in real time, could lead to experimental observation of such exotic dynamics. As before, the dominant oscillation frequencies in Figure 5.63 are unchanged from previous scenarios.

For these parameters, we also conduct a simulation in which we neglect fluctuations. Plots of condensate and molecule number from this mean-field-only simulation look indistinguishable from Figures 5.60b and 5.61b, and the numbers differ in no reliable significant figures between the simulation. The dominant frequencies of oscillation are the same to three significant figures. Note that it is not possible to estimate the rethermalization time of the condensate from the mean-field-only simulation. Still, the quantitative and qualitative agreement of the mean-field-only and HFB simulations and the HFB simulation's estimated rethermalization time of 400

⁵See Appendix F for discussion of the uncertainty.



Figure 5.60: Condensed atoms in a simulation of a single magnetic field pulse: longest hold. (a) Density $|\bar{\phi}_a(R)|^2$ and (b) number N_a of those atoms, about 400 of which are lost to the molecular field during the peak of the oscillations.

 μ s suggest that quantum fluctuations are important only in the much later stages of such an experiment.

Now we compare the number of atoms remaining in the condensate after the pulses of varying shapes have ended. Figure 5.67 shows the number of condensed atoms during t_{tail} , which was 1.00 μ s. We see that the remnant number increases with increasing t_{hold} , in contradiction to the experimental findings [2], where a t_{hold} of 5 μ s decreased the remnant number from about 13,000 to 11,000 compared to a t_{hold} of 1 μ s.⁶ Comparison of the number remaining in the $t_{\text{ramp }1} = t_{\text{ramp }2} = 12.5 \,\mu$ s and $t_{\text{ramp }1} = t_{\text{ramp }2} = 16.5 \,\mu$ s cases shows a very slight increase for the larger ramp times. Experimentally, for the parameters we simulated, the remnant number

⁶These experimental values are for $B_{\text{hold}} = 156.7$ G and an initial condensate number of 16,500 atoms, rather than our simulated parameters of $B_{\text{hold}} = 156.0$ G and initial number of 16,600. Again, all of the atomic parameters are those of ⁸⁵Rb.



Figure 5.61: Molecules in a simulation of a single magnetic field pulse: longest hold. (a) Density $|\bar{\phi}_m(R)|^2$ and (b) number N_m of those atoms, about 200 of which formed from condensed atoms during the peak of the oscillations. Two bands of nonzero density persist after the pulse ends.



Figure 5.62: Noncondensed atoms in a simulation of a single magnetic field pulse: longest hold. (a) Density $\bar{G}_N(R,0)$ and (b) number N_{non} of those noncondensed atoms. Only a fraction of a single noncondensed atom is formed.



Figure 5.63: Frequency components of atom numbers during a simulation of a single magnetic field pulse: longest hold. Same as Figure 5.32, but for the longest hold time.

$t_{\rm hold} \ (\mu {\rm s})$	$N_{\rm non}$
1.0	0.00097
4.0	0.0052
12	0.031

Table 5.2: *Remaining noncondensed number as a function of hold time*. The noncondensed number increases by orders of magnitude as the hold time in a single-pulse simulation increases.

the remnant number increases but does not exceed the $t_{\text{ramp 1}} = t_{\text{ramp 2}} = 12.5 \ \mu\text{s}$ figure for even the largest ramp time considered in the experiments, about 252 μ s. Our simulations qualitatively reproduce the counterintuitive experimental result that longer ramp times can result in increased remnant number, but overestimate by at least 240 μ s the ramp time for which the increased remnant number appears.

One significant difference between our simulations and the experiments is the experimental imaging process, in which the magnetic field is slowly ramped to a



Figure 5.64: Condensate number when $t_{hold} = 12 \ \mu s$, including error estimates. The solid curve is the same number data that appears in Figure 5.60, and the dotted curves bound the maximum numerical error, as described in Appendix F.

value near the resonance, expanding the condensate to a size larger than the imaging system's resolution. The results of the simulation with the longer first ramp suggest that this mean field imaging expansion has a significant effect on the measured number of atoms in a condensate. Realistically, the imaging ramp is much slower than what we have simulated, and would allow for losses due to three-body recombination, as well.

None of our simulations reproduced anything resembling the observed bursts of noncondensed atoms. Our small noncondensed fraction occupied the center of the trap, rather than expanding in one or more rings. This disagreement implies that our model does not include whatever mechanism is responsible for the observed bursts in the single-pulse experiments, but the following two-pulse simulations (see Section



Figure 5.65: Molecule number when $t_{hold} = 12 \ \mu s$, including error estimates. Same as Figure 5.64, but for the molecular field.

5.3) suggest that the burst behavior emerges later, after a pulse, while the magnetic field is constant.

We observe that the size of the peak in molecule number appears to be independent of pulse shape. Only the strength of the magnetic field determines how many molecules are produced at the height of the atom-molecule oscillations.

Lastly, we compare the dependence of condensed particle velocities on pulse shape. Figures 5.68, 5.69, 5.70, 5.71, and 5.72 show the radial velocities of condensed atoms and molecules for the simulations having a long hold time, the longest hold time, a long first ramp, a long second ramp, and two long ramps, respectively. Comparing the figures for various hold times with Figure 5.41 shows that the outward velocities of the atoms during the second ramp is highly dependent on the hold time,



Figure 5.66: Noncondensed number when $t_{hold} = 12 \ \mu s$, including error estimates. Same as Figure 5.64, but for noncondensed atoms.

while Figures 5.70, 5.71, and 5.72 show that this quantity is largely independent of ramp times. Molecular velocities are also mostly independent of ramp times, but the number of molecules having the largest inward velocity during the second ramp increases whenever the second ramp is longer, likely because this longer transition to a magnetic field far from resonance is more adiabatic, allowing more molecules to persist. In both cases of extended hold times, regions of varying but large molecular velocities exist, reminiscent of that seen in Figure 5.42b for the pulse to resonance. When the hold time is the longest, two such regions simulatenously exist, one about 1.5 μ m from the origin and the other centered near 4 μ m. In Figure 5.61a we see faint molecular oscillations in these regions, suggesting that the bands of high molecular velocity in the second ramp do correspond to the dissociation of molecules.



Figure 5.67: Pulse shape dependence of condensate number in single-pulse simulations. Number of condensed atoms during t_{tail} , when the magnetic field is constant, after the pulse is over. (The horizontal axis is labeled from the start of the simulation.) Here, $B_{hold} = 156$ G in every data set. (a) $t_{ramp 1} = t_{ramp 2} = 12.5 \ \mu s$ and $t_{hold} = 1 \ \mu s$. (b) Long hold. $t_{ramp 1} = t_{ramp 2} = 12.5 \ \mu s$ and $t_{hold} = 4 \ \mu s$. (c) Long ramp 2. $t_{ramp 1} = 12.5 \ \mu s$, $t_{ramp 1} = 16.5 \ \mu s$, and $t_{hold} = -\mu s$. (d) Long ramp 1. $t_{ramp 1} = 16.5 \ \mu s$, $t_{ramp 2} = 12.5 \ \mu s$, and $t_{hold} = -\mu s$. (e) Two long ramps. $t_{ramp 1} = t_{ramp 2} = 16.5 \ \mu s$ and $t_{hold} = 1 \ \mu s$. (f) Longest hold. $t_{ramp 1} = t_{ramp 2} = 12.5 \ \mu s$ and $t_{hold} = 12 \ \mu s$.

We may estimate an effective temperature of the molecules with the equipartition theorem. This estimate is strictly only valid when the molecular condensate is in equilibrium, which it likely is not, as evidenced by the rapid oscillations. We nonetheless make this estimate, assuming that each grid point in the simulation represents a region where the molecular condensate is in local equilibrium. If no rotational or vibrational molecular modes are excited, equating the equipartition theorem to the kinetic energy gives an effective temperature of

$$T = \frac{2}{3k_B}mv^2,\tag{5.4}$$

where k_B is Boltzmann's constant, m is the mass of a single *atom*, and v is the flow velocity of the molecular condensate at a point. Figure 5.73 gives the estimated effective temperature of the molecules in the case of the $t_{\text{hold}} = 12.0 \ \mu\text{s}$ simulation. As the plot of molecular velocities suggests, two distinct regions of high temperature persist at the end of the experiment.

5.3 Two-Pulse Simulations

In the spirit of Donley *et al.* [3], we perform simulations using all the same computational parameters as in the above one-pulse simulations, but now with two magnetic field pulses of the shape shown in Figure 5.74. Figure 5.75 shows the corresponding behavior of the effective scattering length. The noninteracting initial state is found using imaginary time relaxation with 16,500 atoms, and all other fields are initialized to zero. The magnetic field then ramps linearly to $B_{\text{hold 1}}$ in a time $t_{\text{ramp 1}}$, and stays at this field for an amount of time $t_{\text{hold 1}}$. The field then rises in $t_{\text{ramp 2}}$ to a constant value of B_{ev} , where it remains for the "free evolution time" t_{ev} . Another pulse follows, after which the field remains at a final and constant



Figure 5.68: *Condensed particle velocities for a long hold time*. The radial velocities of (a) atoms and (b) molecules. A region of moderate molecular velocities appears far from the origin.



Figure 5.69: Condensed particle velocities for the longest hold time. The radial velocities of (a) atoms and (b) molecules. Two distinct regions of large molecular velocities persist during the second ramp, and atomic velocities are much larger in this case than for shorter hold times.



Figure 5.70: *Condensed particle velocities for a long first ramp.* The radial velocities of (a) atoms and (b) molecules. These data are little different from case of the shorter first ramp.



Figure 5.71: *Condensed particle velocities for a long second ramp*. The radial velocities of (a) atoms and (b) molecules. Notice that the maximum velocity of the molecules is the same as in the case of the longer first ramp, but more molecules have this largest velocity.



Figure 5.72: Condensed particle velocities for two long ramps. The radial velocities of (a) atoms and (b) molecules. Notice that the maximum velocity of the molecules is the same as in the case of the longer first ramp, but more molecules have this largest velocity. These data are little different from the case where only the second ramp is longer.



Figure 5.73: Effective temperature of molecules. During the simulation where $t_{\text{hold}} = 12.0 \ \mu\text{s}$, the molecules' temperatures may be estimated by Equation (5.4), which assumes that each grid point represents a region of local equilibrium and no rotational or vibrational molecular modes are excited.



Figure 5.74: Computational model of magnetic field pulses. In practice, the pulses are symmetric and the free evolution time t_{ev} is varied between simulations.

value B_{tail} for t_{tail} . In practice, $B_{\text{hold }1} = B_{\text{hold }2} = 156.65$ G, $B_{\text{ev}} = 157.6$ G, and $B_{\text{tail}} = B_{\text{ini}} = 166.0$ G, with $t_{\text{ramp }1} = t_{\text{ramp }2} = t_{\text{ramp }3} = t_{\text{ramp }4} = 14.0 \ \mu\text{s}$ and $t_{\text{hold }1} = t_{\text{hold }2} = 15.0 \ \mu\text{s}$. We consider three evolution times, $t_{\text{ev}} = 10$, 25, and 40 μ s, in an attempt to reproduce some of the results of Donley *et al.*'s [3] Figure 4, showing that the number of atoms remaining in the condensate after the pulses does not increase or decrease monotonically with t_{ev} .

In every simulation, the average error in number behaves erratically and never exceeds 1.3×10^{-13} in magnitude, suggesting stability and convergence. Figure 5.76 shows the error for the $t_{\rm ev} = 40 \ \mu {\rm s}$ simulation.



Figure 5.75: *Behavior of effective scattering length during magnetic field pulses.* The linear ramps in magnetic field result in nonlinear ramps in effective scattering length.

We first consider $t_{ev} = 10 \ \mu$ s. Figures 5.77, 5.78, and 5.79 show the time evolution of the density and number of condensed atoms, molecules, and noncondensed atoms, respectively. The first pulse closely resembles one of the long hold time single-pulse simulations, with rapid, damped oscillations. A cloud of noncondensed density forms at and around the center of the trap during the first hold time, and radiates outward during the free evolution time. During this time and the second hold time, the atommolecule oscillations take on a much smaller amplitude, and a second, dense burst of noncondensed atoms (or rather, fractions of atoms) forms at and near the origin, radiating outward during the final magnetic field ramp. It is during the hold times



Figure 5.76: Example of number conservation during a two-pulse simulation. The average error for every simulation (above, for the $t_{\rm ev} = 40 \ \mu s$ simulation) exhibits seemingly random behavior, suggesting stability and convergence.

that the noncondensed number increases the most. Figure 5.80 shows the diagonal parts of the anomalous fluctuations, which qualitatively mimics the noncondensed density.

Figure 5.81 shows the prominent frequencies in atom number during the four ramp times. The condensed atom number is dominated in every case by the low frequencies associated with the overall rise and fall of condensed number, but the noncondensed number has a prevalent higher frequency of 50 kHz during the first and fourth ramps. Compare this to the characteristic frequency $f_U = 11.2$ kHz. Figure 5.82 shows the dominant frequencies in number during the hold times and free evolution time. The noncondensed number has no distinct higher frequencies, but the condensed number oscillations have prominent contributions from 3 MHz during the



Figure 5.77: Condensed atoms in a simulation of a two magnetic field pulses: 10 µs evolution time. (a) Density $|\bar{\phi}_a(R)|^2$ and (b) number N_a of those atoms, about 45 of which are lost to the molecular field during the peak of the oscillations.

hold times and 6 MHz during the free evolution time, or 20 and 40 MHz, respectively, in terms of angular frequency. Compare these to detuning-dependent characteristic frequencies of $f_{\nu} = 18.6$ MHz and $f_{\nu} = 37.2$ MHz, computed from the magnetic fields during the hold and evolution times, respectively.

Next, we simulate $t_{\rm ev} = 25 \ \mu$ s. The qualitative behavior of the densities and numbers shown in Figure 5.83, 5.84, 5.85, and 5.86 is the same as the $t_{\rm ev} = 10 \ \mu$ s case, though a noticeable burst of noncondensed density is starting to form near the origin towards the end of the evolution time. Note that by about $t = 100 \ \mu$ s, this burst, now centered slightly more than 1 μ m from the origin, has a higher density than the burst originating from the first hold time, even though the second burst developed later. The frequency data from Figures 5.87 and 5.88 has the same peaks as the $t_{\rm ev} = 10 \ \mu$ s scenario, matching well with the frequencies derived from our model's detuning.

Lastly, we simulate an evolution time of $t_{\rm ev} = 40 \ \mu s$. The condensed atomic



Figure 5.78: Molecules in a simulation of two magnetic field pulses: 10 μ s evolution time. (a) Density $|\bar{\phi}_m(R)|^2$ and (b) number N_m of those molecules, about 22 of which are formed from condensed atoms during the peak of the oscillations.



Figure 5.79: Noncondensed atoms in a simulation of two magnetic field pulses: 10 μ s evolution time. (a) Density $\bar{G}_N(R,0)$ and (b) number $N_{\rm non}$ of those atoms. Only a fraction of a noncondensed atom is formed.



Figure 5.80: Diagonal parts of anomalous fluctuations in a simulation of two magnetic field pulses: 10 μ s evolution time. Shown is the magnitude $|\bar{G}_A(R,0)|$.



Figure 5.81: Frequency components of atom numbers during a simulation of four magnetic field ramps: 10 μ s evolution time. Normalized Lomb periodogram for (a) condensed atoms and (b) noncondensed atoms during ramps. A periodogram for the molecular number data looks the same as the condensed atoms' periodogram. A solid curve represents data from $t_{\text{ramp 1}}$, the dashed curve is for $t_{\text{ramp 2}}$, the dotted is for $t_{\text{ramp 3}}$, and the finely dotted is for $t_{\text{ramp 4}}$. Adjacent points are connected with a line, to guide the eye.



Figure 5.82: Frequency components of atom numbers during a simulation of three constant magnetic fields: 10 μ s evolution time. Normalized Lomb periodogram for (a) condensed atoms and (b) noncondensed atoms during hold and evolution times. A solid curve represent data from $t_{\text{hold 1}}$, the dashed curve is for t_{ev} , and the dotted curve is for $t_{\text{hold 2}}$. Adjacent points are connected with a line, to guide the eye.



Figure 5.83: Condensed atoms in a simulation of a two magnetic field pulses: 25 μ s evolution time. (a) Density $|\bar{\phi}_a(R)|^2$ and (b) number N_a of those atoms, about 45 of which are lost to the molecular field during the peak of the oscillations.



Figure 5.84: Molecules in a simulation of two magnetic field pulses: 25 µs evolution time. (a) Density $|\bar{\phi}_m(R)|^2$ and (b) number N_m of those molecules, about 22 of which are formed from condensed atoms during the peak of the oscillations.



Figure 5.85: Noncondensed atoms in a simulation of two magnetic field pulses: 25 μs evolution time. (a) Density $\bar{G}_N(R,0)$ and (b) number N_{non} of those atoms. Only a fraction of a noncondensed atom is formed.



Figure 5.86: Diagonal parts of anomalous fluctuations in a simulation of two magnetic field pulses: $25 \ \mu s$ evolution time. Same as Figure 5.80, but for a longer evolution time.



Figure 5.87: Frequency components of atom numbers during a simulation of four magnetic field ramps: $25 \ \mu s$ evolution time. Same as Figure 5.81, but for a moderate evolution time.



Figure 5.88: Frequency components of atom numbers during a simulation of three constant magnetic fields: $25 \ \mu s$ evolution time. Same as Figure 5.82, but for a moderate evolution time.

density in Figure 5.89 is visibly reduced at the origin by the end of the simulation, indicating that 120 μ s is sufficient time for the condensate to begin spreading due to repulsive interactions. The condensed atom number and the molecular density and number in Figure 5.90 is qualitatively similar to the earlier simulations, while the non-condensed density in Figure 5.91 shows that three bursts have developed, one during the first hold time, the second during the later part of the free evolution time, with the last burst growing near the origin when the simulation ends. Still, the noncondensed number represents only a small fraction of a particle, and so cannot account for the bursts observed in the experiments. As before, the anomalous fluctuations in Figure 5.92 qualitatively mimic the noncondensed density. The dominant frequencies in atom number given in Figures 5.93 and 5.94 are identical to those found earlier. Figures 5.95, 5.96, and 5.97 are identical to the plots of number in Figures 5.89, 5.90, and 5.91, but include estimates of numerical error.

In this case, we also perform a simulation neglecting fluctuations. During the



Figure 5.89: Condensed atoms in a simulation of two magnetic field pulses: 40 μ s evolution time. (a) Density $|\bar{\phi}_a(R)|^2$ and (b) number N_a of those atoms, about 45 of which are lost to the molecular field during the peak of the oscillations.

last hold and ramp times, a plot of molecule number from the mean-field-only simulation starts to visibly differ from Figure 5.90b, with the number consistently lower than that from the HFB simulation by about 0.02. This difference appears in the fourth significant figure, though, and so cannot be considered quantitatively reliable. All oscillation frequencies in atom and molecule number are the same to three significant figures, except during the first hold time, when the frequency measured in the HFB simulation is larger by 0.625 percent. All these differences are too small to be considered reliable, and we conclude that second order quantum fluctuations are unimportant to the pulse-train phase of this experiment.

We now compare the number of atoms remaining in the condensate at the end of the simulations for the various evolution times. Figure 5.98 shows the condensed atom number during t_{tail} , where the magnetic field is a constant $B_{\text{tail}} = 166$ G. The means of the oscillations are 16,499.419, 16,499.415, and 16,499.424 atoms for the $t_{\text{ev}} = 10 \ \mu\text{s}$, $t_{\text{ev}} = 25 \ \mu\text{s}$, and $t_{\text{ev}} = 40 \ \mu\text{s}$ simulations, respectively. As in the experiments, an



Figure 5.90: Molecules in a simulation of two magnetic field pulses: 40 µs evolution time. (a) Density $|\bar{\phi}_m(R)|^2$ and (b) number N_m of those molecules, about 22 of which are formed from condensed atoms during the peak of the oscillations.



Figure 5.91: Noncondensed atoms in a simulation of two magnetic field pulses: 40 μs evolution time. (a) Density $\bar{G}_N(R, 0)$ and (b) number N_{non} of those atoms. Only a fraction of a noncondensed atom is formed.



Figure 5.92: Diagonal parts of anomalous fluctuations in a simulation of two magnetic field pulses: $40 \ \mu s$ evolution time. Same as Figure 5.80, but for the longest evolution time.



Figure 5.93: Frequency components of atom numbers during a simulation of four magnetic field ramps: $40 \ \mu s$ evolution time. Same as Figure 5.81, but for the longest evolution time.



Figure 5.94: Frequency components of atom numbers during a simulation of three constant magnetic fields: $40 \ \mu s$ evolution time. Same as Figure 5.82, but for the longest evolution time.



Figure 5.95: Condensate number when $t_{ev} = 40 \ \mu s$, including error estimates. The solid line is the simulated condensate number, and the dotted lines provide an estimate of numerical error. See Appendix F for a description of this estimate.


Figure 5.96: Molecule number when $t_{ev} = 40 \ \mu s$, including error estimates. Same as Figure 5.95, but for the molecular field.

evolution time of 25 μ s resulted in a lower remnant condensate number than either the 10 μ s or 40 μ s evolution times. However, the numbers in all three cases are much higher than the experimental values, which were between 3500 and 6000 atoms, and are hardly different from the initial condensate number (and are identical is all reliable significant digits). As with the single-pulse simulations, our model does not account for the vast majority of condensate loss.

The velocities of condensed particles look nearly identical between simulations, so we present the data for the 40 μ s evolution time only (see Figure 5.99). In constrast to the single-pulse simulations, the dominant molecular velocity is outwards during the last half of the simulation, while the final ramp exhibits the dramatic variations in velocity that we interpret as an undersampling of the phenomenon observed in Figure



Figure 5.97: Noncondensed number when $t_{ev} = 40 \ \mu s$, including error estimates. Same as Figure 5.95, but for noncondensed atoms.

5.8a. An experiment with a sequence of several such magnetic field pulses could reveal very interesting dynamics. With minor modifications, our code could simulate such an experiment, though the numerics may only conserve number for pulse sequences lasting less than about 150 μ s.



Figure 5.98: Evolution time dependence of condensate number in two-pulse simulations. Number of condensed atoms N_a during t_{tail} , when the magnetic field is constant. The means of the oscillations are 16,499.419, 16,499.415, and 16,499.424 for the $t_{\text{ev}} = 10$, 25, and 40 μ s simulations, respectively, though not all these significant figures are reliable.



Figure 5.99: *Condensed particle velocities during a two-pulse simulation*. These radial velocities of (a) atoms and (b) molecules are representative of the data for the other simulated evolution times, as well. During the final ramp, the molecules acquire rapidly changing and large-magnitude velocities.

Chapter 6

CYLINDRICAL SIMULATIONS

The code, which is provided in Appendix G and numerically approximates solutions to our model, is written in C++. The parallelization scheme used in the cylindrical code lends itself well to an object-oriented programming approach, in which equations defined over (R_{ρ}, R_z) are divided amongst nodes in a cluster and divided amongst cores on each node.

6.1 Parallelization Scheme for Cylindrical Simulation

The cylindrical model consists of Equations (3.56), (3.57), (3.63), and (3.64), where (3.65) is needed to compute the diagonal parts of the normal and anomalous fluctuations. Considering only n = 0 in the cosine series expansions of the correlation functions reduces the number of spatial independent variables to four. The amount of computation per time step required by the cylindrical model may be several times that required by the spherical model, so parallelization on a cluster appears practical and worthwhile.

6.1.1 Data Dependencies

The Runge-Kutta method requires us to calculate K_1 through K_6 , defined in Equation (4.3), in order to calculate the time-stepped solution. Each K term depends on the one that preceded it; for example, K_2 is required to calculate K_3 . Since each field depends in some way on every other field, a given K term must be computed for every field before the next K term can be computed for any field; for example, K_2 must be calculated for the atomic and molecular fields and the normal and anomalous densities before any K_3 term can be calculated. However, the order in which the fields' K_i terms are calculated for a given i is irrelevant; for example, K_2 for $\varphi_a(R_{\rho}, R_z)$ can be calculated before K_2 for $\varphi_m(R_{\rho}, R_z)$, or vice versa. This independence allows several threads to simultaneously calculate a given K term for different fields, but only at one stage of the time stepping process for a single time step; hence, our choice of an explicit Runge-Kutta method for time propagation effectively forbids any temporal parallelization but allows spatial parallelization.

Inspection of Equations (3.56) and (3.57), the equations for the atomic and molecular fields, shows that each depends on both single-particle fields, as well as the diagonal parts of the correlation functions. These diagonal parts are calculated from the correlation functions at every $(R_{\rho}, R_z, k_{\rho}, k_z)$ point. The correlation functions at any such point depend on the same data as the atomic and molecular fields, in addition to each other; that is, $\mathcal{G}_N^0(R_{\rho}, R_z, k_{\rho}, k_z)$ and $\mathcal{G}_A^0(R_{\rho}, R_z, k_{\rho}, k_z)$ both depend on $\varphi_a(R_{\rho}, R_z)$, $\varphi_m(R_{\rho}, R_z)$, $\mathcal{G}_N^0(R_{\rho}, R_z, k_{\rho}, k_z)$, and $\mathcal{G}_A^0(R_{\rho}, R_z, k_{\rho}, k_z)$.¹ We can minimize the amount of internodal communication by ensuring that $\mathcal{G}_N^0(R_{\rho}, R_z, k_{\rho}, k_z)$ is on the same node as $\mathcal{G}_A^0(R_{\rho}, R_z, k_{\rho}, k_z)$ for a given $(R_{\rho}, R_z, k_{\rho}, k_z)$ point. As long as fields are distributed over nodes, the atomic and molecular fields and the diagonal parts of the correlation functions must be transmitted to every other node at least six times per time step.

¹Note that truncating the cosine series expansions at an n > 0 would introduce dependencies among the $\mathcal{G}_N^n(R_\rho, R_z, k_\rho, k_z)$ for different *n*, substantially complicating the communication issues.

6.1.2 Load Balancing

Efficient use of a cluster (again, a group of interconnected multi-core machines) requires careful load balancing, so we attempt to give each node roughly the same number of floating point operations per time step. It is useful to think of a correlation function as a set of equations defined over (R_{ρ}, R_z) for a particular point (k_{ρ}, k_z) . We use a real equation defined over (R_{ρ}, R_z) as a unit of computational work. The atomic and molecular fields each consist of two such equations (one for the real part and one for the imaginary part); the normal fluctuations field consists of $N_{k_z}N_{k_{\rho}}$ such equations, where N_{k_z} is the number of axial relative momentum grid points and $N_{k_{\rho}}$ is the number of radial relative momentum grid points, and we recall that the normal fluctuations are real as long as their initial conditions are real; and the anomalous fluctuations field consists of $2N_{k_z}N_{k_\rho}$ such equations. Each of these units of computational work requires at least one derivative in the R_z direction, which is done in order $N_{R_{\rho}}N_{R_{z}}\log_{2}(N_{R_{z}})$ operations (assuming we take pseudospectral derivatives via fast transforms), where $N_{R_{\rho}} + 1$ and $N_{R_z} + 1$ are numbers of center of mass radial and axial grid points, respectively. Equations other than those for the normal fluctuations also require a derivative in the R_{ρ} direction, making their operation count of order $N_{R_{\rho}}N_{R_{z}}\log_{2}(N_{R_{\rho}}N_{R_{z}})$. The dominant factor is still $N_{R_{\rho}}N_{R_{z}}$, justifying our treatment of the normal fluctuations's equations and the real or imaginary part of any other equation defined over (R_{ρ}, R_z) as equal units of computational work.

The task is now to ensure that each node has nearly the number of floating point operations per time step. The total number of units of computational work in the system is

$$W_{\rm tot} = 4 + 3N_{k_{\rho}}N_{k_{z}}.\tag{6.1}$$

If we use M nodes of a computer, the computational work assigned to each node is

 $W = W_{\text{tot}}/M$, though in practice we round W to the next highest integer divisible by three, since our units of computational work must be whole and are usually assigned in threes (one unit for a normal fluctuations equation and two for the anomalous fluctuations equation with the same values of k_z and k_ρ). One node may have less work than all the others; this node should be burdened with any serial housekeeping duties. See Figure 6.1 for an example arrangement.

6.1.3 Basic Algorithm

Each node has assigned to it several real equations defined over (R_{ρ}, R_z) . Our definition of a unit of computational work fits well into C++'s object-oriented programming paradigm; each equation defined over (R_{ρ}, R_z) residing on a node is an instance of a class. This approach also facilitates loop-level parallelization with OpenMP; for example, calculation of a general number of equations' K terms on a node might be easily programmed as

```
#pragma omp parallel for
for ( int e = 0 ; e < myNumberOfEquations ; e++ )
{
    myEqns[e].CalcKArg();
}</pre>
```

where the member function handles the particulars of the Runge-Kutta method. Since the amount of computation in each equation is considerable, one would have insignificant overhead with dynamic thread scheduling, so that no threads remain idle for long periods of time.

The assignment of equations to nodes is handled during initialization and remains the same for the duration of the simulation. The algorithm for computing a single

$$\begin{array}{l} \mathcal{G}^{0}_{N}(R_{\rho},R_{z},k_{\rho}=0,k_{z}=0) \\ \mathcal{G}^{0}_{A}(R_{\rho},R_{z},k_{\rho}=0,k_{z}=0) \\ \mathcal{G}^{0}_{N}(R_{\rho},R_{z},k_{\rho}=0,k_{z}=0) \\ \mathcal{G}^{0}_{N}(R_{\rho},R_{z},k_{\rho}=1,k_{z}=0) \\ \mathcal{G}^{0}_{A}(R_{\rho},R_{z},k_{\rho}=1,k_{z}=0) \\ \mathcal{G}^{0}_{A}(R_{\rho},R_{z},k_{\rho}=2,k_{z}=0) \\ \mathcal{G}^{0}_{A}(R_{\rho},R_{z},k_{\rho}=2,k_{z}=0) \\ \mathcal{G}^{0}_{A}(R_{\rho},R_{z},k_{\rho}=2,k_{z}=0) \\ \mathcal{G}^{0}_{A}(R_{\rho},R_{z},k_{\rho}=6,k_{z}=0) \\ \mathcal{G}^{0}_{A}(R_{\rho},R_{z},k_{\rho}=6,k_{z}=0) \\ \mathcal{G}^{0}_{A}(R_{\rho},R_{z},k_{\rho}=7,k_{z}=0) \\ \mathcal{G}^{0}_{A}(R_{\rho},R_{z},k_{\rho}=3,k_{z}=0) \\ \mathcal{G}^{0}_{A}(R_{\rho},R_{z},k_{\rho}=8,k_{z}=0) \\ \mathcal{G}^{0}_{A}(R_{\rho},R_{z}) \\ \mathcal{G}^{0}_{A}(R_{\rho},R_{z},k_{\rho}=8,k_{z}=0) \\ \mathcal{G}^{0}_{A}(R_{\rho},R_{z},k_{\rho}=8,k_{z}=0) \\ \mathcal{G}^{0}_{A}(R_{\rho},R_{z},k_{\rho}=8,k_{z}=0) \\ \mathcal{G}^{0}_{A}(R_{\rho},R_{z},k_{\rho}=8,k_{z}=0) \\ \mathcal{G}^{0}_{A}(R_{\rho},R_{z},k_{\rho}=8,k_{z}=0) \\ \mathcal{G}^{0}_{A}(R_{\rho},R_{z},k_{\rho}$$

Figure 6.1: Example of load balancing in parallel cylindrical code. Consider a grid with only one k_z point, 10 k_ρ points, and an arbitrary number of center of mass grid points (R_ρ, R_z) . If we run the simulation on four nodes (represented by the boxes above), each node is assigned at least one pair of correlation function equations defined over (R_ρ, R_z) , for particular values of k_ρ and k_z . A single $\mathcal{G}_N^0(R_\rho, R_z, k_\rho, k_z)$ equation at a (k_ρ, k_z) point is one unit of computational work; a single $\mathcal{G}_A^0(R_\rho, R_z, k_\rho, k_z)$ equation at such a point is two units, as are the atomic and molecular fields. Note that the bottom right node has seven units of computational work, while the others have nine; this node should perform any serial housekeeping duties. If the upper left node has six cores, each of the six equations on that note could be handled simultaneously by a different thread; if equations outnumber threads, OpenMP (the threading standard we use) determines at runtime how equations will be distributes amongst cores.

time step is as follows:

- 1. Each thread computes the argument needed to compute the current K term for a particular set of the fields residing on the node. Each thread waits until every thread on every node has computed its arguments.
- 2. Each thread having an equation corresponding to a (k_{ρ}, k_z) point of a correlation function adds the argument corresponding to that correlation function to one of two accumulators, one of which is for the diagonal parts of the normal fluctuations and the other for the diagonal parts of the anomalous fluctuations. These accumulators are shared by every thread on the node.
- 3. Once every thread on every node has added all correlation function arguments to the proper local accumulators, an MPI collective reduction call adds together the local accumulators (keeping the diagonal parts of the normal and anomalous densities separate) and broadcasts the results to every node. Now every node has access to the diagonal elements of the correlation functions. Simultaneously, using different threads, the arguments corresponding to the atomic and molecular fields are broadcast to all nodes.
- Each thread calculates the current K term for whatever equations it is assigned.
 All nodes block until every equation's K term has been calculated.
- 5. The first four steps are repeated until K_1 through K_6 are available for every field. The master thread on each node determines the highest truncation error on the node.
- 6. An MPI collective reduction call notifies every node of the highest truncation error in the system.

- 7. Each node's master thread determines whether or not to accept the stepped solution, and either refines the current time step size, or recommends a step size to use during the next cycle. Here, it is very important that every core on every node in the computer does arithmetic identically; otherwise, different nodes might use slightly different time step sizes. If the cores are not identical, a single thread in a single node could do this step, but this necessitates more communication and further complicates already complicated code.
- 8. Once a stepped solution is accepted, each thread calculates that solution for whatever equations in the system it is assigned.

This algorithm is slowed by the overhead associated with threading, which is negligible in comparison to the time spent on computation, and the time spent sending data. Only four fields must be passed between nodes; as long as each node has at least four cores, the communication time is that required to accumulate and broadcast $2N_{R_{\rho}}N_{R_{z}}$ double-precision numbers.² The real and imaginary parts of the three complex fields could each be sent by separate threads if at least seven cores exist on each node; then the communication time is halved (neglecting overhead). The barriers and blocking calls in the algorithm are unavoidable due to the time propagation method we have chosen, as the K_{i-1} term must be known for every field before the K_i term can be calculated for any field. Preliminary testing suggests a 370 percent speedup when using four nodes as compared to one, and a 200 percent speedup when using four cores as compared to one.

²While the MPI-2 specification nominally allows for simultaneous inter-process communication by each process' threads, not all implementations are compliant. On the Golden Energy Computing Organization's Ra supercomputer, OpenMPI 1.2.5 does *not* guarantee thread-safety for simultaneous calls to MPI routines by multiple threads in a single process; hence, our code checks for MPI thread safety and serializes all MPI calls when thread safety is not ensured.

6.2 Parallelization Scheme for Spherical Simulation

Considering resource limitations at the time of development and the smaller amount of computation per time as compared to the cylindrical model, we write the spherical code with a multithreaded (OpenMP) parallelization appropriate for use only on an SMP (again, a machine where all cores address the same memory space). In practice, we require q = 0 in the spherical harmonic expansions of the correlation functions for expediency, since this eliminates one independent variable.³ Preliminary testing of the spherical code suggests a speedup of over 200 percent when using four cores as compared to a single core.

6.3 Cylindrical Proof-of-Concept Simulations

Our results thus far have exclusively concerned the spherical model, though a great deal of time and effort is embodied in the cylindrical model and parallel code. As a demonstration that this code functions, we present plots of all fields and total numbers for a simulation with repulsive interactions and one with attractive interactions. Each case uses 17 axial relative momentum grid points ranging from -1.0 to $1.0 \ \mu m^{-1}$, 33 radial relative momentum points ranging from 0 to $6.7 \ \mu m^{-1}$, 17 axial center of mass points ranging from -12.5 to $12.5 \ \mu m$, and 33 radial center of mass points ranging from 0 to $15 \ \mu m$. Imaginary time relaxation works correctly but extremely slowly, requiring several days to approach the ground state, so we use an analytical initial state for expediency.⁴ The repulsive simulation has $a_{\rm eff} = 2000a_0$,

³The simulations of Ref. [11] effectively make the same approximation, however; Milstein et al. make this approximation from the outset, expanding the correlation functions in Legendre polynomials. We retain our spherical harmonic expansion, but only consider q = 0 spherical harmonics. Some terms in our correlation function equations differ from those of Ref. [11] by a constant factor.

⁴A more prudent choice of initial conditions during imaginary time relaxation may result in faster convergence to the ground state.

the attractive simulation has $a_{\text{eff}} = -400a_0$, and both use realistic ⁸⁵Rb parameters. We do not calculate total energy for these simulations, since the nonuniform Gauss-Lobatto grid in the radial center of mass coordinate does not facilitate the necessary transformation to momentum space in a straightforward way.

These parameters, in the attractive case, should simulate a collapse in less than 125 days when using 64 nodes. The repulsive case is more feasible, and would likely produce interesting results within a few (tens of) days, using a more modest number of nodes. For example, the longest two-pulse simulation of Section 5.3 would take approximately 25 days to complete on 16 nodes.

The results are qualitatively similar to spherical simulations, with atom-molecule oscillations of a higher frequency in the attractive, low $|a_{\text{eff}}|$ case than in the repulsive, high $|a_{\text{eff}}|$ case. Average error in number is of a considerable magnitude and exhibits clear trends. Such error could be the result of a lack of convergence, or may be connected to our use of Gauss-Lobatto quadrature in computing the number; preliminary investigations suggest that the method of computing total number, independent of the simulation, has nontrivial implications for number conservation. Note that the noncondensed density has not yet acquired any of the large negative values frequently seen in the spherical collapse simulations.

We show densities taken at $R_z = 0$ for all R_ρ (a "slice in ρ "), and for all R_z for the R_ρ point that is indexed by the integer division quotient $3N_{R_\rho}/4$, which is near the origin (a "slice in z"). Figures 6.2 through 6.7 are the results for the repulsive case, and Figures 6.8 through 6.13 are the results for the attractive case. Each simulation ran in about nine hours on eight nodes having eight cores each. Comparison between a smaller-scale simulation run on four nodes and a single node produced results identical in every significant digit, suggesting an absence of race



Figure 6.2: Condensate density in a repulsive cylindrical simulation. Slices in (a) ρ and (b) z.

 $conditions^5$ due to the parallelization. The four-node simulation ran 370 percent faster than the single-node simulation, and an even smaller simulation on a single node achieved approximately 200 percent speedup when run on four cores instead of one.

 $^{{}^{5}\}mathrm{A}$ race condition is a situation where a calculation's outcome depends on the order in which cores or nodes finish their work.



Figure 6.3: Molecular density in a repulsive cylindrical simulation. Slices in (a) ρ and (b) z.



Figure 6.4: Noncondensed density in a repulsive cylindrical simulation. Slices in (a) ρ and (b) z.



Figure 6.5: Diagonal parts of anomalous fluctuations in a repulsive cylindrical simulation. Slices in (a) ρ and (b) z of $|\bar{G}_A(R,0)|$.



Figure 6.6: Numbers of (a) condensed atoms and (b) molecules in a repulsive cylindrical simulation.



Figure 6.7: (a) Number of noncondensed atoms and (b) average number error in a repulsive cylindrical simulation.



Figure 6.8: Condensate density in an attractive cylindrical simulation. Slices in (a) ρ and (b) z.



Figure 6.9: Molecular density in an attractive cylindrical simulation. Slices in (a) ρ and (b) z.



Figure 6.10: Noncondensed density in an attractive cylindrical simulation. Slices in (a) ρ and (b) z.



Figure 6.11: Diagonal parts of anomalous fluctuations in an attractive cylindrical simulation. Slices in (a) ρ and (b) z of $|\bar{G}_A(R,0)|$.



Figure 6.12: Numbers of (a) condensed atoms and (b) molecules in an attractive cylindrical simulation. Subsequent points are connected by a line, which only serves to guide the eye.



Figure 6.13: (a) Number of noncondensed atoms and (b) average number error in an attractive cylindrical simulation. Subsequent points are connected by a line, which only serves to guide the eye.

Chapter 7

CONCLUSION

We have rigorously derived a Hartree-Fock-Bogoliubov model of dynamic Bose-Einstein condensates. The model accounts for kinetic and potential energies of atoms, collisions between two atoms, and formation and dissociation of quasibound pairs of atoms, or molecules, due to a single Feshbach resonance. So that the model is tractable, we factorize to second order quantum fluctuations via Wick's theorem. This factorization is exact only if the system is in a squeezed state; such an assumption is more general than that implicit in the Gross-Pitaevskii equation, but there is no reason to believe *a priori* that a collapsing BEC or a condensate with significant repulsive interactions must be in such a state. The theory then takes the form of four, coupled, nonlinear partial differential equations, defined over time and six spatial independent variables. Geometrical symmetry assumptions and restrictions reduce the number of spatial independent variables to five in the case of cylindrical symmetry, and four in the case of spherical symmetry. We have written and tested parallelized code for simulations in cylindrical symmetry, and find that insightful simulations are feasible, even with experimental parameters.

Our simulations in spherical symmetry have shown that the HFB model developed in Chapters 2 and 3 qualitatively reproduces condensate contraction and burst formation for realistic collapse parameters. We are able to predict pre-collapse atom-molecule oscillations of frequency ν/h , where ν is the detuning of the Feshbach resonance and h is Planck's constant. In this context we also predict brief periods, on the order of h/ν in duration, of high molecular velocities when molecules dissociate and reenter the atomic condensate. We find that the stength of the trapping potential influences the time to collapse, and stable condensates formed in a strong trap and then suddenly given attractive interactions in a weaker trap develop two spatially distinct regions, one where harmonic oscillator physics dominates, and the other where unstable attractive interactions dominate. Condensates formed in the ground state of their trap contract with a roughly quadratic time dependence when given attractive interactions.

The model predicts small-amplitude atom-molecule oscillations in a single-pulse experiment, regardless of pulse strength, with a molecular condensate remaining after the pulse. The number of molecules in this remnant depends on pulse shape and strength, but the number of molecules produced at the peak of the oscillations depends only on pulse strength. A pulse to resonance produces atom-molecule oscillations which completely dominate the dynamics of every field. Our simulations indicate that the number in the atomic condensate remnant increases with the pulse hold time, in contradiction to experimental observation, and increases slightly with the pulse ramp times, in qualitative agreement (though significant quantitative disagreement) with experiment. We find that increasing the duration of the first pulse ramp decreases the remnant number, implying that the mean field expansion used in imaging could cause a significant loss of atoms from the condensate.

We also predict atom-molecule oscillations with frequency ν/h during the periods of constant magnetic field in the two-pulse experiments, and a small modulation of the total noncondensed fraction by an oscillation \hbar^5/m^3U^2 in angular frequency. This modulation appears during some periods of changing magnetic field, both in oneand two-pulse simulations. Bursts of noncondensed density form quickly when the magnetic field is close to resonance, while denser bursts form slowly when the field is far from resonance. These simulations may indicate that the lack of bursts observed in the single-pulse simulations are a result of the fact that the simulated bursts move radially outward well after the pulse has ended. Our two-pulse simulations qualitatively reproduce the experimental observation that the remnant condensate number does not monotonically increase or decrease with increasing evolution time.

We find that number conservation depends sensitively on temporal resolution and not spatial resolution for situations far from collapse. The reason for this discrepancy is unclear. Collapse simulations have an increasing error in total number as the condensate contracts onto only a few grid points, suggesting numerical instabilities and warranting further experimentation with spatial resolution.

None of our simulations show the dramatic loss from the condensate that is experimentally observed, or that has been simulated using similar methods based on an HFB theory like ours, and Kokkelmans *et al.*'s [14] resonance theory. This disagreement could suggest that our inclusion of the trap, the previously unattempted expansion in terms of spherical harmonics, or the numerical methods we use somehow suppress the mechanism which is responsible for condensate depletion. Conversely, our methods are the most numerically accurate to date. Therefore, the more likely explanation is that the model does not incorporate the correct physics. In particular, we have intentionally neglected three-body and other density-dependent losses in order to isolate the effects of quantum fluctuations. Second-order quantum fluctuations alone do not account quantitatively for experimental results. Subsequent simulations should include phenomenological three-body losses. Still, comparison of some of our simulations to mean-field-only simulations suggests that second-order quantum fluctuations are only important over long time scales, such as the approximately 400 μ s rethermalization time determined in a single-pulse experiment.

Our inclusion of the azimuthal component of the relative momentum in the spherical model would allow one to study collapse in a rotating condensate or a vortex. The quantized nature of rotation in a BEC would lead to exotic, previously unobserved dynamics, and the inclusion of rotation would further strengthen the Bosenova's qualitative analogy with a supernova.

Extensive use of this model of Bose-Einstein condensates would benefit enormously from a more detailed theoretical and analytical treatment. The evaluation of the kinetic energy of the noncondensed component appears intractable, though physical reasoning suggests that the quantum pressure term in the noncondensed gas' kinetic energy should vanish. As mentioned in Section 3.1, if we sacrifice all knowledge of off-diagonal correlations, the general problem with absolutely no symmetry may be reduced from six to three spatial independent variables. Then, by assuming spherical symmetry and using spherical coordinates, simulations would only need a single spatial variable. Quantum fluctuations would still be present in the model in the form of the diagonal parts of the normal and anomalous fluctuations. It may then be practical to include higher-order fluctuations, for example, $\langle \hat{\chi}_a^{\dagger}(R) \, \hat{\chi}_a(R) \, \hat{\chi}_a(R) \, \hat{\chi}_a(R) \rangle$, where $\hat{\chi}_a(R)$ is a fluctuation operator acting at the radial coordinate R, without the approximate factorizations of Wick's theorem. This idea has been explored, to some extent, in ZGN theory [45].

The model lacks realism in a few key aspects. Rubidium-85 has a second Feshbach resonance which we have not accounted for, and the detailed inclusion of a thermal cloud, though perhaps inconsequential [13] to the JILA collapse experiments, would allow for truly insightful simulations of the Rice experiments. Our chosen symmetries also restrict what physical effects we could simulate; for example, jets cannot appear in our spherical simulations, nor can bursts with anisotropy. The cylindrically symmetric case could allow for jets distributed along the axis, but those jets would completely encircle the axis.

More involved analytical PDE methods could give some analytical insight into the model. The method of characteristics (see Section 1.6.1) may lead to an analytical solution, at least under some set of assumptions. Linearization might not yield a realistic model, but could determine stability (or lack thereof). The integrability of our HFB equations or some simplified version has never been examined. Given the disparity of time scales we observe in our simulations and the nondimensionalization procedure of Section 2.6.2, an analytical treatment of our equations by perturbation theory (in the context of PDE's) may be highly insightful, and could be the subject of future work by this group.

Instabilities and computational impracticalities may be the result of the numerics we have used. A solution using finite element methods in the spatial discretization or a solution via finite element discrete variable representation could improve convergence and compute time [105]. Another possibility is the use of implicit Runge-Kutta methods (as opposed to the explicit kind that we use), which more efficiently handle stiff equations [106], and for which many parallelized algorithms exist (see the work of Korch and Rauber, for example). An adaptive spatial grid could be crucial to accurate collapse simulations, since all of the Bosenova's violent dynamics are highly concentrated near the origin, while the initial state is relatively broad.

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APPENDIX A

WICK'S THEOREM FOR SQUEEZED STATES

A particular manifestation of Wick's theorem expresses an expectation value of a product of several field operators as a sum of terms, each of which is an expectation value of a smaller number of field operators and is more amenable to calculation. The theorem is exact if the state $|\lambda\rangle$ is a squeezed state.

We outline a derivation of a form of the theorem given by Blaizot and Ripka [107], and then describe in detail how it is adapted, extended, and interpreted for use in Chapter 3.

A.1 Outline of the Derivation

The derivation begins with a specialization of the Baker-Hausdorf lemma, called Glauber's formula:

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{[\hat{A},\hat{B}]},$$
 (A.1)

true for any two operators \hat{A} and \hat{B} such that $\left[\hat{A}, \left[\hat{A}, \hat{B}\right]\right] = \left[\hat{B}, \left[\hat{A}, \hat{B}\right]\right] = 0$. This is extended by mathematical induction and the requirements that $\left[\hat{A}_i, \hat{A}_j\right] = \left[\hat{B}_i, \hat{B}_j\right] = 0$ for all i and j so that the left-hand side of (A.1) consists of several factors of the form $\exp\left(\hat{A}_i + \hat{B}_i\right)$, where the index i is unique to each factor. The resulting expression can be simplified with the notation of normal- and T-ordered products and contractions. Normal ordering consists of all the \hat{A} factors in a product being written to the left of the \hat{B} factors, while a T-ordered product has the factors put in order of decreasing indices. A contraction of two operators is their T-ordered product minus their normal-ordered product. The extended form of (A.1) can be written in terms of a single T-ordered exponential of a sum of operators, a normal-ordered exponential of the sum, and exponentials of sums of contractions and commutators. These sums go to integrals as the operators' discrete parameter (their summation index) becomes continuous (this parameter later being identified as time), except for the sum over commutators, which vanishes in the continuum limit.

Specializing to field theory, the generic operators are identified as weighted sums of the single-particle momentum-space ladder operators \hat{a}_k and \hat{a}_k^{\dagger} , for which normalordering is defined as a product in which all of the creation operators are written to the left of the destruction operators, and T-ordering is defined as the operators being ordered by decreasing values of their continuous parameter (time). Being interested in expectation values, one then averages this expression, and only obtains any useful simplifications if the average is assumed to be taken with respect to an eigenstate of all annihilation operators, is expanded in power series. Equating coefficients in the series on each side of the equation gives another form of Wick's theorem, in which most contractions vanish.

However, the sums of \hat{a}_k and \hat{a}_k^{\dagger} can be related by a linear transformation (a canonical transformation, in which commutation relations are preserved) to sums of different operators, \hat{b}_j and \hat{b}_j^{\dagger} . Given the \hat{a}_k 's interpretation as momentum-space ladder operators, the \hat{b}_j are Bogoliubov quasiparticle ladder operators, in which the j indexes quasiparticle excitations, or the eigenvalues of the Bogoliubov-de Gennes equations (see [108], for example). Since $|\lambda\rangle$, an eigenstate of all the \hat{a}_k , is not generally an eigenstate of the \hat{b}_j , the contractions that vanished for the \hat{a}_k do not

vanish for the \hat{b}_j .

The general rule for factorization of \hat{b} 's is then: an expectation value of a product of \hat{b} 's and \hat{b}^{\dagger} 's is equal to the product of the expectation values of all the operators individually, plus all the products in which a single contraction of two of the operators multiplies the expectation values of the remaining factors individually, plus all the products in which two contractions multiply the expectation values of the remaining factors individually, etc. This rule is best written schematically:

 $\langle Product \rangle = (Individual averages of each factor)$

$$\begin{aligned} + \sum_{a.p.c.} \left[\text{ (Contraction of two of the factors)} \right. \\ & \times \text{ (Individual averages of the remaining factors)} \right] \\ + \sum_{a.p.c.} \left[\text{ (Contraction of two of the factors)} \right. \\ & \times \text{ (Contraction of two of the remaining factors)} \\ & \times \text{ (Individual averages of the remaining factors)} \right] \\ + \dots \\ & + \sum_{a.p.c.} \left[\text{ (Contraction of two of the factors)} \right. \\ & \times \text{ (Contraction of two of the remaining factors)} \\ & \times \text{ (Contraction of two of the remaining factors)} \\ & \times \dots \\ & \times \text{ (Contraction of two of the remaining factors)} \\ & \times (\text{Contraction of the last two factors)} \\ & \times (\text{Average of the remaining lone factor, if it exists)} \right], \\ & (\text{A.2)} \end{aligned}$$

where a.p.c. stands for "all possible contractions"; for example,

$$\begin{split} \left\langle \hat{A}\hat{B}\hat{C}\hat{D} \right\rangle &= \left\langle \hat{A} \right\rangle \left\langle \hat{B} \right\rangle \left\langle \hat{C} \right\rangle \left\langle \hat{D} \right\rangle \\ &+ \left(\hat{A}^{\bullet}\hat{B}^{\bullet}\left\langle \hat{C} \right\rangle \left\langle \hat{D} \right\rangle + \left\langle \hat{A} \right\rangle \hat{B}^{\bullet}\hat{C}^{\bullet}\left\langle \hat{D} \right\rangle + \left\langle \hat{A} \right\rangle \left\langle \hat{B} \right\rangle \hat{C}^{\bullet}\hat{D}^{\bullet} \\ &+ \hat{A}^{\bullet}\left\langle \hat{B} \right\rangle \hat{C}^{\bullet}\left\langle \hat{D} \right\rangle + \hat{A}^{\bullet}\left\langle \hat{B} \right\rangle \left\langle \hat{C} \right\rangle \hat{D}^{\bullet} + \left\langle \hat{A} \right\rangle \hat{B}^{\bullet}\left\langle \hat{C} \right\rangle \hat{D}^{\bullet}) \\ &+ \left(\hat{A}^{\bullet}\hat{B}^{\bullet}\hat{C}^{\bullet\bullet}\hat{D}^{\bullet\bullet} + \hat{A}^{\bullet}\hat{B}^{\bullet\bullet}\hat{C}^{\bullet\bullet}\hat{D}^{\bullet\bullet} + \hat{A}^{\bullet}\hat{B}^{\bullet\bullet}\hat{C}^{\bullet}\hat{D}^{\bullet\bullet} \right), \end{split}$$
(A.3)

where, in this case, each factor is a \hat{b}_j or \hat{b}_j^{\dagger} , and each factor's subscript and time dependence is not necessarily the same. A contraction of two operators $\hat{A}^{\bullet}\hat{B}^{\bullet} = \langle T(\hat{A}\hat{B}) \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle$, where $T(\ldots)$ indicates T-ordering. If the times at which two contracted factors are evaluated is the same, their T-ordered product is taken to be their ordinary, or unaltered, product. This expansion is exact when the state $|\lambda\rangle$ with respect to which the average is taken is an eigenstate of all the \hat{a}_k , to which the \hat{b}_k are related by a canonical transformation.

A.2 Extension of the Established Result

As in Equation (1.11) in the Introduction (Section 1.2.1),

$$\hat{\Psi}(\mathbf{x}) = \sum_{k} \zeta_k(\mathbf{x}) \,\hat{a}_k,\tag{A.4}$$

where $\hat{\Psi}(\mathbf{x})$ is a field operator and $\zeta_k(\mathbf{x})$ is the wavefunction of the *k*th single-particle energy eigenstate. Let us apply the requirement of Blaizot and Ripka's derivation of Wick's theorem; that is,

$$\hat{a}_k |\lambda\rangle = \lambda_k |\lambda\rangle \,\forall k, \tag{A.5}$$

where $|\lambda\rangle$ is the system's state and λ_k is the eigenvalue of \hat{a}_k acting on $|\lambda\rangle$. Noting that

$$\left\langle \hat{\Psi}(\mathbf{x}) \right\rangle = \left\langle \lambda \right| \sum_{k} \zeta_k(\mathbf{x}) \, \hat{a}_k \left| \lambda \right\rangle = \sum_{k} \zeta_k(\mathbf{x}) \, \lambda_k$$
 (A.6)

(assuming normalized states), we would have

$$G_{N}(\mathbf{x}, \mathbf{x}') = \left\langle \hat{\Psi}^{\dagger}(\mathbf{x}') \, \hat{\Psi}(\mathbf{x}) \right\rangle - \left\langle \hat{\Psi}^{\dagger}(\mathbf{x}') \right\rangle \left\langle \hat{\Psi}(\mathbf{x}) \right\rangle$$
$$= \sum_{k} \left\langle \lambda \right| \, \hat{\Psi}^{\dagger}(\mathbf{x}') \, \zeta_{k}(\mathbf{x}) \, \hat{a}_{k} \left| \lambda \right\rangle - \left\langle \hat{\Psi}^{\dagger}(\mathbf{x}') \right\rangle \left\langle \hat{\Psi}(\mathbf{x}) \right\rangle$$
$$= \left\langle \lambda \right| \, \hat{\Psi}^{\dagger}(\mathbf{x}') \left| \lambda \right\rangle \sum_{k} \zeta_{k}(\mathbf{x}) \, \lambda_{k} - \left\langle \hat{\Psi}^{\dagger}(\mathbf{x}') \right\rangle \left\langle \hat{\Psi}(\mathbf{x}) \right\rangle$$
$$= 0; \qquad (A.7)$$

that is, absolutely no correlations. Since we desire information about correlations, the requirement in Equation (A.5) will not do. Instead, let us interchange the \hat{a}_k and \hat{b}_j in the derivation, so that $|\lambda\rangle$ (now a coherent state in another sense) is an eigenstate of all the \hat{b}_j , and (A.5) now reads

$$\hat{b}_j |\lambda\rangle = \lambda_j |\lambda\rangle \,\forall j, \tag{A.8}$$

where the λ_j is now the eigenvalue of \hat{b}_j acting on $|\lambda\rangle$. The \hat{a}_k are related to the \hat{b}_j by the canonicil transformation

$$\hat{a}_k = \sum_j \left(U_{jk} \hat{b}_j + V_{jk}^* \hat{b}_j^\dagger \right), \tag{A.9}$$

where the U_{jk} and V_{jk} are the (scalar) elements of the matrix that performs the Bogoliubov transformation. Now, $|\lambda\rangle$ is not an eigenstate of \hat{a}_k :

$$\hat{a}_k|\lambda\rangle = \sum_j \left(U_{jk}\lambda_j|\lambda\rangle + V_{jk}^*\hat{b}_j^\dagger|\lambda\rangle \right),\tag{A.10}$$

where the $\hat{b}_j^{\dagger}|\lambda\rangle$ terms cannot be evaluated any further, since \hat{b}_j is not Hermitian, and so $|\lambda\rangle$ is not generally an eigenstate of \hat{b}_j^{\dagger} . Since the transformation of Equation (A.9) is canonical, the state $|\lambda\rangle$ can be shown [4] to be a *squeezed state*, which saturates the number-phase Heisenberg uncertainty relation:

$$\Delta N \,\Delta \phi \ge \frac{1}{2},\tag{A.11}$$

where ΔN and $\Delta \phi$ are the uncertainties in number and phase, respectively.

With the new assumption about $|\lambda\rangle$ and the definition of the \hat{a}_k in terms of the \hat{b}_j and \hat{b}_j^{\dagger} , let us re-write Equation (A.4):

$$\hat{\Psi}(\mathbf{x}) = \sum_{j} \left[u_j(\mathbf{x}) \, \hat{b}_j + v_j^*(\mathbf{x}) \, \hat{b}_j^\dagger \right],\tag{A.12}$$

where

$$u_j(\mathbf{x}) \equiv \sum_k U_{jk} \zeta_k(\mathbf{x}) \tag{A.13}$$

$$v_j^*(\mathbf{x}) \equiv \sum_k V_{jk}^* \zeta_k(\mathbf{x}) \,. \tag{A.14}$$

Now the general rule (A.2) for our desired manifestation of Wick's theorem can be re-written for field operators by letting $\hat{a} \rightarrow \hat{b}$ and $\hat{a}^{\dagger} \rightarrow \hat{b}^{\dagger}$, and then multiplying by and summing over energy eigenstate wavefunctions. Then, the same schematic (A.2) applies, where each factor is a field operator, and each may be evaluated at a different time and point.

A.3 Interpretation of Correlation Functions

In light of our assumption about $|\lambda\rangle$, let us evaluate the correlation functions $G_N(\mathbf{x}, \mathbf{x}')$ and $G_A(\mathbf{x}, \mathbf{x}')$, which are defined in Equations (2.13) and (2.14).¹

The normal fluctuations $G_N(\mathbf{x}, \mathbf{x}')$ in terms of field operators [using the decomposition (2.4)] is

$$G_N(\mathbf{x}, \mathbf{x}') = \left\langle \hat{\Psi}_a^{\dagger}(\mathbf{x}') \, \hat{\Psi}_a(\mathbf{x}) \right\rangle - \left\langle \hat{\Psi}_a^{\dagger}(\mathbf{x}') \right\rangle \left\langle \hat{\Psi}_a(\mathbf{x}) \right\rangle. \tag{A.15}$$

(Note that this is $\left[\hat{\Psi}_{a}^{\dagger}(\mathbf{x}')\right]^{\bullet} \left[\hat{\Psi}_{a}(\mathbf{x})\right]^{\bullet}$.) Assuming normalized states, the first term on the right-hand side, in terms of the \hat{b}_{j} and \hat{b}_{j}^{\dagger} , is

$$\langle \lambda | \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \hat{\Psi}_{a}(\mathbf{x}) | \lambda \rangle = \sum_{j,j'} \langle \lambda | \left[v_{j}(\mathbf{x}') \hat{b}_{j} + u_{j}^{*}(\mathbf{x}') \hat{b}_{j}^{\dagger} \right] \left[u_{j'}(\mathbf{x}) \hat{b}_{j} + v_{j'}^{*}(\mathbf{x}) \hat{b}_{j}^{\dagger} \right] | \lambda \rangle$$

$$= \sum_{j,j'} \left[v_{j}(\mathbf{x}') u_{j'}(\mathbf{x}) \lambda_{j} \lambda_{j'} + v_{j}(\mathbf{x}') v_{j'}^{*}(\mathbf{x}) \delta_{j,j'} + v_{j}(\mathbf{x}') v_{j'}^{*}(\mathbf{x}) \lambda_{j} \lambda_{j'}^{*} + u_{j}^{*}(\mathbf{x}') u_{j'}(\mathbf{x}') \lambda_{j}^{*} \lambda_{j'} + u_{j}^{*}(\mathbf{x}') v_{j'}^{*}(\mathbf{x}) \lambda_{j}^{*} \lambda_{j'}^{*} \right], \qquad (A.16)$$

where we have added and subtracted the same term inside the sum in order to use the commutation relation $\left[\hat{b}_{j}, \hat{b}_{j'}^{\dagger}\right] = \delta_{j,j'}$. The second term on the right-hand side, in terms of the \hat{b}_{j} and \hat{b}_{j}^{\dagger} , is

¹Henceforth, we take the \hat{b}_j and \hat{b}_j^{\dagger} to correspond to the atomic field.

$$\left\langle \hat{\Psi}_{a}^{\dagger}(\mathbf{x}') \right\rangle \left\langle \hat{\Psi}_{a}(\mathbf{x}) \right\rangle = \sum_{j,j'} \left\langle \lambda \right| \left[v_{j}(\mathbf{x}') \hat{b}_{j} + u_{j}^{*}(\mathbf{x}') \hat{b}_{j}^{\dagger} \right] \left| \lambda \right\rangle \left\langle \lambda \right| \left[u_{j'}(\mathbf{x}) \hat{b}_{j'} + v_{j'}^{*}(\mathbf{x}) \hat{b}_{j'}^{\dagger} \right] \left| \lambda \right\rangle$$
$$= \sum_{j,j'} \left[v_{j}(\mathbf{x}') u_{j'}(\mathbf{x}) \lambda_{j} \lambda_{j'} + v_{j}(\mathbf{x}') v_{j'}^{*}(\mathbf{x}) \lambda_{j} \lambda_{j'}^{*} + u_{j}^{*}(\mathbf{x}') u_{j'}(\mathbf{x}) \lambda_{j}^{*} \lambda_{j'} + u_{j}^{*}(\mathbf{x}') v_{j'}^{*}(\mathbf{x}) \lambda_{j}^{*} \lambda_{j'}^{*} \right].$$
(A.17)

Subtracting this from Equation (A.16) leaves

$$G_N(\mathbf{x}, \mathbf{x}') = \sum_j v_j(\mathbf{x}') \, v_j^*(\mathbf{x}) \,. \tag{A.18}$$

Using the same procedure on $G_A(\mathbf{x}, \mathbf{x}')$ (which turns out to be $\left[\hat{\Psi}_a(\mathbf{x}')\right]^{\bullet} \left[\hat{\Psi}_a(\mathbf{x})\right]^{\bullet}$) results in

$$G_A(\mathbf{x}, \mathbf{x}') = \sum_j u_j(\mathbf{x}') v_j^*(\mathbf{x}).$$
(A.19)

Note that neither Blaizot and Ripka's derivation nor our adaption mentions either a vacuum state or a Gaussian distribution.

A.4 Proof of Factorizations

With a considerable amount of algebra, one may use Equations (A.8), (A.12), (A.18), and (A.19) to prove Equations (2.46) to (2.51). We shall henceforth use Einstein's summation convention, in which summation is implied in any term in which a subscript is repeated. We will not explicitly write the \mathbf{x} dependence of any coefficient, and denote a coefficient that depends on \mathbf{x}' with an overbar. For example,

$$\hat{\Psi}_a(\mathbf{x}) = \sum_j \left[u_j(\mathbf{x}) \,\hat{b}_j + v_j^*(\mathbf{x}) \,\hat{b}_j^\dagger \right] = u_j \hat{b}_j + v_j^* \hat{b}_j^\dagger \tag{A.20}$$

$$\phi_a(\mathbf{x}) = \sum_j \left[u_j(\mathbf{x}) \,\lambda_j + v_j^*(\mathbf{x}) \,\lambda_j^* \right] = u_j \lambda_j + v_j^* \lambda_j^* \tag{A.21}$$

$$G_N(\mathbf{x}, \mathbf{x}') = \left\langle \hat{\chi}_a^{\dagger}(\mathbf{x}') \, \hat{\chi}_a(\mathbf{x}) \right\rangle = \sum_j v_j(\mathbf{x}') \, v_j^*(\mathbf{x}) = \bar{v}_j v_j^* \tag{A.22}$$

$$G_A(\mathbf{x}, \mathbf{x}') = \langle \hat{\chi}_a(\mathbf{x}') \, \hat{\chi}_a(\mathbf{x}) \rangle = \sum_j u_j(\mathbf{x}') \, v_j^*(\mathbf{x}) = \bar{u}_j v_j^* \tag{A.23}$$

$$\left\langle \hat{\chi}_a(\mathbf{x}') \, \hat{\chi}_a^{\dagger}(\mathbf{x}) \right\rangle = \sum_j u_j(\mathbf{x}') \, u_j^*(\mathbf{x}) = \bar{u}_j u_j^*$$
(A.24)

It will also be important to recall that the Bogoliubov transformation is canonical, so that we have the following commutation relations:

$$\left[\hat{b}_j, \hat{b}_k\right] = 0 \tag{A.25}$$

$$\left[\hat{b}_{j},\hat{b}_{k}^{\dagger}\right] = \delta_{j,k},\tag{A.26}$$

where $\delta_{j,k}$ is the Kronecker delta symbol.

We first prove Equation (2.46). Substitute Equation (A.20) and its Hermitian conjugate into the left hand side of Equation (2.46), substitute Equations (A.21), (A.22), and (A.23) into Equation (2.46)'s right hand side, recall the assumption (A.8), and take care to use distinct summation indices when multiplying two or more sums. In this proof and others, we frequently encounter expectation values of the form $\langle b_j b_k^{\dagger} \rangle$, which we cannot simplify with the assumption (A.8). These averages are handled with the commutation relation (A.26); for example,

$$\left\langle \hat{b}_{j}\hat{b}_{k}^{\dagger}\right\rangle = \left\langle \hat{b}_{j}\hat{b}_{k}^{\dagger} - \hat{b}_{k}^{\dagger}\hat{b}_{j} + \hat{b}_{k}^{\dagger}\hat{b}_{j}\right\rangle = \delta_{j,k} + \lambda_{k}^{*}\lambda_{j}.$$
(A.27)

The commutator (A.26) can be used as many times as necessary in an expectation value so that we only have averages of delta symbols and normal-ordered products of quasiparticle ladder operators, which *can* be simplified using (A.8).

Both sides of Equation (2.46), when written with the aforementioned substitutions, reduce to the expression²

$$v_{j}u_{k}u_{l}\lambda_{j}\lambda_{k}\lambda_{l} + v_{j}v_{j}^{*}u_{l}\lambda_{l} + v_{j}v_{k}^{*}u_{l}\lambda_{l}\lambda_{k}^{*}\lambda_{j} + u_{j}^{*}u_{k}u_{l}\lambda_{j}^{*}\lambda_{k}\lambda_{l} + u_{j}^{*}v_{k}^{*}u_{l}\lambda_{j}^{*}\lambda_{k}^{*}\lambda_{l}$$
$$+ v_{j}u_{k}v_{k}^{*}\lambda_{j} + v_{j}v_{j}^{*}u_{k}\lambda_{k} + v_{j}u_{k}v_{l}^{*}\lambda_{k}\lambda_{l}^{*}\lambda_{j} + v_{j}v_{j}^{*}v_{l}^{*}\lambda_{l}^{*} + v_{j}v_{j}^{*}v_{k}^{*}\lambda_{k}^{*}$$
$$+ v_{j}v_{k}^{*}v_{l}^{*}\lambda_{k}^{*}\lambda_{l}^{*}\lambda_{j} + u_{j}^{*}u_{k}v_{k}^{*}\lambda_{j}^{*} + u_{j}^{*}u_{k}v_{l}^{*}\lambda_{j}^{*}\lambda_{l}^{*}\lambda_{k} + u_{j}^{*}v_{k}^{*}v_{l}^{*}\lambda_{j}^{*}\lambda_{k}^{*}\lambda_{l}^{*}, \qquad (A.28)$$

indicating that (2.46) is true. The factorization (2.47) is found more quickly by taking the Hermitian conjugate of (2.46) and replacing **x** with **x**'.

One can prove Equation (2.48) by substituting Equation (A.20) and its Hermitian conjugate (and taking $\mathbf{x} \to \mathbf{x}'$ where appropriate) into the left hand side of Equation (2.48), and then by substituting (A.21), (A.22), and (A.23) into the right hand side of (2.48). Simplifying as described above, both the right and left hand sides of (2.48)

 $^{^2 \}rm We$ do not combine like terms, since some one who reproduces the calculations is likely to encounter these length ier expressions first.

result in the expression

$$\bar{v}_{j}\bar{v}_{k}\bar{u}_{l}u_{m}\lambda_{j}\lambda_{k}\lambda_{l}\lambda_{m} + \bar{v}_{j}\bar{v}_{k}\bar{u}_{l}v_{l}^{*}\lambda_{j}\lambda_{k} + \bar{v}_{j}\bar{v}_{k}\bar{u}_{l}v_{k}^{*}\lambda_{l}\lambda_{j} + \bar{v}_{j}\bar{v}_{k}\bar{u}_{l}v_{j}^{*}\lambda_{l}\lambda_{k}$$

$$+\bar{v}_{j}\bar{v}_{k}\bar{u}_{l}v_{m}^{*}\lambda_{l}\lambda_{k}\lambda_{m}^{*}\lambda_{j} + \bar{v}_{j}\bar{v}_{k}\bar{v}_{k}^{*}u_{m}\lambda_{m}\lambda_{j} + \bar{v}_{j}\bar{v}_{k}\bar{v}_{j}^{*}u_{m}\lambda_{m}\lambda_{k} + \bar{v}_{j}\bar{v}_{k}\bar{v}_{l}^{*}u_{m}\lambda_{m}\lambda_{k}\lambda_{j}\lambda_{l}^{*}$$

$$+\bar{v}_{j}\bar{v}_{k}\bar{v}_{k}^{*}v_{j}^{*} + \bar{v}_{j}\bar{v}_{k}\bar{v}_{k}^{*}v_{m}^{*}\lambda_{j}\lambda_{m}^{*} + \bar{v}_{j}\bar{v}_{k}\bar{v}_{j}^{*}v_{m}^{*}\lambda_{m}^{*}\lambda_{k}$$

$$+\bar{v}_{j}\bar{v}_{k}\bar{v}_{k}^{*}v_{k}^{*}\lambda_{l}^{*}\lambda_{j} + \bar{v}_{j}\bar{v}_{k}\bar{v}_{k}^{*}v_{m}^{*}\lambda_{j}\lambda_{m}^{*} + \bar{v}_{j}\bar{v}_{k}\bar{v}_{l}^{*}v_{m}^{*}\lambda_{l}^{*}\lambda_{k}\lambda_{m}^{*}\lambda_{k}$$

$$+\bar{v}_{j}\bar{u}_{k}^{*}\bar{u}_{l}u_{m}\lambda_{l}\lambda_{m}\lambda_{j}\lambda_{k}^{*} + \bar{v}_{j}\bar{u}_{j}^{*}\bar{u}_{l}v_{m}^{*}\lambda_{m}^{*}\lambda_{l} + \bar{v}_{j}\bar{u}_{k}^{*}\bar{u}_{l}v_{m}^{*}\lambda_{k}^{*}\lambda_{l}\lambda_{m}$$

$$+\bar{v}_{j}\bar{u}_{k}^{*}\bar{u}_{l}v_{m}^{*}\lambda_{k}^{*}\lambda_{l} + \bar{v}_{j}\bar{u}_{k}^{*}\bar{u}_{l}v_{m}^{*}\lambda_{k}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{j} + \bar{v}_{j}\bar{u}_{k}^{*}\bar{v}_{l}^{*}v_{m}^{*}\lambda_{k}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{l}$$

$$+\bar{v}_{j}\bar{u}_{k}^{*}\bar{v}_{l}^{*}v_{m}^{*}\lambda_{k}^{*}\lambda_{l} + \bar{v}_{j}\bar{u}_{k}^{*}\bar{v}_{l}v_{m}\lambda_{m}^{*}\lambda_{k}^{*}\lambda_{l}\lambda_{m}^{*} + \bar{v}_{j}\bar{u}_{k}^{*}\bar{v}_{l}^{*}v_{m}^{*}\lambda_{k}^{*}\lambda_{l}\lambda_{m}^{*}$$

$$+\bar{v}_{j}\bar{u}_{k}^{*}\bar{v}_{l}^{*}v_{m}^{*}\lambda_{k}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l} + \bar{v}_{j}\bar{u}_{k}^{*}\bar{v}_{l}v_{m}^{*}\lambda_{k}^{*}\lambda_{m}^{*} + \bar{v}_{j}\bar{u}_{k}^{*}\bar{v}_{l}v_{m}^{*}\lambda_{k}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m$$

indicating that Equation (2.48) is true. The factorization (2.49) is found by taking the Hermitian conjugate of (2.48) and interchanging \mathbf{x} and \mathbf{x}' .

One can prove Equation (2.50) by substituting Equation (A.20) and its Hermitian conjugate into the left hand side of (2.50), and Equations (A.21), (A.22), and (A.23) into (2.50)'s right hand side. Both sides of Equation (2.50) then reduce to the

expression

$$\bar{v}_{j}\bar{u}_{k}\bar{u}_{l}u_{m}\lambda_{j}\lambda_{k}\lambda_{l}\lambda_{m} + \bar{v}_{j}\bar{u}_{k}\bar{u}_{l}v_{l}^{*}\lambda_{j}\lambda_{k} + \bar{v}_{j}\bar{u}_{k}\bar{u}_{l}v_{k}^{*}\lambda_{l}\lambda_{j} + \bar{v}_{j}\bar{u}_{k}\bar{u}_{l}v_{k}^{*}\lambda_{l}\lambda_{j} + \bar{v}_{j}\bar{u}_{k}\bar{u}_{m}\bar{v}_{j}^{*}\lambda_{m}\lambda_{k} + \bar{v}_{j}\bar{u}_{k}u_{m}\bar{v}_{l}^{*}\lambda_{m}\lambda_{k}\lambda_{l}^{*}\lambda_{j} \\ + \bar{v}_{j}\bar{u}_{k}\bar{v}_{k}^{*}v_{j}^{*} + \bar{v}_{j}\bar{u}_{k}\bar{v}_{k}^{*}v_{m}^{*}\lambda_{m}^{*}\lambda_{j} + \bar{v}_{j}\bar{u}_{k}\bar{v}_{j}^{*}v_{k}^{*} + \bar{v}_{j}\bar{u}_{k}\bar{v}_{l}^{*}v_{k}^{*}\lambda_{j}\lambda_{l}^{*} \\ + \bar{v}_{j}\bar{u}_{k}\bar{v}_{j}^{*}v_{m}^{*}\lambda_{m}^{*}\lambda_{k} + \bar{v}_{j}\bar{u}_{k}\bar{v}_{l}^{*}v_{m}^{*}\lambda_{l}^{*}\lambda_{k} + \bar{v}_{j}\bar{u}_{k}\bar{v}_{l}^{*}v_{k}^{*} + \bar{v}_{j}\bar{u}_{k}\bar{v}_{l}^{*}v_{k}^{*}\lambda_{j}\lambda_{l}^{*} \\ + \bar{v}_{j}\bar{u}_{k}\bar{v}_{j}^{*}v_{m}^{*}\lambda_{m}^{*}\lambda_{k} + \bar{v}_{j}\bar{u}_{k}\bar{v}_{l}^{*}v_{m}^{*}\lambda_{l}^{*}\lambda_{k} + \bar{v}_{j}\bar{v}_{j}^{*}\bar{u}_{l}v_{m}^{*}\lambda_{l}^{*}\lambda_{k}\lambda_{m}^{*}\lambda_{j} + \bar{v}_{j}\bar{v}_{k}^{*}\bar{u}_{l}u_{m}\lambda_{l}\lambda_{k}\lambda_{k} \\ + \bar{v}_{j}\bar{v}_{k}^{*}\bar{u}_{l}u_{j}^{*}\lambda_{k}^{*}\lambda_{l} + \bar{v}_{j}\bar{v}_{k}^{*}\bar{u}_{l}v_{m}^{*}\lambda_{k}^{*}\lambda_{l} + \bar{v}_{j}\bar{v}_{j}^{*}\bar{u}_{l}v_{m}^{*}\lambda_{k}^{*}\lambda_{l} + \bar{v}_{j}\bar{v}_{k}^{*}\bar{u}_{l}v_{m}^{*}\lambda_{k}^{*}\lambda_{l} \\ + \bar{v}_{j}\bar{v}_{k}^{*}\bar{u}_{l}v_{m}^{*}\lambda_{k}^{*}\lambda_{l}^{*}\lambda_{j} + \bar{v}_{j}\bar{v}_{j}^{*}\bar{v}_{l}^{*}v_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*} + \bar{v}_{j}\bar{v}_{k}^{*}\bar{v}_{l}^{*}v_{m}^{*}\lambda_{k}^{*}\lambda_{l}^{*}\lambda_{k}^{*} \\ + \bar{v}_{j}\bar{v}_{k}^{*}\bar{v}_{l}v_{m}^{*}\lambda_{k}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}} + \bar{v}_{j}\bar{v}_{k}\bar{v}_{l}^{*}v_{m}^{*}\lambda_{k}^{*}\lambda_{l}^{*}\lambda_{l}^{*}\lambda_{l}^{*}\lambda_{l}^{*}\lambda_{l}^{*}\lambda_{l}^{*}\lambda_{l}^{*}\lambda_{l}^{*}\lambda_{l}^{*}\lambda_{l}^{*}\lambda_{l}^{*}\lambda_{l}^{*}\lambda_{l}^{*}\lambda_{l}^{*}\lambda_{l}^{*}\lambda_{l}^{*}\lambda_{l}^{*}\lambda_{l}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{l}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}$$

Thus, Equation (2.50) is true.

The last factorization we use is Equation (2.51). We substitute Equation (A.20) and its Hermitian conjugate into the left hand side of (2.51), and Equations (A.21), (A.23), (A.22), and (A.24) into the right hand side of (2.51). Then both sides of

Equation (2.51) reduce to the expression

$$\bar{u}_{j}v_{k}u_{l}u_{m}\lambda_{j}\lambda_{k}\lambda_{l}\lambda_{m} + \bar{u}_{j}v_{k}u_{l}v_{l}^{*}\lambda_{j}\lambda_{k} + \bar{u}_{j}v_{k}u_{l}v_{k}^{*}\lambda_{l}\lambda_{j} + \bar{u}_{j}v_{k}u_{l}v_{j}^{*}\lambda_{l}\lambda_{k}$$

$$+\bar{u}_{j}v_{k}u_{l}v_{m}^{*}\lambda_{l}\lambda_{k}\lambda_{m}^{*}\lambda_{j} + \bar{u}_{j}v_{k}v_{k}^{*}u_{m}\lambda_{m}\lambda_{j} + \bar{u}_{j}v_{k}v_{j}^{*}u_{m}\lambda_{m}\lambda_{k} + \bar{u}_{j}v_{k}v_{l}^{*}u_{m}\lambda_{m}\lambda_{k}\lambda_{l}^{*}\lambda_{j}$$

$$+\bar{u}_{j}v_{k}v_{k}^{*}v_{j}^{*} + \bar{u}_{j}v_{k}v_{k}^{*}v_{m}^{*}\lambda_{m}^{*}\lambda_{j} + \bar{u}_{j}v_{k}v_{j}^{*}v_{k}^{*} + \bar{u}_{j}v_{k}v_{l}^{*}v_{k}^{*}\lambda_{l}^{*}\lambda_{j}$$

$$+\bar{u}_{j}v_{k}v_{j}^{*}v_{m}^{*}\lambda_{m}^{*}\lambda_{k} + \bar{u}_{j}v_{k}v_{l}^{*}v_{j}^{*}\lambda_{k}^{*}\lambda_{l} + \bar{u}_{j}v_{k}v_{l}^{*}v_{m}^{*}\lambda_{l}^{*}\lambda_{k}\lambda_{l}^{*}\lambda_{j}$$

$$+\bar{u}_{j}u_{k}^{*}v_{l}^{*}v_{m}^{*}\lambda_{m}^{*}\lambda_{k} + \bar{u}_{j}v_{k}v_{l}^{*}v_{j}^{*}\lambda_{k}^{*}\lambda_{k} + \bar{u}_{j}v_{k}v_{l}^{*}v_{m}^{*}\lambda_{k}^{*}\lambda_{k}\lambda_{m}^{*}\lambda_{j}$$

$$+\bar{u}_{j}u_{j}^{*}u_{l}u_{m}\lambda_{l}\lambda_{m} + \bar{u}_{j}u_{k}^{*}u_{l}v_{j}^{*}\lambda_{k}^{*}\lambda_{l} + \bar{u}_{j}u_{k}^{*}u_{l}v_{m}^{*}\lambda_{k}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{j}$$

$$+\bar{u}_{j}u_{j}^{*}v_{l}^{*}u_{m}\lambda_{m}\lambda_{l}^{*} + \bar{u}_{j}u_{k}^{*}v_{l}^{*}u_{m}\lambda_{m}\lambda_{k}^{*} + \bar{u}_{j}u_{k}^{*}v_{l}^{*}u_{m}\lambda_{m}\lambda_{k}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{l}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}^{*}\lambda_{m}\lambda_{l}\lambda_{m}^{*}\lambda_{m$$

so Equation (2.51) is true.

APPENDIX B

SCATTERING IN COUPLED SQUARE WELLS

Kokkelmans *et al.* [14] consider scattering in coupled square wells as one step in the derivation of a renormalized contact potential model of a Feshbach resonance. Here, we treat the square well system in some detail.

Similar to Reference [14]'s Figure 3, consider the coupled square well system in our Figure B.1. This model could represent two incident particles of combined energy E with separation r. The open channel potential $V_P(\mathbf{r})$ is zero for r greater than the potentials' range R, while the closed channel potential $V_Q(\mathbf{r})$ is a constant $\epsilon > E > 0$ for r > R. Inside the wells, $V_P(\mathbf{r}) = -V_1$ and $V_Q(\mathbf{r}) = -V_2$, both constant, and the wavefunctions $\psi_P(\mathbf{r})$ and $\psi_Q(\mathbf{r})$ are coupled by the complex constant g. Since there is no coupling for r > R, we write g as a function of r below.

Two coupled Schrödinger equations model the situation:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_P(\mathbf{r})\right]\psi_P(\mathbf{r}) + g(\mathbf{r})\,\psi_Q(\mathbf{r}) = E\psi_P(\mathbf{r}) \tag{B.1}$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_Q(\mathbf{r})\right]\psi_Q(\mathbf{r}) + g^*(\mathbf{r})\,\psi_P(\mathbf{r}) = E\psi_Q(\mathbf{r})\,,\tag{B.2}$$

where we choose to work in spherical coordinates. Assuming no angular dependence of the wavefunctions and making the substitutions

$$\psi_Q(r) = \frac{u_Q(r)}{r} \text{ and } \psi_P(r) = \frac{u_P(r)}{r},$$
 (B.3)



Figure B.1: Coupled square wells. The open $[V_P(\mathbf{r}), \text{ bold red}]$ and closed $[V_Q(\mathbf{r}), \text{ dotted blue}]$ channel potentials are negative for r < R and zero and ϵ , respectively, for r > R. The combined energy of the two colliding particles is E, which is greater than zero but less than ϵ . The open and closed channel wavefunctions are coupled only when r < R.

Equations (B.1) and (B.2) simplify to

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V_P(r)\right]u_P(r) + g(r)u_Q(r) = Eu_P(r) \tag{B.4}$$

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V_Q(r)\right]u_Q(r) + g^*(r)\,u_P(r) = Eu_Q(r)\,. \tag{B.5}$$

B.1 Interior Solutions

We first consider the interior region, where $r \leq R$ and the equations simplify to

$$-\frac{\hbar^2}{2m}u_P''(r) - V_1 u_P(r) + g u_Q(r) = E u_P(r)$$
(B.6)

$$-\frac{\hbar^2}{2m}u_Q''(r) - V_2 u_Q(r) + g^* u_P(r) = E u_Q(r).$$
(B.7)

Solving Equation (B.6) for $u_Q(r)$ and substituting into Equation (B.7) decouples the equations; then

$$u_Q(r) = \frac{1}{g} \left(E + V_1 \right) u_P(r) + \frac{1}{g} \frac{\hbar^2}{2m} u_P''(r)$$
(B.8)

$$u_P^{(4)}(r) + b \, u_P''(r) + c \, u_P(r) = 0, \tag{B.9}$$

where, for brevity, we define

$$b = \frac{2m}{\hbar^2} \left(2E + V_1 + V_2 \right) \tag{B.10}$$

$$c = \frac{4m^2}{\hbar^4} \left[(E + V_1) \left(E + V_2 \right) - |g|^2 \right].$$
 (B.11)

We attempt solutions of the form e^{xr} , where x is a constant to be determined. Substituting this solution into Equation (B.9), we have

$$x^4 + b\,x^2 + c = 0, (B.12)$$

a quadratic equation in x^2 . There are four solutions for x:

$$x_1 = i \frac{1}{\sqrt{2}} \sqrt{b + \sqrt{b^2 - 4c}}, \quad x_2 = -i \frac{1}{\sqrt{2}} \sqrt{b + \sqrt{b^2 - 4c}},$$

$$x_3 = \frac{1}{\sqrt{2}}\sqrt{-b + \sqrt{b^2 - 4c}}, \text{ and } x_4 = -\frac{1}{\sqrt{2}}\sqrt{-b + \sqrt{b^2 - 4c}}.$$
 (B.13)

Notice that, since we are only considering E > 0 (otherwise the open channel would not be open) and V_1 and V_2 both positive (otherwise the potentials would not be wells), b is strictly positive. Requiring

$$b^2 - 4c > 0 \tag{B.14}$$

is not very limiting; substituting Equations (B.10) and (B.11) into (B.14) gives

$$-4|g|^{2} < (V_{1} - V_{2})^{2}, \qquad (B.15)$$

which is true for all nonzero g and V_1 and V_2 both real. We henceforth accept these lenient restrictions.

Now we are assured that x_1 and x_2 are both purely imaginary and complex conjugates. We combine the solutions corresponding to x_1 and x_2 into

$$u_P(r) = A\sin\left(r\frac{1}{\sqrt{2}}\sqrt{b+\sqrt{b^2-4c}}\right) \tag{B.16}$$

$$u_Q(r) = \frac{1}{g} A \left[E + V_1 - \frac{1}{2} \frac{\hbar^2}{2m} \left(b + \sqrt{b^2 - 4c} \right) \right] \sin \left(r \frac{1}{\sqrt{2}} \sqrt{b + \sqrt{b^2 - 4c}} \right), \quad (B.17)$$

where A is a constant to be determined, and we have discarded the cosine solutions, since the wavefunctions $\psi_P(r)$ and $\psi_Q(r)$ must be bounded, and

$$\lim_{r \to 0} \frac{\cos\left(r\right)}{r} \to \infty. \tag{B.18}$$

More solutions exist, but their general form depends on the particular physical

parameters. For the situation we call "weak coupling," where

$$-b + \sqrt{b^2 - 4c} < 0 \implies c > 0 \implies (E + V_1) (E + V_2) > |g|^2$$
, (B.19)

 x_3 and x_4 are imaginary and complex conjugates. The corresponding solutions which are bounded at the origin when divided by r are

$$u_P(r) = B \sin\left(r\frac{1}{\sqrt{2}}\sqrt{b - \sqrt{b^2 - 4c}}\right) \tag{B.20}$$

$$u_Q(r) = \frac{1}{g} B \left[E + V_1 - \frac{1}{2} \frac{\hbar^2}{2m} \left(b - \sqrt{b^2 - 4c} \right) \right] \sin \left(r \frac{1}{\sqrt{2}} \sqrt{b - \sqrt{b^2 - 4c}} \right).$$
(B.21)

Note that these are linearly independent from the everpresent solutions (B.16) and (B.17), since the arguments of the sine functions are different.

For the "strong coupling" situation, where

$$-b + \sqrt{b^2 - 4c} > 0 \implies c < 0 \implies (E + V_1) (E + V_2) < |g|^2,$$
 (B.22)

 x_3 and x_4 are both purely real. Then the corresponding solutions

$$u_P(r) = C \sinh\left(r\frac{1}{\sqrt{2}}\sqrt{-b+\sqrt{b^2-4c}}\right)$$
(B.23)
$$u_Q(r) = \frac{1}{g}C\left[E+V_1 + \frac{1}{2}\frac{\hbar^2}{2m}\left(-b+\sqrt{b^2-4c}\right)\right]\sinh\left(r\frac{1}{\sqrt{2}}\sqrt{-b+\sqrt{b^2-4c}}\right).$$
(B.24)

The remaining case, that of "moderate coupling," concerns

$$-b + \sqrt{b^2 - 4c} = 0 \implies c = 0 \implies (E + V_1) (E + V_2) = |g|^2.$$
 (B.25)

Since c = 0, the differential equation reduces to

$$u_P^{(4)}(r) + b \, u_P''(r) = 0, \tag{B.26}$$

which has linearly independent solutions

$$\sin\left(r\sqrt{b}\right), \ \cos\left(r\sqrt{b}\right), \ r, \ \alpha,$$
 (B.27)

where α is a constant. The cosine and constant solutions diverge at the origin when divided by r. The sine solution is equivalent to that in Equation (B.16), so that (B.16) and (B.17) are still valid. Then the only new solutions are

$$u_P(r) = Dr \tag{B.28}$$

$$u_Q(r) = \frac{1}{g} D \left(E + V_1 \right) r.$$
 (B.29)

B.2 Exterior Solutions

For $r \ge R$, Equations (B.4) and (B.5) simplify to

$$-\frac{\hbar^2}{2m}u_P''(r) - E u_P(r) = 0$$
 (B.30)

$$-\frac{\hbar^2}{2m}u_Q''(r) + (\epsilon - E) = 0, \qquad (B.31)$$

which are uncoupled and may be solved immediately to give

$$u_P(r) = F \sin\left(r\sqrt{\frac{2mE}{\hbar^2}} + G\right) \tag{B.32}$$

$$u_Q(r) = L \exp\left[-r\sqrt{\frac{2m}{\hbar^2}} \left(\epsilon - E\right)\right],\tag{B.33}$$

where we have discarded the $u_Q(r) \sim e^r$ solution because

$$\lim_{r \to \infty} \frac{\mathrm{e}^r}{r} \to \infty. \tag{B.34}$$

B.3 Matching at the Well Boundary

Solutions to the Schrödinger equation must be finite anywhere the potential is bounded. We must also have a continuous wavefunction, even where the potential is discontinuous or has a singularity; that is,

$$\psi_{\text{out}}(R) = \psi_{\text{in}}(R), \qquad (B.35)$$

where ψ_{out} is an exterior solution and ψ_{in} is an interior solution. Using a substitution like those in (B.3), we have

$$\frac{u_{\text{out}}(R)}{R} = \frac{u_{\text{in}}(R)}{R} \Rightarrow u_{\text{out}}(R) = u_{\text{in}}(R).$$
(B.36)

The first derivative of a solution must also be continuous anywhere the potential is bounded; that is,

$$\psi_{\text{out}}'(r)|_{R} = \psi_{\text{in}}'(r)|_{R} \Rightarrow \left[\frac{u_{\text{out}}'(r)}{r} - \frac{u_{\text{out}}(r)}{r^{2}}\right]_{R} = \left[\frac{u_{\text{in}}'(r)}{r} - \frac{u_{\text{in}}(r)}{r^{2}}\right]_{R}$$
$$\Rightarrow u_{\text{out}}'(r)|_{R} = u_{\text{in}}'(r)|_{R}.$$
(B.37)

To be concise, we define

$$k_0 = \frac{1}{\sqrt{2}}\sqrt{b + \sqrt{b^2 - 4c}} = \frac{\sqrt{m}}{\hbar}\sqrt{2E + V_1 + V_2 + \sqrt{(V_1 - V_2)^2 + 4|g|^2}}$$
(B.38)

$$k_W = \frac{1}{\sqrt{2}}\sqrt{b - \sqrt{b^2 - 4c}} = \frac{\sqrt{m}}{\hbar}\sqrt{2E + V_1 + V_2 - \sqrt{(V_1 - V_2)^2 + 4|g|^2}}$$
(B.39)

$$k_{S} = \frac{1}{\sqrt{2}}\sqrt{-b + \sqrt{b^{2} - 4c}} = \frac{\sqrt{m}}{\hbar}\sqrt{-2E - V_{1} - V_{2} + \sqrt{(V_{1} - V_{2})^{2} + 4|g|^{2}}} \quad (B.40)$$

$$k_M = \sqrt{b} = \frac{\sqrt{2m}}{\hbar} \sqrt{2E + V_1 + V_2} \tag{B.41}$$

$$k_P = \sqrt{\frac{2mE}{\hbar^2}} \tag{B.42}$$

$$\tau_Q = \sqrt{\frac{2m}{\hbar^2} \left(\epsilon - E\right)}.$$
(B.43)

Since the overall norm is arbitrary in scattering problems, we take A = 1 for simplicity. Then the matching conditions for weak coupling are

$$\sin(k_0 R) + B\sin(k_W R) = F\sin(k_P R + G)$$

$$k_0 \cos(k_0 R) + Bk_W \cos(k_W R) = Fk_P \cos(k_P R + G)$$

$$\left(E + V_1 - \frac{\hbar^2 k_0^2}{2m}\right) \sin(k_0 R) + B\left(E + V_1 - \frac{\hbar^2 k_W^2}{2m}\right) \sin(k_W R) = Lg e^{-\tau_Q R}$$

$$k_0 \left(E + V_1 - \frac{\hbar^2 k_0^2}{2m}\right) \cos(k_0 R) + Bk_W \left(E + V_1 - \frac{\hbar^2 k_W^2}{2m}\right) \cos(k_W R) = -L\tau_Q g e^{-\tau_Q R}.$$
(B.44)

For strong coupling, the conditions are

$$\sin(k_0 R) + C \sinh(k_S R) = F \sin(k_P R + G)$$

$$k_0 \cos(k_0 R) + Ck_S \cosh(k_S R) = Fk_P \cos(k_P R + G)$$

$$\left(E + V_1 - \frac{\hbar^2 k_0^2}{2m}\right) \sin(k_0 R) + C \left(E + V_1 + \frac{\hbar^2 k_S^2}{2m}\right) \sinh(k_S R) = Lg e^{-\tau_Q R}$$

$$k_0 \left(E + V_1 - \frac{\hbar^2 k_0^2}{2m}\right) \cos(k_0 R) + Ck_S \left(E + V_1 + \frac{\hbar^2 k_S^2}{2m}\right) \cosh(k_S R) = -L\tau_Q g e^{-\tau_Q R}.$$
(B.45)

For moderate coupling, the conditions are

$$\sin(k_0 R) + DR = F \sin(k_P R + G)$$

$$k_0 \cos(k_0 R) + D = F k_P \cos(k_P R + G)$$

$$\left(E + V_1 - \frac{\hbar^2 k_0^2}{2m}\right) \sin(k_0 R) + D(E + V_1) R = Lg e^{-\tau_Q R}$$

$$k_0 \left(E + V_1 - \frac{\hbar^2 k_0^2}{2m}\right) \cos(k_0 R) + D(E + V_1) = -L\tau_Q g e^{-\tau_Q R}.$$
(B.46)

Note that in each case the constants k_0 , F, and G are different.

B.4 Example

One can solve the systems (B.44), (B.45), and (B.46) for the necessary constants [the identities $F \sin (k_P R + G) = F \cos (G) \sin (k_P R) + F \sin (G) \cos (k_P R)$ and $F \cos (k_P R + G) = F \cos (G) \cos (k_P R) - F \sin (G) \sin (k_P R)$ are useful], but the complicated expressions are not especially edifying, so we proceed immediately to an example.

We use parameters appropriate on an atomic scale:

$$R = a_0$$

$$V_1 = 13.6 \text{ eV}$$

$$V_2 = 1.1 \times 13.6 \text{ eV}$$

$$\epsilon = 0.1 \times 13.6 \text{ eV}$$

$$E = 0.05 \times 13.6 \text{ eV}$$

$$m = 2m_P,$$
(B.47)

where a_0 is the Bohr radius and m_P is the mass of a proton. For the case of weak coupling, we use $g = 0.1 \times \sqrt{(E+V_1)(E+V_2)}$; for strong coupling, $g = 10 \times \sqrt{(E+V_1)(E+V_2)}$; and for moderate coupling, $g = \sqrt{(E+V_1)(E+V_2)}$. The phase shifts G calculated from the matching conditions are then 2.2808, 2.1999, and 2.3088 for weak, strong, and moderate coupling, respectively. Figures B.2 through B.7 show the wavefunctions $\psi_P(r)$ and $\psi_Q(r)$ for the three different coupling regimes. Only in the case of moderate coupling are the amplitudes of the open and closed channel wavefunctions comparable, and only in this case are the oscillations of the two wavefunctions perfectly out of phase within the inner region. In every plot, the wavefunction is finite for r = 0 (though this does not appear in the plots, since the vertical axes do not encompass the full range of the wavefunctions) and the wavefunctions and their first derivatives are continuous.



Figure B.2: Weak coupling, open channel.



Figure B.3: Weak coupling, closed channel.



Figure B.4: Strong coupling, open channel.



Figure B.5: Strong coupling, closed channel.



Figure B.6: Moderate coupling, open channel.



Figure B.7: Moderate coupling, closed channel.

APPENDIX C

RECURRENCE RELATIONS IN EIGENFUNCTION EXPANSIONS

When expanding the correlation functions in a basis of eigenfunctions, we have in mind equating the expansion coefficients on each side of equations involving those correlation functions. To do so, each side of the equation must be summed over exactly the same linearly independent eigenfunctions.

C.1 Laplace Series

As described in [84], for example, a well-behaved and generally complex scalar function $G(\theta, \phi)$ of polar and azimuthal angles θ and ϕ , respectively, can be expanded in a Laplace series, an infinite sum over spherical harmonics $Y_l^m(\theta, \phi)$:

$$G(\theta,\phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} G^{l,m} Y_l^m(\theta,\phi) , \qquad (C.1)$$

where $G^{l,m}$ is a complex expansion coefficient. The series (C.1) is uniformly convergent, allowing summation to commute with both integration and differentiation.

A spherical harmonic is a normalized product of an associated Legendre polynomial and a complex exponential:

$$Y_l^m(\theta,\phi) = N_l^m P_l^m(\cos\theta) e^{im\phi}, \qquad (C.2)$$

where

$$N_l^m \equiv (-1)^m \sqrt{\frac{(2l+1)}{4\pi} \frac{(l-m)!}{(l+m)!}}.$$
 (C.3)

The spherical harmonics are eigenfunctions of the angular part of the Laplacian in spherical coordinates; that is,

$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]Y_l^m(\theta,\phi) = -l\left(l+1\right)Y_l^m(\theta,\phi).$$
(C.4)

Using the recurrence relations for associated Legendre polynomials found in [84] and [109], a constant multiple or an angular derivative of a Laplace series can often be reduced to some algebraic manipulation of the original series. Consider

$$\cos\theta \sum_{l=0}^{\infty} \sum_{m=-l}^{l} G^{l,m} Y_l^m(\theta,\phi); \qquad (C.5)$$

using a recurrence relation for associated Legendre polynomials,

$$\cos\theta P_{l}^{m}(\cos\theta) = \frac{l+m}{2l+1} P_{l-1}^{m}(\cos\theta) + \frac{l-m+1}{2l+1} P_{l+1}^{m}(\cos\theta), \quad (C.6)$$

the series (C.5) becomes

$$\cos \theta \sum_{l=0}^{\infty} \sum_{m=-l}^{l} G^{l,m} Y_{l}^{m}(\theta, \phi) = S_{1} + S_{2}, \qquad (C.7)$$

where

$$S_{1} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} N_{l}^{m} \frac{l+m}{2l+1} P_{l-1}^{m}(\cos\theta) e^{im\phi} G^{l,m}$$
(C.8)

$$S_2 = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} N_l^m \frac{l-m+1}{2l+1} P_{l+1}^m(\cos\theta) e^{im\phi} G^{l,m}.$$
 (C.9)

In the sum (C.8), observe that $l = 0 \Rightarrow m = 0 \Rightarrow l + m = 0$, so we can start the sum over l at 1. Also, $m = -l \Rightarrow l + m = 0$, so the sum over m can start at -l + 1. Then, defining an associated Legendre polynomial in terms of its Rodrigues' formula,

$$P_l^m(\cos\theta) \equiv \left(1 - \cos^2\theta\right)^{m/2} \frac{\mathrm{d}^m}{\mathrm{d}\left(\cos\theta\right)^m} P_l(\cos\theta), \qquad (C.10)$$

we see that $P_l^m(\cos\theta) \equiv 0$ for any |m| > l, since $P_l(\cos\theta)$ (an ordinary Legendre polynomial) is an l^{th} order polynomial. (The negative values of m are handled by defining the ordinary Legendre polynomials in terms of their own Rodrigues' formula.) This fact entitles us to end the sum over m at l - 1, giving

$$S_1 = \sum_{l=1}^{\infty} \sum_{m=-l+1}^{l-1} N_l^m \frac{l+m}{2l+1} P_{l-1}^m(\cos\theta) e^{im\phi} G^{l,m}.$$
 (C.11)

Now allowing $l \to l+1$ throughout the series (C.11) and defining \mathcal{N}_{l+1}^m such that $\mathcal{N}_{l+1}^m = N_{l+1}^m/N_l^m$, we have

$$S_1 = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \mathcal{N}_{l+1}^m \frac{l+m+1}{2l+3} Y_l^m(\theta,\phi) G^{l+1,m}.$$
 (C.12)

No terms are obviously zero in the series (C.9), so begin by letting $l \rightarrow l - 1$:

$$S_2 = \sum_{l=1}^{\infty} \sum_{m=-l+1}^{l-1} N_{l-1}^m \frac{l-m}{2l-1} P_l^m(\cos\theta) e^{im\phi} G^{l-1,m}.$$
 (C.13)

Now the m = l term vanishes, so the sum over m can end at l. We would like to start the sum over m at -l, but this would result in extra, non-zero terms, so we introduce a step function u_{-l+1}^m such that¹

¹This is different from the usual Heaviside step function (as defined in [84], for example), which

$$u_{-l+1}^{m} = \begin{cases} 1, & m \ge -l+1\\ 0, & m < -l+1 \end{cases}$$
(C.14)

Notice that multiplying S_2 by this factor will also allow us to include the l = 0 term, since both $u_1^0 = 0$ and $l = 0 \Rightarrow m = 0 \Rightarrow l - m = 0$. Now Equation (C.13) can be written

$$S_2 = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} u_{-l+1}^m \mathcal{N}_{l-1}^m \frac{l-m}{2l-1} Y_l^m(\theta,\phi) G^{l-1,m}.$$
 (C.15)

Using Equations (C.12) and (C.15), one could now express (C.5) without any mention of the angle θ outside of a spherical harmonic, just altering the coefficient on each spherical harmonic in the Laplace series.

Next, consider the Laplace series

$$\sin\theta \frac{\partial}{\partial\theta} \sum_{l=0}^{\infty} \sum_{m=-1}^{l} G^{l,m} Y_l^m(\theta,\phi) = S_3 + S_4, \tag{C.16}$$

where

$$S_3 = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} N_l^m \left(l+m\right) \left(\frac{l}{2l+1} - 1\right) P_{l-1}^m(\cos\theta) e^{im\phi} G^{l,m}$$
(C.17)

$$S_4 = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} N_l^m \frac{l(l-m+1)}{2l+1} P_{l+1}^m(\cos\theta) e^{im\phi} G^{l,m},$$
(C.18)

which is obtained from a recurrence relation for associated Legendre polynomials. The strategy for dealing with S_3 is identical to the one we used for S_1 ; the l = 0 and |m| = l terms vanish. Then re-indexing with $l \rightarrow l + 1$, one obtains

would be undefined at the point m = -l + 1.

$$S_3 = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \mathcal{N}_{l+1}^m \left(l+m+1\right) \left(\frac{l+1}{2l+3}-1\right) Y_l^m(\theta,\phi) \, G^{l+1,m}. \tag{C.19}$$

In a treatment similar, though not identical, to that for S_2 , we notice that the l = 0 term contributes nothing to the series (C.18), and then let $l \to l - 1$. With this substitution, the m = l and l = 1 terms vanish and so may be included. Then we can include the non-zero m = -l terms if we multiply S_4 by the step function (C.14). Including the l = 0 term, since both $u_1^0 = 0$ and $l = 0 \Rightarrow m = 0 \Rightarrow l - m = 0$, we have

$$S_4 = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} u_{-l+1}^m \mathcal{N}_{l-1}^m \frac{(l-1)(l-m)}{2l-1} Y_l^m(\theta,\phi) G^{l-1,m}.$$
 (C.20)

Again, Equations (C.19) and (C.20) allow us to express a multiple and derivative of a Laplace series as some algebraic manipulation and shifting of the coefficient on each spherical harmonic in the series.

C.2 Cosine Series

A continuous, generally complex scalar function $G(\phi)$ of an angle $\phi \in [0, 2\pi]$ can be expanded in a series of cosines,

$$G(\phi) = \sum_{n=0}^{\infty} G^n \cos(n\phi) , \qquad (C.21)$$

where G^n is the n^{th} generally complex expansion coefficient. We will assume that the series is uniformly convergent, which will be true if $\frac{\partial}{\partial \phi}G$ is continuous, so that we may differentiate term-by-term. If the condition for uniform convergence does not hold, we will still differentiate term-by-term, with the knowledge that we will truncate the series.

$$S_5 = \cos\phi G(\phi); \qquad (C.22)$$

using $2\cos A\cos B = \cos (A - B) + \cos (A + B)$, we have

$$S_5 = \frac{1}{2} \sum_{n=0}^{\infty} G^n \cos\left[(n-1)\phi\right] + \frac{1}{2} \sum_{n=0}^{\infty} \cos\left[(n+1)\phi\right].$$
 (C.23)

Reindexing the sums in (C.23) gives

$$S_5 = \frac{1}{2} \sum_{n=-1}^{\infty} G^{n+1} \cos(n\phi) + \frac{1}{2} \sum_{n=1}^{\infty} G^{n-1} \cos(n\phi) \,. \tag{C.24}$$

Recalling that cosines are even, we can use convenient notation to start both sums at n = 0:

$$S_5 = \sum_{n=0}^{\infty} \frac{1}{2} \left(G^{n+1} + G^{n-1} + G^0 \,\delta_{1,n} \right) \cos\left(n\phi\right). \tag{C.25}$$

Next, consider

$$S_6 = \sin \phi \frac{\partial}{\partial \phi} G(\phi) \,. \tag{C.26}$$

As noted above, we formally differentiate term-by-term, and use $2 \sin A \sin B = \cos (A - B) - \cos (A + B)$ to write

$$S_6 = \frac{1}{2} \sum_{n=0}^{\infty} G^n n \cos\left[(n+1)\phi\right] - \frac{1}{2} \sum_{n=0}^{\infty} G^n n \cos\left[(n-1)\phi\right].$$
 (C.27)

Reindexing the sums and applying convenient notation as before, we have

$$S_6 = \frac{1}{2} \sum_{n=0}^{\infty} \left[G^{n-1} u_1^n \left(n-1 \right) - G^{n+1} \left(n+1 \right) \right] \cos\left(n\phi \right).$$
 (C.28)

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Finally,

$$S_7 = \frac{\partial^2}{\partial \phi^2} G(\phi) \tag{C.29}$$

requires no trigonometric identities; we differentiate term by term twice and get

$$S_7 = -\sum_{n=0}^{\infty} G^n n^2 \cos(n\phi) \,.$$
 (C.30)

APPENDIX D

DERIVATION OF A RUNGE-KUTTA METHOD

We want to solve the ordinary differential equation

$$\frac{\mathrm{d}\psi}{\mathrm{d}x} = f(\psi, x) \tag{D.1}$$

for $\psi(x)$, with the initial condition $\psi_n = \psi(x_n)$. Assuming analytical methods are unavailable or unfeasible, we intend to find an approximation to the solution at some point, $\psi(x_n + h)$. We could use a truncated Taylor series expansion

$$\psi(x_n + h) \approx \sum_{i=0}^{4} \left. \frac{h^i}{i!} \frac{\mathrm{d}^i}{\mathrm{d}x^i} \psi(x) \right|_{x=x_n},\tag{D.2}$$

but cannot or wish not to use analytical derivatives of $\psi(x)$. We will attempt to find constants w_i , a_i , and B_{ij} such that

$$\psi(x_n + h) \approx \psi(x_n) + \sum_{i=1}^4 w_i k_i, \qquad (D.3)$$

where

$$k_i = hf\left(x_n + a_ih, \psi_n + \sum_{j=1}^{i-1} B_{ij}k_j\right).$$
 (D.4)

Such a method is a fourth order Runge-Kutta method. The extensive algebra required by a brute-force calculation is somewhat alleviated by using convenient, though perhaps non-obvious, notation. To this end, the derivation will closely follow that given by Ralston [110].

D.1 Taylor Series Expansion of the Approximate Solution

Substituting Equation (D.1) into (D.2) and re-indexing gives

$$\psi(x_n + h) \approx \psi_n + \sum_{i=0}^3 \frac{h^{i+1}}{(i+1)!} \frac{\mathrm{d}^i}{\mathrm{d}x^i} f(\psi, x) \Big|_{x=x_n}.$$
 (D.5)

Note that evaluating everything at x_n includes evaluating ψ at x_n . Applying the chain rule and again using Equation (D.1), we have

$$\psi(x_n+h) \approx \psi_n + \sum_{i=0}^3 \frac{h^{i+1}}{(i+1)!} \left(\frac{\partial}{\partial x} + f\frac{\partial}{\partial \psi}\right)^i f(\psi, x) \Big|_{x=x_n}.$$
 (D.6)

Here is an important opportunity for expedient notation. Define a differential operator D such that

$$D = \frac{\partial}{\partial x} + \psi_n \frac{\partial}{\partial \psi},\tag{D.7}$$

where we are careful to note that ψ_n is simply a constant and thus can be factored out of any differentiation.

Equation (D.6) can be expanded in terms of D. For example, observe that

$$\left(\frac{\partial}{\partial x} + f \frac{\partial}{\partial \psi} \right) f \Big|_{x=x_n} = Df$$

$$(f_x + f f_{\psi}) \Big|_{x=x_n} = (f_x + f_n f_{\psi}) \Big|_{x=x_n},$$

$$(D.8)$$

where f_x means the partial derivative of f with respect to x. Also,

$$\left(\frac{\partial}{\partial x} + f\frac{\partial}{\partial \psi}\right)^2 f\Big|_{x=x_n} = D^2 f + f_{\psi} D f\Big|_{x=x_n}$$
(D.9)

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial x} f \frac{\partial}{\partial \psi} + f \frac{\partial}{\partial \psi} \frac{\partial}{\partial x} + f \frac{\partial}{\partial \psi} f \frac{\partial}{\partial \psi} \right) \Big|_{x=x_n}$$

$$= \left[\left(\frac{\partial^2}{\partial x^2} + 2f_n \frac{\partial}{\partial x} \frac{\partial}{\partial \psi} + f_n^2 \frac{\partial^2}{\partial \psi^2} \right) f + f_\psi \left(\frac{\partial}{\partial x} + f_n \frac{\partial}{\partial \psi} \right) f \right] \Big|_{x=x_n}$$
(D.10)

$$\left(f_{xx} + f_x f_{\psi} + 2f f_{x\psi} + f f_{\psi}^2 + f^2 f_{\psi\psi} \right) \Big|_{x=x_n}$$

= $\left(f_{xx} + f_x f_{\psi} + 2f_n f_{x\psi} + f_n f_{\psi}^2 + f_n^2 f_{\psi\psi}^2 \right) \Big|_{x=x_n},$ (D.11)

where we have carefully applied the product rule and assumed that the order of partial differentiation is unimportant; e.g., $f_{x\psi} = f_{\psi x}$. This is not a very restrictive assumption, and is reasonable for most functions encountered in the modeling of nature. With identical methods and much more work, one can prove

$$\left(\frac{\partial}{\partial x} + f\frac{\partial}{\partial \psi}\right)^3 f\Big|_{x=x_n} = \left(D^3f + f_{\psi}D^2f + f_{\psi}^2Df + 3DfDf_{\psi}\right)\Big|_{x=x_n}, \qquad (D.12)$$

and Equation (D.6) expands to

$$\psi(x_n + h) - \psi_n \approx \left[hf + \frac{h^2}{2} Df + \frac{h^3}{6} \left(D^2 f + f_{\psi} Df \right) + \frac{h^4}{24} \left(D^3 f + f_{\psi} D^2 f + f_{\psi}^2 Df + 3Df Df_{\psi} \right) \right] \Big|_{x=x_n}.$$
 (D.13)

D.2 Series Expansion of the Runge-Kutta Approximation

We wish to match the coefficients on each factor of h in Equation (D.13) to those in (D.3). To do this we need to expand each k_i as a Taylor series. Taking $a_1 = 0$, we can immediately write

$$k_1 = h f_n. \tag{D.14}$$

That result gives for k_2

$$k_2 = hf \left(x_n + a_2 h, \psi_n + B_{21} h f_n\right). \tag{D.15}$$

 k_3 and k_4 , like k_2 , will have right-hand sides of the form

$$f\left[x_n + a_i h, \psi_n + h f_n \sum_{j=1}^{i-1} B_{ij}\right],$$
 (D.16)

which, expanded as a Taylor series in two variables, is

$$\sum_{l=0}^{\infty} \frac{h^l}{l!} \left[a_i \frac{\partial}{\partial x} + \left(f_n \sum_{j=1}^{i-1} B_{ij} \right) \frac{\partial}{\partial \psi} \right]^l f(x, \psi) \Big|_{x=x_n}.$$
 (D.17)

Here is the second important opportunity for concise notation. Define another differential operator D_i such that

$$D_i = a_i \frac{\partial}{\partial x} + \left(f_n \sum_{j=1}^{i-1} B_{ij} \right) \frac{\partial}{\partial \psi}.$$
 (D.18)

Note that this operator is slightly different from D, defined earlier, in that D_i is exactly the operator appearing in the Taylor series expansion of the given function, while D was a slightly modified version. Now we can write Equation (D.15), truncated after fourth order in h, as

$$k_2 = hf + h^2 D_2 f + \frac{1}{2} h^3 D_2^2 f + \frac{1}{6} h^4 D_2^3 f.$$
 (D.19)

We wish to get k_3 in a form resembling (D.16), so we write it as

$$k_3 = hf \left[x_n + a_3 h, \psi_n + (B_{31} + B_{32}) hf_n + B_{32} \left(k_2 - hf_n \right) \right].$$
 (D.20)

Taylor expanding that expression gives

$$k_{3} = h \sum_{i=0}^{\infty} \frac{1}{i!} \left[h D_{3} + B_{32} \left(k_{2} - h f_{n} \right) \frac{\partial}{\partial \psi} \right]^{i} f(x, \psi) \Big|_{x=x_{n}}.$$
 (D.21)

Note that D_i and $\partial/\partial y$ commute, since we have assumed the order of partial differentiation to be unimportant. Careful application of the product rule to (D.21) leads to

$$k_{3} = \left[hfh^{2}D_{3}f + hB_{32}\left(k_{2} - hf_{n}\right)f_{y} + \frac{1}{2}h^{3}D_{3}^{2}f + h^{2}B_{32}\left(k_{2} - hf_{n}\right)D_{3}f_{\psi} + \frac{1}{2}hB_{32}^{2}\left(k_{2} - hf_{n}\right)^{2}f_{\psi\psi} + \frac{1}{6}h^{4}D_{3}^{3}f + \frac{1}{2}h^{3}B_{32}\left(k_{2} - hf_{n}\right)D_{3}^{2}f_{\psi} + \frac{1}{2}h^{2}B_{32}^{2}\left(k_{2} - hf_{n}\right)^{2}D_{3}f_{\psi\psi} + \frac{1}{6}hB_{32}^{3}\left(k_{2} - hf_{n}\right)^{3}f_{\psi\psi\psi}\right]\Big|_{x=x_{x}}.$$
 (D.22)

In deriving that equation, we treated k_2 as a constant, since it has been evaluated at x_n . The next step is to substitute k_2 , Equation (D.19), into Equation (D.22). Evaluating the resulting expression at x_n allows a great deal of terms to either combine or cancel, and the result is

$$k_{3} = \left[hf + h^{2}D_{3}f + h^{3}\left(\frac{1}{2}D_{3}^{2}f + B_{32}f_{\psi}D_{2}f\right) + h^{4}\left(\frac{1}{6}D_{3}^{3}f + \frac{1}{2}B_{32}f_{\psi}D_{2}^{2}f + B_{32}D_{2}fD_{3}f_{\psi}\right) \right] \Big|_{x=x_{n}}.$$
 (D.23)

Even though evaluating at x_n was an important step in reaching Equation (D.23), we leave the evaluation-at- x_n pipe symbol on the end of (D.23) to simplify the notation. The derivation of the expression for k_4 follows the same method, but with more algebra and product rules. The result is

$$k_{4} = \left[hf + h^{2}D_{4}f + h^{3}\left(\frac{1}{2}D_{4}^{2}f + B_{42}f_{\psi}D_{2}f + B_{43}f_{\psi}D_{3}f\right) + h^{4}\left(\frac{1}{6}D_{4}^{3}f + \frac{1}{2}B_{42}f_{\psi}D_{2}^{2}f + B_{32}B_{43}f_{\psi}^{2}D_{2}f + \frac{1}{2}B_{43}f_{\psi}D_{3}^{2}f + B_{42}D_{2}fD_{4}f_{\psi} + B_{43}D_{3}fD_{4}f_{\psi}\right) \right]_{x=x_{n}} (D.24)$$

D.3 Determining the Constants

The next step is to plug our new expressions for the k_i into Equation (D.3) and equate the resulting coefficients on each power of h with those in Equation (D.13). The first two equations are

$$w_1 + w_2 + w_3 + w_4 = 1 \tag{D.25}$$

and

$$w_2 D_2 f + w_3 D_3 f + w_4 D_4 f = \frac{1}{2} D f.$$
 (D.26)

For this last equation to be generally true, some restrictions must be placed on $f(x, \psi)$. This undesirable necessity if alleviated if we require

$$a_i = \sum_{j=1}^{i-1} B_{ij}, \ i = 2, 3, 4,$$
 (D.27)

so that $D_i f/Df = a_i$, i = 2, 3, 4. Equation (D.26) becomes

$$a_2w_2 + a_3w_3 + a_4w_4 = \frac{1}{2}.$$
 (D.28)

Equating coefficients on the h^3 terms gives

$$\frac{1}{2} \left(w_2 D_2^2 f + w_3 D_3^2 f + w_4 D_4^2 f \right) + f_{\psi} \left(B_{32} w_3 D_2 f + B_{42} w_4 D_2 f + B_{43} w_4 D_3 f \right) = \frac{1}{6} \left(D^2 f + f_{\psi} D f \right). \quad (D.29)$$

We equate terms on the left- and right-hand sides that are second order in D, and do the same for terms that are first order in D and proportional to f_{ψ} . Using the proportionality of D and D_i , we obtain

$$a_2^2 w_2 + a_3^2 w_3 + a_4^2 w_4 = \frac{1}{3}$$
 (D.30)

and

$$a_2 B_{32} w_3 + a_2 B_{42} w_4 + a_3 B_{43} w_4 = \frac{1}{6}.$$
 (D.31)

Equating coefficients on the h^4 terms gives

$$\frac{1}{6} \left(w_2 D_2^3 f + w_3 D_3^3 f + w_4 D_4^3 f \right) + \frac{1}{2} f_{\psi} \left(B_{32} w_3 D_2^2 f + B_{42} w_4 D_2^2 f + B_{43} w_4 D_3^2 f \right)
+ B_{32} w_3 D_2 f D_3 f_{\psi} + B_{42} w_4 D_2 f D_4 f_{\psi} + B_{43} w_4 D_3 f D_4 f_{\psi} + B_{32} B_{43} w_4 f_{\psi}^2 D_2 f
= \frac{1}{24} \left(D^3 f + f_{\psi} D^2 f + 3D f D f_{\psi} + f_{\psi}^2 D f \right). \quad (D.32)$$

By the same logic used to obtain Equations (D.30) and (D.31) from (D.29), we obtain from (D.32)

$$a_2^3 w_2 + a_3^3 w_3 + a_4^3 w_4 = \frac{1}{4}$$
 (D.33)

$$a_2^2 B_{32} w_3 + a_2^2 B_{42} w_4 + a_3^2 B_{43} w_4 = \frac{1}{12}$$
(D.34)

$$a_2 a_3 B_{32} w_3 + a_2 a_4 B_{42} w_4 + a_3 a_4 B_{43} w_4 = \frac{1}{8}$$
(D.35)

and

$$a_2 B_{32} B_{43} w_4 = \frac{1}{24}.\tag{D.36}$$

To summarize these 11 equations in 13 unknowns:

$$B_{21} = a_2$$
 (D.37)

$$B_{31} + B_{32} = a_3 \tag{D.38}$$

$$B_{41} + B_{42} + B_{43} = a_4 \tag{D.39}$$

$$w_1 + w_2 + w_3 + w_4 = 1 \tag{D.40}$$

$$a_2w_2 + a_3w_3 + a_4w_4 = \frac{1}{2} \tag{D.41}$$

$$a_2^2 w_2 + a_3^2 w_3 + a_4^2 w_4 = \frac{1}{3}$$
(D.42)

$$a_2 B_{32} w_3 + a_2 B_{42} w_4 + a_3 B_{43} w_4 = \frac{1}{6}$$
(D.43)

$$a_2^3 w_2 + a_3^3 w_3 + a_4^3 w_4 = \frac{1}{4}$$
(D.44)

$$a_2^2 B_{32} w_3 + a_2^2 B_{42} w_4 + a_3^2 B_{43} w_4 = \frac{1}{12}$$
(D.45)

$$a_2 a_3 B_{32} w_3 + a_2 a_4 B_{42} w_4 + a_3 a_4 B_{43} w_4 = \frac{1}{8}$$
(D.46)

$$a_2 B_{32} B_{43} w_4 = \frac{1}{24}.$$
 (D.47)

D.3.0 The Common Method

Two constants must be chosen before one can solve the above nonlinear set of equations. The typical choice is $a_2 = a_3 = 1/2$, which leads to

$$a_4 = 1$$

$$B_{21} = B_{32} = \frac{1}{2}$$
$$B_{43} = 1$$
$$B_{31} = B_{41} = B_{42} = 0$$
$$w_1 = w_4 = \frac{1}{6}$$
$$w_2 = w_3 = \frac{1}{3}.$$

In practice, other solutions may have better properties [80]. In any case, since the method was derived from a Taylor series that was truncated after the h^4 term, the method has an error proportional to h^5 and so is considered fourth order accurate.

Given a known function value $\psi_n = \psi(x_n)$, one can then find an approximate solution to the differential equation in Equation (D.1) at the point $x_n + h$:

$$\psi(x_n+h) \approx \psi_n + \frac{1}{6} \left(k_1 + 2k_2 + 2k_3 + k_4\right),$$
 (D.48)

where

$$k_{1} = hf(x,\psi) \Big|_{x=x_{n}}$$

$$k_{2} = hf\left(x + \frac{1}{2}h,\psi + \frac{1}{2}k_{1}\right) \Big|_{x=x_{n}}$$

$$k_{3} = hf\left(x + \frac{1}{2}h,\psi + \frac{1}{2}k_{2}\right) \Big|_{x=x_{n}}$$

$$k_{3} = hf(x + h,\psi + k_{3}) \Big|_{x=x_{n}}.$$

APPENDIX E

DERIVATION OF PSEUDOSPECTRAL DERIVATIVES

Spectral solutions to PDE's generally involve expanding the solution in some basis. In Galerkin and tau (or Lanczos tau) spectral methods, one works exclusively with the expansion coefficients. These approaches are usually impractical in nonlinear equations, requiring difficult convolutions. Pseudospectral methods use the expansion coefficients solely for computing derivatives; all other computations are carried out in physical space. Depending on the choice of basis, fast transform algorithms may allow for rapid computation of pseudospectral derivatives; otherwise, one must resort to differentiation matrices (though this is not always crippling) [90, 97, 98, 100, 101, 99].

E.1 Sinusoidal Basis

Let the function f be defined over a continuous variable $x \in [0, \pi]$ such that $f(0) = f(\pi) = 0$. Approximate f(x) by a truncated expansion in a basis of sines:

$$f(x) \approx \sum_{k=1}^{N-1} \tilde{f}_k \sin(kx), \qquad (E.1)$$

where \tilde{f}_k is the expansion coefficient corresponding to the basis function $\sin(kx)$. Then the approximate first and second derivatives are

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x} \approx \sum_{k=1}^{N-1} k \tilde{f}_k \cos\left(kx\right) \tag{E.2}$$

$$\frac{\mathrm{d}^2 f(x)}{\mathrm{d}x^2} \approx \sum_{k=1}^{N-1} \left(-k^2\right) \tilde{f}_k \sin\left(kx\right).$$
(E.3)

Now require the approximation in (E.1) to be exact at N-1 points $x_j = j\pi/N$, $j \in \{1, \ldots, N-1\}$:

$$f(x_j) = \sum_{k=1}^{N-1} \tilde{f}_k \sin\left(\frac{\pi jk}{N}\right), \ j \in \{1, \dots, N-1\},$$
(E.4)

which is a common form of a discrete sine transform. Then

$$f(x_j) = \mathcal{S}_j\left(\tilde{f}_k\right), \ j \in \{1, \dots, N-1\}$$
(E.5)

and

$$\tilde{f}_k = \frac{2}{N} S_k[f(x_j)], \ k \in \{1, \dots, N-1\},$$
(E.6)

where S_k denotes the value of the discrete sine transform at a particular value of k, and we have used the fact that the discrete sine transform is nearly its own inverse, apart from a factor of 2/N [80].

Interpolation does not commute with differentiation [97], so the requirement (E.4) does not imply that the derivatives (E.2) and (E.3) are exact at the points x_j . Our pseudospectral approximations to the first and second derivatives of f at the points x_j are then

$$\frac{\mathrm{d}f(x_j)}{\mathrm{d}x} \approx \sum_{k=1}^{N-1} k \tilde{f}_k \cos\left(\frac{\pi jk}{N}\right) = \mathcal{C}_j\left(k \tilde{f}_k\right), \ j \in \{1, \dots, N-1\}$$
(E.7)

and

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$$\frac{\mathrm{d}^2 f(x_j)}{\mathrm{d}x^2} \approx \sum_{k=1}^{N-1} \left(-k^2\right) \tilde{f}_k \sin\left(\frac{\pi jk}{N}\right) = \mathcal{S}_j\left(-k^2 \tilde{f}_k\right), \ j \in \{1, \dots, N-1\}, \quad (\mathrm{E.8})$$

where C_j denotes the value of the (type 1, in the language of Reference [80]) discrete cosine transform at a particular value of k. The identification of the sum in Equation (E.7) as a discrete cosine transform is only true if we take $\tilde{f}_0 = \tilde{f}_N = 0$.

If the function f is instead defined over a continuous variable $y \in [a, b]$, we can use the results above if we also use the chain rule. Since

$$x = \frac{y-a}{b-a}\pi,\tag{E.9}$$

we have

$$\frac{\mathrm{d}f}{\mathrm{d}y} = \frac{\mathrm{d}f}{\mathrm{d}x}\frac{\mathrm{d}x}{\mathrm{d}y} = \frac{\mathrm{d}f}{\mathrm{d}x}\frac{\pi}{b-a},\tag{E.10}$$

for example.

Alternatively, we may take $f(x_j)$ to be a discrete function from the outset. In this case, derivatives are replaced by finite differences; the analogy of Equation (E.2) might be

$$\frac{\Delta f(x_j)}{\Delta x_j} = \frac{f(x_{j+1}) - f(x_{j-1})}{2\pi/N} \\ = \frac{1}{2\pi/N} \sum_{k=1}^{N-1} \tilde{f}_k \left\{ \sin\left[\frac{\pi k}{N} \left(j+1\right)\right] - \sin\left[\frac{\pi k}{N} \left(j-1\right)\right] \right\}, \quad (E.11)$$

where $\frac{\Delta}{\Delta x_j}$ is the operator that takes the centered finite difference at the x_j . Using $\sin(A) - \sin(B) = 2\cos\left[\frac{1}{2}(A+B)\right]\sin\left[\frac{1}{2}(A-B)\right]$,

$$\frac{\Delta f(x_j)}{\Delta x_j} = \frac{1}{\pi/N} \sum_{k=1}^{N-1} \tilde{f}_k \sin\left(\frac{\pi k}{N}\right) \cos\left(\frac{\pi jk}{N}\right) = \frac{1}{\pi/N} \mathcal{C}_j \left[\tilde{f}_k \sin\left(\frac{\pi k}{N}\right)\right]. \quad (E.12)$$

Likewise, the analogy of Equation (E.3) might be

$$\frac{\Delta^2 f(x_j)}{\Delta x_j^2} = \frac{1}{(\pi/N)^2} \left[f(x_{j+1}) - 2f(x_j) + f(x_{j-1}) \right] \\
= \frac{1}{(\pi/N)^2} \sum_{k=1}^{N-1} \tilde{f}_k \left\{ \sin \left[\frac{\pi k}{N} \left(j + 1 \right) \right] - \sin \left(\frac{\pi k}{N} j \right) \right\} \\
+ \frac{1}{(\pi/N)^2} \sum_{k=1}^{N-1} \tilde{f}_k \left\{ \sin \left[\frac{\pi k}{N} \left(j - 1 \right) \right] - \sin \left(\frac{\pi k}{N} j \right) \right\}, \quad (E.13)$$

where $\frac{\Delta^2}{\Delta x_j^2}$ is the operator that takes the three-point, second order finite difference at the point x_j . Using the same trigonometric identity as in the previous case as well as $\sin^2(A) = \frac{1}{2} [1 - \cos(2A)]$, we eventually get

$$\frac{\Delta^2 f(x_j)}{\Delta x_j^2} = \frac{2}{(\pi/N)^2} \sum_{k=1}^{N-1} \tilde{f}_k \left[\cos\left(\frac{\pi k}{N}\right) - 1 \right] \sin\left(\frac{\pi j k}{N}\right)$$
$$= \frac{2}{(\pi/N)^2} \mathcal{S} \left\{ \tilde{f}_k \left[\cos\left(\frac{\pi k}{N}\right) - 1 \right] \right\}.$$
(E.14)

Again, if the discrete function is defined over a set of N + 1 points y_j , where $y_0 = a$ and $y_N = b$, we can apply the chain rule and get, for instance

$$\frac{\Delta f(y_j)}{\Delta y_j} = \frac{1}{(b-a)/N} C_j \left[\tilde{f}_k \sin\left(\frac{\pi k}{N}\right) \right].$$
(E.15)

E.2 Chebyshev Basis

With sines, the basis functions individually satisfy the box boundary conditions. Chebyshev polynomials of the first kind $T_k(x)$ are 1 at x = 1 and $(-1)^k$ at x = -1. The most popular method of using Chebyshev polynomials in pseudospectral methods directly enforces the box boundary conditions, but we also mention basis recombination, frequently used in Galerkin spectral methods, in which one creates a new set of basis functions that *do* individually satisfy the boundary conditions, nominally reducing the amount of computation.

E.2.1 Direct Enforcement

Let the function f be defined over a continuous variable $x \in [-1, 1]$. We do not need f(-1) = f(1) = 0; practically, those boundary conditions are enforced sometime other than during differentiation. Approximate f(x) by a truncated expansion in a basis of first-kind Chebyshev polynomials:

$$f(x) \approx \sum_{k=0}^{N} \tilde{f}_k T_k(x) , \qquad (E.16)$$

where \tilde{f}_k is an expansion coefficient. We can use fast transform algorithms if we require the approximation to be exact at N + 1 interpolation nodes $x_j = \cos\left(\frac{\pi j}{N}\right)$, $j \in \{0, \ldots, N\}$:

$$f(x_j) = \sum_{k=0}^{N} \tilde{f}_k T_k(x_j) \,. \tag{E.17}$$

With the chosen nodes (which are the nodes of Chebyshev-Gauss-Lobatto quadrature), the first-kind Chebyshev polynomials obey the discrete orthogonality relation [100]

$$\sum_{j=0}^{N} T_k(x_j) T_l(x_j) = b_l N \delta_{k,l}, \ 0 \le l \le N,$$
(E.18)

where $b_l = 1/2$ if 0 < l < N and $b_0 = b_N = 1$, and the double-prime on the sum indicates that the first and last terms are halved. Multiplying both sides of Equation (E.17) by $T_l(x_j)$ and summing over j as indicated in (E.18), we see that

$$\tilde{f}_k = \frac{1}{Nb_k} \sum_{j=0}^{N} f(x_j) T_k(x_j) .$$
(E.19)

At the chosen nodes, the Chebyshev polynomials are $T_k(x_j) = \cos\left(\frac{\pi jk}{N}\right)$, so Equation (E.19) is proportional to a cosine transform:

$$\tilde{f}_k = \frac{1}{N} \mathcal{C}_k[f(x_j)], \qquad (E.20)$$

which gives

$$f(x_j) = \frac{2}{N} C_j \left(N b_k \tilde{f}_k \right) = C_j \left(2 b_k \tilde{f}_k \right)$$
(E.21)

for the back transform.

Now we wish to express the derivative of f as another Chebyshev expansion; that is,

$$\sum_{k=0}^{N} \tilde{f}_k T'_k(x) = \sum_{k=0}^{N} \tilde{f}'_k T_k(x) , \qquad (E.22)$$

where \tilde{f}'_k is an expansion coefficient in the derivative's Chebyshev series. The task now is to find the \tilde{f}'_k in terms of the \tilde{f}_k . Using

$$2T_k(x) = \frac{1}{k+1}T'_{k+1}(x) - \frac{1}{k-1}u_2^kT'_{k-1}(x), \ k \ge 1$$
(E.23)

[the step function u is defined in C.14] on Equation (E.22) gives

$$2\sum_{k=0}^{N} \tilde{f}_{k}T_{k}'(x) = 2\tilde{f}_{0}'T_{0}(x) + \sum_{k=1}^{N} \frac{\tilde{f}_{k}'}{k+1}T_{k+1}'(x) - \sum_{k=2}^{N} \frac{\tilde{f}_{k}'}{k-1}T_{k-1}'(x)$$
$$= 2\tilde{f}_{0}'T_{0}(x) + \sum_{k=2}^{N} \frac{\tilde{f}_{k-1}'}{k}T_{k}'(x) - \sum_{k=1}^{N} \frac{\tilde{f}_{k+1}'}{k}T_{k}'(x)$$
$$+ \frac{\tilde{f}_{N}'}{N+1}T_{N+1}'(x) + \frac{\tilde{f}_{N+1}'}{N}T_{N}'(x), \qquad (E.24)$$

where in the last step we re-indexed the sums and added and subtracted terms so that the sums at k = N. Now note that $\tilde{f}'_N = \tilde{f}'_{N+1} = 0$, since the derivative of an Nth degree polynomial is (N - 1)th degree. On the left hand side of (E.24), the k = 0 term is zero, since $T'_0(x) = 0$, so we can start the left hand side's sum at k = 1. Recalling that $T_0(x) = T'_1(x)$ and defining $c_k = 2$ for k = 0 and $c_k = 1$ otherwise, we have

$$2\sum_{k=1}^{N}\tilde{f}_{k}T'_{k}(x) = \sum_{k=1}^{N} \left(\frac{c_{k-1}}{k}\tilde{f}'_{k-1} - \frac{1}{k}\tilde{f}'_{k+1}\right)T'_{k}(x).$$
(E.25)

The sums (E.25) give a recurrence relation,

$$\tilde{f}_{k-1}' = \frac{1}{c_{k-1}} \left(2k\tilde{f}_k + \tilde{f}_{k+1}' \right), \ k \ge 1,$$
(E.26)

which we can use to find the \tilde{f}'_k by starting at k = N and working backwards, using $\tilde{f}'_{N+1} = \tilde{f}'_N = 0$ where necessary. The second derivative is found by applying the recurrence twice, the second time with $\tilde{f}_{N-1} = 0$. Again, differentiation does not commute with interpolation, and the derivatives are only approximate at nodes x_j . The above derivation has been given, in some form, in Canuto *et al.* [97] and Mason and Handscomb [100].

The chain rule may be used to apply these derivatives to a function f defined over $y \in [a, b]$, where now

$$y = \frac{b-a}{2} (x+1) + a,$$
 (E.27)

giving

$$\frac{\mathrm{d}x}{\mathrm{d}y} = \frac{2}{b-a}.\tag{E.28}$$

As with the sine basis, we may use finite differences rather than continuous derivatives. The nodes x_j are not uniformly spaced, though, and we need more complicated difference formulas. Quadratic Lagrange interpolants give [111]

$$\frac{\mathrm{d}f(x_j)}{\mathrm{d}x} \approx \frac{x_j - x_{j+1}}{(x_{j-1} - x_j)(x_{j-1} - x_{j+1})} f(x_{j-1}) + f(x_j) + \frac{x_j - x_{j-1}}{(x_{j+1} - x_{j-1})(x_{j+1} - x_j)} f(x_{j+1})$$
(E.29)

$$\frac{\mathrm{d}^2 f(x_j)}{\mathrm{d}x^2} \approx \frac{2}{(x_{j-1} - x_j) (x_{j-1} - x_{j+1})} f(x_{j-1}) + \frac{2}{(x_j - x_{j-1}) (x_j - x_{j+1})} f(x_j) + \frac{2}{(x_{j+1} - x_{j-1}) (x_{j+1} - x_j)} f(x_{j+1}).$$
(E.30)

As the resulting pseudospectral derivatives are relatively computationally intensive, and the first derivative performs poorly, we merely state the formulas:

$$\frac{\mathrm{d}f(x_j)}{\mathrm{d}x} \approx f(x_j) \\
+ \frac{1}{2} \sin\left(\frac{\pi j}{N} + \frac{\pi}{2N}\right) \csc\left(\frac{\pi j}{N} - \frac{\pi}{2N}\right) \csc\left(\frac{\pi j}{N}\right) \csc\left(\frac{\pi}{N}\right) \\
\times \left\{ \mathcal{C}_j \left[2b_k \tilde{f}_k \cos\left(\frac{\pi k}{N}\right) \right] + \mathcal{S}_j \left[\tilde{f}_k \sin\left(\frac{\pi k}{N}\right) \right] \right\} \\
- \frac{1}{2} \sin\left(\frac{\pi j}{N} - \frac{\pi}{2N}\right) \csc\left(\frac{\pi j}{N} + \frac{\pi}{2N}\right) \csc\left(\frac{\pi j}{N}\right) \csc\left(\frac{\pi}{N}\right) \\
\times \left\{ \mathcal{C}_j \left[2b_k \tilde{f}_k \cos\left(\frac{\pi k}{N}\right) \right] - \mathcal{S}_j \left[\tilde{f}_k \sin\left(\frac{\pi k}{N}\right) \right] \right\} \tag{E.31}$$

$$\frac{\mathrm{d}^{2}f(x_{j})}{\mathrm{d}x^{2}} \approx -\frac{1}{2}\csc\left(\frac{\pi j}{N} - \frac{\pi}{2N}\right)\csc\left(\frac{\pi j}{N} + \frac{\pi}{2N}\right)\csc^{2}\left(\frac{\pi}{2N}\right)f(x_{j}) \\
+ \frac{1}{2}\csc\left(\frac{\pi j}{N} - \frac{\pi}{2N}\right)\csc\left(\frac{\pi j}{N}\right)\csc\left(\frac{\pi j}{2N}\right)\csc\left(\frac{\pi}{n}\right) \\
\times \left\{\mathcal{C}_{j}\left[2b_{k}\tilde{f}_{k}\cos\left(\frac{\pi k}{N}\right)\right] + \mathcal{S}_{j}\left[\tilde{f}_{k}\sin\left(\frac{\pi k}{N}\right)\right]\right\} \\
+ \frac{1}{2}\csc\left(\frac{\pi j}{N} + \frac{\pi}{2N}\right)\csc\left(\frac{\pi j}{N}\right)\csc\left(\frac{\pi}{2N}\right)\csc\left(\frac{\pi}{N}\right) \\
\times \left\{\mathcal{C}_{j}\left[2b_{k}\tilde{f}_{k}\cos\left(\frac{\pi k}{N}\right)\right] - \mathcal{S}_{j}\left[\tilde{f}_{k}\sin\left(\frac{\pi k}{N}\right)\right]\right\}.$$
(E.32)

Division by zero at j = 0 and N restricts us to the interior of the grid.

E.2.2 Basis Recombination

Several modifications of Chebyshev polynomials give functions that are zero at x = -1 and x = 1, but we seek one that has a somewhat straightforward recurrence of the kind in Equation (E.26). Following Reference [100], we expand f as

$$f(x) \approx \sum_{k=0}^{N-2} \tilde{f}_k \left[T_k(x) - T_{k+2}(x) \right] = 2 \sum_{k=0}^{N-2} \tilde{f}_k \left(1 - x^2 \right) U_k(x) , \qquad (E.33)$$

where $U_k(x)$ is a Chebyshev polynomial of the second kind. Requiring the approximation to be exact at the nodes $x_j = \cos\left(\frac{\pi j}{N}\right)$ and using the discrete orthogonality of the second-kind Chebyshev polynomials at these nodes gives

$$\tilde{f}_k = \frac{1}{N} \sum_{j=1}^{N-1} f(x_j) U_k(x_j), \ k \in \{0, \dots, N-2\},$$
(E.34)

where we have used $f(x_0) = f(x_N) = 0$. Then with

$$U_k(x_j) = \frac{\sin\left[(k+1)\frac{\pi j}{N}\right]}{\sin\left(\frac{\pi j}{N}\right)},\tag{E.35}$$

the expansion coefficients \tilde{f}_k can be found by fast transforms:

$$\tilde{f}_k = \frac{1}{N} \mathcal{S}_k \left[f(x_j) \cot\left(\frac{\pi j}{N}\right) \right] + \frac{1}{N} \mathcal{C}_k[f(x_j)], \ k \in \{0, \dots, N-2\}.$$
(E.36)

The back transform is most easily found from Equation (E.33) taken at the nodes x_j , which upon re-indexing gives

$$f(x_j) = \sum_{k=0}^{N-2} \tilde{f}_k T_k(x_j) - \sum_{k=2}^{N} \tilde{f}_{k-2} T_k(x_j) = \mathcal{C}_j(\tilde{\mathfrak{f}}_k), \qquad (E.37)$$

where $\tilde{\mathfrak{f}}_k = \tilde{f}_k - \tilde{f}_{k-2}$ for $2 \leq k \leq N-2$ and $\tilde{\mathfrak{f}}_0 = 2\tilde{f}_0$, $\tilde{\mathfrak{f}}_1 = \tilde{f}_1$, $\tilde{\mathfrak{f}}_{N-1} = -\tilde{f}_{N-3}$, and $\tilde{\mathfrak{f}}_N = -2\tilde{f}_{N-2}$.

Now, in the same vein as Equation (E.2), we write

$$\sum_{k=0}^{N-2} \tilde{f}_k T'_k(x) - \sum_{k=0}^{N-2} \tilde{f}_k T'_{k+2}(x) = \sum_{k=0}^{N-2} \tilde{f}'_k T_k(x) - \sum_{k=0}^{N-2} \tilde{f}'_k T_{k+2}(x)$$
(E.38)

and try to find the \tilde{f}'_k in terms of the \tilde{f}_k . Re-indexing Equation (E.38), applying the recurrence in (E.23) to the right hand side, and re-indexing again gives

$$\sum_{k=0}^{N-2} \tilde{f}_k T'_k(x) - \sum_{k=2}^{N} \tilde{f}_{k-2} T'_k(x) = \tilde{f}'_0 T'_1(x) + \sum_{k=2}^{N-1} \frac{\tilde{f}'_{k-1}}{2k} T'_k(x) - \sum_{k=1}^{N-3} \frac{\tilde{f}'_{k+1}}{2k} T'_k(x) - \sum_{k=1}^{N-3} \frac{\tilde{f}'_{k+1}}{2k} T'_k(x) - \sum_{k=3}^{N-3} \frac{\tilde{f}'_{k-1}}{2k} T'_k(x) + \sum_{k=1}^{N-1} \frac{\tilde{f}'_{k-1}}{2k} T'_k(x) \cdot (E.39)$$

Recalling $T'_0(x) = 0$ and using earlier notation, all the sums can run from k = 1 to

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$$k = N + 1;$$

$$\sum_{k=1}^{N+1} \left[\left(1 - u_{N-1}^{k} \right) \tilde{f}_{k} - u_{2}^{k} \left(1 - u_{N+1}^{k} \right) \tilde{f}_{k-2} \right] T_{k}'(x)$$

$$= \sum_{k=1}^{N+1} \left[\left(1 - u_{N}^{k} \right) \frac{c_{k-1} \tilde{f}_{k-1}'}{2k} - \left(1 - u_{N-2}^{k} \right) \frac{\tilde{f}_{k+1}'}{2k} - u_{3}^{k} \frac{\tilde{f}_{k-3}'}{2k} + \left(1 - u_{N}^{k} \right) \frac{\tilde{f}_{k-1}'}{2k} \right] T_{k}'(x),$$
(E.40)

from which we extract the recurrence relation

$$\tilde{f}_{k-3}' = \left(1 - u_N^k\right) \left(c_{k-1} + 1\right) \tilde{f}_{k-1}' - \left(1 - u_{N-2}^k\right) \tilde{f}_{k+1}' - 2k \left[\left(1 - u_{N-1}^k\right) \tilde{f}_k - \left(1 - u_{N+1}^k\right) \tilde{f}_{k-2} \right], \ k = 3, \dots, N+1. \quad (E.41)$$

One finds the \tilde{f}'_k by starting (E.41) with k = N + 1, with \tilde{f}_k and \tilde{f}'_k both zero for $k \ge N - 1$ and $\tilde{f}'_{N-2} = 0$.

Looking at the k = 3 term of the recurrence relation, we have

$$\tilde{f}'_0 = 2\tilde{f}'_2 - \tilde{f}'_4 - 6\left(\tilde{f}_3 - \tilde{f}_1\right).$$
(E.42)

Thus, the approximation to the derivative takes no contribution from the $T_0(x) - T_2(x)$ term in the series (E.33), making this pseudospectral derivative a poor approximation.

APPENDIX F

CONVERGENCE STUDIES

As this thesis is heavily computational, we attempt to determine the accuracy of particular measurements in select simulations, and the effects of grid resolution on number conservation. We find that most measurements are reliable only in a single significant figure (with one exception), and that temporal resolution is more important to number conservation than spatial resolution.

F.1 Accuracy of Simulations

To ensure the accuracy of a numerical solution to a partial differential equation, one typically increases grid resolution until the difference between a simulation conducted on N grid points gives effectively identical results to one conducted on 2Ngrid points. Given time constraints and the computationally intensive nature of our simulations, we are able to perform limited convergence studies for select simulations.

In the cases of the one-pulse simulation in which $t_{\text{hold}} = 12 \ \mu$ s and the two-pulse simulation in which $t_{\text{ev}} = 40 \ \mu$ s, we use grid sizes of $(N_R + 1) \times N_k \times (\ell_{\text{max}} + 1) =$ $65 \times 30 \times 7$ and $33 \times 16 \times 4$. We estimate the maximum value of the absolute error in the higher resolution simulations to be the difference at a given point in time between the higher and lower resolution simulations. The adaptive time stepping algorithm complicates this estimate, though, as the simulations at different spatial resolutions use slightly different time steps. To calculate the error at a particular value of the time in the higher resolution simulation, we choose the two temporally nearest points in the lower resolution simulation, linearly interpolate them, and evaluate that interpolant at the value of the time we desire. The difference between this interpolant and the value of the number of particles in the higher resolution simulation at this point in time is the absolute error at that time; in the case of the higher bound on error, we add this difference to the higher resolution simulation's value of the number of particles, and subtract it for the lower bound on error. Such is the process by which Figures 5.64, 5.65, 5.66, 5.95, 5.96, and 5.97 are calculated. Figure 5.13 is calculated in a similar way, but for different simulations, one of which uses $17 \times 8 \times 2$ grid points and the other uses $33 \times 16 \times 4$ grid points.

For the single-pulse simulation where $t_{\text{hold}} = 12 \ \mu\text{s}$, we also determine the number of reliable significant figures in the frequency of atom-molecule oscillations measured during the hold time. Following Scarborough [112], we calculate the relative error E_r as

$$E_r = \frac{|f_{\rm hi} - f_{\rm lo}|}{f_{\rm hi}},\tag{F.1}$$

where $f_{\rm hi}$ is the frequency measured in the higher resolution simulation and $f_{\rm lo}$ is that measured in the lower resolution simulation. Then

$$\frac{1}{E_r} = (k+1) \, 10^{n-1},\tag{F.2}$$

where $1 \leq (k+1) < 10$ and *n* gives the number of reliable significant digits. For the one-pulse simulation we consider, $f_{\rm hi} = 1.06$ MHz, $f_{\rm lo} = 1.96$ MHz, $E_r = 0.849$, and n = 1. As the single-pulse simulations use as large a number of grid points of any simulations we conduct and have well-conserved number, we apply the one significant figure limit to all frequencies measured in any simulation.

The same procedure is used to find the number of reliable significant figures in

the fit parameters applied to the collapsing condensates having $\kappa = 0.6$. Noteworthy is that for the $\omega = 8\pi \times 12.77$ Hz cases, the relative error indicates that a single significant figure is reliable in the coefficient in the power law for the condensate's width as a function of time, but the power β itself is reliable to three significant figures, as $\beta = 1.932$ in a simulation using a $33 \times 16 \times 4$ grid and $\beta = 1.918$ in a simulation using a $17 \times 8 \times 2$ grid.

The procedure for finding the uncertainty in the estimated rethermalization time $t_{\rm th}$ of the condensate in the one-pulse, $t_{\rm hold} = 12 \ \mu {\rm s}$ simulation is different, even though the calculation of $t_{\rm th}$ uses a power law least-squares fit. In this case, $t_{\rm th}$ is found from

$$t_{\rm th} = \left(\frac{N_0}{\alpha}\right)^{1/\beta},\tag{F.3}$$

where N_0 is the number of atoms initially in the condensate, α is the coefficient in the power law, and β is the power itself. When a quantity is calculated from a function such as $t_{\rm th}$ with parameters α and β having absolute errors $\Delta \alpha$ and $\Delta \beta$, the error $\Delta t_{\rm th}$ in $t_{\rm th}$ is estimated as [112]

$$\Delta t_{\rm th} = \frac{\partial t_{\rm th}}{\partial \alpha} \Delta \alpha + \frac{\partial t_{\rm th}}{\partial \beta} \Delta \beta, \qquad (F.4)$$

which for Equation (F.3) reduces to

$$\Delta t_{\rm th} = -\left(\frac{N_0}{\alpha}\right)^{1/b} \left[\frac{\Delta\alpha}{\alpha\beta} + \frac{\ln\left(N_0/\alpha\right)}{\beta^2}\Delta\beta\right].$$
 (F.5)

We estimate the absolute errors $\Delta \alpha$ and $\Delta \beta$ by taking the differences in α and β as determined by the higher and lower resolution simulations, and all other parameters in Equation (F.5) are taken from the higher resolution simulation, leading to $\Delta t_{\rm th} =$ $150 \ \mu s.$

F.2 Dependence of Number Conservation on Resolution

Finally, we consider the effects of spatial and temporal resolution on number conservation. The sometimes unphysical behavior of the total number, exemplified by Figure 5.5, may be due, in part, to insufficient spatial or temporal resolution. We use the parameters of Section 5.1.2 in exploring this issue, since they allow for quicker simulations.

Figure F.1 compares the average error in total number for such simulations, where the spatial grid resolution is varied. We examine three cases: $N_R = 65$, $N_k = 32$, $l_{\text{max}} = 7$; $N_R = 33$, $N_k = 16$, $l_{\text{max}} = 3$; and $N_R = 17$, $N_k = 8$, and $l_{\text{max}} = 0$, where N_R is the number of center of mass grid points, N_k is the number of noncondensed modes, and l_{max} is the index of the highest spherical harmonic $Y_l^{q=0}$ used in the correlation function expansions. In all cases, the truncation error limit in the adaptive Runge-Kutta integrator is 10^{-16} . With every spatial grid, the error in total number exhibits the jagged and seemingly random behavior, nearly machine precision in magnitude, that we interpret as an indication of a stable and possibly converged simulation.

To compare changes in the temporal resolution, we keep fixed $N_R = 33$, $N_k = 16$, and $l_{\text{max}} = 3$ and vary the truncation error limit. Figure F.2 shows average error in total number for limits of 10^{-16} , 10^{-8} , and 10^{-2} . Only in the case of 10^{-16} , where the truncation error is allowed to be no higher than machine precision, does the error in total number have the desired nearly-zero mean and seemingly random behavior. For next most stringent case of 10^{-8} , the error is still a tolerable 5×10^{-11} by the end of the simulation, but is growingly linearly. In the lax case of 10^{-2} , the error grows faster than linearly and exceeds 0.04 at the end of the simulation. Hence, the



Figure F.1: Comparison of number conservation for different spatial resolutions. The solid red curve is the average error in total number for the highest resolution spatial grid, the dashed green curve is that for a moderate-resolution grid, and the dotted blue for the lowest resolution. All three perform very well.

temporal aspects of our system, including the integration method and its resolution, are key to the accuracy and stability of our approximate solutions. These results, considered in conjunction with those in Figure F.1, suggest that a truncation error limit of 10^{-16} may be appropriate for temporal convergence in most cases.



Figure F.2: Comparison of number conservation for different truncation error limits. Average error in total number for a given spatial grid, where the adaptive time integrator's truncation error is set to (top to bottom) 10^{-16} , 10^{-8} , and 10^{-2} .

APPENDIX G

COMPLETE HARTREE-FOCK-BOGOLIUBOV CODE

The spherical and cylindrical codes have substantial differences, mainly due to their different grids and parallelization schemes. Still, each uses some of the same routines.

G.1 Common Code

The following files are located in the bosenova/ directory.

- ARK.cpp and ARK.h. The files contain adaptive Runge-Kutta integrators. A single routine is appropriate for numerically integrating a system of ODE's where a single function can handle each of the ODE's right-hand sides; that is, a single routine calculates $\frac{df_i}{dx}$ for all *i*. This approach is appropriate for a one-dimensional GPE simulation, for example. Another set of routines numerically integrates a system of ODE's, like the spherical or cylindrical HFB simulations, in which some or all ODE's right-hand sides must be evaluated by different routines.
- ARK_2.cpp. This file contains the same group of Runge-Kutta algorithms as ARK.h and ARK.cpp, except for the single routine that handles ODE's with a common right-hand side. Rather than the procedural programming approach of ARK.h and ARK.cpp, ARK_2.cpp implements a templated class appropriate for the object-oriented parallelization used in the cylindrical code.

- Contig.cpp has several templated routines for assigning a pointer with up to fifth-level indirection to a contiguous chunk of dynamically allocated memory. The result is a multidimensional array, sized at runtime, that is contiguous in memory. Looping calls to the C++ "new" operator with such a pointer usually results in non-contiguous memory allocation, which can result in cache misses. The Message Passing Interface and the HDF5 library, used for writing data to disk, both expect arrays of any dimensionality to be contiguous in memory. Contig.cpp does not allow for deallocation of memory.
- ContigArray.cpp accomplishes the same task as Contig.cpp, but using a templated class. This approach is appropriate for the object-oriented cyldindrical parallelization, allows for deallocation of memory via the class destructor, and easily allows for deep copies of multidimensional arrays. This class is somewhat atypical in that a data member, the name of the multidimensional array, is public, which makes calls to MPI and HDF5 routines simpler.
- Derivatives.cpp and Derivatives.h contain routines for approximating one-dimensional first and second derivatives, assuming box boundary conditions. Finite difference and sine and Chebyshev pseudospectral methods are available, and some functions allow for a derivative to be taken over the first of two array indices. A future revision of these routines should make them templated.
- NRFourier.cpp and NRFourier.h. Fast Fourier transform routines, including fast sine and cosine transforms, are found in these files. All the routines except for the Chebyshev transform routines are adapted from *Numerical Recipes in* C++ [80]. Adaptations include transformation over the first of two array indices, direct transformation of the C++ complex<typename> datatype without

repackaging complex<typename> arrays into two separate arrays,¹ and modifications for thread-safety.

• Utilities.cpp and Utilities.h contain a random number generator and quadrature functions from [80], as well as inline functions for separating arrays of type complex<double> into two arrays of type double.

G.2 Spherical Code

The following files are located in the bosenova/Sphere/ directory and are specific to the HFB simulation in spherical geometry and symmetry.

- macRun.sh and runSph.sh are bash scripts that compile and run a spherical simulation on a personal computer or workstation, storing the data in a uniquelynamed directory.
- Makefile compiles the spherical simulation. Much of this code and the bash scripts mentioned above are particular to the Colorado School of Mines Academic Computing and Networking department's Macintosh cluster.
- Parameters.h is the sole user interface file, where physical and computational parameters are set.
- SphereDriver.cpp makes multi-threaded calls to routines in ARK.h for time propagation, and calls the initialization functions.
- SphIO.h and SphIO.cpp perform output using the platform-independent HDF5 library, reads output files for initial conditions, and initializes all data structures.

¹This ability requires that the compiler and complex number library store a complex number as two memory-adjacent doubles, real part first, with no other members in the data structure.

- RHSSph.h and RHSSph.cpp contain the right hand sides of the ODE's used in the time integration. The condensed and noncondensed atomic, molecular, and anomalous fields each have their own routines, and the diagonal parts of the normal and anomalous fields are calculated by a fifth routine.
- RHSInfo.h defines the data structure which contains all information needed by the right hand side routines other than the fields themselves.

The directory bosenova/Sphere/VizUtils contains Matlab routines for visualization and post-processing. Due to differences between versions of Matlab, these scripts and functions are guaranteed to work only with Matlab version 7.1.0.246 (R13) Service Pack 3 running under Windows XP on a 32-bit machine.

- GetFields.m is a function that retrieves the atomic and molecular fields and the diagonal parts of the normal and anomalous densities. The value of each field at the origin is found by extrapolation.
- GetNoR.m is a function that performs the same task as GetFields.m, but without dividing through by the center of mass grid, and so does not require extrapolation.
- GetNorms.m is a function that performs the same task as GetNoR.m, but returns the squared modulus of the atomic and molecular fields.
- GetNus.m is a function that extracts the detuning from each data file.
- GetParams.m is a function that retrieves metadata such as grids from a simulation's metadata file.
- GetScales.m is a function that calculates the characteristic time and length scales from the parameters appearing in the Hamiltonian.

- getSteps.m finds the square modulus of the atomic and molecular fields returned by GetFields.m, and writes these and the diagonal parts of the normal and anomalous densities to an ASCII file for plotting in gnuplot. getSteps.m also creates an HDF5 file for use by post-processing routines described below.
- getWidths.m fits the condensate width to a Gaussian and writes an array of widths to an ASCII file.
- matPlot.m reads all the data and plots it directly in Matlab, for exploratory purposes.
- octPlot.m reads all the data and plots in directly in Octave, should Matlab be unavailable.
- pcolorPlot.m, written by Ryan Mishmash, creates contour plots of field data.
- SortDataFiles.m is a function that creates a cell array of filenames, ordered according to each data file's "Time" dataset. This function ensures that data is stored chronologically, in case the data file names are corrupted.

G.3 Cylindrical Code

The following files are located in bosenova/Cyl/, and are specific to the HFB simulation in cylindrical geometry and symmetry.

- Makefile compiles the cylindrical simulation or the ITR initialization program, and is mostly specialized to the Golden Energy Computing Organization's Ra supercomputer.
- Eqn.cpp implements a templated Eqn<typename> class. Each Eqn object represents the atomic or molecular field, or the normal or anomalous fluctuations

at a particular point in relative momentum space. This class is the central component of the object-oriented parallelization scheme.

- CylParams.h is the sole user interface, where physical and computational parameters are set.
- CylDriver.cpp initializes MPI, calls the initialization routine particular to a cylindrical simulation, and calls the time propagation routine.
- Initialize.h and Initialize.cpp allocate memory and parse CylParams.h.
- ITROnly.cpp is a minimalistic version of Initialize.cpp that has its own main function, and performs imaginary time relaxation only. ITROnly.cpp is provided so that the relaxation initialization method, which benefits little from parallelization, can run on a workstation without MPI.
- Output.h and Output.cpp write data files in HDF5 format, and read the files created by ITROnly.cpp for initialization.
- TimePropagation.h and TimePropagation.cpp call the routines needed for Runge-Kutta time propagation, and contain all parallelization.
- RHSCyl.h and RHSCyl.cpp have functions for evaluating the right hand sides of the differential equations for the atomic and molecular fields and the normal and anomalous densities.
- RHSInfo.h defines the data structure which contains all information needed by the right hand side routines other than the fields themselves.

The directory bosenova/Cyl/VizUtils contains Matlab visualization routines, guaranteed to run only on a particular version of Matlab, as described above. A C++
program for visualization is included, as well.

- GetMids.m is a function that extracts number densities (values at the origin are found by extrapolation) for a radial slice through the middle of the trap axis, and for an axial slice about a quater of the way from the origin.
- GetRGrid.m is a function that reads the nonuniform radial center of mass grid from the simulation's metedata file.
- getDens.m is a script that takes the densities from GetMids.m and writes them to an ASCII file for plotting in gnuplot.
- SortDataFiles.m is identical to that in bosenova/Sphere/VizUtils, and exists here only for convenience.
- POCDump.cpp is a C++ program that reads ρ and z slices of the atomic and molecular fields and the diagonal parts of the normal and anomalous densities, computes numbers of each kind of particle and average error in total number as a functions of time, and writes the results to an ASCII file.

G.4 Post-Processing Routines

Because a simulation can produce hundreds of thousands of data files and several gigabytes of data, shell scripts and programs for manipulating the files are useful and are found in bosenova/Tools/. All C++ programs in this directory are particular to data from a spherical simulation.

• AvgErr.cpp reads the file created by getSteps.m and creates an ASCII file containing the average error in total number as a function of time.

- PowerSpect.cpp reads the file created by getSteps.m and creates ASCII files containing data on the numbers of particles as a function of time, and computes and outputs data for plotting a Lomb normalized periodogram.
- Currents.cpp reads HDF5 files directly and computes velocities of the atomic and molecular fields. It writes these data to an ASCII file for plotting in gnuplot.
- NumCompare.cpp computes average error in total number as a function of time, using the trapezoid rule and Simpson's rule. The result is written to an ASCII file for plotting and visual comparison.
- ConvNum.cpp computes the error in a high-resolution simulation's number data to that of a low-resolution simulation, using the interpolation procedure described in Appendix F.
- decimate.sh is a bash script that deletes all but every n^{th} data file, in case a simulation produced an unnecessarily large number of files.
- pander.sh is a bash script that calls the h5repack utility for a set of files created on Ra. While the files are perfectly valid, some versions of Matlab are unable to read them unless this script is run first.
- rename.sh is a bash script that renames data files in a consistent way.