Simulating an Anomalous Prediction of the Boltzmann Equation

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Simulating an Anomalous Prediction of the Boltzmann Equation

by

Andrew E. S. Barentine

A thesis submitted to the Faculty of the University of Colorado in partial fulfillment of the requirements for the degree of Bachelors of Arts, Physics

Department of Physics

March 6th, 2015
This thesis entitled:
Simulating an Anomalous Prediction of the Boltzmann Equation
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The final copy of this thesis has been examined by the signatories, and we find that both the content and the form meet acceptable presentation standards of scholarly work in the above mentioned discipline.
There is an anomalous prediction of the Boltzmann equation that monopole motion in an isotropic and harmonic potential will not damp. We have implemented a modification to our Time-Averaged Orbiting Potential (TOP) Trap, which we call the zzTOP Trap. Although this modification allows us to reach unprecedented levels of isotropy, it is still not perfectly isotropic. There are several methods of proving that the monopole motion in isotropic and harmonic potentials is undamped, but there are no analytic descriptions of monopole motion in slightly anharmonic and slightly anisotropic potentials. To this end, I have programmed a semi-classical Monte Carlo simulation to numerically predict dynamics of the monopole motion in slightly arbitrary potentials.

In this thesis I will discuss Boltzmann’s prediction, introduce monopole and quadrupole motion, and describe and validate the simulation. Then I will investigate monopole and quadrupole shape oscillations in isotropic and harmonic potentials, anisotropic and harmonic potentials, and slightly anharmonic potentials. Finally I will compare dynamics of these motions from the simulation with results we have observed in our experiment.
Dedication

To Larry and Dorcas Wilkinson, Julie Hall, and Warren Olson
Acknowledgements

Dan Lobser has been incredibly helpful throughout the process of this thesis. Not only has he taken the time to teach me about the experiment, and how to experiment in general, but he has also taught me how to program, and assisted me greatly when I’ve been stuck.

My advisers Eric Cornell and Heather Lewandowski have been supportive, instructive and patient, and continued to do so after this work was outpaced by our experiment.

Ming-Guan Hu was very generous to give me his code to get me started with the simulation, and Jila Computing was very helpful in getting my code set up to run on the clusters.
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Chapter 1

Introduction

Over one hundred years ago, Ludvig Boltzmann’s kinetic theories were the center of heated debate among physicists. Boltzmann’s theories were derived from kinematics, which has inherent time reversal symmetries; yet he was using them to describe thermodynamics, which is inherently not time-reversible. Physicists Josef Loschmidt, and William Thomson pointed this out, and it become known as the “Reversibility Paradox”[3]. This is still a relevant issue today, as some believe there is a very weak time-reversal violation involved with the interaction of elementary particles that might have created a preferred time axis for the Big Bang [19]. Shortly before experimental confirmation of the existence of atoms, which largely validated Boltzmann’s approach, he committed suicide in 1906. The success of his theories, and in particular the Boltzmann equation have earned Boltzmann the respect of the physics community. The Boltzmann equation is used in plasma physics, calculations of neutron flow in nuclear reactors, and generally when predicting how a gas reaches equilibrium [3, 17].

The validity of the Boltzmann equation stands on a foundation of statistics, but comparison with experiment is required to verify this approach [17]. Some of the Reversibility Paradox arguments centered around a special class of solutions to the Boltzmann equation, including that the monopole motion of a gas in an isotropic and harmonic potential is undamped[2, 4]. Our recent design of a novel trap geometry has finally made this anomalous prediction testable. Analytic solutions of the monopole motion in harmonic and isotropic potentials exist [4, 2, 12, 14, 25]; however, there is no analytic description for the monopole motion in a potential that is slightly anisotropic.
or anharmonic. In this chapter I will introduce monopole and quadrupole motion, discuss analytic solutions of their dynamics in an isotropic and harmonic potential, and describe our experiment that motivated this work.

1.1 Collective Excitations: Monopole Motion

Collective excitations occur when a gas, composed of individual atoms, undergoes motion as a whole; the motion can be generally described without explicitly tracking each individual atom. In a single dimension, monopole motion is analogous to Newton’s Cradle, where an equal number of masses on each side are displaced an equal distance from the center and released. In this analogy, all collisions are occurring at the ‘trap center’ and one can apply conservation of momentum to see that monopole motion would not damp. In three dimensions it becomes less trivial to describe the monopole motion. Monopole motion in three dimensions is a spherically symmetric expansion and contraction of the gas, commonly referred to as breathing oscillations.

Quadrupole motion is very similar to monopole motion, except that two axes are exactly out of phase: As the cloud expands axially, it contracts radially, or vice-versa. In an anisotropic potential, in the limit of zero collisions, an initial monopole excitation will couple into quadrupole motion as the single particle trajectories dephase. Eventually the quadrupole motion will dephase as the phases of axial and radial motion realign, and a revival in monopole motion can be observed, as depicted in figure 1.1. The larger the anisotropy, the faster the motions along different axes dephase, and the frequency of monopole-quadrupole coupling increases. In an isotropic potential, this mechanism does not couple the monopole and quadrupole motion because the motion never dephases.

1.2 Our Experiment

We experimentally examine monopole and quadrupole motion of $^{87}\text{Rb}$ atoms in a modified time-averaged orbiting potential (TOP) trap. The standard TOP trap consists of a set of anti-Helmholtz coils that create a magnetic quadrupole potential and two sets of Helmholtz coils
Figure 1.1: An initial excitation of pure monopole motion in an isotropic and harmonic potential is undamped. However, in an anisotropic potential the monopole excitation will couple into quadrupole motion. This coupling between the two motions is the damping mechanism for monopole motion in a perfectly harmonic, yet slightly anisotropic potential. Image modified from Dan Lobser[22].

positioned orthogonally to each other as drawn in figure 1.2a. The quadrupole (hourglass) potential has a magnetic zero at the trap center. This is problematic because cold atoms in a magnetic spin state that is trapped, find themselves in a super-position of trapped, untrapped, and anti-trapped states when they oscillate through the region of zero magnetic field. When they leave the magnetic-zero point, they lose their super-position and can undergo Majorana spin flip, becoming untrapped or even anti-trapped. The TOP trap avoids unwanted Majorana spin flip by keeping the magnetic zero point away from the center of the trap and the atoms. The Helmholtz coils provide a linear offset, shifting the position of the magnetic zero in the $xy$-plane. Changing the current through one of the Helmholtz coils rapidly pushes the potential, and the atoms then start to move toward the new magnetic zero. To keep the atoms from ever reaching the magnetic zero, two pairs of Helmholtz coils are positioned orthogonal to each other, and driven sinusoidally out of phase fast enough that the atoms are unaffected [26, 9]. This removes the magnetic zero point from the trap center, provides a means of variably forcing evaporation, and makes the time-average potential very harmonic, as shown in 1.2b.
Figure 1.2: a) Diagram of the standard TOP trap. b) The TOP coils in the $xy$-plane offset the quadrupole potential. When driven out of phase sinusoidally this causes the trap center to trace out a circle, which smoothes out the trap center and results in a nearly harmonic potential near the center. Adapted from Dan Lobser[22].

In order to test Boltzmann’s prediction of undamped monopole motion, our potential must be very isotropic. We can think about the 3D parabaloid of our potential, traced out by a vector starting from the trap center. With the standard TOP potential, we can control the radius of the circle in the $xy$-plane with the TOP coil amplitude. By varying the current through the quadrupole coils, we can also control the aspect ratio of the trap: $\lambda = \frac{\omega_{x,y}}{\omega_z}$. Which means our controllable potential is

$$U_c \propto Ax^2 + Ay^2 + Cz^2.$$

Unfortunately, there are cross-terms in the potential due to the fact that our coils are not perfectly orthogonal, and these cross-terms limit how isotropic the potential can be with a standard TOP configuration. In order to access the $xy$ cross-term, we implement a counter-rotating field in the $xy$-plane. Adjusting the phase of this field relative to the TOP field allows us to add to or subtract
from the TOP field strength at various parts of its rotation. Doing so allows us to correct for any $xy$ cross-terms, which in past experiments has allowed us to create a potential that is one part per thousand out of round in the $xy$-plane [5]. The TOP trap requires another modification in order to control the $xz$, and $yz$ cross-terms. To access the $xy$ cross-terms we implemented a rotating bias field in the $xy$-plane. If we had instead implemented our rotating bias field in the $xz$-plane, we would have access to the $xz$ cross-term, and likewise with the $yz$-plane and the $yz$ cross-term. In order to access all three cross-terms simultaneously we implement a superposition of all three by adding a third rotating bias field aligned axially, as illustrated in figure 1.3.

Figure 1.3: The zzTOP Configuration employs the standard TOP configuration, with an additional third oscillating bias field along the axial direction. Our zzTOP also employs a counter-rotating field in the $xy$-plane.

The three-rotating bias field approach has been done before and is referred to as the stiff zTOP trap. Previously, the Christopher Foot group at Oxford achieved an aspect ratio of $\lambda = 1.6$ with their stiff zTOP trap [15, 16]. As we will discuss, this is not spherically symmetric enough to observe an undamped monopole motion because there is significant coupling between monopole and quadrupole motion in a $\lambda = 1.6$ potential. The Oxford experiment did not implement a counter-rotating bias field. Our potential, which we call the zzTOP trap, is the combination of a quadrupole field, three rotating, linear-bias fields, and one counter-rotating linear-bias field. We have reached out-of-sphericity levels as low as three parts per thousand with our zzTOP trap [7], significantly
improving the observability of undamped monopole motion.

1.3 Motivation for a Simulation

Experimenters have previously been unable to produce very isotropic potentials. As previously mentioned, the predictions for undamped monopole motion and the damping rate of quadrupole motion require a perfectly isotropic potential. We have produced a Monte Carlo simulation to develop a model for monopole and quadrupole damping in a slightly anisotropic potential. Starting with a Maxwell-Boltzmann distribution of several thousand atoms and evolving time while propagating hard-sphere isotropic (s-wave) collisions, we can predict the dynamics of our gas in arbitrary potentials without needing a perturbative-analytic solution to the Boltzmann equation. Not only would it be very difficult to arrive at a perturbative-analytic description of monopole and quadrupole motion in anisotropic potentials, but it would be especially difficult to include anharmonic effects present in our experiment. Our simulation can be made to include approximations of the anharmonic aspects of our experimental potential. We can assert the validity of our simulation by demonstrating conservation of energy, agreement with equipartition theorem, conservation of momentum for collisions, and a similar number of collisions needed to relax a cross-dimensional temperature anisotropy. It has been numerically, and experimentally shown that 2.7 collisions per atom are required to relax a cross-dimensional temperature anisotropy [25, 6, 30].

\[ \Gamma_T = \frac{1}{2.7} \gamma_{Coll} \]  

(1.2)

This relation can be used to compare relaxation rates of temperature anisotropies with the damping rate of quadrupole motion, and is a good metric for comparison between simulations and experiments.
Chapter 2

Analytic Theory

2.1 Analytic Solutions in Isotropic Harmonic Potentials

The Boltzmann equation describes changes to the single-particle phase-space distribution function, and can be written in the form

$$\frac{d}{dt}f(v, r) = I_{coll}(f), \quad (2.1)$$

where $f(v, r)$ is the single-particle phase space distribution, and $I_{coll}(f)$ is the classical collision integral. The classical collision integral can be written as

$$I_{coll} = \frac{\sigma_o}{4} \int d^2\Omega d^3v_2 |v_2 - v_1|[f(v'_1)f(v'_2) - f(v_1)f(v_2)], \quad (2.2)$$

where $\sigma_o$ is the collision cross-section and the primed velocities are the velocities after the collision [14]. The easiest way to responsibly handle an integral of this nature is to show that the integrand is actually equal to zero. If $I_{coll}$ goes to zero, then the gas should be in equilibrium. We can test this by substituting a distribution that we know should be at equilibrium: The Maxwell-Boltzmann distribution,

$$f(r, v) = n_o(2\pi mk_bT)^{-3/2}e^{-\frac{1}{2}mv^2/k_bT}, \quad (2.3)$$

where $k_b$ is the Boltzmann constant, $T$ is temperature, and $n_o$ is the peak density. Assuming $U(r)$ is harmonic,

$$U(r) = \frac{1}{2}m\omega^2r^2. \quad (2.4)$$
Substituting (2.3) and (2.4) into \[ f(v_1')f(v_2') - f(v_1)f(v_2) \] from the collision integral, and dropping the constant yields
\[
[f(v_1')f(v_2') - f(v_1)f(v_2)] = e^\beta r_1'^2 e^{\alpha v_1'^2} e^\beta r_2'^2 e^{\alpha v_2'^2} - e^\beta r_1^2 e^{\alpha v_1^2} e^\beta r_2^2 e^{\alpha v_2^2},
\] (2.5)
where \( \alpha = m/2k_bT \) and \( \beta = m\omega^2/2 \) and we have assumed each atom has the same mass. By conservation of energy we require \( E_1 + E_2 = E_1' + E_2' \) and consequently
\[
\beta r_1'^2 + \alpha v_1'^2 + \beta r_2'^2 + \alpha v_2'^2 = \beta r_1^2 + \alpha v_1^2 + \beta r_2^2 + \alpha v_2^2.
\] (2.6)
This causes \( f(v_1')f(v_2') - f(v_1)f(v_2) \), and therefore (2.2) to go to zero. This matches our intuition: An equilibrium distribution has a zero collision integral, and therefore has no time dependence. Although not necessary for this example, we assume that the collisions are point-like, such that \( r_1 = r_2 = r_1' = r_2' \).

The monopole motion of a thermal gas can be written as a Maxwell-Boltzmann distribution with a time-dependent width-scaling \( b(t) \) [29],
\[
f(v, r, t) \propto e^{-m|v - b(t)r|^2/2k_bT}.
\] (2.7)
Starting with the Maxwell-Boltzmann distribution, (2.3), ten differential equations can be found by setting the collision integral equal to zero and requiring a constant, harmonic potential with no external forces [4]. These differential equations have non-trivial solutions for the monopole motion only for the case that the potential is isotropic. This same result has been shown by several groups including Boltzmann himself, using several approaches [2, 13, 14].

2.2 Method of Averages

The Method of Averages relies on the Conservation Theorem, which states that quantities of certain forms are conserved by the Boltzmann equation [17]. Let \( \chi(r, v) \) represent certain dynamical quantities that are conserved during collisions, so
\[
\chi_1 + \chi_2 = \chi_1' + \chi_2'.
\] (2.8)
These quantities include
\[ \chi = a(r) + b(r) \cdot v + c(r)v^2, \]
(2.9)
where the first term corresponds to number conservation, the second is a result of conservation of momentum, and the third is due to conservation of energy [14]. The conservation theorem then states that
\[ \int d^3v d^3r \chi I_{\text{coll}} = 0. \]
(2.10)

Multiplying the Boltzmann equation (2.1) by \( \chi \) and expanding yields,
\[
\chi I_{\text{coll}} = \chi \frac{df}{dt} - f \frac{d\chi}{dt} - \nabla_r (\chi f) + \frac{F}{m} \nabla_v (\chi f) - f (v \cdot \nabla_r) \chi - f \frac{F}{m} \nabla_v \chi.
\]
(2.11)
(2.12)

Taking the average in phase-space, \( \langle A \rangle = \frac{1}{N} \int d^3r d^3v f A \), gets us to the useful relation
\[
\frac{d\langle \chi \rangle}{dt} - \langle v \cdot \nabla_r \chi \rangle - \langle \frac{F_{\text{trap}}}{m} \cdot \nabla_v \chi \rangle = \langle \chi I_{\text{coll}} \rangle,
\]
(2.15)
as in [14], which can then be used to calculate the time evolution of \( \chi \).

The quantities \( \chi = r^2 \), \( r \cdot v \), and \( v^2 \) each satisfy (2.9), so \( \langle \chi I_{\text{coll}} \rangle \) goes to zero in each instance.

The time dependence of \( r^2 \), \( r \cdot v \), and \( v^2 \) can then be found using (2.15), and are
\[
\frac{d\langle r^2 \rangle}{dt} = 2\langle r \cdot v \rangle,
\]
(2.16)
\[
\frac{d\langle r \cdot v \rangle}{dt} = \langle v^2 \rangle - \omega_0^2 \langle r^2 \rangle,
\]
(2.17)
and
\[
\frac{d\langle v^2 \rangle}{dt} = \omega_0^2 \langle r^2 \rangle.
\]
(2.18)
The solution to this closed system of equations is an undamped monopole motion at twice the trap frequency [14].
This approach can be used to describe both monopole and quadrupole motion. Quadrupole motion involves the quantity \( \chi = v_r^2 - 2v_z^2 \), which does not satisfy (2.9) and is the source of quadrupole damping [14]. The quadrupole damping rate for a collisionless gas can be calculated from the results of [14] and [25], and is

\[
\Gamma_{\text{Quad}} = \frac{1}{5} \gamma_{\text{Coll}},
\]

(2.19)

where \( \gamma_{\text{Coll}} \) is the classical collision rate. Therefore we expect an average of five collisions per atom in order to see \( \frac{1}{e} \) decay of the quadrupole amplitude. This result can also be produced using variational techniques [20].

### 2.3 Collisionless and Hydrodynamic Regimes

There are two collisional limits of the Boltzmann equation. The collisionless limit describes the situation of a low density thermal gas, where the mean-free path is long relative to the size of the gas. This is the regime where our experiment operates. The hydrodynamic limit is the opposite of the hydrodynamic regime, where atoms collide so frequently the gas can be mathematically treated as a continuous medium. The difference in regimes is relevant because the frequency of monopole and quadrupole oscillations change between these two limits [14, 12, 25].
3.1 History and Structure

To investigate dual-species evaporative cooling of $^{87}\text{Rb}$ and $^{40}\text{K}$, John Goldwin programmed a Monte Carlo simulation [11]. When I was starting to program our Monte Carlo simulation, Ming-Guang Hu, a graduate student currently working in the lab Goldwin was a student in, generously lent me the current version of their software to help me get started. The general structure of generating a distribution, evolving it in time, and saving the results is very much the same. Although I have essentially rewritten the entire program, Ming-Guang and Goldwin’s code was a very helpful starting point.

3.2 Creating the Distribution

The Maxwell-Boltzmann distribution, eq. 2.3, takes the functional form of a gaussian, and the standard deviation in position space and velocity space is

$$\sigma_x = \sqrt{\frac{k_b T}{m \omega_T}},$$  \hspace{1cm} (3.1)

and

$$\sigma_{v_x} = \sqrt{\frac{k_b T}{m}},$$  \hspace{1cm} (3.2)

respectively. Here, $k_b$ is Boltzmann’s constant, $T$ is temperature, $m$ is the mass of a $^{87}\text{Rb}$ atom, and $\omega_T$ is the trap frequency. In order to create a Maxwell-Boltzmann distribution, we simply generate vectors for position and velocity space in each dimension. These vectors are then filled
with normally-distributed random numbers, with a standard deviation of 1, and then multiplied by the standard deviations shown above.

Ideally, we would be able to simulate the same number of atoms as we typically use in our experiment, but unfortunately this is computationally expensive, as the most time consuming calculation in the simulation scales as $N^2$. Minimal error in distribution initialization is important because it allows us to create distributions with little to no residual monopole or quadrupole motion. The percent error in $\sigma_x$ is less than 0.1% for $N = 2000$ atoms, which is the standard number of atoms we simulate.

### 3.3 Time Propagation

Various time propagation schemes are necessary for numerical simulations involving differential equations due to the fact that time cannot necessarily be regarded as continuous in these simulations. For instance, propagating the motion of a simple pendulum using the Euler method causes the amplitude of the oscillation to diverge. This can be solved by using the Euler-Cromer method, as described in [1], which is the time propagation technique I used in my simulation.

The accuracy of the time evolution depends on size of the time steps used in the simulation. I found that $\Delta t = 50\mu s$ was accurate enough for our purposes. This can be checked by simulating a single atom with some initial displacement, $x_o$ along one dimension. Subtracting the difference between the initial position and the position of the atom after exactly one period, $x_T$, can be used to determine the accuracy of the calculation. At $50\mu s$, the difference is $|x_o - x_T| = (1.846 \pm 0.005) \times 10^{-13} m$, which is about 28,000 times smaller than the $s$-wave scattering length of a $^{87}$Rb atom [8].

A more imposing constraint on the time step is that it must be small enough that a significant amount of collisions are not missed because atoms only would have been close enough to collide in-between time steps.
3.4 Collision Function

The function that propagates collisions in Ming-Guang’s code relied on calculating a probability of a collisional event between a given pair of atoms, and then generating a random number to determine if the event occurs. My collision function however, employs a hard-sphere assumption. In other words, if two atoms are within a certain distance of each other, they undergo a perfectly elastic collision. In order to account for s-wave collisions, the outgoing scattering angle is chosen to be random such that scattering is isotropic. This allows for a drastic simplification in the calculation of final velocities of colliding atoms, as pointed out by Dan Lobser, because the impact parameter and scattering angle do not need to be explicitly calculated.

For each eligible pair, the collision function begins by calculating a randomly generated unit vector, \( \mathbf{u} \). Then, we move to the center of mass frame, where

\[
\mathbf{v}_{cm} = \frac{1}{2} (\mathbf{v}_1 + \mathbf{v}_2).
\]  

(3.3)

The relative velocity is then calculated,

\[
v_{rel} = \sqrt{(v_{2,x} - v_{1,x})^2 + (v_{2,y} - v_{1,y})^2 + (v_{2,z} - v_{1,z})^2}
\]

(3.4)

Next, the outgoing velocities are determined by adding half of the relative velocity in the direction of the normalized random unit vector \( \mathbf{u} \) to \( \mathbf{v}_{cm} \) for one atom, and subtracting half of the relative velocity from \( \mathbf{v}_{cm} \) atom along the direction of \( \mathbf{u} \) for the other atom,

\[
\mathbf{v}'_1 = \mathbf{v}_{cm} + \frac{v_{rel} \cdot \mathbf{u}}{2},
\]

(3.5)

and

\[
\mathbf{v}'_2 = \mathbf{v}_{cm} - \frac{v_{rel} \cdot \mathbf{u}}{2}.
\]

(3.6)

Finite time steps require several book-keeping tasks to be completed by the collision function in order to ensure that the pair selection is physically correct. The first step in the collision function is to create a matrix containing the distance between each atom with every other atom: the separation matrix. This matrix is an upper triangular \( N \times N \) matrix, where the \( [n,m]^{th} \) element
corresponds to the distance between the \( n^{th} \) and \( m^{th} \) atoms. The next step is to create another upper triangular matrix in order to keep track of which atom pairs are available to collide with each other; I call this the availability matrix. This is necessary because with finite time steps, pairs can sometimes be within a collision distance of each other and collide during one time step, yet still be within a collision distance of each other on the following time step. Colliding the pair twice would not be physical, so once a pair collides, it is set unavailable until the pair separate by at least a collision distance. When a pair is unavailable the two atoms cannot collide with each other, but they can still collide with other atoms. At each time step, a list is compiled of all pairs within a collision distance of each other that are also available to collide. This list is then sorted and the pairs are collided in order of least separation. If an available atom is within a collision distance of more than one other available atom, it will only be collided with the one that it is closest to during that time step.

If the simulation involved several hundred thousand atoms, I would be able to use the physical scattering length of a \(^{87}\text{Rb}\) atom as the maximum distance at which two atoms could collide. However, large \( N \) calculations take an extremely long time to run. For \( N = 2000 \) and \( \Delta t = 50\mu s \) it takes approximately 8 hours to run one second of simulation time with an Intel Xeon processor, and the run-time increases roughly as \( N^2 \). This long run-time is almost entirely due to the collision function, as 1 second of simulation time takes less than a minute to run on a similar processor with no collisions. The \( N^2 \) scaling occurs because of calculating the separation matrix. In order to simulate a collision rate on the order of the collision rate we achieve experimentally with number on the order of \( N = 2000 \), we artificially increase the scattering length of our atoms. Rather than a scattering length of about \( 5nm \) [8], typical scattering lengths in the simulation are on the order of \( \mu m \). This ability to varying the scattering length to arbitrary values allows us to vary the collision rate over a very large range. The finite time steps can also be problematic for the collision function. The collision rate dependence on time step size, \( \Delta t \), is shown in fig. 3.1. We typically operate with \( \Delta t = 50\mu s \), at which we are missing approximately 7.8% of collisions. While it would be nice to increase our accuracy further, run-time increases linearly with \( \Delta t \), and it becomes impractical to
run such long simulations.

Figure 3.1: A linear regression predicts that at $\Delta t = 0$ s, the collision rate would be $\gamma_{coll} = 11.2 \text{ (s}^{-1})$. Taking this as the total collision rate, at $\Delta t = 50\mu s$ we are missing approximately 7.8% of the total number of collisions.

3.5 Connecting Theoretical and Simulated Collision Rates

There are numerous factors of 2 involved in calculating the average collision rate per atom, $\gamma_{coll}$, for a given situation. Factors of two can be added in to take into account effects like Bose-enhancement, collisional events involving two atoms, etc.. In the collisionless regime, the collision rate can be written

$$\gamma_{coll} = \frac{n(0) \nu_{th} \sigma}{2},$$  \hspace{1cm} (3.7)

where $n(0)$ is the peak number density, $\nu_{th}$ is the average magnitude of atoms’ velocities, and $\sigma$ is the scattering cross-section [25]. For a classical Maxwell-Boltzmann distribution, the average velocity magnitude is

$$\nu_{th} = \sqrt{\frac{8k_B T}{\pi m}}.$$ \hspace{1cm} (3.8)
For a classical gas in a harmonic potential, the central density is known [25] to be

$$n(0) = N \omega_x \omega_y \omega_z \left( \frac{m}{2 \pi k_b T} \right)^{3/2}. \quad (3.9)$$

We are implementing a hard-sphere model, in which the scattering cross-section is simply

$$\sigma = 4 \pi \left( \frac{d_c}{2} \right)^2. \quad (3.10)$$

Combining the above equations, we have an expression for the theoretical collision rate in the simulation,

$$\gamma_{\text{coll}} = \frac{N m d_c^2 \omega_x \omega_y \omega_z}{2 \pi k_b T}. \quad (3.11)$$

The collision rate can also be calculated directly in the simulation by counting collision events. In order for $\gamma_{\text{coll}}$ to be the average collision rate per atom, we need to account for the fact that collisions involve two atoms [31]. The theoretical collision rate is a factor of two larger than the counted collision rate, even when we account for both atoms participating in a collision. We are not sure why this is, but are relatively confident in the counted collision rate because of the results discussed in section 3.7.

### 3.6 Dummy Checks

This simulation would be mean nothing if we could not confirm that it agreed with basic laws of physics including conservation of energy, equipartition theorem, etc.. To this end, I did several checks, most of them were incorporated into a script called DummyChecks.m, that I could run to make sure the current version of the simulation still held up to our theoretical expectations.

First, it is useful to write the single atom hamiltonian for our gas:

$$\mathcal{H} = \frac{1}{2} m \left( v_x^2 + v_y^2 + v_z^2 \right) + \frac{1}{2} m \omega^2 \left( x^2 + y^2 + z^2 \right). \quad (3.12)$$

According to the Equipartition Theorem [27], the average energy of an atom in an ideal gas is given by

$$\bar{E}_{\text{atom}} = \frac{f}{2} k_b T, \quad (3.13)$$
where $f$ is the number of quadratic degrees of freedom present in the single particle Hamiltonian. By eq. 3.12, each atom in our gas has $f = 6$ quadratic degrees of freedom, and for a gas at $T = 100nK$ we expect that $E_{\text{atom}} = 4.142 \cdot 10^{-30} J$. Generating a distribution with $N = 2000$ atoms, I calculate the average energy per atom to be $(4.1139 \pm 0.0012) 10^{-30} J$; we do not see a significant violation of the Equipartition Theorem. We can also look at the average magnitude of an atom’s velocity, $\nu_{th}$, as defined in eq. 3.7, which we would expect to equal $4.93 \frac{mm}{s}$. For a distribution of $N = 2000$ atoms, I calculate $\nu_{th} = (4.96 \pm 0.05) \frac{mm}{s}$, in good agreement with theory.

Another check is that the momentum is conserved when the collision function carries out an elastic collision with isotropic scattering. Momentum is conserved, and further, we can look at the derivative of each atom’s motion and use a peak-finding algorithm to confirm that the collision function is counting collisions correctly.

The point of this simulation is to investigate damping rates of various collective excitations in several potentials. In order to verify that we can accurately simulate damping rates of collective motion, we can calculate the number of collisions it takes per atom to relax a cross-dimensional temperature anisotropy in our simulation, and compare to the experimentally known value.

## 3.7 Cross-dimensional Temperature Anisotropy

A cross-dimensional temperature anisotropy occurs when the temperature along each dimension is not the same, and the gas is not in thermal equilibrium with itself, as illustrated in figure 3.2. Analytically, one would expect $\rho = 2.5$ collisions per atom per second to relax a cross-dimensional temperature anisotropy [25], but it has been shown both experimentally and through numeric simulations that $\rho = 2.7$ [6, 30]. Discussing collisions per atom inherently involves a factor of two due to the fact that collision events involve two atoms [31], since we are only considering binary collisions. The simulation counts collision events so we include this factor of two when calculating the average collision rate. By varying the collision distance, $d_c$, we can vary the collision rate, and observe the dependence of the temperature anisotropy relaxation rate on the average collision rate. At each collision rate, several runs are averaged together, and the $x$ and $y$ temperatures are
averaged together. Finally, the average $xy$ and $z$ temperatures are fit to exponentials in time,

$$f(t) = Ae^{-\Gamma_T t} + T_{x,y,z}.$$  \hspace{1cm} (3.14)

Uncertainties were calculated from an approximation of the covariance matrix, which itself was returned from MATLAB®’s built-in fitting function nlinfit. The one-standard-deviation uncertainties for individual trials and fits of $\Gamma_T$ were determined by taking the inverse of the square root of diagonal elements in the covariance matrix approximation. This is how standard deviations were calculated throughout this text, and it appears that these standard deviations are generally under-estimates for the uncertainty.

The decay rates, the inverse of the characteristic damping times, from both the $xy$ and $z$ fits are plotted in figure 3.4; the $xy$ and $z$ points overlap extremely well. We determine $\varrho$ by fitting the decay rates vs. the average collision rates with a linear regression.

We find $\varrho_{\text{sim}} = 2.69 \pm 0.13$ collisions per atom, well within one standard deviation of, and in
Figure 3.3: Cross-Dimensional Temperature Anisotropy Relaxation Rates. These simulations involved 2000 atoms, and the temperature along the $z$ axis was $40nK$ higher than the temperature along the $x$ and $y$ axes, with the average temperature of the gas at $T = 100nK$. The time step was $\Delta t = 50\mu s$. The inverse of the slope corresponds to the average number of collisions per atom per second required to relax the temperature anisotropy.

\[
\frac{1}{\Gamma_T} = \frac{\gamma_{coll}}{d_c} \Rightarrow \frac{1}{\Gamma_T} = \gamma_{coll} \frac{\text{coll/Atom}}{d_c}
\]

\[
\text{Slope} = 0.372 \pm 0.018 \Rightarrow 2.7 \text{ Coll/Atom}
\]

very good agreement with, experiment and previous numerics [6, 30]. There is a finite offset from the origin, which we do not expect, and does not make physical sense. We identified two possible causes that would be practical to check: time step size and collision distance. These are both factors of the same (potential) problem. The gas is equilibrating systematically slow, which might be a result of missing collisions from faster atoms. Our thought was that with finite time steps, some of the faster atoms might be moving fast enough to move through the trap center, which slow atoms spend more time near, without undergoing a collision. This would systematically slow down the temperature anisotropy relaxation rates. We tried varying the time step in order to maintain the same ratio between $d_c$ and the distance the fastest atom would travel in one time step. This did not produce any noticeable change in the relaxation rates or the offset. We then looked at the relative velocities of colliding atoms, to see if smaller collision distances systematically missed high relative velocity collisions. We did not observe any noticeable difference in the relative velocities of
colliding atoms for various collision distances.

Figure 3.4: (left) We binned the relative velocity of colliding atoms to see if smaller collision distances and finite time steps allowed the fastest atoms to punch through the trap center without colliding with slower atoms that spend more time near the trap center. We do not see a noticeable difference between collision distances of $d_c = 2$, 3.2, and 3.6$\mu$m. (right) Varying the time step from $50\mu s \leq \Delta t \leq 500\mu s$ also does not yield a change in the offset in $\Gamma_T$ vs. $\gamma_{coll}$; the slope is consistent with our previously stated result.

3.8 Too Many Collisions

As discussed in section 2.3, we start leaving the truly collision-less regime if atoms are on average colliding at least once each time they pass through the gas. For a 10Hz trap, this occurs when $\gamma_{coll} = 10\ (s^{-1})$. If we run simulations with very large collision distances, and very large average collision rates, we see a breakdown of exponential temperature anisotropy relaxation, as seen in figure 3.5. This breakdown occurs when the characteristic relaxation time, $(1/\Gamma_T)$, is on the order of several trap periods.
Figure 3.5: (left) The collision rate for this temperature anisotropy relaxation is $\gamma_{\text{coll}} = 338 \, (s^{-1})$, which is not in the collisionless regime. In fact, the expected characteristic time for this collision rate would roughly be a tenth of the trap period (0.1 seconds). (right) Exponential fits for temperature anisotropy relaxation with collision rates higher than roughly $\gamma_{\text{coll}} = 60 \, (s^{-1})$ start to break down because the temperature anisotropy relaxation is no longer purely exponential.
Chapter 4

Isotropic and Harmonic Potentials

4.1 Monopole Motion

As mentioned in the introduction, Boltzmann predicted that monopole motion of a thermal gas in a perfectly isotropic and harmonic potential would be undamped [2, 4], where monopole motion is an oscillation of symmetric expansion and contraction of the gas. We can simulate monopole motion by creating our distribution of atoms out of equilibrium. The method we use to create a distribution undergoing monopole motion is slightly modified from what is described in 3.2. To initiate monopole motion, with normalized amplitude

\[ A_m = \frac{\sigma_x^2 + \sigma_y^2 + \sigma_z^2}{\langle \sigma_x^2 + \sigma_y^2 + \sigma_z^2 \rangle} - 1, \]  

(4.1)

the initial distribution is created so that is larger than its canonical equilibrium state. We want our initial distribution to dictate that

\[ \sigma_{x,y,z}^2 - \sigma_{eq}^2 = \alpha \sigma_{eq}^2 \]

where \( \alpha \) is a unit-less scaling parameter. To accomplish this we multiply the position space standard deviation, \( \sigma_{x,y,z} \) by a factor of \( \sqrt{1 + \alpha} \), so

\[ \sigma_{x,y,z} = \sqrt{\frac{k_B T}{m \omega_{x,y,z}^2}} \sqrt{1 + \alpha}. \]  

(4.2)

We typically run simulations with \( \alpha = 0.3 \), which corresponds to amplitudes of \( A_m = 0.3 \), and is typical of our experimental monopole amplitudes. The momentum space standard deviation also needs to be modified to reflect that the monopole excitation is at its peak amplitude, and velocities should typically be smaller in magnitude. This is accomplished by scaling the standard deviation
of the velocity by a factor \( \sqrt{1 - \alpha} \), or

\[
\sigma_{v_x, v_y, v_z} = \sqrt{\frac{k_B T}{m}} \sqrt{1 - \alpha}.
\]  

(4.3)

In accordance with Boltzmann’s prediction, we observe undamped monopole motion in isotropic and harmonic potentials in the simulation. One interesting feature is that the 1-dimensional monopole motion is not necessarily conserved along any given axis, yet these thermal fluctuations are always exactly suppressed such that the total, 3-dimensional monopole motion is robustly undamped. This is illustrated in figure 4.1. Note that due to finite time step effects and rounding errors, there is a finite loss in monopole amplitude at a rate of less than 0.06% per second with \( \Delta t = 50\mu s \).

### 4.2 Quadrupole Motion

To drive quadruple motion we again deviate from the routine described in 3.2 by initializing a distribution out of equilibrium from its potential. Our perturbations to the standard deviations of the distribution in position and velocity space cannot be symmetrically applied to all three dimensions as they were for monopole excitations. Quadrupole motion is effectively monopole motion with the monopole motion along one axis exactly out of phase with the monopole motion along the other two axes, and the normalized quadrupole amplitude can be written

\[
A_Q = \frac{\sigma_x^2 + \sigma_y^2 - 2\sigma_z^2}{(\sigma_x^2 + \sigma_y^2 + \sigma_z^2)}.
\]  

(4.4)

In order to drive a pure quadrupole motion, with no monopole component in position space or velocity space, we need to set up distributions so that \( \sigma_x^2 + \sigma_y^2 + \sigma_z^2 - 3\sigma_{eq}^2 = 0 \) and \( \sigma_{v_x}^2 + \sigma_{v_y}^2 + \sigma_{v_z}^2 - 3\sigma_{v_{eq}}^2 = 0 \). Scaling the standard deviation of our distributions by \( \sqrt{1 \pm \beta} \) or \( \sqrt{1 \pm 2\beta} \) satisfies this constraint, where \( \beta \) is a unit-less parameter. We produce monopole motion along the \( xy \) axes that is exactly out of phase with the monopole motion along the \( z \) axis by creating distributions that follow

\[
\sigma_{x, y} = \sqrt{\frac{k_B T}{m\omega_{x, y}^2}} \sqrt{1 + \beta},
\]  

(4.5)
Figure 4.1: Components of a monopole excitation with $N = 2000$, $T_{avg} = 100nK$, and $\gamma_{coll} = 5.4\, (s^{-1})$ in a harmonic and isotropic potential with trap frequency $\omega_T = 10\,(2\pi)\,Hz$. (top) Monopole motion along any single dimension is not typically constant in amplitude. There is also $y$-axis monopole motion, which is not shown for the sake of space. (bottom) Despite the thermal fluctuations in amplitude along single dimensions, the 3-dimensional monopole motion is robustly undamped and the thermal fluctuations are suppressed.

\[\sigma_z = \sqrt{\frac{k_B T}{m \omega_z^2}} \sqrt{1 - 2\beta}, \quad (4.6)\]

\[\sigma_{v_x, v_y} = \sqrt{\frac{k_B T}{m}} \sqrt{1 - \beta}, \quad (4.7)\]
\[ \sigma_{vz} = \sqrt{\frac{k_b T}{m}} \sqrt{1 + 2\beta}, \]  

which result in a normalized quadrupole amplitude of \( 2\beta \).

In order to analyze the quadrupole data, we first average trials together that have the same collision rate. We then normalize our quadrupole data in the same manner as we normalize the monopole data: dividing by \( \langle \sigma_x^2 + \sigma_y^2 + \sigma_z^2 \rangle \). We fit the averaged, normalized data to an exponentially decaying sine wave with the functional form,

\[ f(t) = A \sin(2\omega_T t + \phi) \left( e^{-\Gamma_Q t} + C \right), \]

where \( A \) is the amplitude, \( \omega_T \) is the isotropic trap frequency, \( C \) is a constant, \( \Gamma_Q \) is the quadrupole damping rate, and \( t \) is time measured in seconds.

Figure 4.2: This example of quadrupole decay fit to an exponentially damped sine wave was simulated with \( N = 2000 \) atoms, \( T = 100\,\text{nK} \), and \( \gamma_{\text{coll}} = 39\,(\text{s}^{-1}) \) in a \( \omega_T = 10(2\pi)\,\text{Hz} \) potential.

Quadrupole damping is very similar to cross-dimensional temperature anisotropy relaxation in that the quadrupole damping rate also depends linearly on the average collision rate, \( \gamma_{\text{coll}} \). The
relation is expected to be
\[ \Gamma_Q = \xi \gamma_{\text{coll}} = \frac{1}{5} \gamma_{\text{coll}}, \] (4.10)
or in other words, one expects approximately twice as many collisions \((5)\) to exponentially damp quadrupole motion in an isotropic and harmonic trap than it takes to exponentially relax a temperature anisotropy in the same potential with the same collision rate \([25, 14]\).

In figure 4.3 I plot the damping rate against the collision rate, and fit to a line going through the origin. This yields a slope of \(\xi = 0.139 \pm 0.009\), which is 30.5% away from the \(\frac{1}{5}\) slope we were expecting.

Figure 4.3: These quadrupole motion simulations were done using \(\beta = 0.1\), a time step of \(\Delta t = 50\mu s\), and \(N = 2000\) atoms. The damping rates were plotted against the collision rates they occurred at, then fit using a linear regression that passes through the origin. The expected slope is \(\xi = 0.2\).

4.3 Comparison With Experiment

Experimentally we drive quadrupole motion as described in [7]. Examining the relationship between our experimental quadrupole damping rates and their respective collision rates yields good
agreement with our theoretical expectations. The linear regression of $\Gamma_{Q_{\text{exp}}}$ vs. $\gamma_{\text{exp}}$ has a slope of $\xi = 0.197 \pm 0.005$, which is within one standard deviation of the expected result. Our simulation result differs from this slope by 29.4%. We spent quite a while trying to determine the source of this systematic error in the simulation, but have been unable to figure out why it is present.

Figure 4.4: Results of simulations in an isotropic and harmonic potential for quadrupole damping rates are plotted with the experimentally observed monopole and quadrupole damping rates. While the experimental quadrupole damping rates agree quite well with theory, the monopole motion is unexpected for an isotropic and harmonic potential.

This finite monopole damping we observe is not predicted by either the simulation, or Boltzmann’s equation. There are three assumptions required in Boltzmann’s proof of undamped monopole motion: the potential is isotropic, the potential is harmonic, and collisions are point like, as discussed previously. Observing a non-zero monopole damping rate experimentally indicates that one or more of our model’s assumptions is not accurate for our system. The next chapter will investigate whether breaking the trap isotropy can account for the finite damping we observe.
Chapter 5

Anisotropic and Harmonic Potentials

5.1 Setup

Setting up an anisotropic potential is very simple to do in our simulation. In implementing time propagation (see section 3.3), the acceleration due to the potential is calculated for each atom in cartesian coordinates. Changing the potential along the $x$-, $y$-, or $z$-axis is therefore quite trivial. Following [7], we define the residual anisotropy as

$$\Lambda = \frac{f_{\text{max}} - f_{\text{min}}}{f_{\text{avg}}}.$$  \hspace{1cm} (5.1)

As shown in section 3.11, the collision rate of a classical thermal gas in the simulation is given by

$$\gamma_{\text{coll}} = \frac{N m d_c^2 \omega_x \omega_y \omega_z}{2 \pi k_b T}.$$  \hspace{1cm} (5.2)

Breaking the isotropy of the potential changes the collision rate because the collision rate depends on the density of the gas, which in turn depends on the trap frequencies along each principal axis. We confirmed that varying $\Lambda$ while keeping all other parameters constant demonstrates a collision rate that is linearly dependent on $\Lambda$.

We can use eq. 5.2 to varying the collision distance, $d_c$, used in the simulation in order to keep a constant collision rate over various anisotropies. Solving for $d_c$ yields

$$d_c = \sqrt{\frac{2 k_b T \pi \gamma_{\text{coll}}}{m N \omega_x \omega_y \omega_z}}.$$  \hspace{1cm} (5.3)

Using eq. 5.3 we can achieve a relatively constant collision rate, as shown in figure 5.1, for any given anisotropy.
5.2 Monopole Motion

Looking at just the monopole motion, we see what looks like a beating motion between two distinct frequencies, where the slower envelope frequency is determined by the trap anisotropy and the faster carrier frequency is the monopole motion itself. As one would expect, changing the collision rate relative to the trap anisotropy will change the dynamics of the gas. For a given collision rate, breaking the isotropy more severely will result in more shape oscillations between monopole and quadrupole motion. This can be seen in figure 5.2.

In order to simplify fitting this data, and look at the data in a more model independent way, we first fit each individual period of monopole motion to an undamped sine wave. We extract the amplitude from this fit, and then look at the single period amplitudes in time, fitting to the functional form

\[ f(t) = A e^{-\Gamma_m t} \left( \cos^2 \left[ 2\pi (f_{max} - f_{min}) t + \phi \right] + C \right), \]  

(5.4)
where $A$ is related to the amplitude, $\Gamma_m$ is the monopole damping rate, $\phi$ is a phase offset, and $C$ is a constant. At first the constant $C$ in this fitting function might appear non-physical, but it is there to account for the fact that at any given time there is still some fraction of the excitation undergoing monopole motion (before it is completely damped out). In other words, not all of the monopole motion is coupled into quadrupole motion at the same time, this can be seen in figure 5.2.

Figure 5.2: These monopole simulations were run with an average collision rate of $\gamma_{coll} = 8.4 \ (s^{-1})$, and their individual collision rates are shown in figure 5.1. For each of the four simulations shown, the top plot is shows the single period amplitude fits and the original monopole motion, while the bottom plot shows the amplitudes fit to eq. 5.4, which were cut off when the amplitude consistently remained below 20% of its initial value or at $t = 15$ seconds. The fits are shown in red.

\[
\Lambda = 0.051724
\]

\[
\Lambda = 0.030612
\]

\[
\Lambda = 0.0080429
\]

\[
\Lambda = 0.0010007
\]

Varying the residual anisotropy and fitting the resulting monopole motion to eq. 5.4 we are...
able to look at the damping rate with respect to \( \Lambda \). In agreement to one’s physical intuition, when

Figure 5.3: Monopole damping rates with varying amounts of residual anisotropy, \( \Lambda \). The collision rates for these data are relatively constant, and are shown in figure 5.1.

![Monopole Damping with Anisotropy](image)

the residual anisotropy, \( \Lambda \), is large, we expect the dynamics of the gas to be undergoing monopole motion half of the time, and quadrupole motion the other half. In the large \( \Lambda \) limit the damping rate approaches half of the canonical quadrupole damping rate, which for the collision rate in figure 5.3 would be \( \frac{1}{2} \Gamma_Q (\gamma_{\text{coll}} = 8.4) = 0.58 \).

### 5.3 Not The Droids We’re Looking For

Comparison with experimental data reveals that anisotropy is not the source of monopole damping we see experimentally. First, we use the unit-less parameter \( \Lambda \) as defined in eq. 5.1. We then define a second unit-less parameter \( \kappa \), which is the monopole damping divided by the expected quadrupole damping rate at a given collision rate,

\[
\kappa = \frac{\Gamma_m}{\Gamma_Q}. \tag{5.5}
\]
We would expect that in the limit of large $\Lambda$, $\kappa$ should tend to $\frac{1}{2}$, because the monopole excitation is spending approximately half of its time in the quadrupole mode. We would also expect to see $\kappa$ go to zero as $\Lambda$ goes to zero. In figure 5.4 we see that in the simulation, $\kappa$ goes to zero in the small $\Lambda$ limit. As mentioned above, at larger $\Lambda$ we see the simulated monopole damping rate approach half of the expected quadrupole rate. We know that anisotropy is not the cause of the finite monopole damping we observe experimentally because in the nearly-isotropic limit, we still see finite damping. This can be seen in 5.4. The next step in investigating the source of this damping is to simulate a potential that models our experimental anharmonicities.

Figure 5.4: (left) Monopole damping in potentials with various residual anisotropies. $\kappa$ is the monopole damping divided by the quadrupole damping rate at a given collision rate, and in the limit of larger anisotropy one would expect $\kappa$ to be $\frac{1}{2}$. (right) This is the same data plotted to the left, but focused on $\kappa$ at very small residual anisotropies, $\Lambda$. 

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5.4.png}
\caption{(left) Monopole damping in potentials with various residual anisotropies. $\kappa$ is the monopole damping divided by the quadrupole damping rate at a given collision rate, and in the limit of larger anisotropy one would expect $\kappa$ to be $\frac{1}{2}$. (right) This is the same data plotted to the left, but focused on $\kappa$ at very small residual anisotropies, $\Lambda$.}
\end{figure}
Chapter 6

Isotropic and Anharmonic Potentials

6.1 Simulating Our Trap Anharmonicities

The analytic form of the instantaneous potential created by the standard TOP Trap can be found in [9]. Dan Lobser provides an integrated analytic form for the potential of our zzTOP Trap in [22], as well as a Taylor expansion of the potential. Applying $F = -\nabla U$ and $F = ma$, we are able to implement the Taylor expanded potential in the simulation.

The TOP trap potential can be written

$$U(x, y, z, t) = \mu \sqrt{\left( B_0 \cos(\omega_{top} t) + \frac{B_z' x}{2} \right)^2 + \left( B_0 \sin(\omega_{top} t) + \frac{B_z' y}{2} \right)^2 + (B_z'(r_{min} + z))^2 + mg(r_{min} + z)}, \quad (6.1)$$

where $B_0$ is the TOP coil amplitude, and $B_z'$ is the quadrupole field gradient. The time-averaged potential can be found by Taylor expanding and integrating $U(x, y, z, t)[22, 9]$, which yields

$$U_{TOP}(x, y, z) = \frac{\omega}{2\pi} \int_0^{2\pi/\omega} U(x, y, z, t) dt, \quad (6.2)$$

and

$$U_{TOP}(x, y, z) = \varrho_{0,0} + \varrho_{2,0} (x^2 + y^2) + \varrho_{4,0} (x^2 + y^2)^2 + \varrho_{2,1} (x^2 + y^2) z + \varrho_{4,1} (x^2 + y^2)^2 + \ldots \quad (6.3)$$

The coefficients $\varrho_{r,z}$ are indexed by their orders of $r$, $|r| = \sqrt{x^2 + y^2}$, and $z$, and are shown in table 6.1. These coefficients are in terms of $\eta = \frac{mg}{\mu g z}$ as defined in [9]. In this context $\mu$ is the magnetic moment, given in [28]. In an isotropic configuration we typically operate with $B_0 = 130 \mu T$ and $B_z' = 0.346 \frac{\mu T}{m}$, which are the values used in the simulation. It is still convenient to calculate the
acceleration of each atom due to the potential in cartesian coordinates because only the even powers of $r$ survive the expansion. The acceleration is then

$$a_x = -\frac{1}{m} \left( 2q_{2,0}x + 4q_{4,0}x \left( x^2 + y^2 \right) + 2q_{2,1}xz + 4q_{4,1}x \left( x^2 + y^2 \right) z + \ldots \right), \quad (6.4)$$

$$a_z = -\frac{1}{m} \left( q_{0,1} + q_{2,1} \left( x^2 + y^2 \right) + q_{4,1} \left( x^2 + y^2 \right)^2 + 2q_{0,2}z + \ldots \right). \quad (6.5)$$

The potential generated by this expansion is shown in figure 6.1. The validity of this approximated potential is discussed in section 6.4.

Figure 6.1: The Taylor expanded zzTOP potential approximates the anharmonic aspects of our experimental potential. Note that the potential is more isotropic and harmonic near the trap center. Typically the FWHM of the simulated clouds are 133$\mu$m.

6.2 Quadrupole Motion in Anharmonic Potentials

With the experiment we observed quadrupole damping rates consistent with theory, so we expect that the anharmonic terms introduced to the potential with the Taylor expansion will only have a small perturbative effect on quadrupole damping rates. The finite monopole damping we observe in the experiment is significantly smaller than the quadrupole damping rates in an isotropic
Table 6.1: This table contains the coefficients up to 4th order in r and z [22]. The coefficients of odd orders of r are zero.

<table>
<thead>
<tr>
<th></th>
<th>$x^0 + y^0$</th>
<th>$x^2, y^2$</th>
<th>$(x^2 + y^2)^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$z^0$</td>
<td>$B_o \sqrt{1 - \eta^2} \mu$</td>
<td>$B_o^2 \sqrt{1 - \eta^2 (\eta^2+1)} \mu$</td>
<td>$B_o^2 \sqrt{1 - \eta^2 (\eta^2+1)(\eta^2+5) \mu}$</td>
</tr>
<tr>
<td>$z^1$</td>
<td>$0$</td>
<td>$-B_o^3 \eta (3 \eta^4 - 4 \eta^2 + 1) \mu$</td>
<td>$-\frac{3B_o^5 \eta (\eta^2 - 1)^2 (35 \eta^4 - 30 \eta^2 + 3 \mu}{1024 B_o^4}$</td>
</tr>
<tr>
<td>$z^2$</td>
<td>$\frac{B_o^2 (1 - \eta^2)^{3/2} \mu}{2B_o}$</td>
<td>$\frac{B_o^4 (1 - \eta^2)^{3/2} (15 \eta^4 - 12 \eta^2 + 1)}{32 B_o^2}$</td>
<td>$-\frac{3B_o^6 (1 - \eta^2)^{3/2} (35 \eta^4 (9 \eta^4 - 11 \eta^2 + 3) - 3 \mu}{2048 B_o^4}$</td>
</tr>
<tr>
<td>$z^3$</td>
<td>$\frac{B_o^3 \eta (\eta^2 - 1)^2 \mu}{2B_o^3}$</td>
<td>$\frac{B_o^5 \eta (\eta^2 - 1)^2 (35 \eta^4 - 40 \eta^2 + 9) \mu}{32 B_o^3}$</td>
<td>$\frac{5B_o^7 \eta (\eta^2 - 1)^2 (7 \eta^2 (99 \eta^4 - 153 \eta^2 + 65) - 45 \mu}{2048 B_o^6}$</td>
</tr>
<tr>
<td>$z^4$</td>
<td>$\frac{B_o^4 (1 - \eta^2)^{3/2} (5 \eta^2 - 9 \eta^2 \eta^2 + 33 - 9) \mu}{8B_o^4}$</td>
<td>$\frac{B_o^6 (1 - \eta^2)^{3/2} (5 \eta^2 (63 \eta^4 - 91 \eta^2 + 33) - 9) \mu}{128 B_o^4}$</td>
<td>$\frac{-15B_o^8 (1 - \eta^2)^{3/2} (7 (429 \eta^4 - 792 \eta^4 + 450 \eta^2 - 80) \eta^2 + 15) \mu}{8192 B_o^6}$</td>
</tr>
</tbody>
</table>

potential, for all but very small collision rates.

In figure 6.2 we plot the quadrupole damping rates against their collision rates for simulations run in the Taylor expanded potential. The slope is $\xi = 0.157 \pm 0.006$ for quadrupole motion with a drive strength of $A_Q = 0.2$, but for drive strengths of $A_Q = 0.8$, $\xi$ increases slightly to $\xi = 0.171 \pm 0.006$, which is reasonable given that the anharmonic aspects of the potential increase at larger radii. The quadrupole damping rates for this larger drive strength in the Taylor expanded potential is about 23% larger than quadrupole damping rates in a perfectly harmonic and isotropic potential. The experimental quadrupole damping ($\xi = 0.197 \pm 0.005$), was observed with quadrupole amplitudes of roughly $A_Q = 1$. The simulated slope is still substantially less than the experimental value; however, adding in the anharmonic effects does edge the simulation closer to agreement with experiment.

### 6.3 Monopole Motion in Anharmonic Potentials

We excite monopole motion the same way that we do for an isotropic and harmonic potential, described in section 4.1, except that the trap frequency is no longer analytically known. We approximate $\omega_T$ by simulating a single atom in the taylor expanded potential, with no initial velocity and an initial displacement along one axis of 1 FWHM of a typical cloud ($N = 2000$, etc.)
Figure 6.2: Quadrupole damping rates increase with larger size quadrupole drives in the Taylor expanded potential. The experimental drive amplitude was typically $A_Q = 1$. (left) Quadrupole damping rates driven with an initial amplitude of $A_Q = 0.2$. The slope is $\xi = 0.157 \pm 0.006$. (right) Quadrupole damping rates driven with an initial amplitude of $A_Q = 0.8$. The slope is $\xi = 0.171 \pm 0.006$.

$T = 100 nK$), in a $9Hz$ harmonic potential. Fitting the atom’s motion reveals trap frequencies of $f_{x,y} = 8.826Hz$ and $f_z = 8.718Hz$.

The monopole amplitude was extracted using single period fits as described in 5.2, and are fit to the same functional form as the monopole simulations in anisotropic and harmonic potentials, eq. 5.4, except that the $\cos^2$ frequency is allowed to float. The monopole amplitudes also fit well to a simple exponential, but the lower collision rate simulations appear to initially have a slight $\cos^2$ functional form. The monopole damping of simulations using the taylor expanded potential does not appear to depend largely on collision rate, as shown in figure 6.3, in agreement with our experimental observations.

We can now compare both monopole and quadrupole damping with anharmonic effects to our experimental values. The weighted average of experimental monopole damping rates is $\bar{\Gamma}_m = 0.15 \pm 0.01$. The weighted average of simulated monopole damping rates is $\bar{\Gamma}_m = 0.1469 \pm 0.0004$, and is well within one standard deviation of the experimentally determined value. Is it a happy coincidence that our model predicts similar damping effects to what we observe experimentally? Possibly; the cloud size was similar between the simulation and the experiment (133$\mu m$ and 115$\mu m$
Figure 6.3: Simulations including approximated anharmonic effects in the experiment by implementing a Taylor’s expansion of the TOP potential demonstrate finite monopole damping that does not appear to depend on collision rate.

\[
\text{Anharm. Monopole, } FWHM = 132.8932 \mu m
\]

FWHM, respectively). In order to determine the accuracy of our simulation model, we need to examine monopole damping at various cloud sizes.

### 6.4 Monopole Damping for Different Cloud Sizes

The anharmonic effects present in the Taylor expanded potential increase with displacement from trap center, as seen in figure 6.1. Since we have shown that anharmonic effects cause finite monopole damping, we should observe changes in the amount of monopole damping as we change the size of the gas we are simulating. As in chapter 5, we can again use eq. 5.3 to maintain a constant collision rate, only this time we are varying the temperature. The anharmonic monopole data are again fit to eq. 5.4 with a floating \( \cos^2 \) frequency, and the fit cut off when the monopole amplitude drops below 5% of its initial value. Example data with fits are shown in figure 6.5.

We do not take experimental data at smaller cloud sizes than listed in 6.2 because this would
Figure 6.4: Running simulations with the Taylor expanded potential to approximate anharmonic effects present in the experiment substantially improves agreement between the simulation and the experiment. Average cloud sizes for these simulations are 133µm in the simulation and 115µm in the experiment.

Monopole and Quadrupole Damping

cause the temperature of our gas to drop below twice the critical temperature, which we avoid in order not to invoke mean-field effects or Bose-Einstein condensation of our gas. We have established that the anharmonic monopole damping does not vary significantly with collision rate. Still, the simulated collision rates for each datum are shown in table 6.2, and are at least the same order of magnitude as the experimental data. Data simulated in the Taylor expanded potential and experimental observations of monopole damping rates vs. cloud size are plotted in figure 6.6.

We learn here that the Taylor expanded model of our potential is not as accurate model as we might have hoped after seeing similar monopole damping in section 6.3. We only observe similar damping for cloud sizes near 115µm FWHM. Although the simulated damping appears to have a similar functional form to the experimental damping, the simulated damping results underestimate the damping we observe experimentally. This might have been expected because
Figure 6.5: Simulations at different cloud sizes demonstrate different larger damping rates for larger cloud sizes. At some cloud sizes there also appears to be enough anisotropy for small monopole-quadrupole coupling.

Figure 6.6: The simulation appears to systematically underestimate the monopole damping we observe in the experiment at larger cloud sizes. We do not take experimental data at smaller cloud sizes than shown because we would start to run the risk of Bose-condensing our gas.

Anharmonic Monopole Damping

the TOP potential, eq. 6.1, and the Taylor expansion do not take into account constructional asymmetries present in the experiment. These constructional asymmetries could be slight angles between magnetic coils, slight misalignments between coil pairs, small kinks in the wires wound in the coils, residual magnetization of the optics table, etc.. It is reasonable that these slight blemishes
Table 6.2: This table contains parameters for both the simulated and experimental data showed in figure 6.6. We previously showed that the anharmonic monopole damping does not depend on the collision rate. The collision rates are the same order of magnitude for each datum, and the cloud sizes are very similar.

<table>
<thead>
<tr>
<th>Datum</th>
<th>FWHM (µm)</th>
<th>$\gamma_{coll}$ (s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experiment 1</td>
<td>115</td>
<td>5.8</td>
</tr>
<tr>
<td>Simulation 1</td>
<td>115.9(4)</td>
<td>5.86(9)</td>
</tr>
<tr>
<td>Experiment 2</td>
<td>147</td>
<td>0.1780</td>
</tr>
<tr>
<td>Simulation 2</td>
<td>147.8(8)</td>
<td>0.1014(9)</td>
</tr>
<tr>
<td>Experiment 3</td>
<td>192</td>
<td>0.1108</td>
</tr>
<tr>
<td>Simulation 3</td>
<td>195.4(1)</td>
<td>0.051(2)</td>
</tr>
<tr>
<td>Experiment 4</td>
<td>236</td>
<td>0.0621</td>
</tr>
<tr>
<td>Simulation 4</td>
<td>241(1)</td>
<td>0.0220(8)</td>
</tr>
</tbody>
</table>

might increase the trap anharmonicities, particularly at larger radii.

6.5 Anharmonic Adjustment to Anisotropic Data

We have shown that the residual monopole damping can be attributed to anharmonic effects. Earlier, in section 5.2, the experimental data did not agree very well with the anisotropic simulations run in perfectly harmonic potentials. It is instructive to see that if we modify the anisotropic monopole damping rate by subtracting the weighted mean experimental damping rate in an isotropic potential (0.15 Hz), the data matches quite well with our expectations. In other words, for the experimental data,

$$\kappa = \frac{\Gamma_m - \Gamma_{anharm}}{\Gamma_Q},$$

(6.6)

where $\Gamma_Q$ is in this case the expected quadrupole damping rate for the collision rate at each individual point. This modified $\kappa$ is plotted in figure 6.7.
Figure 6.7: Here we have modified the experimental data by subtracting the experimental average monopole damping in an isotropic potential from the experimental monopole damping before dividing by the expected quadrupole damping, as written in eq. 6.6. The agreement between simulation and experiment is greatly improved, as well as between the experiment and our expectations.
Chapter 7

Conclusion

We have investigated the anomalous prediction of the Boltzmann equation that monopole motion in an isotropic and harmonic potential will not damp, both in our experiment and through the Monte Carlo simulation described in this text. Our zzTOP trap enabled us to reach new levels of isotropy while maintaining a relatively harmonic potential. A lack of analytic theory for monopole motion in slightly anisotropic and slightly anharmonic potentials motivated the creation of this simulation. In order to verify the accuracy of the simulation we examined cross-dimensional temperature anisotropy relaxation rates, and found that $1/e$ relaxation in the simulation requires an average of $2.69 \pm 0.13$ collisions per atom, in close agreement with the experimentally proven\cite{6} value of $2.7$. There is however, an offset from the origin when looking at $\Gamma_T$ vs. $\gamma_{coll}$, which we cannot account for. Quadrupole motion was relevant to our interests because of the monopole-quadrupole coupling that occurs in anisotropic potentials. We found experimentally that the quadrupole damping rate dependence on collision rate is linear with a slope of $\xi = 0.197 \pm 0.005$, within one standard deviation of the theoretical prediction of $\xi = 0.2$ \cite{25, 14}. This slope, according to simulations in an isotropic and harmonic potential, is $\xi = 0.139 \pm 0.009$, which is 30.5% smaller than the expected value. We are not sure of the cause for this systematic discrepancy.

While finite monopole damping was not predicted by the Boltzmann equation or our simulation for an isotropic and harmonic potential, we experimentally observed a damping effect, and this damping effect did not depend on the average collision rate. With controlled isotropy breaking of our zzTOP trap, we investigated whether the finite, $\Lambda \leq 0.003$ anisotropy and resulting
monopole-quadrupole coupling was the root of the finite monopole damping we observed. At very small residual anisotropies the monopole motion still damps significantly more than we can account for by anisotropy alone. Implementing a Taylor expanded model of our potential allowed us to account for the anharmonic effects present in our experiment. We did not expect including these anharmonic effects to have a large perturbative effect on quadrupole damping effects, and the slope relating the quadrupole damping in this potential to the collision rate was $\xi = 0.171 \pm 0.006$, slightly closer to the experimental slope. Simulations involving this new model of our zzTOP trap demonstrate monopole damping in an isotropic potential that is not dependent on collision rate. The residual monopole damping rate in the simulation matches what we observe in the experiment for cloud sizes roughly between $115\mu m$ and $135\mu m$, which are typical of our experiment. While this would indicate agreement between our model and the experiment, we found this agreement to be limited. The anharmonic effects increase at larger displacements from trap-center. Investigating the dependence of residual monopole damping rates on average cloud size revealed that at larger FWHM, the simulation model significantly underestimates the monopole damping present in the experiment. It is reasonable for our model not to match the anharmonic effects we see experimentally, since it does not take into account construction flaws inherent to any experiment, including our own. While this limits the utility of the Monte Carlo simulation, it has still been a helpful tool for investigating collective excitations in our experiment.

### 7.1 A Number Game

While our simulation has been very accurate in qualitative predictions, there are several systematic discrepancies, as mentioned above, that hinder quantitative agreement with experimental and analytic results. We have checked whether changing $\Delta t$ has a significant effect on these discrepancies, and for the range of $\Delta t$ we have looked at, limited to 10s of microseconds or larger, it has not.

There is one assumption in analytic theory which we have not discussed so far, and that is whether the collisions are point-like. The analytic theory available requires collisions be point-like;
however, this is not the case in our simulation. The small atom number we can simulate in a reasonable amount of time forces us to use artificially huge collision distances in our simulations in order to run with collision rates similar to our experiment. This larger collision distance means that when atoms are colliding in our simulation, they are still a micron or more apart from each other. This is quite different from the physical case, where the scattering length, $a_{Rb^{87}}$ is on the order of nanometers. Using (3.11), we can look at the discrepancy factor between the simulated collision distance and the physical scattering length as a function of number, for a given collision rate. This discrepancy factor is plotted in figure 7.1 for $\gamma_{coll}=5 \, (s^{-1})$, where the leftmost point plotted is $N = 2000$, the number of atoms typically used in this simulation.

Figure 7.1: One of the assumptions made in Boltzmann’s prediction of undamped monopole motion is that collisions can be regarded as point-like. Because of the small number of atoms involved in our simulation, we artificially increase the collision distance to obtain collision rates similar to those we observe in our experiment. Based on (3.11), the discrepancy factor between $d_c$ and the physical scattering length, $a_{Rb^{87}}$ is plotted below, for a collision rate of $\gamma_{coll}=5 \, (s^{-1})$.

As previously mentioned, we are limited to small atom number because the simulation is generally slow, and the run-time scales as $N^2$ due to the separation matrix. At one point, I converted
the code to run in parallel using parfor loops to calculate the separation matrix. Unfortunately, the
time it took to transfer memory between processors was longer than the time saved by calculating
the matrix across several processors. There are other methods physicists use to simulate collective
excitations, and while they may be less straightforward, they allow for rapid computation. One of
these methods is Birds method, and is described in [30]. Rather than calculating the separation
between every possible pair of atoms, Birds method divides position space into small volumes called
cells, and acts out collisions between atoms within each cell according to probability based on their
relative velocities. This allows for the simulation of large $N$ gases, and has been shown to accurately
predict gas dynamics. Since we are closing down our experiment, we do not have any future plans
involving this simulation. If we were to pursue numeric simulations of our experiment further,
using the Bird Monte Carlo method of molecular gas dynamic simulations might be preferable to
continuing with our own Monte Carlo model.


