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Collisional Interactions in an Ultracold Lithium Gas

by

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A Thesis Submitted
in Partial Fulfillment of the
Requirements for the Degree

Doctor of Philosophy

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ABSTRACT

Collisional Interactions in an Ultracold Lithium Gas

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William Ian McAlexander

Laser cooling and atom trapping techniques have enabled atomic physicists to attain temperatures on the order of 100 nK. In this regime, a trapped gas must be described within the framework of quantum statistical mechanics. In 1995, Bose-Einstein condensation (BEC) was achieved for the first time in such a system by three independent groups. The success of attaining BEC has encouraged research in quantum degenerate Fermi gases (DFG). One of the most exciting opportunities for a DFG is the prospect for Cooper pairing in a two-component gas. The experimental techniques for obtaining degenerate gases, as well as the mechanism for Cooper pairing, hinges on understanding and characterizing ultracold collisional interactions.

This thesis is a twofold study in this exciting field. The first section is an in-depth treatment of collisions in atomic lithium. Lithium has two isotopes, $^6$Li which is a fermion and $^7$Li which is a boson. This makes it an ideal candidate for studying quantum degenerate gases. In a series of experiments using a magneto-optical trap, we have spectroscopically measured the ground and excited state molecular potentials for both isotopes. From this work we have been able to obtain the most accurate potentials for lithium to date. These precise measurements have enabled us to extract the most accurate value to date for the 2P atomic radiative lifetime of lithium. Furthermore, we have developed a coupled-channel treatment of two-body collisions.
which has enabled us to calculate the scattering amplitude, elastic cross section, and rate of spin-exchange decay for any ground state collision in lithium as a function of temperature and magnetic field.

Armed with this knowledge, we have made progress on the design and construction of an electromagnetic trap for lithium. This trap will enable the study of a degenerate Fermi gas of $^6\text{Li}$ as well as the possibility of observing a Cooper pairing transition. The trap performance has been characterized for each isotope and current work is focussed on cooling lithium down to degeneracy. Measurements of spin-exchange decay have been made and compare well with the collisional theory that has been developed.
Acknowledgments

This thesis marks the end of an eight year journey through graduate school. I could not have gotten even half this far without the effort and support of more people than I can possibly list here. To everyone who has helped to shape my graduate school career and my life in Houston, I extend my sincere thanks and appreciation. In the short space I have here, I would like to specifically acknowledge those people who have directly influenced the work described in this thesis.

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My advisor, Randy Hulet, deserves credit for arranging a talented group and guiding the lab to the forefront of atomic physics. I thank him for the opportunity to do such exciting work. We have enjoyed a productive collaboration with Marianne Houbiers and Henk Stoof. I am particularly indebted to Henk for his efforts in helping me to understand the nuances of scattering theory.

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I wish to particularly thank my mother and father, sister and brother. This work is dedicated to them.

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Chapter 1
Introduction

Since the late 1970s and early 1980s, atomic physics has witnessed the growth of an almost entirely new field of ultracold physics known these days as laser cooling [1]. This new field of study was made possible with the advent of the laser which has allowed physicists and scientists to manipulate matter on a scale that was only dreamed of 50 years ago. Through the techniques of laser cooling, atomic physicists have been able to confine and cool samples of atoms at temperatures that are about a millionth of a degree above absolute zero temperature Kelvin. At these low temperatures, the classical description of the gas breaks down. One can no longer think of the gas as being an ensemble of point-like particles, instead a more quantum mechanical description is needed. The purpose of this work has been to both experimentally and theoretically explore this regime and to develop a better understanding of the physics involved with these systems. I will begin this thesis with a summary of the overall goals and techniques of this field as well as the long term projects that are on the horizon.

1.1 Quantum Degenerate Gases

Ultimately, we are interested in using ultracold atoms to study various aspects of quantum statistical mechanics. Statistical mechanics, in general, is used to describe the macroscopic properties of large numbers of particles [2, 3]. For the case of a gas, statistical mechanics can be used to describe macroscopic quantities such as density, temperature, and pressure to name a few. As long as one assumes that the various particles in the gas are able to exchange energy, statistical mechanics says that the gas will thermalize to a steady-state condition. If the gas can be treated classically (consisting of point-like particles), then the energy distribution of the gas is described
by the famous Boltzmann relation [2, 3],

\[ f(E) = A \exp \left( -\frac{E}{k_B T} \right) . \]  \hspace{1cm} (1.1)

Here \( f(E) \) gives the probability of finding atoms with energy between \( E \) and \( E + dE \) (\( k_B \) is the Boltzmann constant and \( T \) is the temperature). The normalization constant \( A \) is chosen so that,

\[ N = \int_0^\infty dE \, f(E) \, \rho(E) , \]  \hspace{1cm} (1.2)

where \( N \) is the total number of particles and \( \rho(E) \) is the energy density of states [2]. This is an extraordinarily powerful and useful description of the system, and while it does rely on some sort of interaction to allow for the exchange of energy, it ignores the quantum mechanical details of the particles. If conditions in the system are such that this assumption fails, then this description of the gas must be modified. Specifically, if the density gets too high, or if the particles get too “big” (large de Broglie wavelength), then the point-like description breaks down. This is the regime of quantum statistical mechanics and it is these conditions which we try to achieve using the techniques of laser cooling and atom trapping.

Quantum statistical mechanics (QSM) goes a step further than classical statistical mechanics by considering the quantum description of the particles. Interestingly there is only one additional variable that is considered, the intrinsic “spin” of the particle. Spin is a variable that allows us to label the internal state of a particle and which has all the properties of angular momentum [4, 5]. This spin variable can take on either integer or half-integer values depending on the exact particle in question. An integer spin particle is called a “boson”, while a half-integer particle is called a “fermion”.

The consequences of these two different types of spin are enormous. Unlike classical statistical mechanics, QSM must address the issue of identical particles. Quantum mechanics describes an N-body system with an N-body wavefunction by the time de-
pendent Schrödinger equation [4, 5],

\[ i\hbar \frac{\partial \Psi(1, 2, ..., N)}{\partial t} = H(1, 2, ..., N) \Psi(1, 2, ..., N) , \]  

(1.3)

where \( H \) is the Hamiltonian and \( \Psi \) is the \( N \)-body wavefunction. If two particles are exchanged \((1 \leftrightarrow 2 \text{ for example})\), the physics described by this equation cannot change if the particles are truly identical. To all observation this is the same system. The consequence of this is that the many-body wavefunction \( \Psi \) must have a symmetry associated with the exchange operation. In fact, the exchange operator \( P_{12} \) which switches particle ‘1’ for particle ‘2’ must have one of two eigenvalues,

\[ P_{12} \Psi = \pm 1 \Psi , \]  

(1.4)

since the operation \( P_{12}^2 \) must return the identity relation. If the wavefunction has a \( +1 \) eigenvalue due to exchange, we say that the wavefunction is symmetric to exchange. If the eigenvalue is \(-1\), then the wavefunction is anti-symmetric. There is a remarkable connection which exists between the intrinsic spin of a particle and whether the particle is symmetric or anti-symmetric to exchange. Spin-statistics says,

- half-integer spin particles are anti-symmetric
- integer spin particles are symmetric

This spin-statistics connection is an exact law of nature which can be painstakingly proven within the details of relativistic quantum theory [5]. One stark difference between anti-symmetric particles (fermions) and symmetric particles (bosons) is that a purely anti-symmetric many-body wavefunction cannot have two particles in the same quantum state (the wavefunction vanishes if this occurs). This is a mathematical verification of the Pauli-exclusion principle and leads to radically different behavior between fermions and bosons.

QSM must treat the statistical descriptions of Bose and Fermi systems differently. Since bosons are symmetric particles, numerous bosons can occupy the same quantum
mechanical state. In contrast, since fermions are anti-symmetric they are forbidden to do so. QSM takes this property into account by modifying the classical Boltzmann distribution function. The modified energy distribution function has the form [2, 3],

\[ f(E) = \frac{A}{\exp(E/k_BT)} \pm 1, \]  

where the + sign refers to fermions and the − sign refers to bosons (the details of this function will be discussed later on). When we are looking at large energies compared to \( k_BT \) (a typically classical condition), then the distribution for either bosons or fermions reduces to the Boltzmann distribution. How does one determine whether a given particle is a boson or a fermion? To some extent, this is “hard-wired” by nature. All particles fall into one of these two categories. Fundamental bosons include photons and high energy/particle field propagators such as the W and Z. Fermions include electrons as well as protons and neutrons (actually protons and neutrons are composed of quarks which have spin multiples of 1/3, but that is dealt with separately within the regime of quantum-chromodynamics). An atom can be treated as either a boson or a fermion depending on whether all the constituent particles in the atom add up to give net integer or half-integer spin; this is certainly a good assumption when the characteristic binding energy of these particles in the atom is significantly larger than the thermal energy of the atomic gas.

In order to study both Bose and Fermi statistics, we have elected to use lithium as our gas constituent. Naturally occurring lithium comes in two isotopes, \(^7\)Li which is a composite boson (total ground state angular momentum is \( f = 1 \) or \( f = 2 \)), and \(^6\)Li which is a composite fermion (total ground state angular momentum is \( f = 3/2 \) or \( f = 1/2 \)). This makes it an ideal candidate for studying quantum statistical mechanics. Furthermore, since lithium is an alkali atom, it has a single valence electron and consequently a convenient laser transition at 671 nm which can be used for laser cooling.

A convenient parameter for describing whether the gas is classical or quantum
degenerate is the phase space density. The phase space density is a measure of the number of atoms present in a given quantum state in the system [2]. Normally, the full classical distribution of a gas is given by \( f(\vec{r}, \vec{p}) \) which describes the number of atoms present in the range \( \vec{r} \) to \( \vec{r} + d\vec{r} \) with momentum in the range \( \vec{p} \) to \( \vec{p} + d\vec{p} \). This distribution function is related to the energy distribution function described earlier by,

\[
N = \int d^3r \int d^3p f(\vec{r}, \vec{p}) = \int dE \, f(E) \rho(E),
\]

where \( \rho(E) \) is the energy density of states [2]. The phase space density is essentially \( f(\vec{r}, \vec{p}) \) which gives the value of \( dN \) for the region of phase space \( (d^3r \, d^3p) \) centered at \( \vec{r}, \vec{p} \). Since phase space has both spatial and momentum coordinates, this quantity can also be expressed as a spatial density times a momentum density,

\[
f(\vec{r}, \vec{p}) = n(\vec{r}) \times \tilde{n}(\vec{p}) = n(\vec{r}) \times \Lambda^3(\vec{p}),
\]

where the momentum density \( \tilde{n} \sim 1/p^3 \) has been expressed as the cube of the de Broglie wavelength \( (\Lambda = h/p) \). Even though this is a classical definition since it assumes that both the spatial and momentum variables are known exactly, it nevertheless gives a measure of the number of particles per "state" as the state spacing goes to zero \( (h \to 0) \). For a classical gas, this phase space density is normally quite small. This is our figure-of-merit for describing the quantum degeneracy of our gas, when \( \rho_o \equiv n_o \Lambda^3 \sim 1 \) (where \( n_o \) is the peak density of the gas), then we are in the quantum regime. At this point, the de Broglie wavelength of the gas is comparable to the inter-particle spacing. Depending on whether we are observing a bosonic or fermionic gas when this regime is achieved, we expect to observe strikingly different macroscopic behavior.

1.1.1 Bosons

A fundamental and interesting aspect of a quantum degenerate Bose gas is the formation of a Bose-Einstein condensation (BEC). BEC is a term describing the sud-
den, macroscopic occupation of the lowest energy state of the Bose gas as the system becomes degenerate. This is a direct consequence of the fact that multiple bosons can occupy the same quantum state, and that these particles are indistinguishable. In fact, as the degenerate regime is attained, the occupation of the ground state is described by a sudden phase transition [2]. The indistinguishable property of the gas causes the statistical probability of occupying the ground state to increase rapidly with increasing BEC population. This is known as Bose enhancement.

In the zero temperature limit, all the bosons will be in the ground state of the system. The distribution function looks like,

\[
f(E) = \frac{1}{\exp[(E - \mu)/k_B T] - 1},
\]

where \( \mu \) is the chemical potential [2, 3]. As the temperature goes to zero, we know that \( f(0) = N \) for \( N \) bosons. This implies that,

\[
\lim_{T \to 0} f(0) = N \approx -\frac{k_B T}{\mu}.
\]

This shows that the chemical potential, which is defined to be the change in the internal energy divided by the change in particle number \( (\mu = \partial U / \partial N) \), must be negative for a Bose gas and goes to zero as the temperature goes to zero. No energy can be extracted from a zero-temperature Bose gas which gives rise to interesting superfluid behavior (no viscosity) [2, 3].

Figure 1.1  Formation of BEC in an harmonic trap. As the bosons in the harmonic trap on the right are cooled to zero temperature, we expect to see all of the gas particles in the ground state of the trap.
Since each boson is indistinguishable from the next, this BEC is described by one unique wavefunction with one unique energy (the ground state energy). BEC was predicted 75 years ago, but was only just observed in a dilute gas in 1995 by three different groups [6–8]. The realization of BEC has allowed scientists to observe quantum mechanical properties of matter on a macroscopic scale. For example, two separate BECs have been formed and allowed to interfere resulting in observable interference fringes in the density distribution [9], in much the same way that two laser beams in an interferometer can be overlapped to produces fringes. This begs a direct comparison of BEC with a laser. Since the atoms which comprise a BEC are in a sense “in phase”, the properties which differentiate a laser from a flashlight also differentiate a BEC from a normal gas. The concepts of atom/matter lasers and coherent atomic sources have been a topic of discussion in the field of quantum gases and has even led to the realization of a pulsed type of “atom laser” [10]. Other topics of interest related to the properties of BEC include the study of non-zero angular momentum states or vortices [11], multi-component BECs or spinor condensates [12], and solitons [13–15].

1.1.2 Fermions

The physics of a degenerate Fermi system is in many ways a polar opposite from Bose physics. In contrast to bosons, fermions are forbidden to occupy the same quantum state. Instead of a macroscopic occupation of the ground state, as a Fermi gas is cooled the atoms will “stack up” into the lower lying levels, filling them all up to some energy known as the Fermi energy. The distribution function which describes this behavior is,

\[ f(E) = \frac{1}{\exp[(E - \mu)/k_BT] + 1}, \]

where the Fermi energy is defined to be the chemical potential at zero temperature (\(\lim_{T\to0}\mu = E_F\)). In the limit of zero-temperature, we know that the ground state
Figure 1.2 Fermions in a trapping potential. As the fermions are cooled to zero temperature, we expect to see each of the lowest quantum levels occupied by one particle. The energy of the highest occupied energy state is called the Fermi energy.

will have only one particle \( f(0) = 1 \), and that each successive level will be similarly occupied until the lowest \( N \) levels are filled (assuming \( N \) particles are present). The Fermi energy will correspond to the highest occupied energy state. Upon inspecting the form of \( f(E) \), one can see that as \( T \to 0 \) the exponential in the denominator will be zero if \( E < E_F \) and infinite otherwise. This gives the desired functionality,

\[
\begin{align*}
  f(E) &= 1 \quad (E < E_F) \\
  &= 0 \quad (E > E_F). 
\end{align*}
\]

So the Fermi energy is a function of both the number of particles as well as the geometry of the trap. For example, in the case of a 3D harmonic trap with mean frequency \( \bar{\nu} = (\nu_x\nu_y\nu_z)^{1/3} \) we have [16],

\[
E_F = \hbar \bar{\nu}(6N)^{1/3}. \tag{1.13}
\]

For the case of \( 10^6 \) \( ^6 \)Li atoms confined in our trapping potential (\( \bar{\nu} = 133 \) Hz), this amounts to a Fermi temperature of \( 1.2 \) \( \mu \)K. If the gas isn’t at zero temperature, then the Fermi surface will acquire a width proportional to the finite temperature. In the high temperature limit, the distribution function reduces to the classical Boltzmann distribution with extremely small occupation, \( f(E) \), for given values of energy \( E \).

Unlike the Bose gas, the degenerate Fermi gas (DFG) does not have a clear and sudden phase transition. In fact, the difference between a classical density distribution
in an harmonic trap and a DFG distribution is relatively small, unlike for a Bose gas. Getting to a phase space density of order one will start to produce deviations from the classical result, but these deviations will be small. Only when the temperature starts to be small compared to the Fermi energy will we see distinctions. In the fall of 1999, a group at JILA in Boulder, Colorado was able to trap and cool a fermionic atom (\(^{40}\)K) into the DFG regime \cite{17}. They saw significant deviations from classical theory at a temperature of around 0.5 \(T_F\) where \(T_F\) is the temperature that corresponds to the Fermi temperature of the gas. One goal of the apparatus and project that is described in this thesis is to observe similar behavior with a degenerate sample of \(^6\)Li.

### 1.1.3 Cooper Pairing

The ultimate goal of the apparatus described in this thesis is to observe a Bardeen-Cooper-Schrieffer (BCS) transition in a degenerate gas of \(^6\)Li \cite{18, 19}. A BCS transition is a mechanism which has been successful in describing the behavior of things like superconductivity and superfluid \(^3\)He \cite{20, 21}. A BCS transition can occur for a degenerate system of fermions in which an attractive interaction exists between the Fermi particles. For the case of a superconductor, this interaction is mediated by phonons within the crystal lattice which "screen" the normal coulombic repulsion between conduction electrons and instead cause pairs of electrons to be attracted to one another. Once a mechanism exists which allows two fermions to form a pair, the composite particle obeys Bose statistics since two anti-symmetric particles add to give a symmetric particle. The BCS phase transition can be viewed as a BEC phase transition of Cooper pairs resulting in a coherent superfluid of Cooper paired fermions.

The collisional interactions between ultracold \(^6\)Li have been measured and calculated in a series of experiments which are summarized in this thesis. Fortuitously, nature has allowed for a large, attractive interaction within the \(^6\)Li two-body inter-
action potential which would aid greatly in the formation of Cooper paired \(^6\)Li. The transition temperature for this BCS process has been calculated to be around 40 nK based upon the result of this scattering calculation [19]. We are hoping to ultimately achieve these conditions and observe the phase transition. The BCS phase transition will not have a clear density signature like the BEC transition in \(^7\)Li [19]. However, we are hoping to observe the effect of pair formation by observing an increase in wide angle scattering of a probe laser passing through the cloud [22].

1.2 Path to Degeneracy

What I want to present here is the basic process and techniques that are used to trap and cool an atomic gas down to degeneracy. This is an overview where details will be addressed in various chapters further on in the thesis. This is a complicated and multi-step process where each stage must be carefully designed and peaked in order to be successful. In order to cool and contain atoms at the temperatures of interest, we must isolate the atoms from outside heat sources. This requires an ultrahigh vacuum apparatus where the background gas pressure has been minimized as much as possible.

1.2.1 Laser Cooling/Magneto-Optical Trapping

The first stage of the experiment requires cooling and confining atoms from an atomic oven through the techniques of laser cooling and magneto-optical trapping. Basic laser cooling of atoms seeks to remove thermal energy from an atom by creating conditions where the atom absorbs less energy than it emits through spontaneous decay. The way this is typically done is by using the Doppler shift of a moving atom; the process is illustrated in figure 1.3. In this example, the atom has some velocity component which opposes a laser beam that is detuned red of the atom's atomic transition. If the frequency of the laser is just right, the atom will Doppler shift the frequency into resonance and absorb the photon. Some time later (27 ns for lithium),
Figure 1.3  Basic laser cooling. This figure shows the characteristic excitation energy of the lithium atom. If we expose a thermal beam of lithium to a counter-propagating laser beam with a frequency that is less than what is needed to excite the atoms, the atoms can still be excited if their Doppler shift $\Delta_V$ is equal to the difference between the laser frequency and the atomic transition frequency. In this way, an atom can absorb a lower energy photon, and then spontaneously emit a higher energy photon around 27 ns later. This leads to a reduction in the thermal energy of the atom.
the atom will emit a photon with higher energy thereby lowering its thermal energy. One can think of the atom receiving a lot of momentum kicks from the laser against its motion, meanwhile the spontaneous emission is in random directions and has zero net contribution to the mean atomic velocity. This mechanism works fine for slowing an atomic beam as long as the laser frequency is continually adjusted to take into account the changing Doppler shift of the atom as it slows down. The other way of compensating for this is to appropriately change the energy structure of the atom as it slows down. We do the latter by Zeeman shifting the atoms with an external magnetic field. This is discussed in more detail in chapter 4.

Once we have slowed some fraction of the atomic beam, the atoms need to be confined. We start by confining the atoms in a magneto-optical trap (MOT) [23]. A MOT in many ways is the 3D analogy of the basic laser cooling scheme. One can imagine having 3 pairs of counter-propagating beams which are detuned as described above in order to cool the atoms in every direction. An atom with an appreciable velocity in any direction will be cooled in this “optical molasses”. Of course, damping the atoms’ motion does not give us a trap; we need some type of spatial restoring force. This is provided in the MOT by introducing a quadrupole magnetic field, generated by a set of anti-Helmholtz coils, as well as choosing appropriate polarizations for the laser beams. By choosing counter-propagating beams with $\sigma^+\sigma^-$ polarization, this allows the damping seen by the atoms to be spatially dependent in such a way that as the atom is further removed from the magnetic field zero, it will witness a larger damping force. The end result is a robust atom trap which both confines and cools. The MOT does have limitations. The number of atoms that can be trapped is limited by the optical density of the cloud as well as collisional losses that are induced by the laser [24]. The temperature of the atoms in the MOT is limited by the energy width of the atomic transition used for the laser cooling (this is called the Doppler limit and it is 140 $\mu$K for lithium) [1]. For our lithium MOTs, we find that in order
Figure 1.4  Basic magneto-optical trap (MOT). This figure shows a schematic of the trapping region with suitable anti-Helmholtz coils and 3 counter-propagating pairs of $\sigma^+\sigma^-$ circularly polarized beams. These beams are detuned red of the atomic transition in order to get the needed damping/cooling. The figure on the right shows a basic schematic of how the polarizations and the magnetic field work together to achieve a spatial restoring force as well. Even though the spin structure of lithium is not a $J = 0$ ground state and $J = 1$ excited state, the spin structure shown illustrates how the relative Zeeman shifting of the ground and excited states can favor excitation from one beam instead of the other. Since $\sigma^+$ light can only drive $\Delta m = +1$ transitions and $\sigma^-$ light can only drive $\Delta m = -1$ transitions, if an atom happens to be displaced from the magnetic field minimum then it will preferentially absorb photons from only one of the beams in the pair. Assuming that the circular polarizations have been chosen correctly with respect to the magnetic field direction, this will cause atoms to collect at the center of the MOT.
to get more trapped atoms we need to compromise on the temperature. This is done by using a larger detuning for the lasers and results in MOT temperatures of around 1.5 mK with about $3 \times 10^{10}$ trapped atoms for our best case. The phase space density of this sample is of the order of $10^{-6}$, a long ways off from the quantum degenerate regime. In order to get colder and denser, we need a trap which can overcome the optical limitations of the MOT.

1.2.2 Magnetic Trapping

The next stage towards degeneracy in our experiment is to transfer the atoms from the MOT to a purely magnetic trap. A magnetic trap works by using the Zeeman interaction that exists between an atom with magnetic moment $\vec{\mu}$ and an external magnetic field $\vec{B}$. A suitable choice of magnets (or electromagnetic coils) can be arranged to give a local minimum of magnetic field inside the vacuum/trap chamber. Nearly all atoms, including lithium, have a non-zero magnetic moment $\vec{\mu}$ due to the intrinsic spin of the atom,

$$\vec{\mu} = g \mu_B \vec{F} ,$$  \hspace{1cm} (1.14)

where $g$ is the gyromagnetic ratio, $\mu_B$ is the Bohr magneton, and $\vec{F}$ is the angular momentum of the atom. In the presence of a magnetic field, the atom will see an energy shift which goes like,

$$U = \vec{\mu} \cdot \vec{B} = g \mu_B m_F B ,$$  \hspace{1cm} (1.15)

where $m_F$ is the projection of $\vec{F}$ along the axis defined by $\vec{B}$. This energy will increase or decrease with increasing magnetic field depending on whether the atomic angular momentum is aligned or anti-aligned with the magnetic field. Figure 1.5 shows both a trapping and anti-trapping magnetic interaction based on the atomic spin orientation. This type of trap circumvents the optical limitations of the MOT and ultimately is the trap in which a degenerate gas will be confined. However, a rather large field
Figure 1.5 Magnetic trapping and anti-trapping potentials. By creating a magnetic field minimum in space, atoms with a magnetic moment $\mu$ can be trapped by the minimum if their orientation with respect to the magnetic field is correct. If the moment (or spin) of the atom were flipped (for example by an RF transition) then the atom would see a potential maximum and would accelerate away from the region. This anti-trap is utilized for evaporatively cooling the atoms.

Gradient is needed to trap atoms of reasonable energies. The trapping force is given by the magnitude of the Bohr magneton, $\mu_B = 67 \, \mu K/G$. In order to confine a 1 mK cloud within a space of a few mm, we need to generate field gradients on the order of 100 G/cm, this is not an easy task. It is for this reason that we start with a MOT before moving to a magnetic trap. The MOT is able to capture atoms with energies of 0.5 K and cool them to around 1 mK allowing us to collect a sizeable number for transferring to the magnetic trap. The details of creating this magnetic field as well as the transfer/switching of the trap will be discussed in chapter 4.

At this point, the phase space density of the gas has not changed. Transferring the MOT atoms to the magnetic trap ideally should not heat or cool assuming that the trap geometries are well matched. Because only certain spin states are trapped in the magnetic trap, only a fraction of the optically trapped atoms will be successfully transferred (assuming the atoms are not optically pumped). However, this does not change the phase space density of the spin-polarized atoms in the magnetic trap.
because we have decreased the number of possible microstates (fewer atoms in a smaller phase space). Certainly if we can optically pump the atoms into the correct spin state before transfer, then we could increase the phase space density.

1.2.3 Evaporative Cooling/Sympathetic Cooling

Once the atoms have been transferred to the magnetic trap, we need to cool them the rest of the way into degeneracy. This is done in our experiment by using evaporative cooling. Evaporative cooling is a technique where the most energetic atoms in the gas are removed thereby leaving the remaining atoms to re-thermalize and cool. This process is indicated in figure 1.6. To achieve this in the magnetic trap, we make use of the anti-trapping potential that was described earlier. We can use carefully tuned microwaves to spin-flip certain atoms thereby causing them to become untrapped and leave. Only the most energetic atoms will travel the furthest up the side of the magnetic trap and therefore undergo the largest Zeeman energy shift. We can preferentially remove these atoms and rely on collisions between the trapped atoms to re-thermalize and cool the gas. Since the colder atoms will sit further down in the trapping potential, this technique helps to increase density as well as increase the de Broglie wavelength (by lowering temperature). In this fashion, evaporative cooling can increase the phase space density of the gas from $10^{-6}$ all the way to 1 even though the process reduces the number of atoms in the trap.

In order to understand evaporative cooling and how to appropriately change the microwaves during cooling, we need to have a full understanding of our initial conditions as well as collisional interactions. A large part of this thesis deals with understanding collisional interactions in ultracold gases. The basic theory behind describing collisions in these systems is discussed in chapter 2. The actual potential interactions which describe collisions in $^6\text{Li}$ and $^7\text{Li}$ are discussed in chapter 3. Finally, the process of evaporative cooling and how it can be optimized for the type of atom trap
Figure 1.6  Basic process of evaporative cooling. Atoms can be selectively removed from the magnetic trap by using RF to spin-flip atoms to the anti-trap. The idea of evaporative cooling is to remove the hottest atoms from the distribution. The remaining atoms will re-thermalize and cool to a new distribution which will have a lower temperature (given by the peak of the \( f(E) \) curve). These hotter atoms are those atoms which travel the furthest up the side of the trap, and so have the largest spin-flip transition frequency. By carefully tuning the RF spin-flip frequency and waiting for the cloud to thermalize, the distribution can be made quite cold and dense (since colder atoms occupy a smaller region of the trap) even though we are removing atoms.
discussed in this thesis is described in chapter 5.

One important point needs to be made concerning the cooling of fermions. Since the Pauli-exclusion principle keeps fermions from occupying the same quantum state, it also prevents identical fermions from undergoing low-energy collisions. This presents a problem when trying to evaporatively cool fermionic $^6$Li since evaporation relies on collisional thermalization. Since we are ultimately interested in cooling $^6$Li, we plan to do this by using $^7$Li as a cooling buffer. Our apparatus will eventually load both isotopes simultaneously. The $^7$Li will be evaporatively cooled as described above while the $^6$Li will be cooled through sympathetic collisions with the $^7$Li. This is also discussed in chapter 5.

1.2.4 Imaging

Once the gas has been cooled to degeneracy, we need to take a picture of the cloud and analyze it. There are a number of ways in which this can be done. For the work presented in this thesis, we use fluorescence imaging as well as absorption imaging. Both techniques rely on exposing the atoms in the trap to near resonant laser light. The data is discussed in chapter 6 although the basic techniques are outlined below.

For the case of fluorescence imaging, the atoms in the trap are exposed to a 3D molasses for a short period of time (typically $\sim 200$ $\mu$s). Some distance away from the cloud, we have a lens which collects some amount of the fluorescence and images it onto a CCD camera. As long as one assumes that the transition is saturated and that the cloud is not optically thick, then by counting the number of photons produced during the pulse, one can determine the number of atoms present.

$$\text{number of photons} = N \rho_{ee} \Gamma t = \frac{N \Gamma t}{2} ,$$  \hspace{1cm} (1.16)

where $N$ is the number of atoms, $\rho_{ee}$ is the fraction of excited-state atoms ($= 1/2$ if saturated), $\Gamma$ is the rate of spontaneous emission, and $t$ is the time interval of the exposure. It is also necessary to know the quantum efficiency of the CCD and the
Figure 1.7  Schematic of fluorescence imaging. The atoms in the magnetic trap are exposed to a brief flash of near resonant light from all directions. Photons are emitted from the cloud, some of which are collected by a lens system and imaged onto a CCD camera. Assuming that all the atoms are saturated by the beams and emit at the same rate, the number of collected photons can be directly related to the number of atoms in the trap. The size of the cloud is related to the temperature and this can also be measured from the image.

collection efficiency of the lens system. The temperature of the cloud is ascertained by calculating the physical size of the cloud from the image (assuming a measured magnification); a hotter cloud will appear larger in a spatially varying trapping potential such as a linear or harmonic trap. Since the trapping potential which holds the atoms is well characterized, we can directly calculate the temperature from the images. Fluorescence imaging is a robust means of measuring atom number and temperature for optically dilute clouds.

Once the trapped cloud gets optically thick, then another means of imaging is necessary. For the work presented in this thesis, we used absorption imaging. In this technique, a collimated beam of near resonant light is passed through the cloud. The cloud will absorb light from the probe beam resulting in a shadow which can be imaged onto a CCD camera. The peak absorption is directly related to the peak column density of the cloud, and so this absorption, \( A \), can be related to the density

Figure 1.8  Schematic of absorption imaging. A near-resonant probe beam is sent through the atom cloud and the absorption shadow created by the atoms propagates through an imaging system onto a CCD camera. The peak absorption signal is related to the column density of the cloud, so the peak density of atoms can be measured. The temperature is found by measuring the width of the absorption image and relating that to the width of the actual cloud.

distribution:

\[ A(x,y) = 1 - \exp(-\alpha(x,y)) = 1 - \exp\left(-\sigma \int_{-\infty}^{\infty} n(x,y,z) \, dz \right), \]  

(1.17)

where \( \alpha \) is the optical density, which is the light scattering cross section \( \sigma \) times the integral of the density along the probe axis (column density). Just as with fluorescence imaging, the size of the absorption image can be related to the temperature. As the cloud is cooled further via evaporation, one would expect it to get smaller and more optically thick. The absorption probe can be detuned in order to avoid "flat-topping" the absorption signal, but ultimately a better imaging technique, such as phase contrast imaging, will be needed.

In the future, we hope to use phase-contrast imaging for looking at degenerate atomic clouds. Besides creating a shadow in the probe beam due to absorption, the cloud also refracts an appreciable amount of the beam due to the fact that the atomic cloud has an index of refraction. In fact, as the cloud gets cold and small, it can severely distort the near-resonant probe beam since it will act like a small lens. Figure 1.9 shows both the absorption and phase shift which results from being
near an atomic resonance. Phase contrast imaging is a technique which allows us
to be sensitive to the phase shift induced in the probe laser by the atoms. This is
based on techniques developed for imaging small transparent objects like biological
cells [25]. The advantage in phase contrast imaging is that it allows us to detune
the probe by a large amount, the phase signal only falls off like $1/\Delta$ as opposed to
the absorption signal which falls off as $1/\Delta^2$. This could ultimately lead to non-
destructive imaging since the atoms may end up absorbing a small amount of the
light while their phase shift is imaged [26]. We plan to implement phase contrast
imaging by using a phase plate which shifts the relative phase of the unscattered

Figure 1.9 Absorption and phase shift in near-resonant probe beam. The detuning $\Delta$ is
the difference between the laser frequency and the frequency of the atomic transition. The
frequency scale is set by the natural linewidth of the transition, $\Gamma = 5.9$ MHz for lithium.
When probing at large detunings, sensitivity to phase shift is actually a better probe since
it functionally falls off as $1/\Delta$ whereas absorption falls off as $1/\Delta^2$. 
light in relation to the scattered light. Figure 1.10 shows the basic set-up. A relay telescope is used to focus the unscattered light to a point whereas the light which is scattered by the cloud is nearly collimated and only a tiny portion of it goes through this point. At this focal point, a phase plate is inserted which shifts the phase of the unscattered light by \( \lambda/4 \) (as well as attenuating the unscattered light by some amount). At the image plane an interference pattern is formed which is sensitive to the phase information imprinted in the scattered beam by the atomic cloud. The phase shift signal (in the small signal limit) is related to the column density of the cloud as follows,

\[
\frac{\text{signal}}{\text{background}} = 1 + \frac{\alpha_o}{2\Delta} \exp(\delta/2),
\]

(1.18)

where \( \alpha_o \) is the on-resonance optical density, \( \Delta \) is the detuning (which can be positive or negative with respect to the atomic transition), and \( \delta \) is related to the phase plate.

**Figure 1.10** Basic optical set-up for phase-contrast imaging. A relay telescope is used to focus the unscattered light to a point where a phase plate (\( \lambda/4 \)) is introduced to shift the unscattered light relative to the scattered light. The interference image produced at the CCD camera is a measure of the optical density of the cloud and can be analyzed to determine the atomic density and temperature.
transmission intensity coefficient $T$ by $\delta = -\ln T$. A variation of this technique has been used in our lab and is discussed in detail in [27, 28].
Chapter 2
Low Energy Collisional Theory

The physics of scattering is enormously important and has generated numerous volumes and papers on the subject. In fact, even for the relatively simple case of describing low-energy collisions in ultracold gases, I find that it is not too difficult to write another volume or two. What I hope to present in this chapter is a sampling of the key elements and concepts that help in describing collisions of ultracold gases. While it may seem rather long, I found it useful in helping to read the literature of the field as well as fully understanding the underlying rich physics associated with this topic.

2.1 Two-Body Scattering

The physical process of scattering one particle off of another can be described quantum mechanically by solving the Schrödinger equation for the entire system. Assume that particle 1 has a mass $m_1$ located at $\vec{r}_1$, and particle 2 has a mass $m_2$ located at $\vec{r}_2$. Quantum mechanics says that there exists a two-body wavefunction, $\Psi(\vec{r}_1, \vec{r}_2, t)$, that describes the entire system where its evolution obeys the equation, $H \Psi = i\hbar \frac{\partial \Psi}{\partial t}$, and the Hamiltonian is given by [29],

$$H = -\frac{\hbar^2}{2m_1} \nabla_1^2 - \frac{\hbar^2}{2m_2} \nabla_2^2 + V(\vec{r}_1, \vec{r}_2, t).$$

(2.1)

An immediate simplification can be made by assuming that the potential is time independent. In the physical case of two atoms scattering off one another, the interaction potential depends only on the relative separation of the two atoms, $V = V(\vec{r}_1 - \vec{r}_2)$, and not on the time coordinate. This implies that the time dependence in $\Psi$ can be separated out so that $\Psi(\vec{r}_1, \vec{r}_2, t) = \psi(\vec{r}_1, \vec{r}_2) \exp(-iEt/\hbar)$, where the variable $E$
describes the total energy and $\psi$ solves the time independent Schrödinger equation,

$$\left[ -\frac{\hbar^2}{2m_1} \nabla_1^2 - \frac{\hbar^2}{2m_2} \nabla_2^2 + V(\vec{r}_1 - \vec{r}_2) \right] \psi = E \psi .$$ (2.2)

While this enables one to ignore the time coordinate, this also raises an interesting question. Namely, is it appropriate to describe the scattering of two particles, which seems to be a “delta-function” type of event in time, by a time-independent picture? This question is dealt with in the literature [5], so I will address it briefly. The formal treatment of scattering presented here and elsewhere [5, 29–31], ends up describing the process as an incident plane wave which is scattered by the potential into outgoing spherical waves. In this simple picture one needs to remember that plane waves and spherical waves are infinite in extent in both space and time. A more “realistic” treatment could involve looking at wave-packets where the two atoms are localized at certain points far away from each other, then come close together at some time $t_0$. Sakurai treats this problem and finds that the answer is identical to the case where infinite plane/spherical waves are used in a time-independent picture [5]. In fact, as long as the wave packet used to describe the particles has a characteristic dimension that is large compared to the range of the potential, which is the case for low-energy scattering, then the time-independent picture works fine.

Now the approach to solving a two-body, time-independent problem like this is to reduce it to an equivalent one-body problem. One-body problems in quantum mechanics have been studied extensively and have well known solutions. In the case of this problem, since we know that the potential energy is spherically symmetric and only dependent on one-coordinate, the relative separation $r = |\vec{r}_1 - \vec{r}_2|$, this allows us to change our variables where we can separate out two new coordinates [29, 30]. We define two new coordinates, $\vec{r} = \vec{r}_1 - \vec{r}_2$ and $\vec{R} = (m_1 \vec{r}_1 + m_2 \vec{r}_2)/(m_1 + m_2)$. By defining the reduced mass of the system to be $\mu = m_1 m_2/(m_1 + m_2)$, one can let $\psi(\vec{R}, \vec{r}) = \psi_R(\vec{R}) \psi_r(\vec{r})$ and thereby separate the two-body equation into two one-body
equations,

\[ -\frac{\hbar^2}{2(m_1 + m_2)} \vec{\nabla}_R^2 \psi_R = E_{CM} \psi_R \]  \hspace{1cm} (2.3)

\[ -\frac{\hbar^2}{2\mu} \vec{\nabla}_r^2 \psi_r + V(r)\psi_r = E_{rel} \psi_r \]  \hspace{1cm} (2.4)

where $\psi_R$ governs the free propagation of the center-of-mass of the two particles (with energy $E_{CM}$), while $\psi_r$ governs the relative motion of the two particles with the appropriate interaction $V(r)$ and relative energy $E_{rel}$. All of the physics of the scattering process is contained in the relative one-body Schrödinger equation. Solving this equation will be the basis for the rest of the chapter.

### 2.1.1 Formal Treatment of Scattering

In solving a quantum scattering problem, one usually starts with knowledge about the system in the absence of the scatterer. For the case of two atoms colliding, we know the basis sets that describe each atom when they are far apart. In this sense, we know the Hamiltonian and the solution set,

\[ H_o \ |\phi\rangle = E \ |\phi\rangle , \]  \hspace{1cm} (2.5)

where $H_o$ describes the system with $V(r) = 0$ and the wavefunction $\phi(r) = \langle r | \phi \rangle$ is the appropriate one-body wavefunction that describes the relative behavior of the two atoms.

If the scattering is treated by perturbation theory, then the scattered state must be close to the unscattered state, $|\psi\rangle \approx |\phi\rangle$, or

\[ |\psi\rangle = |\phi\rangle + |\chi\rangle , \]  \hspace{1cm} (2.6)

where $|\chi\rangle$ is understood to be "small" and the state $|\psi\rangle$ must solve the Schrödinger equation,

\[ (H_o + V - E) |\psi\rangle = 0 . \]  \hspace{1cm} (2.7)
But since the unscattered state solves,

\[(H_o - E) |\phi\rangle = 0 ,\]  

(2.8)

we can equate the two equations,

\[(H_o + V - E) |\psi\rangle = (H_o - E) |\phi\rangle ,\]  

(2.9)

to find an expression for the scattered state,

\[|\psi\rangle = |\phi\rangle + \frac{1}{E - H_o} V |\psi\rangle .\]  

(2.10)

This is the *Lippman-Schwinger Equation* [5,31]. While it is rather straightforward to derive, it is not so simple to solve. There are two immediate problems with the Lippman-Schwinger equation, first how does one treat the singular operator \(1/(E - H_o)\), and then how can the state \(|\psi\rangle\) be written completely in terms of the known state \(|\phi\rangle\).

Attacking the first problem requires a bit of math and this is presented in appendix A. The singular operator \(1/(E - H_o)\) is the operator representation of the Green’s function which solves Schrödinger’s equation in the absence of the scattering potential. In the case of no potential we have,

\[(H_o - E) |\phi\rangle = 0 ,\]  

(2.11)

or

\[\left( -\frac{\hbar^2}{2\mu} \nabla^2 - E \right) |\phi\rangle = 0 .\]  

(2.12)

But this is equivalent to the Helmholtz equation where,

\[(\nabla^2 + k^2) |\phi\rangle = 0 ,\]  

(2.13)

and \(k^2 = 2\mu E/\hbar^2\). There is a Green’s function \(G(\vec{r}, \vec{r}')\) which solves the Helmholtz equation [32],

\[(\nabla^2 + k^2) G(\vec{r}, \vec{r}') = \delta(\vec{r} - \vec{r}') ,\]  

(2.14)
that has the form,

\[ G(\vec{r}, \vec{r}') = -\frac{1}{4\pi} \frac{e^{\pm i k (|\vec{r}| - |\vec{r}'|)}}{|\vec{r} - \vec{r}'|}. \]  \hfill (2.15)

For the case of the Lippman-Schwinger equation, we find that the operator

\[ \left( \frac{1}{E - H_0} \right) \phi = G_0^\pm (\vec{r}, \vec{r}') \frac{2\mu}{\hbar^2} \left( \frac{1}{4\pi} \frac{e^{\pm i k (|\vec{r}| - |\vec{r}'|)}}{|\vec{r} - \vec{r}'|} \right), \]  \hfill (2.16)

where the \( \pm \) sign of the operator corresponds to the boundary condition of outgoing/incoming spherical waves and the subscript refers to the fact that this is a Green’s function solution to the unperturbed Hamiltonian \( H_0 \). Using this Green’s function, we can write the solution to the scattering equation as an integral equation,

\[ \phi = \phi + \int d\vec{r}' G_0^\pm (\vec{r}, \vec{r}') \left( \frac{1}{E - H_0} \right) \phi . \]  \hfill (2.17)

This defines the integral representation of Schrödinger’s equation, but still leaves the problem of having the solution \( |\psi\rangle \) appearing on both sides of the equation.

Finding ways of removing the \( |\psi\rangle \) state from the right-hand side of the scattering equation is one of the central problems of scattering theory. Of course one can always solve the equation self-consistently using a computer, and that has been done for lithium in this thesis. Attacking the problem algebraically can lead to some insights even if an analytic answer cannot be found. One such approach involves a slight re-writing of the Lippmann-Schwinger equation. I have shown that for the equation,

\[ (H_o + V - E) |\psi\rangle = 0 \],

the solution is,

\[ |\psi\rangle = |\phi\rangle + G_0^\pm V |\psi\rangle . \]  \hfill (2.19)

By redefining a new type of scattering operator \( G^\pm \), the equation for \( |\psi\rangle \) can be rewritten entirely in terms of \( |\phi\rangle \),

\[ |\psi\rangle = |\phi\rangle + G^\pm V |\phi\rangle , \]  \hfill (2.20)
where the new operator is,

\[ G^\pm = \frac{1}{E - H_\circ - V}, \]  \tag{2.21}

and contains all of the physics of the scattering since it is defined in terms of the scattering potential. Unfortunately, unlike the free resolvent \( G^\pm_\circ \) where the solution can be found, the perturbed resolvent \( G^\pm \) is unknown. In fact, it is the entire scattering problem! I have just rewritten the problem so that all the physics of the scattering is in the operator \( G^\pm \) and not the state vector \( |\psi\rangle \). What does this gain us? Having the physics contained in the operator allows us to functionally describe a number of things such as the Born series, the T-matrix, and the S-matrix. All of these concepts are important to scattering and can be understood simply in this operator picture.

### 2.1.2 S-matrix, T-matrix, and Born Series

For the moment, let us consider two different scattering states \( a \) and \( b \) which couple through the scattering potential. This is exactly the basis of coupled-channel scattering which I will discuss in more detail later. In this sense, there are two scattering problems with two solutions. One can talk about state \( a \) scattering off the potential,

\[ |\psi_a^+\rangle = |\phi_a\rangle + \frac{1}{E_a - H_\circ - V + i\epsilon} V |\phi_a\rangle, \]  \tag{2.22}

\[ = \left[ 1 + G_a^+ V \right] |\phi_a\rangle, \]  \tag{2.23}

where I am using the perturbed resolvent \( G_a^+ \) which operates on state \( a \) and has a + sign corresponding to scattering outgoing spherical waves as is physically expected. Likewise, there is a similar scattering equation for state \( |\psi_b^+\rangle \) that can be written. The vanishing complex piece \( i\epsilon \) of the resolvent has been explicitly shown and should be treated the same way as it is with the free resolvent in appendix A. In talking about transitions occurring between states \( a \) and \( b \) as a result of the scattering, we
define the $S$-matrix to be,
\[ \langle b | S | a \rangle \equiv \langle \psi_b^- | \psi_a^+ \rangle , \] (2.24)
which describes the overlap of an initial state $a$ with the time-reversal of state $b$ [31]. Both state vectors are a combination of an incident plane wave with outgoing spherical waves in the respective states $a$ and $b$. The S-matrix can be written out as,
\[ \langle b | S | a \rangle = \langle \psi_b^+ | \psi_a^+ \rangle + \langle \psi_b^- | \psi_a^+ \rangle \]
\[ = \delta_{ba} + \langle \psi_b^- | \psi_a^+ \rangle . \] (2.26)

Note that,
\[ |\psi_b^+\rangle = |\phi_b\rangle + \frac{1}{E_b - H_o - V + i\epsilon} V |\phi_b\rangle \] (2.27)
\[ |\psi_b^-\rangle = |\phi_b\rangle + \frac{1}{E_b - H_o - V - i\epsilon} V |\phi_b\rangle \] (2.28)
\[ \langle \psi_b^- | = \langle \phi_b| + \langle \phi_b| V \frac{1}{E_b - H_o - V + i\epsilon} \] (2.29)
so we find that,
\[ \langle b | S | a \rangle = \delta_{ba} + \langle \phi_b| \left[ 1 + V \frac{1}{E_b - H_o - V + i\epsilon} - V \frac{1}{E_b - H_o - V - i\epsilon} - 1 \right] \psi_a^+ \rangle \]
\[ = \delta_{ba} + \langle \phi_b| V \psi_a^+ \rangle \left[ \frac{1}{E_b - E_a + i\epsilon} - \frac{1}{E_b - E_a - i\epsilon} \right] \]
\[ = \delta_{ba} + \langle \phi_b| V \psi_a^+ \rangle \lim_{\epsilon \to 0} \frac{E_b - E_a - i\epsilon - E_b + E_a - i\epsilon}{(E_b - E_a)^2 + \epsilon^2} \]
\[ = \delta_{ba} + \langle \phi_b| V \psi_a^+ \rangle \lim_{\epsilon \to 0} \frac{-2i\epsilon}{(E_b - E_a)^2 + \epsilon^2} . \] (2.30)

The $\lim_{\epsilon \to 0}$ expression acts like a delta function. If $E_b = E_a$ then the limit goes as $1/\epsilon$ which goes to $\infty$, otherwise the limit goes zero. We can write,
\[ \lim_{\epsilon \to 0} \frac{-2i\epsilon}{(E_b - E_a)^2 + \epsilon^2} = C \delta(E_b - E_a) , \] (2.31)

and proceed to solve for the constant $C$ by writing out the expression as an integral,
\[ \int_{E_b}^{\infty} \frac{\epsilon dE_b}{(E_b - E_a)^2 + \epsilon^2} = \int_{E_b - E_a}^{\infty} \frac{\epsilon^2 dx}{\epsilon^2(1 + x^2)} = \frac{\pi}{2} - \tan^{-1} \left( \frac{E_b - E_a}{\epsilon} \right) \] (2.32)
\[
\int_{-\infty}^{\infty} C \, \delta(E_b - E_a) = \int_{-\infty}^{\infty} \frac{\epsilon \, dE_b}{(E_b - E_a)^2 + \epsilon^2} = \int_{-\infty}^{E_b \leq E_a} \frac{\epsilon \, dE_b}{(E_b - E_a)^2 + \epsilon^2} + \int_{E_b > E_a} \frac{\epsilon \, dE_b}{(E_b - E_a)^2 + \epsilon^2} = \frac{\pi}{2} \quad \text{if } E_b = E_a
\]
\[
= 0 \quad \text{otherwise ,}
\]

which implies that \( C = \pi \). So the final expression for the \( S \)-matrix becomes,
\[
\langle b | S | a \rangle = \delta_{ba} - 2\pi i \, \delta(E_b - E_a) \langle \phi_b | V | \psi_a^+ \rangle .
\]

This also defines the \( T \)-matrix,
\[
\langle b | T | a \rangle \equiv \langle \phi_b | V | \psi_a^+ \rangle ,
\]

where we can see that the two are related by \( S = 1 - 2\pi i \delta(E_b - E_a)T \). The transition matrix element \( T_{ba} \) is the probability amplitude that an incoming, scattering state \( a \) makes a transition to an outgoing, pure state \( b \) as a result of the scattering potential.

We still have the problem that the \( T \)-matrix has the unknown state \( \psi_a^+ \) buried in it, but that can be removed by rewriting its definition using the perturbed resolvent.

\[
T_{ba} = \langle \phi_b | V | \psi_a^+ \rangle = \langle \phi_b | V + VG^+V | \phi_a \rangle ,
\]

where the \( T \)-operator looks like \( T = V + VG^+V \). One can define the \( T \)-operator recursively in order to get rid of the perturbed resolvent so that \( T = V + VG_s^+T \), this is the expression that is used in the coupled-channel scattering treatment found
in the literature [33] Using this recursive form, we can write the T-operator as an infinite series with the free resolvent,

\[ T = V + V G^+_0 V + V G^+_0 V G^+_0 V + \ldots = V + V G^+_0 T, \quad (2.40) \]

which is known as the Born series [31]. If the potential \( V \) is a small perturbation, you can ignore the higher order terms and keep only the first one. This is equivalent to saying that \( |\psi^+\rangle \approx |\phi\rangle \) and constitutes the first order Born approximation. It turns out that this is a bad approximation for ultracold atomic collisions because the energy associated with the interatomic potential is much larger than the thermal energies of the atoms. For a dilute ultracold gas, this series does converge to an answer which can be approximated by a \( \delta \)-function type of interaction which gives the correct low-energy two-body answer. This is the method of pseudo potentials and is important for constructing the non-linear Schrödinger equation [28].

### 2.1.3 Scattering Solution in Position Basis

Armed with the language and formal treatment of quantum scattering, we are now able to re-examine the Lippmann-Schwinger equation and find its solution in a position basis. Scattering theory tells us that in the presence of a potential \( V \), the two-body scattering wavefunction becomes,

\[ \langle \vec{r} | \psi \rangle = \langle \vec{r} | \phi \rangle + \int d\vec{r}' G^+_0 (\vec{r}, \vec{r}') \langle \vec{r}' | V | \psi \rangle, \quad (2.41) \]

or,

\[ \psi(\vec{r}) = \phi(\vec{r}) + \int d\vec{r}' G^+_0 (\vec{r}, \vec{r}') \langle \vec{r}' | V | \psi \rangle, \quad (2.42) \]

where the wavefunction \( \phi(\vec{r}) \) solves the Schrödinger equation in the absence of a potential \( V \). The Green’s function and the matrix element involving \( V \) have been discussed in detail in appendix A, but we really need to develop an understanding of the free wavefunction \( \phi(\vec{r}) \) and then ask how the potential changes it.
For the case of \( V(\vec{r}) = 0 \), where there is no potential, Schrödinger's equation has been solved explicitly in the position basis in 3-dimensions. The wavefunction can be written in spherical coordinates as a product of two functions,

\[
\phi(\vec{r}) = \phi(r, \theta, \phi) = R_l(r)Y_{lm}(\theta, \phi) ,
\]

(2.43)

where the \( Y_{lm} \) functions are spherical harmonics and the radial function \( R_l \) is a function of only \( r \) and the angular momentum quantum number \( l \) [5, 29, 30]. Since the potential we will introduce is only a function of \( r \), it ends up that all of the scattering physics will be contained in the radial function \( R_l \). We have been able to reduce a 2-body, 3-dimensional problem into a 1-body, 1-dimensional problem! In order to simplify the radial equation further, the common substitution of \( u_l(r) = rR_l(r) \) is made so that the radial part of the Schrödinger equation becomes,

\[
\left[ -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V(r) + \frac{l(l + 1)\hbar^2}{2\mu r^2} \right] u_l(r) = E u_l(r) ,
\]

(2.44)

where I have shown the potential term and the familiar centrifugal barrier.

Treating the case of \( V(r) = 0 \), this is simply a form of Bessel's equation and the solutions are known [32]. The solution for \( u_l(r) \) is a linear combination of Bessel and Neumann functions. This make the overall radial wavefunction,

\[
R_l(r) = c_1 j_l(kr) + c_2 n_l(kr) ,
\]

(2.45)

a linear combination of spherical Bessel functions \( j_l(kr) \) and spherical Neumann functions \( n_l(kr) \) with momentum \( k = \sqrt{2\mu E/\hbar^2} \). If the origin \( r = 0 \) is included, then the coefficient \( c_2 \) must be zero since the Neumann function has a singularity there. So with no potential, \( R_l(r) = c_1 j_l(kr) \). However, even in the presence of a potential, this general form holds if the potential \( V(r) \) falls off faster than \( 1/r^2 \). As long as the centrifugal barrier is the dominant long-range part of the radial equation, then the long-range portion of the solution will look like an appropriate Bessel function. What we will find is that one effect of the potential is to introduce an effective phase
shift into the spherical Bessel function that would normally not be there if \( V(r) = 0 \). For the case of low-energy s-wave collisions, \( l = 0 \) and the wavefunction looks like \( j_0(kr) \sim \sin(kr)/kr \) so that \( u_0(kr) \sim \sin(kr) \) at large \( r \).

Since our picture of scattering involves incoming and outgoing waves, it is better to redefine our radial basis functions. Also, since the interatomic potential \( V(r) \) prevents the atoms from getting to \( r = 0 \), we also need to take into account the Neumann solutions to the radial Schrödinger equation. What are commonly used are the spherical Hankel functions,

\[
h_i^{(1)}(kr) = j_i(kr) + in_i(kr) \sim \frac{e^{ikr}}{r} \quad \text{outgoing} \tag{2.46}
\]

\[
h_i^{(2)}(kr) = j_i(kr) - in_i(kr) \sim \frac{e^{-ikr}}{r} \quad \text{incoming} , \tag{2.47}
\]

where there are two types, one that is a spherical outgoing wave, and the other which is an incoming wave.

### 2.1.4 Phase Shift and Scattering Length

As was alluded to earlier, the presence of the potential will introduce a phase shift to the long range portion of the wavefunction. In discussing the Green’s function operator (appendix A) we have seen that the form of the scattered wavefunction looks like,

\[
\psi(\vec{r}) = A \left[ e^{ikz} + \frac{e^{ikr}}{r} f \right] , \tag{2.48}
\]

which is comprised of a non-scattered plane wave plus an outgoing spherical wave with amplitude \( f \). This notation, though commonly used, is strange since it is a mixture of cartesian coordinates and spherical coordinates. To examine this form of the wavefunction more closely, let us rewrite the plane wave portion in a spherical basis. This is known as Rayleigh’s formula [29]

\[
e^{ikz} = A \sum_l c_l j_l(kr) Y_{lm}(\theta, \phi) , \tag{2.49}
\]
and shows that a plane wave looks like a sum of spherical Bessel functions (the Neumann functions do not contribute since a plane wave includes the origin \( r = 0 \)). This expression can be further simplified since there is no \( \phi \)-dependence for a plane wave,

\[
e^{ikz} = A \sum_{l} i^{l}(2l + 1) j_{l}(kr) P_{l}(\cos(\theta))
\]

where \( P_{l} \) are the associated Legendre polynomials of the spherical harmonics. At large distances where \( r \to \infty \), we find that

\[
e^{ikz} \approx A \sum_{l} (2l + 1) P_{l}(\cos(\theta)) \left( \frac{e^{ikr} - e^{-i(kr-\pi/2)}}{2ikr} \right),
\]

since the spherical Bessel function has the long-range behavior,

\[
\lim_{r \to \infty} j_{l}(kr) = \frac{e^{i(kr-\pi/2)} - e^{-i(kr-\pi/2)}}{2ikr}.
\]

Finally we can see that a plane wave looks like a particular superposition of incoming and outgoing spherical waves at large \( r \).

Now looking at the scattered wavefunction, we can begin to see the effect of the potential on the free plane-wave state. We know from the Green's function analysis that,

\[
\psi(\vec{r}) = A \left[ e^{ikz} + \frac{e^{ikr}}{r} f \right],
\]

where \( f \) is the amplitude of the spherical waves and is shown in appendix A to be,

\[
f = - \int d\vec{r}' \frac{e^{-i\vec{k} \cdot \vec{r}'}}{4\pi} \hat{V}(\vec{r}') \langle \vec{r}' | \psi \rangle.
\]

The scattered amplitude is a function of \( \theta \) only \((f = f(\theta))\) since the momentum vector \( \vec{k} \) is chosen to lie along the z-axis. This allows us to expand the scattering amplitude in a partial wave basis as \([5]\),

\[
f(\theta) = \sum_{l} (2l + 1) f_{l}(k) P_{l}(\cos(\theta))
\]
Using this form of \( f \), as well as the spherical wave expansion of the plane wave at large \( r \), allows us to write the scattered wavefunction as,

\[
\psi(\mathbf{r}) = A \sum_l (2l + 1) P_l(\cos(\theta)) \left( \frac{e^{i k r} - e^{-i (k r - l \pi)}}{2 i k r} \right) + \\
A \sum_l (2l + 1) f_l(k) P_l(\cos(\theta)) \frac{e^{i k r}}{r}
\]

\[
= A \sum_l (2l + 1) \frac{P_l(\cos(\theta))}{2 i k} \left[ (1 + 2 i k f_l(k)) \frac{e^{i k r}}{r} - \frac{e^{-i (k r - l \pi)}}{r} \right]
\]

(2.56)

Examining the long range form of \( \psi(\mathbf{r}) \), we see that the presence of the potential \( V(r) \) scatters outgoing spherical waves and introduces a change in the outgoing coefficient of a free plane wave as,

\[
1 \to 1 + 2 i k f_l(k) 
\]

(2.58)

This coefficient is equivalent to the S-matrix element for this scattering event (note, this is a scalar quantity since only one channel is involved) [5, 31]. We make the identification that,

\[
S_l(k) = 1 + 2 i k f_l(k)
\]

(2.59)

In this partial wave basis, the S-matrix is a function of both the channel momentum \( k \) and the angular momentum \( l \) ie, s-wave, p-wave, d-wave, etc.

There are some properties regarding the S-matrix that are apparent in this position representation of the scattered state \( |\psi\rangle \). First of all, since the particle flux between the incoming and outgoing parts of the wavefunction are assumed to be conserved, this implies that,

\[
|S_l(k)| = 1
\]

(2.60)

and the S-matrix must be unitary. The implication of this is that the S-matrix is nothing more than a phase shift which is commonly defined as [5, 31],

\[
S_l(k) \equiv e^{2 i \delta_l(k)}
\]

(2.61)
where $\delta_l$ is the phase shift associated with the $l$ partial wave and the factor of 2 is inserted by convention. To understand this convention, let us re-insert this form of $S_l$ back into the wavefunction and assume that $l = 0$ (s-wave),

\[
\psi_{l=0}(r) = \frac{A}{2ik} \left[ e^{2i\delta} \frac{e^{ikr}}{r} - \frac{e^{-ikr}}{r} \right] \quad (2.62)
\]

\[
= \frac{A e^{i\delta}}{2ik} \left[ \frac{e^{i(kr+\delta)}}{r} - \frac{e^{-i(kr+\delta)}}{r} \right] \quad (2.63)
\]

\[
\sim \sin(kr + \delta). \quad (2.64)
\]

So we see that the convention makes the s-wave piece of the wavefunction look like a sine wave with a phase shift $\delta$.

We can solve for the partial wave amplitude $f_l(k)$ as a function of $S_l(k)$. The result is,

\[
f_l(k) = \frac{S_l(k) - 1}{2ik}, \quad (2.65)
\]

which leads to the full expression for $f(\theta)$,

\[
f(\theta) = \sum_l (2l + 1) \left( \frac{S_l - 1}{2ik} \right) P_l(\cos(\theta)) \quad (2.66)
\]

\[
= \frac{1}{k} \sum_l (2l + 1)e^{i\delta} \sin(\delta)P_l(\cos(\theta)) \quad (2.67)
\]

The cross section for the collision is defined to be $[5, 31]$,

\[
\sigma_{\text{tot}} = \int |f(\theta)|^2 d\Omega, \quad (2.68)
\]

where the integration is taken over solid angle $d\Omega$. We find that the cross section becomes,

\[
\sigma_{\text{tot}} = \frac{1}{k^2} \int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos(\theta)) \sum_{ll'} (2l + 1)(2l' + 1)e^{i\delta} \sin(\delta)e^{-i\delta} \sin(\delta)P_lP_{l'} \quad (2.69)
\]

\[
= \frac{4\pi}{k^2} \sum_l (2l + 1) \sin^2(\delta) \quad (2.70)
\]

\[
= \frac{\pi}{k^2} \sum_l (2l + 1)|S_l - 1|^2, \quad (2.70)
\]
where we use the orthogonality of the Legendre polynomials,

\[ \int_{-1}^{1} P_l(x) P_m(x) \, dx = \frac{2}{2l+1} \delta_{lm}. \]  

(2.71)

There are a number of important properties about the phase shift \( \delta \) that need to be discussed. For the case of a single channel problem where there is only one possible scattering state, the phase shift \( \delta \) must be real. This is a direct consequence of the unitarity of the S-matrix; the fact that particle flux must be conserved. In the case of multi-channel (or coupled-channel) scattering, this condition is relaxed. While the S-matrix for the entire process involving all possible channels must be unitary, the particle flux of a single channel isn’t necessarily conserved since a transition can occur to another channel. The consequence of this is that the phase shift \( \delta \) associated with a particular channel will be complex where the imaginary bit corresponds to loss to another channel. Let us assume that the phase shift \( \delta \) has real and imaginary parts,

\[ S = e^{2i\delta} = e^{2i(\delta_r + i\delta_i)} = e^{-2\delta_i}e^{2i\delta_r}. \]  

(2.72)

The real part of the complex phase gives the “normal” phase shift associated with elastic scattering. The imaginary part makes \(|S| \neq 1\) which implies the inelastic process of either gain or loss in particle flux depending on the sign of \( \delta_i \). The numerical calculations that are carried out in this thesis solve for the complex S-matrix explicitly. Since knowledge of the complex phase shift \( \delta \) is important for describing collisions, I use the following relationships to solve for \( \delta \),

\[ \delta_r = \frac{1}{2} \tan^{-1} \left( \frac{S_i}{S_r} \right) \]  

(2.73)

\[ \delta_i = -\frac{1}{4} \ln \left( S_r^2 + S_i^2 \right) \]  

(2.74)

where \( S_r \) and \( S_i \) refer to the real and imaginary parts of the S-matrix. Diagonal elements of the S-matrix give elastic scattering amplitudes while the off-diagonal elements give inelastic channel-changing amplitudes. More about this will be discussed in section 2.2.
The behavior of the phase shift at low temperatures or energies is extremely important for describing the behavior of an ultracold gas. The low-energy limit of $\delta$ can be found by equating the expression for the partial wave amplitude $f_l$ to the actual expression for $f$ given in appendix A,

$$f_l = \frac{S_l - 1}{2ik} = \frac{e^{i\delta}}{k} \sin(\delta) = -\int d\vec{r}' \frac{e^{-i\vec{k} \cdot \vec{r}'}}{4\pi} \hat{V}(\vec{r}') \langle \vec{r}' | \psi \rangle .$$ (2.75)

The left-hand side of the expression goes as $\delta/k$ in the low energy $k \rightarrow 0$ limit since $\delta$ gets small as the energy goes to zero. The integral on the right-hand side has a plane wave piece that looks like $j_l(kr')$ at large $r'$ as well as the state $\langle \vec{r}' | \psi \rangle$ which looks like a spherical Bessel function, $j_l(kr')$ as well (with some phase shift). So we find that for large $r$ and small $k$,

$$\frac{\delta}{k} \sim \int d\vec{r}' j_l(kr')j_l(kr') \sim (kr)^{2l+1} \sim k^{2l+1},$$ (2.76)

which implies the threshold behavior $\delta \sim k^{2l+1}$. The importance of this for low-energy scattering comes from the fact that as $k \rightarrow 0$, the only partial wave that matters is the $s$-wave ($l = 0$). The scattering amplitude goes as,

$$f_l = \frac{\sin(\delta)}{k} \rightarrow \frac{\sin(k^{2l+1})}{k} \sim k^{2l}$$ (2.77)

where all partial waves of $l > 0$ have vanishing amplitude $f_l$. This is a consequence of the centrifugal barrier which prevents low-energy partial waves of $l > 0$ from getting to small $r$. Since the low-energy scattering amplitude is purely $s$-wave and proportional to $k$, it is customary to define a quantity called the scattering length $a$ as follows,

$$a \equiv \lim_{k \rightarrow 0} -\frac{\tan(\delta)}{k} .$$ (2.78)

This implies that $\delta \approx -ka$, a dimensionless quantity, and says that the radial wavefunction for $u_0(r)$ looks like,

$$u_0(r) \sim \sin(kr + \delta) \sim \sin(kr - ka) \sim \sin(k(r - a)) .$$ (2.79)
So a negative phase shift corresponds to a wavefunction which looks to be shifted by an amount \(+a\) with respect to a free wavefunction which sees no potential. This is identical to the behavior of a system where the potential \(V(r)\) looks to be infinite at \(r < a\) and zero for \(r > a\) \([5, 29]\). So for this situation, the collision is identically described by a hard-sphere repulsive potential of radius \(a\). On the other hand, a positive phase shift corresponds to a negative \(a\). While a little harder to visualize, it nevertheless corresponds to a collision which is attractive, effectively "pulling" the probability amplitude of the particle closer towards \(r = 0\). The elastic s-wave cross section looks like,

\[
\sigma_{l=0} = \frac{4\pi}{k^2} \sin^2(\delta_0) \approx \frac{4\pi}{k^2} \sin^2(-ka) \approx 4\pi a^2 ,
\]

for the case where \(k\) is small and consequently \(\delta_0\) is assumed to be small. So amazingly all of elastic scattering for an ultracold gas can be described by a single parameter, the s-wave scattering length \(a\). The magnitude of this number is related to the elastic cross section while the sign tells you whether the net collision looks to be attractive or repulsive.

There are some difficulties with this simple picture of low-energy scattering. In particular, since the definition of a scattering length depends on having a small, real-valued phase shift, any time this breaks down then the scattering length description is not valid. This can occur for finite temperatures when large inelastic processes might be occurring to other channels. In this case, the phase shift has a significant imaginary component to it so the idea of taking the tangent of the number becomes difficult. Also, even at low temperatures with purely elastic scattering, there is always a problem if the phase shift is not small. In this case, you cannot say that \(\tan(\delta)\) is small and equal to \(-ka\). This is the case with a \textit{collisional resonance} where conditions within the Schrödinger equation allow for very large phase shifts. I will outline a few instances of this shortly. In the end, all that matters in describing a collision is the square of the amplitude, i.e., the cross section. While it is convenient and handy to
approximate the low energy amplitude with $a$ and say that $\sigma = 4\pi a^2$, one needs to keep in mind that it is an approximation. The full proper description of scattering is given by the S-matrix and the cross section by $\sigma = \frac{\pi}{k^2} \sum_i (2l + 1)|S_i - 1|^2$.

2.1.5 Collisional Resonance

Resonant scattering occurs when the phase shift $\delta_i(k)$ goes through the value $\pi/2$. When this occurs, the value for the s-wave scattering length becomes undefined,

$$a = -\frac{\tan(\delta_0)}{k} = \pm\infty.$$  \hspace{1cm} (2.81)

while the elastic cross section achieves its maximum value,

$$\sigma_i = \frac{4\pi}{k^2} \sin^2(\delta_i) = \frac{4\pi}{k^2}.$$  \hspace{1cm} (2.82)

In this circumstance, the value for the cross section would grow without limit as $k \to 0$ (assuming that $\delta(k)$ does not change value which is unlikely), hence the reason for referring to this as resonant scattering. There are a number of physical circumstances in which the phase shift can become $\pi/2$ which I will touch on briefly.

A zero-energy resonance occurs when the potential $V(r)$ supports a bound state at the dissociation limit. To get the simple idea of this and avoid math, let us consider a square well potential where $V(r) = -V_o$ for $r < r_o$, and $V(r) = 0$ for $r > r_o$.

![Simple square well potential](image)

**Figure 2.1** Simple square well potential.

Normally as the energy goes to zero ($k \to 0$), the Schrödinger equation says that
the wavefunction solution $u(r)$ in the region where $V(r) = 0$ obeys the relation,

$$\frac{d^2 u(r)}{dr^2} = 0.$$  \hfill (2.83)

Of course this implies that the simple solution for large $r$ is a straight line where $u(r) = A(r - a)$. This is the large wavelength limit of a sine function, the known solution for $U(r)$ in s-wave scattering,

$$u(r) = \lim_{k \to 0} \sin(kr + \delta) = \lim_{k \to 0} \sin(k(r - a)) \approx k(r - a).$$  \hfill (2.84)

So we can see the wavefunction approaches something that looks like a straight line which intersects the $r$-axis at the scattering length value $a$. This is consistent with the scattering length description given earlier. The behavior of $u(r)$ for $r < r_o$ is described by an oscillating function characterized by,

$$\frac{d^2 u(r)}{dr^2} = -\frac{2\mu}{\hbar^2} V_o \cdot u(r)$$  \hfill (2.85)

where the inner and outer wavefunctions must join smoothly at $r = r_o$. The number of nodes in the wavefunction indicates the number of bound states that must be present in the square well potential. Figure 2.2 shows the zero-energy wavefunction for a square well potential which supports one bound state.

The single node indicates that the well supports one bound state, but I should point out that the location of the node has little to do with the spatial extent of the potential. For figure 2.2, the square well potential extends to $r_o = 1$ while the node in the wavefunction clearly occurs at a larger range and indicates the scattering length.

In a similar fashion, the scattering length for a given potential can be located at a very large value of $r$ despite the limited extent of the interatomic potential. As the potential well depth is decreased, the node will be pushed out to larger and larger values of $r$ until the well cannot support a bound state. At this point, the effective scattering length changes sign and the long range wavefunction appears to cross the
Figure 2.2  Low-energy wavefunction for a square well potential with one bound state. The potential goes from $-V_0$ to 0 at $r_0 = 1$.

$r$ axis at a large, negative value. This change in the wavefunction as a function of changing well depth is shown in figure 2.3.

This is a situation that exists in $^6\text{Li}$, the triplet potential of this isotope supports a virtual level, a level which is barely unbound. This leads to a large, negative scattering length for $^6\text{Li}$ and has made it an interesting candidate for observing Cooper pairing [18, 19]. The key element of a collisional resonance is the existence of a bound state which can couple with the scattering state. For the case of a zero-energy resonance, this coupling occurs because of the existence of a bound state near the dissociation limit, however other types of bound states can also cause resonant collisions.

A shape resonance occurs when the centrifugal barrier of the scattering potential supports a quasi-bound state near the scattering energy (see figure 2.4). In this example, a resonance in the scattering can be observed as the scattering energy is lowered through the energy position of the bound state. This type of scattering is usually limited to higher order partial waves and can only be seen in s-wave scattering if the interatomic potential has some type of local maximum in it similar to the centrifugal barrier.
Figure 2.3  Low-energy wavefunctions for various square wells where the bound state of the square well is removed by decreasing the well depth. As the bound state goes through zero-energy, one can see the low-energy wavefunction has a node which vanishes and its long-range slope goes from negative to positive. This is indicative of the scattering length becoming large and positive before changing sign and becoming large and negative.

The final case of resonant scattering that I will discuss is the Feshbach Resonance. A Feshbach resonance occurs due to coupling between the scattering state and a bound state, though contrary to zero-energy scattering this bound state does not exist in the scattering potential [34]. A Feshbach resonance involves coupling to another potential, usually weakly, and this can be done in a number of ways. For the case of ultracold atomic collisions in traps, this coupling is usually manifested by a mixing between the singlet and triplet potentials through the hyperfine interaction [35]. Atoms that are confined in traps are usually spin aligned and therefore interact mainly along the triplet ($S = s_1 + s_2 = 1$) interatomic potential. For certain values of magnetic field, this triplet potential can be Zeeman shifted with respect to the singlet potential in such a way that a bound state of the singlet potential becomes resonant with the scattering state. This results in resonant scattering with a scattering amplitude that changes as a function of the applied magnetic field. These resonances have been observed in traps [36-40] and could play an important role in adjusting the scattering
Figure 2.4  Quasi-bound state in an interatomic potential with a large centrifugal barrier ($l > 0$).

length for experiments such as BCS pairing [19]. Alternatively, rather than using the hyperfine/Zeeman interaction to set up a resonance, one could also use a laser tuned to an excited molecular state to alter the scattering. This has been called an optical Feshbach resonance and has been studied in the literature [41].
2.2 Coupled-Channel Treatment

The coupled-channel treatment of scattering is necessary for the case where the two atoms undergoing a collision have internal degrees of freedom which allow for more than one possible interaction potential. In the case of ultracold atomic collisions, these degrees of freedom are associated with the electronic and nuclear spin. For alkali atoms where there is one valence electron, a collision can be described as either triplet \( S = s_1 + s_2 = 1 \) or as singlet \( S = 0 \), or as some linear-combination of the two. I will ignore the nuclear spins for now, they will be treated in the full calculation later on. Since electrons are fermions, the product of their spin and spatial wavefunctions must be antisymmetric. So the collision between electrons will have different spatial wavefunctions depending on the symmetry of the spin-wavefunctions. Since the interaction potential is a function of van der Waals forces as well as electronic coulomb repulsion, the energy associated with the interaction will be a function of the spatial-state (and therefore the spin-state) of the collision. This is referred to as the exchange interaction and this leads to two possible spin-dependent interactions, the triplet potential \( V_T(r) \) and the singlet potential \( V_S(r) \), where \( r \) is the interatomic distance in the collision. The nuclear spin manifests itself as a higher-order correction to these potentials in the form of molecular hyperfine structure. This hyperfine interaction will lead to mixing between the singlet and triplet interactions as will be seen.

An approximation that has been talked about in the field of ultracold collisions is the degenerate internal states approximation, or DIS [42]. This approximation is equivalent to assuming that the hyperfine interaction is zero. The consequence of this is that no mixing occurs between the singlet and triplet potentials during the collision, so each part can be treated separately. In that sense, if two atoms are colliding and the collision is 75% triplet and 25% singlet, then the overall scattering length is simply 75% of the pure triplet scattering length plus 25% of the pure singlet. Usually this
type of approximation is only valid when the hyperfine energy is much smaller than the thermal energy of the collision. For the case of ultracold atoms, this is far from the truth; the hyperfine energy is usually much larger than the thermal energy. One would expect this approximation to be a poor one, and it is. An exception can be made for special cases, such as hydrogen/deterium [42], where spin symmetries forbid the types of collisions which would mix the hyperfine energy with the thermal energy. This example is the exception rather than the rule, and so the DIS approximation should be avoided.

Taking the hyperfine energy into account, the full Hamiltonian for the coupled-channel problem has the form,

\[ H = -\frac{\hbar^2}{2\mu} \nabla^2 + A^{HF} \sum_{i=1}^{2} \mathbf{s}_i \cdot \mathbf{\tilde{r}}_i + P_T V_T(r) + P_S V_S(r), \quad (2.86) \]

where the sum is taken over the two constituent atoms and their corresponding hyperfine energies \( A^{HF} \), and \( P_T/S \) is the corresponding triplet and singlet projection operator. The overall wavefunction will have the form of a radial part times an angular piece just as was described earlier,

\[ \Psi(r) = R_l(r) Y_{lm}(\theta, \phi). \quad (2.87) \]

By using the usual substitution, \( F(r) = r R_l(r) \), the radial Schrödinger equation becomes,

\[ \left[ -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + A^{HF} \sum_{i=1}^{2} \mathbf{s}_i \cdot \mathbf{\tilde{r}}_i + P_T V_T(r) + P_S V_S(r) + \frac{l(l+1)\hbar^2}{2\mu r^2} \right] F(r) = E F(r), \quad (2.88) \]

which contains all of the scattering information that we are interested in. The important thing to notice is that the hyperfine interaction given by the \( \mathbf{s} \cdot \mathbf{\tilde{r}} \) term cannot be diagonalized in the same basis as the spin projection operators \( P_T/S \). The hyperfine interaction wants to couple \( \mathbf{s} \) and \( \mathbf{\tilde{r}} \) together to form \( \mathbf{\tilde{f}} = \mathbf{s} + \mathbf{\tilde{r}} \). This angular momentum vector cannot commute with the total spin given by \( \mathbf{\tilde{S}} = \mathbf{\tilde{r}}_1 + \mathbf{\tilde{r}}_2 \) which is where
the projection operators are diagonal. It is the off-diagonal nature of this Hamiltonian which requires that multiple scattering states must be solved for simultaneously leading to the term "coupled-channels" where a particular collisional channel is labeled by its internal state. However, since the potential is central, regardless of the mixing of the basis functions the total angular momentum of the system cannot change during the interaction. This implies that in particular the total spin projection given by \( m_T = m_{f_1} + m_{f_2} = m_S + m_I \) must be conserved (\( \vec{S} = \vec{s}_1 + \vec{s}_2 \) and \( \vec{l} = \vec{l}_1 + \vec{l}_2 \)).

There is freedom in picking the basis set to use for solving the scattering problem. The full scattering solution (angular part as well) will look like

\[
|\psi\rangle = |rlm\alpha\beta\rangle = |rlm\rangle \otimes |\alpha\beta\rangle , \quad (2.89)
\]

where the variables \( r, l, \) and \( m \) characterize the spatial piece of the wavefunction while the internal states of the two atoms are described by \( \alpha \) and \( \beta \). Ignoring any magnetic fields (for now), there are two natural choices for describing the \( \alpha \) and \( \beta \) states. You could elect to work in the molecular basis where total \( \vec{S} \) and \( \vec{l} \) are good quantum numbers,

\[
|\alpha\beta\rangle = |(s_1s_2)Sm_s(i_1i_2)Im_i\rangle = |Sm_sIm_i\rangle , \quad (2.90)
\]

and are formed from a respective coupling of the individual atomic \( s \)'s and \( i \)'s. This is the basis that was used by our collaborators [43]. I have elected to use the hyperfine basis which was described in an earlier coupled-channel work [33],

\[
|\alpha\beta\rangle = |(s_1i_1)f_1m_1(s_2i_2)f_2m_2\rangle = |f_1m_1f_2m_2\rangle . \quad (2.91)
\]

In this basis, the hyperfine interaction \( \vec{s} \cdot \vec{i} \) is diagonal while the triplet and singlet projection operators are not. Ignoring the spatial labelling (\( |rlm\alpha\beta\rangle \equiv |\alpha\beta\rangle \)), I can rewrite the radial Hamiltonian matrix element as,

\[
\langle \alpha'\beta'|H|\alpha\beta\rangle = \left( -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + E_{\alpha}^{HF} + E_{\beta}^{HF} + \frac{l(l+1)\hbar^2}{2\mu r^2} \right) \delta_{\alpha\beta,\alpha'\beta'} \\
+ \langle \alpha'\beta'|P_T V_T(r) + P_S V_S(r)|\alpha\beta\rangle , \quad (2.92)
\]
where the potential term will have off-diagonal elements connecting different spin channels \( \alpha' \beta' \) to \( \alpha \beta \).

Up to now, I have not taken into account whether the atoms are identical, in fact I have not specified whether state \( \alpha \) is on atom ‘1’ or ‘2’ and likewise for state \( \beta \). For the purpose of notation, when writing the ket \( |\alpha \beta\rangle \) this assumes that atom ‘1’ is in state \( \alpha \) and atom ‘2’ is in state \( \beta \). This is different than the state \( |\beta \alpha\rangle \) where the situation is reversed. Why is this important? When considering collisions between identical Bose and Fermi atoms, then the appropriate symmetries must be correctly represented and so the atom “labels” must be explicitly kept track of. To properly represent Bose/Fermi symmetry, the basis kets must be redefined [33],

\[
|rlm\{\alpha \beta\}\rangle \equiv |\{\alpha \beta\}\rangle \equiv |rlm\rangle \otimes \left[ \frac{|\alpha \beta\rangle \pm (-1)^l |\beta \alpha\rangle}{\sqrt{2(1 + \delta_{\alpha \beta})}} \right], \quad (2.93)
\]

where the \( \pm \) refers to bosons or fermions and is dependent on the partial wave symmetry of the spatial part of the wavefunction through the quantum number \( l \). If the atoms are distinguishable, as is the case for a mixed \( ^6\text{Li}^7\text{Li} \) collision, then the original state \( |\alpha \beta\rangle \) is correct where I label atom ‘1’ as the \( ^6\text{Li} \) atom and atom ‘2’ as the \( ^7\text{Li} \) atom (or visa versa). If the atoms are identical, then I need to use the symmetrized state \( |\{\alpha \beta\}\rangle \). We can already see the effect of the statistics when the identical atoms are in the same internal state \( \alpha = \beta \). For bosons undergoing s-wave \( (l = 0) \) collisions, the state looks like \( |\{\alpha \alpha\}\rangle = |\alpha \alpha\rangle \) while the corresponding case for fermions is \( |\{\alpha \alpha\}\rangle = 0 \). Fermions are not able to undergo symmetric collisions as dictated by the Pauli exclusion principle. So the final Schrödinger equation for the scattering looks like,

\[
\langle r'r'l'm'|\alpha' \beta'|H - E|rlm\{\alpha \beta\}\rangle = 0, \quad (2.94)
\]

for a given collision energy \( E \) which can be written out as,

\[
\left( -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + E_{\alpha}^{HF} + E_{\beta}^{HF} + \frac{l(l+1)\hbar^2}{2\mu r^2} - E \right) \delta_{\{\alpha' \beta'\}, \{\alpha \beta\}} \delta_{ll'} \delta_{mm'} F(r) + \langle \{\alpha' \beta'\}|P_T V_T(r) + P_S V_S(r)|\{\alpha \beta\}\rangle F(r) = 0 \quad (2.95)
\]
So the interatomic potentials couple various $F(r)$ together where the total spin projection $m_\alpha + m_\beta$ must be conserved since the potential is central.

At this point I think it is instructive to use an example and from there lead into the numerics of solving the coupled-channel equation. Let us consider the collision between two $^7\text{Li}$ atoms which are in the spin states $|\{f_1m_1f_2m_2\}| = |\{1121\}|$. Since the total spin projection is $m_T = 1 + 1 = 2$, we know that the coupled-channel Hamiltonian will only couple this channel to those channels with the same total spin projection. For this system, there are 5 different possibilities:

$|\{2220\}|$
$|\{2210\}|$
$|\{2121\}|$
$|\{2111\}|$
$|\{1111\}|$

I should point out that even though the channel $|\{2220\}|$ could have higher energy than the incoming channel (and consequently is referred to as a "closed" channel), its wavefunction is non-trivial and must be included in the calculation. So we know that the Hamiltonian is a 5x5 matrix and that $F(r)$ will be a 5-component vector where each element corresponds to a wavefunction in each channel,

$$F(r) = \begin{pmatrix}
\psi_1(r) \\
\psi_2(r) \\
\psi_3(r) \\
\psi_4(r) \\
\psi_5(r)
\end{pmatrix}.$$  \hspace{1cm} (2.96)

At this point the equations seem to have too many unknowns. The non-diagonal Hamiltonian forces us to solve for 5 different channels simultaneously which would lead to 5 different phase shifts or scattering amplitudes, but there is only one equation. To get around this, we must solve for 5 different initial conditions which are orthogonal
to each other. This would enable us to solve for the 5 unknown phase shifts with the corresponding 5 orthogonal Schrödinger equations, a 5x5 matrix equation. Since the scattering process is thought of as one pure incoming channel which undergoes a collision to form outgoing products (elastic and inelastic), the obvious orthogonal choice is to solve for the 5 initial conditions where the incoming channel is one of the 5 coupled channels. So the incoming piece looks like,

$$\psi_{\text{incoming}} = \psi_1(r) \text{ or } \psi_2(r) \text{ or } \psi_3(r) \ldots \quad (2.97)$$

If the scattering probability to other channels (ie, spin-exchange) is small, then the corresponding outgoing parts of the wavefunction will look like,

$$\psi_{\text{incoming}} = \psi_1(r) \text{ , then } \rightarrow \psi_{\text{outgoing}} \sim (1 - \epsilon)\psi_1 + \epsilon\psi_2 + \epsilon\psi_3 + \epsilon\psi_4 + \epsilon\psi_5$$
$$\psi_{\text{incoming}} = \psi_2(r) \text{ , then } \rightarrow \psi_{\text{outgoing}} \sim \epsilon\psi_1 + (1 - \epsilon)\psi_2 + \epsilon\psi_3 + \epsilon\psi_4 + \epsilon\psi_5$$

etc ,

where \( \epsilon \) is simply understood to be “small”. So now the coupled-channel scattering equation looks like

$$\frac{d^2}{dr^2} F_{sxs}(r) = \frac{2\mu}{\hbar^2} C_{sxs}(r) F_{sxs}(r) , \quad (2.98)$$

or,

$$\frac{d^2}{dr^2} F_{\{\alpha',\beta\},\{\alpha\beta\}}(r) = \frac{2\mu}{\hbar^2} C_{\{\alpha',\beta\},\{\alpha\beta\}}(r) F_{\{\alpha',\beta\},\{\alpha\beta\}}(r) , \quad (2.99)$$

where \( C_{\{\alpha',\beta\},\{\alpha\beta\}} \) looks like,

$$C_{\{\alpha',\beta\},\{\alpha\beta\}} = (E^{HF}_\alpha + E^{HF}_\beta - E)\delta_{\{\alpha',\beta\},\{\alpha\beta\}}$$
$$+ V_T(r) \langle \{\alpha'\beta'\} | P_T | \{\alpha\beta\} \rangle$$
$$+ V_S(r) \langle \{\alpha'\beta'\} | P_S | \{\alpha\beta\} \rangle . \quad (2.100)$$

The 5x5 matrix \( F(r) \) is understood to have mutually orthogonal columns where each one corresponds to the incoming channel being one of 5 possibilities. The projection
operators $P_{TIS}$ are straightforward to derive using angular algebra, their derivation is given in appendix B. The hyperfine energy $E_{\alpha}^{HF}$ for state $\alpha$ is given by the appropriate atomic hyperfine constants $A_{\alpha}^{HF}$ where,

$$E_{\alpha}^{HF} = \frac{A_{\alpha}^{HF}}{2} (f_{\alpha}^2 - s_{\alpha}^2 - i_{\alpha}^2) .$$

(2.101)

These hyperfine constants are given in appendix E. So now that the equation has been established and should have a unique solution, how do we solve it?

### 2.2.1 Numerical Integration

To solve for the coupled-channel system, I use a variation of the Numerov-Cooley routine [44, 45] and apply it to a matrix system. This is essentially an iterative equation where, for a given step-size ‘$h$’, the solution of $F(r+h)$ is related to $F(r)$ and $F(r-h)$. The details of the actual Numerov routine are given in appendix C. To start the integration, one begins at a small enough value of $r$ such that the wavefunctions involved are within the classically forbidden regions of both the singlet and triplet potentials. In this region, the scattering wavefunctions are exponentially approaching zero as $r$ goes to zero. Calling this point $r_o$, we assume that

$$F_{\alpha\beta}(r_o - h) = 0 \cdot I_{\alpha\beta} \quad \text{and} \quad F_{\alpha\beta}(r_o) = \epsilon \cdot I_{\alpha\beta} ,$$

(2.102)

where $I_{\alpha\beta}$ is the identity matrix, and $\epsilon$ is a “small” number. The Numerov routine is then used to generate the solution at $F(r_o + h)$ which is then used to generate the solution at $F(r_o + 2h)$ and so on.

Any numerical routine requires some care and attention to ensure that round-off errors do not cause any problems. There are a number of “tricks” that are needed to keep the integration accurate. First off, since the integration starts in the classically forbidden region, as the wavefunctions are constructed at larger and larger values of ‘$r$’, the error in them will grow exponentially. One effect of this is to cause the $F(r)$ matrix to lose its orthogonality as the integration progresses. In order to counteract
this, the solution $F(r)$ is periodically re-diagonalized. This is done by finding a 
transformation matrix $D$ such that $D \cdot F(r) =$diagonal matrix at a particular value
of ‘$r$’. One then transforms all the stored values of $F(r)$ by the matrix and then
continues the integration. Another problem of round-off can occur if the values of
$F(r)$ get either too large or too small. As this occurs, we simply re-scale $F(r)$ and
continue. The integration is carried out until $F(r)$ is known at long range where the
singlet and triplet potentials are essentially zero on the scale of the thermal energy;
this is the asymptotic region. Details concerning the execution of this calculation are
detailed in appendix H.

2.2.2 Computing the S-matrix, $a$, $\sigma$, $G_{\text{exc}}$

To solve for the S-matrix, I need to transform the asymptotic form of $F(r)$ into the
appropriate sum of incoming and outgoing wavefunctions as described by scattering
theory. To do this, I would like to write $F(r)$ as

$$F(r) = I(r) \cdot A + O(r) \cdot B ,$$

where the matrices $I(r)$ and $O(r)$ are diagonal and have the form of the appropriate
incoming ($I$) and outgoing ($O$) wavefunctions one would expect in the absence of
any scattering potential. I have talked about these wavefunctions in the first part
of this chapter, they will look like spherical Hankel functions [33]. The incoming
wavefunction has the form,

$$I_{mn}(r) = -\delta_{mn} \sqrt{k_m r} h^{(2)}_l(k_m r) ,$$

where $k_m$ is the appropriate channel momentum ($k_m = \sqrt{2\mu(E - E^{HF}_\alpha - E^{HF}_\beta)}$) and
$h^{(2)}_l$ is a spherical Hankel function of type (2). The outgoing wavefunction is simply
the complex conjugate of the incoming,

$$O_{mn}(r) = I_{mn}^*(r) .$$

(2.105)
The effect of the transformation requires that the matrices $A$ and $B$ are now complex.

A complication occurs when the value of the incoming energy causes the channel momentum to become imaginary. This leads to the distinction between open and closed channels. An open channel is one in which the momentum is real-valued, $E > E^H_\alpha + E^H_\beta$, so that the scattering wavefunction looks like an oscillating Hankel function. A closed channel is one in which the momentum is purely imaginary, $E < E^H_\alpha + E^H_\beta$. For the case of a closed channel, the wavefunction looks exponentially damped and is equivalent to finding the Hankel function of a complex argument,

$$I_{mn}(r)|_{\text{closed}} \sim h_i^{(2)}(|k_m|i r).$$

The closed channel wavefunction is equivalent to a modified Bessel function. This is a rather tedious thing to figure out, and so it is presented in appendix D. Suffice to say, depending on whether a given channel is open or closed dictates a particular form of $I(r)$ and $O(r)$ to fit to.

The S-matrix can be solved for once the matrices $A$ and $B$ are known. The solution $F(r)$ can be written as,

$$F(r) = I(r) \cdot A + O(r) \cdot B = [I(r) + O(r) \cdot S] \cdot A,$$

where the S-matrix is related to $A$ and $B$ by $S = BA^{-1}$. Since there are two constants to solve for, $A$ and $B$, I need to know $F(r)$, $O(r)$, and $I(r)$ at two different locations. This is trivial since I can carry out the integration to some long range value of 'r' and 'r + x'. So given,

$$F(r) = I(r) \cdot A + O(r) \cdot B$$

$$F(r + x) = I(r + x) \cdot A + O(r + x) \cdot B,$$

I have two equations and two unknowns, which enables me to solve for $S$.

The S-matrix has been discussed earlier in chapter 2 so I will not spend too much time with it here. The diagonal elements are related to elastic scattering and
scattering lengths while the off-diagonal elements are related to inelastic, channel-changing spin-exchange collisions. The elastic cross section of channel $|\alpha \beta \rangle$ is given by [31],

$$\sigma_{l}^{\alpha \beta} = \frac{\pi}{k_{m}^{2}} (2l + 1) |S_{\alpha \beta, \alpha \beta}(l) - 1|^{2} .$$  \hspace{1cm} (2.110)

The scattering length is defined as,

$$a_{l} = \lim_{k_{m} \to 0} - \frac{\tan(\delta_{r})}{k_{m}} ,$$  \hspace{1cm} (2.111)

where the phase shift $\delta_{r}$ is understood to be the real-part of the phase shift as defined by $S_{\alpha \beta, \alpha \beta} \equiv e^{2i\delta}$. Finally, the spin-exchange rate between two different channels $|\alpha' \beta'\rangle$ and $|\alpha \beta\rangle$ is given by [33],

$$G_{\alpha \beta \rightarrow \alpha' \beta'} = \frac{\pi \hbar S_{\alpha' \beta', \alpha \beta} \cdot S_{\alpha' \beta', \alpha \beta}^{*}}{\mu k_{\alpha \beta}} .$$  \hspace{1cm} (2.112)

I should point out that only the sub-matrix of the S-matrix which corresponds to open channels has any meaning in the scattering picture. When I solve for $S$ using $A$ and $B$, I only consider the open-channel elements. This is important since the closed channel wavefunctions have vanishing values in the asymptotic limit and the inversion routines used to find $S$ have problems with those elements.

### 2.2.3 Adding the Zeeman Interaction, Feshbach Resonances

So now that the framework of coupled-channel theory has been developed, it is time to consider the effects of having a magnetic field present during the collision. This field will modify the Hamiltonian of the system and give Zeeman terms which must be dealt with. The radial Hamiltonian becomes,

$$H = -\frac{\hbar^{2}}{2\mu} \frac{d^{2}}{dr^{2}} + \sum_{i=1}^{2} \left[ A_{i}^{HF} \mathbf{s}_{i} \cdot \mathbf{r}_{i} + g_{s} \mu_{B} m_{s}^{(i)} B + g_{i} \mu_{N} m_{i}^{(i)} B \right]$$

$$+ P_{T} V_{T}(r) + P_{S} V_{S}(r) + \frac{l(l + 1) \hbar^{2}}{2\mu r^{2}} ,$$  \hspace{1cm} (2.113)
with the easily recognizable Zeeman terms that account for the separate coupling of
the electronic and nuclear spins to the external field $B$.

I can still solve for this Hamiltonian equation using the hyperfine basis that I have
developed in the previous sections. Now the Zeeman terms are off-diagonal in the
same fashion as the singlet and triplet projection operators. If the complete hyperfine
plus Zeeman interaction for a given atom labelled ‘1’ is given by,

$$H_{1}^{HZ} = A_{1}^{HF} \vec{s}_1 \cdot \vec{i}_1 + g_s \mu_B m_{s_1}^{(1)} B + g_i \mu_N m_{i_1}^{(1)} B,$$

then the Hamiltonian for the coupled-channel system becomes

$$H = -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + H_{1}^{HZ} + H_{2}^{HZ} + P_T V_T(r) + P_S V_S(r) + \frac{l(l+1)\hbar^2}{2\mu r^2},$$

and I am now having to solve for,

$$\langle \{\alpha' \beta'\} | H_{1}^{HZ} + H_{2}^{HZ} | \{\alpha \beta\} \rangle,$$

using the symmetrized hyperfine states I have discussed before. This has been done
in detail in appendix E so I will only discuss the results here.

It is clear that in the long-range, asymptotic region the various wavefunctions
that make up $F(r)$ will be coupled due to the off-diagonal nature of the Zeeman
Hamiltonian. This is equivalent to saying that the hyperfine basis I have chosen
to calculate the problem in, $|\{f_1 m_1 f_2 m_2\}\rangle$, does not represent a good quantum la-
belling of the states ($f m_f$ are not well defined). However, there exists a basis in
which the hyperfine plus Zeeman interaction is diagonal. This basis will be a function
of the magnetic field and can be used to re-diagonalize $F(r)$ such that it appears
to be composed of uncoupled wavefunctions, restoring our picture of scattering. In
the limit as $B$ gets large, the individual electronic and nuclear spins will completely
de-couple implying that the scattering states can be labelled by the strong-field num-
bers $|s_1 m_{s_1} i_1 m_{i_1}\rangle \otimes |s_2 m_{s_2} i_2 m_{i_2}\rangle$. Interestingly, this is the same basis in which the
projection operators $P_S$ and $P_T$ are diagonal. This illustrates quite nicely how the
hyperfine coupling between atomic \( \bar{s} \) and \( \bar{t} \) cause the scattering triplet and singlet states to couple.

Given that the magnetic field is not zero, I need to change the basis description of \( F(r) \) in the asymptotic limit after carrying out the usual numeric integration. To do this, I need to find a matrix \( D \) such that,

\[
D^{-1} \cdot \begin{bmatrix} H_1^{HZ} + H_2^{HZ} \end{bmatrix} \cdot D = \text{diagonal},
\]

(2.117)

where the diagonal elements correspond to the various Breit-Rabi energies one would normally get when diagonalizing the hyperfine and Zeeman interactions of an atom in a magnetic field [46]. I then transform \( F(r) \),

\[
F^{\text{dia}}(r) = D^{-1} \cdot F^{f_1m_1/2m_2}(r) \cdot D = I(r) \cdot A + O(r) \cdot B,
\]

(2.118)

and then carry out the normal analysis that has been discussed to calculate the S-matrix and the scattering properties of the system.

Now that magnetic field effects are included in the coupled-channel calculation, we are in a position to predict and study Feshbach resonances. These resonances occur when the Zeeman shifted scattering state becomes degenerate with a Zeeman shifted (or unshifted) bound molecular state. As a result, resonances occur at certain values of magnetic field. These locations can be approximately found by considering the Zeeman shift of bound molecular states within the singlet and triplet potentials and seeing at what field values they become degenerate with the scattering state. I use this approximation to narrow down my range of \( B \) values before using the coupled-channel code to find the exact resonances. The Breit-Rabi formulas and molecular hyperfine/Zeeman structure calculation that was used to do this is also detailed in appendix E.

As a general rule, since the bound molecular states are usually lower in energy than the scattering state at zero field, this usually means that these resonances will only be seen in a scattering state which Zeeman shifts to lower energy with increasing
magnetic field (high field seeking). Figure 2.5 shows the energy level structure of the ground state of $^6\text{Li}$ as a function of field. As an example, let me consider the collision between two $^6\text{Li}$ atoms in the lower two hyperfine states which are labelled at zero field by the quantum numbers $|\{f_1m_1,f_2m_2\} \rangle = |\{1\frac{1}{2},-\frac{1}{2}\}\rangle$. Figure 2.6 shows how the total Zeeman energy of both these atoms shifts to lower energy at higher field. This figure also shows the location of the highest bound states in the singlet and triplet potentials and how their respective hyperfine structure shifts with magnetic field. From examining the figure, one can see that the singlet molecular state does not shift since the dominant Zeeman interaction, $\sim \vec{S} \cdot \vec{B}$, is zero. In contrast, the triplet level does shift with an energy given by $\sim m_S \mu_B B$ for the different total electronic spin projections of $m_S = -1,0,1$. The scattering state crosses the singlet level at $B \sim 850 \text{ G}$ and the triplet state at $B \sim 4360$ and 8700 G. One would expect to see Feshbach resonances at these field values and the coupled-channel calculation shows

![Figure 2.5: Zeeman structure splitting of $^6\text{Li}$.](image)
Figure 2.6  Zeeman energy of $|{\frac{1}{2}\frac{1}{2}\frac{1}{2}-\frac{1}{2}}\rangle$ scattering state compared with the molecular Zeeman structure of the highest lying triplet and singlet bound states. The states shown are those states which have the same total spin projection and are thus coupled through the coupled-channel equations.

This. Figure 2.7 shows the coupled-channel result for this scattering state. The large resonance at 850 G is due to the scattering state crossing two degenerate molecular singlet states resulting in stronger resonance behavior. This makes the resonance wide as well as shifts it a bit from where simple arguments would say otherwise. The triplet resonances are substantially weaker because at the larger field values there is less coupling since the Zeeman energy is much larger than the hyperfine energy making the scattering basis more and more diagonal. I should point out that in the range of 500 G to 1000 G the scattering length is changing to the pure triplet value for $^6$Li. This directly shows the de-coupling of atomic $\tilde{s}$ and $\tilde{t}$ as expected. This resonance could play an important role in helping to observe BCS pairing in a
Figure 2.7 $^6\text{Li} - ^6\text{Li}$ scattering in state $|\{\frac{1}{2}\frac{1}{2} \frac{1}{2} \frac{1}{2} \frac{3}{2} \frac{1}{2} \}|$.

degenerate gas of $^6\text{Li}$. We hope to observe this resonance in the future and use it to "tune" the scattering length to even larger, negative values than the pure triplet value seen at large field values.

2.2.4 Treating Dipolar Decay

In order to achieve degenerate conditions in a magnetic trap through evaporative cooling, it is critical to minimize two-body losses. Most magnetic traps capture atoms in either the lower hyperfine states, or the stretched state, to eliminate spin-exchange loss. For the specific case of $^7\text{Li}$, we trap in the $f = 2, m = 2$ state so that collisions are characterized by $|\{2222\}|$ which is pure triplet and has no spin-exchange. Unfortunately, there is another loss mechanism which has not been included in the coupled-channel Hamiltonian, but which is large enough for $^7\text{Li}$ that it must be considered during evaporation. This mechanism is dipolar decay. The
Hamiltonian for this process is,

\[ H_{\text{dipolar}} = \frac{\vec{\mu}_1 \cdot \vec{\mu}_2}{r^3}. \]  

(2.119)

The reason that this term is not included in the coupled-channel Hamiltonian is because it mixes the spin and spatial degrees of freedom making the entire calculation significantly more complicated. The common approach is to calculate its effect perturbatively since it is a small interaction compared to the molecular interactions. This has been done in the literature [47] and while I have not done it explicitly, I will outline the procedure that one would have to follow.

To first order, I will assume that the dominant dipolar interaction is due to electronic spin. In this assumption, \( \vec{\mu} \sim \mu_B \vec{s} \) so then the dipolar Hamiltonian looks like,

\[ H_{\text{dipolar}} \sim \frac{\mu_B^2 \vec{s}_1 \cdot \vec{s}_2}{r^3} \sim \frac{\mu_B^2 (S^2 - s_1^2 - s_2^2)}{2r^3}. \]  

(2.120)

Since the \( \vec{s}_1 \cdot \vec{s}_2 \) interaction is diagonal in the \( |Sm_S \rangle \) basis, this implies the selection rule that \( \Delta S = 0 \). Since the parity of the dipolar Hamiltonian is even (\( H(\vec{r}_1, \vec{r}_2) = H(-\vec{r}_1, -\vec{r}_2) \)), this implies the spatial selection rule \( \Delta l = 0, \pm 2, \pm 4, \) etc. Finally, since the dipolar Hamiltonian is central (\( H = H(|r|) \)) angular momentum must be conserved and consequently the total angular momentum projection cannot change, \( \Delta m_{\text{tot}} = \Delta m_S + \Delta m_l = 0 \) (ignoring nuclear spin 'i'). These selection rules can be summarized in table 2.1. I assume that an s-wave collision undergoing dipolar spin

<table>
<thead>
<tr>
<th>\Delta S</th>
<th>\Delta m_S</th>
<th>\Delta l</th>
<th>\Delta m_l</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 spin flip</td>
<td>0</td>
<td>±1</td>
<td>+2</td>
</tr>
<tr>
<td>2 spin flip</td>
<td>0</td>
<td>±2</td>
<td>+2</td>
</tr>
</tbody>
</table>

**Table 2.1** Dipolar selection rules.

flips will have the greatest overlap with the d-wave. While the selection rules do not rule out transitions to higher order partial waves, it seems that this will be the dominant one to consider. Of course if any spin-flip process is to occur, then the
spatial angular momentum must change ($\Delta l \neq 0$) in order to conserve total angular momentum.

To calculate this process perturbatively, I need to calculate the incoming s-wave wavefunction as well as those outgoing d-wave wavefunctions which satisfy the mentioned selection rules. Since the spin-flip will release hyperfine energy into the thermal energy of the product wavefunction, I would need to calculate the d-wave at the appropriately conserved collisional energy. The dipolar interaction could then be found,

$$\langle \psi_{\text{out}}(r) \left| \frac{\vec{s}_1 \cdot \vec{s}_2}{r^3} \right| \psi_{\text{in}}(r) \rangle ,$$

where for an s-wave, spin triplet incoming state,

$$|\psi_{\text{in}}(r)\rangle \sim |lm_1S m_s\rangle \sim |0011\rangle$$

(2.122)

$$|\psi_{\text{out}}(r)\rangle \sim |2110\rangle$$

(2.123)

or

$$\sim |221 - 1\rangle ,$$

(2.124)

the outgoing state is a d-wave with either 1 or 2 spin flips, and so both product states must be summed over. As I said earlier, I have not done the calculation but the result for the $|2222\rangle$ state of $^7$Li is known to be $10^{-14}$ cm/s [47,48]. This decay is one to two orders of magnitude larger than the dipolar loss seen in other alkalis, and consequently must be taken into account when optimizing the trajectory used to evaporatively cool $^7$Li. This is discussed in more detail in chapter 5.
Chapter 3
Lithium Potentials

Despite the complex, molecular interaction that exists between two atoms, having an ultracold gas allows this interaction to be enormously simplified. The previous chapter shows how an arsenal of math can reduce the problem to a single parameter, the S-matrix. For the case of a gas which cannot undergo spin-exchange, this problem reduces even more to a single variable, the s-wave scattering length. Being able to describe arbitrary collisions in an ultracold gas by a single, scalar number is quite powerful and allows for relatively easy modelling of the dynamics. Unfortunately, while this single number is all that you need to describe the gas, actually obtaining this number does require a full knowledge of the interatomic potential. For the case of an atomic species with various internal degrees of freedom (spin), this requires knowing the details of both the spin triplet potential as well as the singlet potential. These potentials are necessary inputs into the coupled-channel calculation of the S-matrix. I was part of a four-year study of these potentials, which have been characterized and studied in great detail through the technique of photoassociative spectroscopy [49–55]. This work has been covered in detail in previous theses [56–58]. What I hope to do in this chapter is present an overview of the work and focus the discussion on how the singlet and triplet ground state potentials have been ascertained from these experiments.

3.1 Photoassociation

Photoassociative spectroscopy of ultracold atoms was first proposed by Thorsheim et al. [59] and has quickly become one of the most powerful means of exploring the highest vibrational levels of excited diatomic molecules as well as high lying ground states. It differs from conventional bound-bound spectroscopic methods in that ex-
cited diatomic molecules are formed from free atoms. Figure 3.1 shows typical attrac-

tive ground state and excited state adiabatic potentials for a hypothetical diatomic
system composed of two identical atoms.

The ground state is asymptotic to two free, ground state atoms \((S + S)\) while
the excited molecular potential correlates to one ground state atom plus one singly
excited atom \((S+P)\). As identical excited state and ground state atoms approach each
other, their \(S\) and \(P\) characteristics mix. Finite dipole moments become associated
with each atom as a result of this mixing and can give rise to an attractive dipole-
dipole interaction that follows the functional form \(-C_3/r^3\) where \(C_3\) is a constant and
\(r\) is the internuclear separation of the atoms [56]. This is the dominant interaction
of the excited state and allows it to extend over a longer range in \(r\) than the ground state,
which is typically characterized by a shorter range \(-C_6/r^6\) van der Waals interaction
[60].
Since the excited state is long-range, the higher lying vibrational levels tend to have appreciable quantum mechanical overlap with unbound atoms colliding along the ground state potential. By tuning a laser between the scattering ground state atoms and a vibrational level in the excited state manifold, one can effectively "glue" the colliding atoms together forming a singly-excited diatomic molecule. In contrast to bound-bound state spectroscopy, photoassociative spectroscopy allows for the study of extremely excited vibrational levels which normally have poor overlap with bound states of the diatomic ground state manifold. Photoassociative spectroscopy also has the advantage of connecting observed vibrational structure with the excited state dissociation limit since the laser is usually reference to the atomic $S \leftrightarrow P$ transition.

Photoassociation of ultracold atoms also introduces other benefits. The spectral resolution of the technique is highly sensitive to the thermal distribution of the initial free state. Having ultracold atoms allows this width to be extremely small allowing for spectral resolution that is of the order of bound-bound spectroscopy. The Boltzmann constant $k_B$ has the equivalent units in frequency of 20.837 GHz/K; so a 1 mK sample of gas would have a frequency width of about 21 MHz. Advances in the fields of laser cooling and atom trapping have enabled photoassociative spectroscopy to develop into a powerful tool.

The detection of photoassociation in an ultracold atom trap has been realized through two basic methods. The first involves using photoassociation as an intermediate step in the ionization of one of the atoms. The ions produced in the ultracold atomic vapor can then be directly linked to photoassociation processes. This has been done with sodium [61–63]. The second method, one which we utilized, uses photoassociation as a means of catalyzing trap loss. Our initial studies used a magneto-optical trap (MOT) to trap ultracold samples of $^6\text{Li}$ and $^7\text{Li}$. In a MOT, atoms are confined by interacting and exchanging momentum with the trapping laser fields [23]. Since the atoms are constantly going from the ground state (S) to the excited state (P),
there is always a chance that such a transition will occur while a collision is occurring between two atoms. If two ground state atoms are close enough when one atom becomes excited, then a bound excited diatomic can be formed. The chance of this occurring is based on the collision rate, normally ultracold trapped gases are quite dilute. For example, a trap density of $10^{10}$ atoms/cm$^3$ leads to an average separation between atoms of about $9 \times 10^4 \ a_o$, where $a_o$ is the Bohr radius; the typical range of the excited state interaction shown in figure 3.1 spans hundreds of $a_o$.

Once an excited state diatomic is formed, two things can occur which lead to an observable trap loss. First, it can decay into a bound, ground state molecule which typically no longer interacts with the trap's confining laser field. Otherwise, it can decay back into two free atoms, but these atoms may have increased their kinetic energy due to the attractive nature of the excited molecular potential. Since our MOT is usually quite shallow (< 1 K), these newly accelerated atoms can typically escape the confining fields. Given this physical picture, it is clear that photoassociation leads to overall trap loss. This loss process can be induced by introducing an appropriately tuned laser ($\omega_{PA}$ in figure 3.1) which connects the free ground state atoms to a vibrational level in the excited state. The vibrational levels of the excited diatomic can then be mapped out by tuning the laser red of the excited dissociation limit and monitoring the trap loss. This is the essence of this novel spectroscopic technique.

For the lithium diatomic molecule, there are two attractive, excited molecular potentials that are asymptotic to the $2S_{1/2} + 2P_{1/2}$ free atoms and which have electronically allowed transitions to the ground states. These are shown in figure 3.2. Since there are two possible electronic manifolds to excite into, one would expect to see two distinct vibrational series using the photoassociative method outlined above. The actual apparatus is described in detail in reference [58] so I will not discuss it here. In essence, the trap loss was observed as a reduction in MOT fluorescence levels. This loss was mapped out as a function of the photoassociation laser detuning.
Figure 3.2  Molecular states of Li$_2$ which are asymptotic to two ground state atoms and one ground plus one excited state atom. Both electronic states have two manifolds which are described by a spin triplet and spin singlet interaction.
Panoramic views of the spectra are shown in figures 3.3 and 3.4. These figures show two distinct vibrational series which correspond to the spin triplet $1^3\Sigma_g^+$ and spin singlet $1^1\Sigma_u^+$ excited diatomic states.

3.2 Analysis of the First Excited States

The basis of this analysis involves the construction of model potentials for the attractive $1^3\Sigma_g^+$ and $1^1\Sigma_u^+$ excited diatomic states. Once accurate models are obtained,
Figure 3.4  Panoramic view of $^7\text{Li}_2$ one-photon photoassociation data. The laser detuning is referenced from the $2S_{1/2} \rightarrow 2P_{1/2}$ atomic transition.
a numerical integration similar to the Numerov routine discussed in chapter 2 can be used to find eigenvalues and compare with experiment. Since this work has been discussed in great detail in a previous thesis, [56], I will just touch upon the basic concepts and references.

Each potential model is comprised of three basic regions. The first involves a Rydberg-Klein-Rees (RKR) representation of the inner region of the potential surrounding the minimum (at \( r = r_{\text{min}} \)). The details of this type of analysis are discussed elsewhere [64, 65] and relies on fitting to observed spectra. As a result, this is one of the most accurate regions of the model potential. The second region of the potential involves representing the innerwall where \( r < r_{\text{min}} \) and \( V(r) \) > dissociation. Since this is in a regime where the atoms are close together, it can only be reliably treated through a full ab initio calculation. While not as accurate as the experimentally based RKR region, the atoms sample this portion of the potential for a relatively short period of time resulting in only a small error in the eigenvalue spectrum. The final region, and the most important for ultracold photoassociation, is the long-range portion of the potential \( r \gg r_{\text{min}} \). This region can be analytically modelled and has the most pronounced effect on the high-lying eigenvalue spectrum. For the excited states, \( ^1\Sigma_g^+ \) and \( ^1\Sigma_u^+ \), the dominant interaction is a resonant dipole-dipole interaction which is proportional to the dipole matrix element between the atomic ground (2S) and excited (2P) states. Both excited state potential models will be discussed in detail.

\subsection{1^3\Sigma_g^+}

In the first set of photoassociation data, the \( ^1\Sigma_g^+ \) data was the largest obtained. The analysis of this state led to our first measurement of the \( 2S \leftrightarrow 2P \) atomic transition matrix element (atomic lifetime) [49]. In the time that has followed, more data and more detailed analysis of the singlet state, \( ^1\Sigma_u^+ \), has made that state the
most accurately known. It will be discussed in the next section. The $^1\Sigma_g^+$ model has systematic uncertainties associated with it due to the fact that its middle region from $r = 8\ a_o$ to $r = 20\ a_o$ has not been experimentally measured, and so we must rely on \textit{ab initio} calculations. Figure 3.5 shows a schematic of the $^1\Sigma_g^+$ model construction.

\begin{figure}[h]
\centering
\includegraphics[width=0.7\textwidth]{potential_model.png}
\caption{$^1\Sigma_g^+$ potential model construction.}
\end{figure}

The RKR region is taken from the work of Linton \textit{et al.} who used Fourier transform spectroscopy of the $^1\Sigma_g^+$ - $^3\Sigma_u^+$ transition of Li$_2$ [66]. The data that was used in this analysis corresponded to observed vibrational levels $v = 0 - 7$ in the $^1\Sigma_g^+$ manifold. Taking the results from both isotopes, this gives a total of 33 discrete points which describe the model in this region. The main parameter in this region is $D_e$, the dissociation energy which is used to reference the RKR points to the long-range asymptote.

The \textit{ab initio} region was studied in detail since there are two primary sources that can be used. The work of Schmidt-Mink \textit{et al.} [67] is considered to be a standard and
was used during the initial analysis. The calculated potentials of Schmidt-Mink et al. (SM) for the $1^3\Sigma_g^+$ and $1^1\Sigma_u^+$ molecular states produce the best comparison with spectroscopically known constants. The work of Konowalow et al. [68–71] presents two different \textit{ab initio} calculations with expected errors of opposite sign. An average of these respective potentials forms a \textit{composite} potential (KC) which is expected to be a reasonable approximation to the true $1^3\Sigma_g^+$ and $1^1\Sigma_u^+$ states [71]. We have found that the KC potentials tend to give a better fit to the long-range data than the SM potentials. Both sets of \textit{ab initio} values were used to get estimates of the error involved in this part of the potential. This is discussed in detail in [56]. The main source of error is the middle region from $r = 8 \ a_o$ to $20 \ a_o$. Starting with the KC values, I adjust this region by a polynomial form, $V(r) \to V(r) \times [1 + A + B/r + C/r^3]$ where the parameters $A$, $B$, and $C$ are adjusted to yield the best fit to our photoassociation data. This is discussed in appendix G.

The final region consists of the long-range portion of the potential which can be analytically represented as a function of $r$. In this regime, the molecular interaction can be well understood and characterized. As stated earlier, the dominant term is a dipolar interaction of the form $V(r) \sim -C_3/r^3$. There are higher order terms which represent the various van der Waals interactions and these are also included. The full form of the potential at long range looks like,

$$ V(r) = \frac{C_3}{r^3} - \frac{C_6}{r^6} - \frac{C_8}{r^8} + FS, \tag{3.1} $$

where $C_6$ and $C_8$ are the van der Waals terms [60] and ‘FS’ represents corrections to the potential due to fine structure interactions. The fine structure mixes the singlet and triplet potentials at long range resulting in Hund’s case (c) basis states [72]. Specifically, the $1^3\Sigma_g^+$ triplet state correlates to either a $1_g$ or $O_g^-$ Hund’s case (c) state. Both states are a function of the dominant $C_3$ coefficient as well as the fine-structure energy splitting. This work has been covered in detail in [72] as well as [56]. The analytic form of the $1^3\Sigma_g^+$ is splined into the $0_g^-$ potential at long range, but this
is not entirely accurate since the observed data will be a mixture of $0_g^-$ and $1_g$. The slight change in the eigenvalue spectrum depending on whether the $1_g$ or $O_g^-$ state is used represents the uncertainty associated with fine-structure mixing of the triplet $1^3\Sigma_g^+$ state.

Armed with all this information, the eigenvalue spectrum of the $1^3\Sigma_g^+$ model potential can be calculated and compared to the photoassociation data. The parameters that are adjusted in this fit include $C_3$, $C_6$, $D_e$, as well as the changes to the ab initio regions and the very-long range fine-structure mixing. The effect of all these uncertainties is tabulated in my previous thesis [56]. A working model of the potential with binding energies is presented in appendix G for both isotopes. Recently work in the lab has extended the range of observed binding energies deeper into the well; level $v = 58$ for $^7\text{Li}_2$ has been seen and has a classical turning point at 27 $a_o$. Unfortunately, until a better mapping of the middle region 8 $a_o$ to 20 $a_o$ is available, the ab initio of this region will be the major source of error in the model eigenvalue spectrum.

3.2.2 $1^1\Sigma_u^+$

Following the work done in 1995, more data was obtained for the $1^1\Sigma_u^+$ state as well as more RKR information making this excited state the most accurately known of the two. We found that the $1^1\Sigma_u^+$ vibrational series goes through a node in its transition strength and then re-occurs at much deeper binding energies [54]. In fact, the location of this node is related to a node in the singlet projection of the ground state scattering wavefunction. This node position can be used to ascertain information about the singlet scattering length, this is discussed later on in this chapter. Since the excited singlet data extends to deeper binding energies than the triplet data, this presents two advantages. First, the high-lying levels that are observed now "overlap" with the deeper levels that make up the RKR portion of the potential; this enables
us to eliminate the middle \textit{ab initio} region which was a major source of error in the $1^3\Sigma_u^+$ analysis. Second, since we have a better measure of the $C_3$ coefficient by having more data, this also enabled us to get a far more precise measure of the atomic dipole matrix element and consequently the atomic lifetime. Figure 3.6 shows a schematic of the $1^1\Sigma_u^+$ model construction.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure3_6.png}
\caption{$1^1\Sigma_u^+$ potential model construction.}
\end{figure}

The RKR region of the $1^1\Sigma_u^+$ potential model is taken from the revised work of Linton \textit{et al.} \cite{73}. The RKR potential covers the range of internuclear separation from $r = 3.8 \ a_o$ to $r = 97.3 \ a_o$. This corresponds to vibrational levels $v = 0$ to $v = 84$. In analyzing our data, we elected to use those points up to $r = 25.4 \ a_o$, which encompass the energy range from the bottom of the well up to our lowest-lying observed vibrational level. This RKR potential is assumed to be the best possible representation of the inner portion of the potential with the only parameter being $D_0$, the dissociation energy, which locates the bottom of the RKR well with respect to the asymptotic $2S_{1/2} + 2P_{1/2}$ limit. Since the publication of our work, the group of Linton
et al. have revised their analysis of the $1^1\Sigma_u^+$ state of $^6\text{Li}_2$ [74]. They incorporate our photoassociation data as well as a more complete treatment of the Hund’s case (c) long range basis.

The ab initio portion of the model is minimal. Two points from the work of Schmidt-Mink el al are used at $r = 3.25 \ a_o$ and $r = 3.50 \ a_o$ [67]. Other ab initio values were used to check for uncertainties, but the effect of this portion of the model on the calculated eigenvalue spectrum was small [52].

The long-range analytic form of the $1^1\Sigma_u^+$ potential shares the same basic form as that of the $1^3\Sigma_g^+$ but more complexity has been added since the photoassociation data is more precise. The full form of the potential is dominated by the dipolar $C_3$ term just as the $1^3\Sigma_g^+$:

$$V(r) = -\frac{C_3}{r^3} - \frac{C_6}{r^6} - \frac{C_8}{r^8} + \text{FS} + \langle T_{\text{nuc}} \rangle ,$$

(3.2)

where $C_6$ and $C_8$ are the van der Waals terms, ‘FS’ is a fine-structure correction, and $\langle T_{\text{nuc}} \rangle$ is the first order correction to the Born-Oppenheimer approximation [75]. The fine structure mixes the singlet and triplet potentials, but it turns out that the $1^1\Sigma_u^+$ manifold correlates to a single Hund’s case (c) state, the $0_u^+$ [72].

The Born-Oppenheimer correction has three terms,

$$\langle T_{\text{nuc}} \rangle = Q(r) + P(r) + S(r) ,$$

(3.3)

where,

$$Q(r) = -\frac{\hbar^2}{2\mu} \left\langle \frac{\partial^2}{\partial r^2} \right\rangle$$

(3.4)

$$P(r) = \frac{\hbar^2}{2\mu r^2} \left\langle L_x^2 + L_y^2 \right\rangle$$

(3.5)

$$S(r) = -\frac{\hbar^2}{8\mu} \left[ \left\langle \sum_i \nabla_i^2 \right\rangle + \left\langle \sum_{i \neq j} \nabla_i \nabla_j \right\rangle \right] .$$

(3.6)

The internuclear axis defines the $z$-axis, $L_x$ and $L_y$ are the corresponding projections of the total electronic orbital angular momentum, the individual electrons making
up the molecule are indexed by \( i \) and \( j \), and the reduced mass of the system is
given by \( \mu \). The \( \langle \rangle \) brackets indicate expectation values taken over the electronic
wavefunctions. The details of these various terms are described in [52]. The terms
which are important in the long-range basis are \( P(r) \) and \( S(r) \). The term \( P(r) \) goes
as,
\[
P(r) \approx \frac{\hbar^2}{2\mu r^2} \left[ l_s(l_s + 1) + l_p(l_p + 1) \right] = \frac{2\hbar^2}{2\mu r^2},
\]
where \( l_s = 0 \) and \( l_p = 1 \) are the orbital angular momenta of the atomic electrons.
The term \( S(r) \) goes as,
\[
S(r) \approx \frac{m_e}{4\mu} \langle T_e \rangle = \frac{m_e}{4\mu} \left[-V(r) - r \frac{\partial}{\partial r} V(r) \right],
\]
where \( m_e \) is the electron mass and the Virial theorem has been used to expressed the
average electronic kinetic energy \( \langle T_e \rangle \) as a function of the adiabatic potential \( V(r) \).
A Numerov-Cooley algorithm is used to compute the eigenvalue spectrum of the \( 1^1\Sigma_u^+ \)
model potential. This model is a function of \( C_3 \), \( C_6 \), and \( D_\infty \). A working model of
this potential with binding energies is also presented in appendix G for each isotope.

### 3.2.3 Radiative Lifetime and Radiation Retardation in the \( 1^1\Sigma_u^+ \)

The \( 1^1\Sigma_u^+ \) photoassociation data allowed us to construct and fit a model where
\( C_3 \) could be found to unprecedented precision. This is the result of the large amount
of RKR data available [73], the large amount of vibrational spectra at long-range
which we observed [52, 54], and the molecular hyperfine analysis which allowed the
center-of-gravity of each line to be found to high accuracy [53]. This work is extensive
and is discussed in detail in references [52, 58] so I will not go into too much detail
here.

The \( C_3 \) coefficient is directly related to the atomic dipole matrix element, and so
is related to the atomic lifetime. The relation is,
\[
C_3 = \frac{3\hbar}{2\tau} \left( \frac{\lambda}{2\pi} \right)^3,
\]
(3.9)
where \( \tau \) is the 2P atomic radiative lifetime and \( \lambda \) is the wavelength of the atomic transition. Atomic radiative lifetimes are known to be sensitive tests of atomic-structure calculations. The relatively simple structure of atomic lithium makes it a viable candidate for testing the various \textit{ab initio} techniques which, in recent years, have grown in both sophistication and accuracy [76–83]. Experimentally, prior to this work, the most precisely-stated measurement of this lifetime was by Gaupp \textit{et al.} [84]. This result and the theory disagreed by more than four standard deviations. Our work was able to resolve this discrepancy, we find the 2P_{1/2} radiative lifetime of \textsuperscript{7}Li to be 27.102(2)(7) ns [52]. The first uncertainty corresponds to one statistical standard deviation, while the second represents the systematic uncertainty. The revised RKR potential by Linton \textit{et al.}, that was modified in light of our data, reports a radiative lifetime which agrees with our number [74].

At the current level of precision, radiation retardation effects in the long-range portion of the potential become important and must be accounted for. An exact quantum electrodynamic expression for this effect has been obtained for the case of a \( S + P \) resonance without spin [86,87]. This treatment was incorporated into the \( 1^1\Sigma_u^+ \) analysis. The \( C_3 \) term was multiplied by an \( r \)-dependent term, \( C_3 \rightarrow C_3 \alpha(r) \), where

\[
\alpha(r) = \cos\left(\frac{2\pi r}{\lambda}\right) + \left(\frac{2\pi r}{\lambda}\right) \sin\left(\frac{2\pi r}{\lambda}\right),
\]

and \( \lambda \) is the wavelength of the 2S \( \leftrightarrow \) 2P transition. The effect of whether this term is included in the long-range analytic form of the \( 1^1\Sigma_u^+ \) potential model is shown in figure 3.8. This was the first time that radiative retardation in the force between two atoms was observed, an effect which was simultaneously seen by a group at NIST with Na [88].
Figure 3.7  Comparison of the recent measurements and some theoretical calculations of the Li $2P_{1/2}$ radiative lifetime. Experiments are from references [49, 52, 73, 84, 85] and theory are references [76–83]. The errors bars given for Gaupp et al. and Carlsson et al. correspond to one standard deviation. Linton et al. report a value for $C_3$ from their 1996 work [73] which we have converted to the lifetime value shown; the error bar represents their estimate of the uncertainty taken from the quality of their fit. The error bar for our previous work with the $1^3\Sigma_g^+$ state represents an estimated systematic error. For the present result, the error bar is a combination of a one standard deviation statistical uncertainty and the systematic uncertainty.
Figure 3.8  Radiation retardation effects in the fit to the $1^1\Sigma_u^+$ photoassociation spectrum. Residuals from the fit are shown.
3.3 Analysis of the Ground States

Similar to the excited state analysis, we make use of photoassociation data to help in the construction of accurate models of the ground state potential interactions. Once the ground state potentials are known, then the coupled-channel calculation from chapter 2 can be used to derive the appropriate S-matrix and scattering parameters for any type of low-energy, ground state collision in the lithium system. This relies on knowing both the ground state triplet and singlet potentials. The triplet potentials were obtained by extending the technique of photoassociation to two-photon transitions [50]. The singlet potentials were obtained by using the coupled-channel treatment to model the node seen in the one-photon singlet photoassociation spectra and relating this to the ground-state scattering wavefunction [54, 55]. Both these techniques will be discussed in the following sections.

3.3.1 \( a^3\Sigma_u^+ \) State

Construction of the triplet ground state potentials are facilitated by locating the highest-lying bound state in the \( a^3\Sigma_u^+ \) potential using two-photon photoassociation. In two-photon photoassociation, a second laser is introduced which causes an excited diatomic (from one-photon photoassociation) to undergo a transition to a bound, ground state molecule. The process is illustrated in figure 3.9. This was carried out in a magneto-optical trap and has been discussed in previous papers [50, 55, 58]. The normal photoassociation laser, \( \omega_{P,1} \), is tuned to an excited vibrational level which has appreciable overlap with the bound ground state molecule. The bound-bound laser, \( \omega_{BB} \), is introduced to drive this transition. Without the bound-bound laser, normal photoassociative loss is seen in the trap. When the bound-bound laser is introduced and tuned to the correct frequency, the bound-bound laser will shift the energy of the free-bound transition (Autler-Townes effect) causing fewer atoms to photoassociate. This has the observable effect of reducing the loss seen by the single photon transition.
Figure 3.9  Two-photon photoassociation.
In practice, as the difference frequency between the two lasers becomes equal to the binding energy of a ground-state vibrational level, we see the loss in the MOT reduced and the fluorescence level increases. This two-photon resonance was seen in both $^7$Li$_2$ and $^6$Li$_2$ [50, 55]. Figures 3.10 and 3.11 show this resonance and the observed binding energy.

As with the excited state potentials, an accurate model of the $a^3\Sigma_u^+$ potential can be constructed and adjusted so that its eigenvalue spectrum fits to this observed binding energy. The model has the same form as has been discussed previously and is diagrammed in figure 3.12. The inner portion of the potential surrounding the minimum is constructed from dense RKR points that are reported in reference [89]. These points span the range from $r = 6.4 \ a_0$ to $r = 17.5 \ a_0$. The inner wall is constructed from an OVC ab initio calculation [71] and spans $r = 3.0 \ a_0$ to $r = 6.0 \ a_0$. The analytic form of the potential beyond the RKR region has the form,

$$V(r) = -\frac{C_6}{r^6} - \frac{C_8}{r^8} - \frac{C_{10}}{r^{10}} + V_{\text{exc}}(r), \quad (3.11)$$

where the dispersion coefficients can be found in reference [90] and the exchange portion, $V_{\text{exc}}$, is discussed in [91]. This exchange piece has the form,

$$V_{\text{exc}}(r) = \gamma r^\alpha \exp(-\beta r), \quad (3.12)$$

where the coefficients were found to be,

$$\alpha = 4.558 \quad (3.13)$$

$$\beta = 1.259 \quad (3.14)$$

$$\gamma = 0.01288. \quad (3.15)$$

The dominant parameter in this model is the dissociation energy, $D_e$, which is used to reference the RKR portion of the model to the long-range asymptote. The effect of using different ab initio calculations was studied and used to help estimate the
Figure 3.10 Two-photon photoassociation resonance in $^7$Li$_2$. (a) One-photon photoassociation of the $v = 64$ vibrational level of the $1^3\Sigma_g^+$ of $^7$Li$_2$. The frequency is relative to the $2S_{1/2} - 2P_{1/2}$ atomic transition frequency. The structure is due to the hyperfine interaction. (b) Two-photon photoassociation of the $v = 10$ vibrational level of the $a^3\Sigma_u^+$ state. The baseline corresponds to the reduction of the fluorescence level due to the photoassociation laser beam. As $\omega_{BB}$ is tuned over the bound-bound transition frequency, the rate of photoassociative loss is reduced, thereby increasing the trap-laser-induced fluorescence. The observed binding energy of the $v = 10$ level is $12.47 \pm 0.04$ GHz.
Figure 3.11  Two-photon photoassociation resonance in $^6$Li$_2$. (a) One-photon photoassociation of the $v = 59$, $N = 1$ vibrational level of the $1^3\Sigma^+_y$ state of $^6$Li$_2$. The trap laser-induced fluorescence, scaled to its value in the absence of photoassociation, is plotted versus $\omega_{PA}$. The initial- and intermediate-state quantum numbers of the states involved in the transitions are indicated by the notation $|N f_1 f_2 G\rangle \rightarrow |NSIG\rangle$, where $G$ is the sum of all spin angular momentum ($f_1 + f_2$ or $S + I$). The $v = 59$, $N = 1$ vibrational level has a binding energy of 1787 GHz and an outer turning point of 35 $a_o$. (b) Two-photon photoassociation of the $v = 9$, $N = 0$ vibrational level of the $a^3\Sigma^+_u$ state of $^6$Li$_2$. The quantum numbers of the final state are $|NSIG\rangle = |0111\rangle$. The photoassociation laser frequency $\omega_{PA}$ is fixed on the peak of the one-photon spectra while a second laser of frequency $\omega_{BB}$ is tuned. The observed binding energy of the $v = 9$ level is $24.43 \pm 0.02$ GHz.
uncertainty in $D_e$. For each set of data, $^6\text{Li}_2$ and $^7\text{Li}_2$, $D_e$ was adjusted to find a model which matched the observed binding energies ($v = 9$ for $^6\text{Li}_2$ and $v = 10$ for $^7\text{Li}_2$). The resulting models and eigenvalue spectrum are tabulated in appendix G.

Recently, the group of Linton et al. have measured vibrational levels $v = 0$ to $v = 9$ in the $a^3\Sigma_u^+$ state of $^7\text{Li}_2$ using a perturbation-facilitated optical-optical double resonance (PFOODR) scheme [92]. Their previous work [66], which is the basis of the dense RKR of Zemke and Stwalley [89], measured levels $v = 0$ to $v = 7$. The new spectroscopy has enabled them to reconstruct a better RKR curve which they discuss in reference [92]. They were unable to observe the $v = 10$ level which would have enabled them to completely determine the potential and the dissociation energy. Instead, they use our measurement to extrapolate the RKR curve. They report a dissociation energy of $333.69 \pm 0.10 \text{ cm}^{-1}$ which agrees with our result of $333.78 \pm 0.20 \text{ cm}^{-1}$. However, their new RKR potential predicts a $v = 10$ binding energy of $11.81 \text{ GHz}$ as opposed to our measured value of $12.47 \pm 0.04 \text{ GHz}$. This
indicates that the RKR curve is not the best match to our data. By increasing the
dissociation energy of their RKR curve, we could get a better match to the observed
\( v = 10 \) and our reported \( D_e \). A change of \( \sim 0.02 \) cm\(^{-1} \) in \( D_e \) will change the \( v = 10 \) binding energy by \( \sim 0.04 \) GHz. This indicates a total needed change of \( \sim 0.3 \) cm\(^{-1} \) in \( D_e \) for the new RKR curve which is still within the range we report.

Since the time the two-photon photoassociation data for \( ^7\)Li\(_2\) has been published,
a new measurement of the \( v = 10 \) binding energy has been made using a quantum
degenerate gas [93]. The preliminary result gives \( 12420.161 \pm 0.005 \) MHz; the effect
of this number on the scattering length extraction is discussed in section 3.3.3.

### 3.3.2 \( X^1\Sigma^+_g \) State

The potential model for the \( X^1\Sigma^+_g \) state was found indirectly by analyzing the node
seen in the one-photon singlet photoassociation transition strength. This minimum
results from a node that exists in the ground-state scattering wavefunction. Since
the ground-state wavefunction for two colliding atoms is a combination of singlet
and triplet interactions, this analysis required using the triplet \( a^3\Sigma^+_u \) model which
was obtained through two-photon photoassociation. Having assumed that the triplet
potential is known, a coupled-channel wavefunction, \( \psi_{gnd} \), for the scattering state was
calculated as a function of the singlet potential. This wavefunction was normalized
such that its amplitude was equal to one in the asymptotic limit. Wavefunctions
for the various bound states in the excited \( 1^1\Sigma^+_u \) state were then calculated and
normalized such that

\[
\int \psi_{exc}^* \psi_{exc} \, dr = 1. \tag{3.16}
\]

Then the Frank-Condon overlap was calculated between the singlet projection of the
ground-state wavefunction and the singlet excited state wavefunction,

\[
\text{Frank Condon} = \left| \int \psi_{exc} P_S \psi_{gnd} \, dr \right|^2, \tag{3.17}
\]
where $P_S$ is the singlet projection operator (see appendix B). The excited state wavefunction, $\psi_{\text{exc}}$, is always real-valued while $P_S\psi_{\text{gnd}}$ is complex. Since the electronic dipole moment should be constant over the energy scale of the various bound states observed in the singlet photoassociation spectra, this overlap probability can be directly compared with the relative transition strengths that were observed.

We observed nodes in the singlet photoassociation spectra for both $^7\text{Li}_2$ and $^6\text{Li}_2$ [54]. The data is shown in figures 3.13 and 3.14 as a function of the vibrational quantum number of the excited state. The data for $^6\text{Li}_2$ was averaged over all the

![Graph showing photoassociation signal vs vibrational level for $^6\text{Li}_2$](image)

**Figure 3.13** Node observed in singlet photoassociation spectra for $^6\text{Li}_2$. The binding energies vary from 220 GHz for $v = 79$ to 3.5 THz for $v = 62$. The photoassociation signal is the fractional decrease in the observed fluorescence due to the presence of the photoassociation laser on a photoassociation resonance. The solid line is a polynomial fit used to help identify the node.

hypersensitive features and so represents an average transition strength from all possible collisional channels, this was taken into account in the analysis. The data for $^7\text{Li}_2$
Figure 3.14  Node observed in singlet photoassociation spectra for $^7$Li$_2$. (a) Spectrum of the $v = 81, N = 1$ level of the $1^1\Sigma_u^+$ state of $^7$Li$_2$. Three features, separated by the atomic ground-state hyperfine splitting, are observed corresponding to collisions with both atoms having $f = 2$, one atom with $f = 1$ and the other with $f = 2$, and both atoms having $f = 1$. The fluorescence is given in arbitrary units. (b) Photoassociation signals for each hyperfine feature of each vibrational level of the $1^1\Sigma_u^+$ state of $^7$Li$_2$. The lines are a polynomial fit to the data to help identify the node for each hyperfine series. The resulting minimum in the photoassociation signal occurs at a different location for the different collision channels.
was able to distinguish slightly different node positions for various collisions involving channels with \( |f_1 f_2| = |22\), \( |21\), or \( |11\) (here \( f \) labels the total angular momentum in the zero magnetic field limit). These different channel possibilities were calculated in the Frank-Condon overlap (with appropriate averaging of the \( m_f \)'s).

The model potential for the singlet \( X^1\Sigma_g^+ \) interaction is constructed from various sources in a similar fashion to the other models. A schematic of this construction is shown in figure 3.15. The RKR portion of the potential comes from the work of Barakat \textit{et al.} [94] and covers the range from \( r = 3.4 \ a_0 \) to \( r = 23.9 \ a_0 \). The dissociation energy, \( D_e \), which is used to reference the RKR data to the asymptotic limit is the only parameter and is adjusted to fit the calculated Frank-Condon factors with the observed nodes seen in the singlet spectra for either isotope. The inner wall of the model is made up of three \textit{ab initio} points, two at \( r = 2.75 \ a_0 \) and \( r = 3.00 \ a_0 \) from reference [69], and one at \( r = 3.25 \ a_0 \) from reference [67]. The analytic portion of the \( X^1\Sigma_g^+ \) model is identical to the triplet \( a^3\Sigma_u^+ \) ground state with the exception of

![Graph showing the \( X^1\Sigma_g^+ \) potential model.](image)

**Figure 3.15** Schematic of the \( X^1\Sigma_g^+ \) potential model.
the sign of the exchange term [91]. The form looks like,

\[ V(r) = -\frac{C_6}{r^6} - \frac{C_8}{r^8} - \frac{C_{10}}{r^{10}} - V_{\text{exc}} , \]

where the exchange term looks like,

\[ V_{\text{exc}}(r) = \gamma r^\alpha \exp(-\beta r) , \]

and,

\[ \alpha = 4.558 \]
\[ \beta = 1.259 \]
\[ \gamma = 0.01288 . \]

The dispersion coefficients, \( C_6, C_8, \) and \( C_{10} \) can be found in reference [90]. A working model of the \( X^1\Sigma_g^+ \) potential can be found in appendix G with the appropriate value of \( D_e \) needed to fit to either isotope. The fits to the observed nodes are shown in figures 3.16 and 3.17.

### 3.3.3 Scattering Lengths

Now that the ground state potentials for \( \text{Li}_2 \) have been accurately determined, I want to finish out this chapter by reporting the appropriate scattering lengths and dissociation energies for the \( a^3\Sigma_u^+ \) and \( X^1\Sigma_g^+ \) states for each possible isotope. The reported uncertainties take into account both experimental uncertainty in the photoassociation data as well as systematic uncertainties in the model potentials. In order to determine the mixed isotope properties (\( ^6\text{Li} + ^7\text{Li} \)), I took the average of the dissociation energies found for the pure isotopes and calculated the scattering lengths with the appropriate reduced mass.

The new \( \nu = 10 \) measurement (reference [93]) of the \( ^7\text{Li}_2 \ a^3\Sigma_u^+ \) does not significantly change the results presented. While the measurement of the binding energy is
Figure 3.16  Fit to the node observed in the $^6$Li$_2$ singlet photoassociation spectra. The calculated Frank-Condon factor is shown as a function of vibrational level. The calculation was carried out for three different values of dissociation energy, $D_e$, for the singlet potential. The region of the observed node is indicated showing the level to which $D_e$ can be obtained. We found that a $D_e = 8516.70$ cm$^{-1}$ gives the best fit.
Figure 3.17  Fit to the node observed in the $^7$Li$_2$ singlet photoassociation spectra. (a) Shows the result of the Frank-Condon calculation for the three different collisional channels observed (averaged over $m_f$). (b) Shows the behavior of the nodes for each channel as a function of the dissociation energy, $D_e$, of the singlet potential used in the calculation. The observed nodes from the $^7$Li$_2$ spectra are indicated. The $|f_1,f_2\rangle = |11\rangle$ channel has the highest precision and was therefore given the most weight in the fit. We found that a $D_e = 8516.75$ cm$^{-1}$ gives the best fit.
almost 4 orders of magnitude better, the scattering length would still vary by ±0.03 \( a_o \) due to the uncertainty in the innerwall \textit{ab initio} points. This is a factor of 16 improvement in the uncertainty of \( a_T \) and would make the scattering length closer to \(-27.02 \pm 0.03 \ a_o \). The value of the extracted dissociation energy \( D_e \) is already limited by the \textit{ab initio} uncertainty and would not change given the new measurement.

\[
\begin{array}{c|ccc}
\hline
& ^6\text{Li}+^6\text{Li} & ^7\text{Li}+^7\text{Li} & ^6\text{Li}+^7\text{Li} \\
\hline
a_T & -2160 \pm 250 & -27.6 \pm 0.5 & 40.9 \pm 0.2 \\
a_S & 45.5 \pm 2.5 & 33 \pm 2 & -20 \pm 10 \\
\hline
\end{array}
\]

\textbf{Table 3.1} Singlet and triplet scattering lengths, in units of Bohr (\( a_o \)), for various isotopes of Li.

\[
\begin{array}{c|ccc}
\hline
& ^6\text{Li}_2 & ^7\text{Li}_2 & ^6\text{Li}^7\text{Li} \\
\hline
a^3\Sigma^+_u & 333.74 \pm 0.2 & 333.78 \pm 0.2 & 333.76 \pm 0.2 \\
X^1\Sigma^+_g & 8516.70 \pm 0.10 & 8516.75 \pm 0.10 & 8516.73 \pm 0.10 \\
\hline
\end{array}
\]

\textbf{Table 3.2} Dissociation energies for the ground molecular states of lithium. Values are given in units of cm\(^{-1}\).
Chapter 4
Electromagnetic Trap Design

Much of our previous work with lithium and photoassociation suggests a number of interesting experiments that could be carried out in a suitable magnetic trap. For the past two years, I have been part of an effort to develop an electromagnetic trap which will be used to investigate the collisional properties of ultracold lithium. Specifically, we are interested in finding ways to measure the large resonant scattering length in the $a^3\Sigma_u^+$ potential of $^6$Li with the ultimate goal of observing BCS pairing of an ultracold, trapped gas of $^6$Li [19]. Since our electromagnetic trap has an adjustable bias field, we can study various collisional properties of a trapped gas as a function of magnetic field. This allows for the study of Feshbach resonances, some of which have been discussed in chapter 2. Also, by operating at sufficiently low magnetic field we can trap certain spin states of Li which are normally high-field seeking (untrapped) at larger field values. For $^6$Li at $B < 27$ G, the $|f m_f\rangle = |1/2 - 1/2\rangle$ state can be trapped. For the case of $^7$Li at $B < 127$ G, the $|1 - 1\rangle$ state is trapped and actually has a positive scattering length of $5 a_o$ at the low field limit (see appendix F). This is significant because it suggests that this spin state could be Bose-condensed and would be stable to density fluctuations, unlike the stretched state ($|2 2\rangle$) where the condensate number is severely limited due to attractive interactions [95]. Given the number of interesting experiments on the horizon, it seems appropriate to discuss the major features of the new trap and how it has been designed to achieve these goals.

4.1 Overview

The purpose of this apparatus is to ultimately observe BCS-pairing in an ultracold gas of $^6$Li. There are difficulties in achieving this due to the Fermi statistics associated with $^6$Li. Ideally one would like to trap $^6$Li in its stretched state, $|f m_f\rangle = |3/2 \ 3/2\rangle$,,
where the trap confinement is the tightest. Unfortunately, by having all the atoms in the same state, no s-wave collisions can occur (see chapter 2). This restriction prevents evaporative cooling from working. In order to circumvent this, two proposals were considered. In the first case, one could imagine having two different trapped spin states, for example the $|3/2 \ 3/2\rangle$ and the $|3/2 \ 1/2\rangle$, where s-wave collisions are allowed between the two spin species in the $|\{3/2 \ 3/2, \ 3/2 \ 1/2\}\rangle$ channel. This is the technique that was used to evaporatively cool $^{40}$K to Fermi degeneracy [17]. It turns out that this cannot work for $^6$Li because there is a large spin exchange rate which causes the channel to decay to the $|\{3/2 \ 3/2, \ 1/2 \ 1/2\}\rangle$ channel (see appendix F). This decay effectively flips the spin state of the $m_f = 1/2$ atom causing a release of hyperfine energy which ejects both atoms from the trap. The rate for this is of order $10^{-9}$ cm$^3$/s which makes the lifetime of the trap far too short for any kind of evaporative cooling.

The second means of cooling the fermion is to use sympathetic cooling. In this technique, we plan to trap both fermionic $^6$Li as well as bosonic $^7$Li. Both atoms will be in their respective stretched states allowing for maximum confinement in the magnetic trap. Even though collisions between the $^6$Li atoms are forbidden, they are not restricted between $^6$Li and $^7$Li; the scattering length for this collision is $40.9 \ a_0$ ($|\{3/2 \ 3/2, \ 2 \ 2\}\rangle$ channel) [55]. Since this is a stretched channel, there is no spin-exchange decay that would limit the trap lifetime. We could also use the $|\{1/2 \ -1/2, \ 1 \ -1\}\rangle$ channel which is trapped below 27 G and does not undergo spin-exchange. Its scattering length in low magnetic field is $\sim 39 \ a_0$, but the trap confinement is reduced by a factor of 8 since the effective magnetic moment of these states is $1/2 \ \mu_B$. This severe limitation makes the stretched states much more appealing for initial evaporation, however, once degeneracy is obtained there is a problem. In the degenerate regime, the $^7$Li will Bose condense and become unstable since the $|\{2 \ 2, \ 2 \ 2\}\rangle$ channel is attractive [96, 97]. This effectively limits the obtainable tem-
perature $T$ to just around the critical temperature $T_c$ and prevents obtaining $T \ll T_c$ which is needed for BCS pairing. If we start evaporation with $^6$Li and $^7$Li in the stretched states, we will need to change the spin states at or before degeneracy to avoid this problem. The $\{|1 - 1, 1 - 1\}$ channel has a positive scattering length of 5 a$_0$ which would allow for $T \ll T_c$.

For sympathetic cooling, we plan to load a large amount of $^7$Li and a smaller amount of $^6$Li. The $^7$Li can be cooled by normal evaporative cooling while relying on sympathetic elastic collisions between the two isotopes to cool the $^6$Li. With this in mind, we have designed the apparatus and electromagnetic trap to handle dual isotopes. Figure 4.1 shows a schematic of the apparatus.

![Overall schematic of the EMTRAP apparatus.](image)

**Figure 4.1** Overall schematic of the EMTRAP apparatus.

The main feature that should be pointed out are the two atomic sources, one for each isotope. The $^7$Li source uses a laser slowed atomic beam of high flux. The $^6$Li source has lower load requirements and so relies on a laserless slow atom source based on magnetic guiding. Both these sources will be discussed in detail later on. The main chamber possesses re-entrant windows which allow the electromagnetic coils to be close together, $\sim 3$ cm. This allows for the high field gradients which are necessary for trapping. In order to minimize trap loss due to background gas collisions, an ultrahigh vacuum must be maintained at pressures $< 10^{-11}$ torr. The main chamber is pumped by a Varian 230 l/s ion pump followed by a titanium sublimation pump. The
source chambers are pumped by Pfeiffer turbo-molecular pumps. Additional pumping is provided along the Zeeman-slowed atomic beam path in order to help remove hot atoms.

4.2 Zeeman Slowed Source

The $^7$Li source starts with a re-circulating oven in which $^7$Li metal is heated to about 550°F C. A thin tube connects the oven to the vacuum system allowing for a collimated beam of atoms to emerge and travel towards the trapping region. Part of the velocity distribution is slowed by exposing the beam to a counter-propagating laser beam tuned about 1.25 GHz red of the atomic transition $(2S, F = 2) \leftrightarrow 2P_{3/2}$ to make up for the Doppler shift of the moving atoms. In addition, an electro-optic modulator is used to add an additional 804 MHz sideband to the beam so that atoms which are pumped into the $(2S, F = 1)$ ground state are repumped back into the cooling cycle. Atoms travelling at $\sim 500$ m/s out of the oven come into resonance with the Doppler-shifted laser beam and absorb photons. As they slow down, they enter the interior of a tapered solenoid which Zeeman shifts the atomic transition in such a way as to compensate for the changing Doppler shift of the laser. The technique of Zeeman slowing has been discussed in previous publications [98] and theses [56, 99]; this particular slower and its construction is discussed in references [100, 101]. In the end, about 1% of the atomic beam with velocity $< 500$ m/s is slowed to about 50 m/s, a velocity within the capture range of a magneto-optical trap. The $^7$Li source is able to load optimally $\sim 5 \times 10^{10}$ atoms into a magneto-optical trap in about 5 seconds.

The atomic beam passes about 1 cm below the trapping region. Those background atoms which are not slowed, continue through the region and are either captured by non-evaporative getters (SAES Getter St-707) which line the vacuum system beyond the trap region, or are pumped by a 30 l/s Varian Star-Cell ion pump. The window through which the Zeeman slowing beam passes is made of sapphire and is heated
to about 245° C to prevent lithium from coating the surface. Since the window introduces significant birefringence to the beam, we use a half-wave and quarter-wave plate to compensate for the effect.

To further aid in loading efficiency, a two-dimension magneto-optical trap is located at the exit of the Zeeman slower. This device helps to transversely cool and collimate the atomic beam as well as steer the slow atoms into the trap region. Since the thermal beam passes below the trapping region, a slight tilt in the vertical alignment of the 2D-MOT is needed to guide the atoms into the center. Re-entrant

![Diagram](image)

**Figure 4.2** 2D-MOT for Zeeman beam collimation.

windows contain the necessary anti-Helmholtz coils which are capable of providing an axial magnetic field gradient of about 30 G/cm with a current of 1 A. We usually run the coils around this value, but the exact value seems strongly coupled to other run conditions and must be continually adjusted to peak the MOT performance. The 2D-MOT is split off from the main MOT beams and so has two frequencies, one for trapping (driving \( f = 2 \) atoms) and one for repumping (driving \( f = 1 \) atoms). The power ratio and frequency splitting of these two components are described in the optics set-up towards the end of this chapter. The 2D-MOT operates at a detuning of about -36 MHz (-6 \( \Gamma \)) for the trapping frequency with a total beam power of 12 mW (including all frequencies). Despite using a spatial filter, the beam profile is not Gaussian and so it is difficult to define a quantitative waist to the beam. The beam size is chosen so as to fill the full aperture of the re-entrant windows of the
2D-MOT (about 1 cm diameter) with a fairly flat profile.

In operation we find that the 2D-MOT will boost the load rate of the magneto-optical trap by roughly a factor of 3 even though the equilibrium fluorescence level of the MOT may only increase by 20-30%. Normally, the number of atoms in the MOT is described by the equation,

\[ \dot{N} = L - \gamma N - \beta n N, \tag{4.1} \]

where \( L \) is the load rate, \( \gamma \) is the one-body loss due to background, and \( \beta \) is the two-body loss rate (such as radiative decay and photoassociative loss) which is density \((n)\) dependent. Assuming that the background loss rate is small (good vacuum), the equilibrium number \((\dot{N} = 0)\) of atoms will be,

\[ N_{\text{equil}} = \frac{L}{\beta n}. \tag{4.2} \]

If the MOT density does not change (this happens when the MOT “flat-tops”), then the factor of 3 increase in load rate would indicate a factor of three increase in the equilibrium number. On the other hand, if the density increases then the two-body loss could limit the ultimate number of trapped atoms despite the increased load rate. The lower limit of performance is given by the 20-30\% increase in fluorescence which indicates that the total number is at least increased by that amount. However, optical density effects could limit the reliability of the fluorescence measurement and CCD imaging does indicate that flat-topping of the density is occurring for large MOT clouds. In the end, the actual increase in the number of trapped atoms probably lies somewhere between both extremes.

4.3 Skimmer Source

The \(^6\text{Li}\) source was designed around a magnetic guiding system so that a slowing laser was not necessary. While this sacrifices flux, compared to a Zeeman slower, we find the load rate fulfills the requirements for sympathetic cooling. Since the
sympathetic cooling will only remove $^7$Li and not $^6$Li, as long as we can load around $10^6$ $^6$Li atoms into the magnetic trap, that should be sufficient for the experiments we wish to perform. Figure 4.3 shows a schematic of the device. The device, acting as a low-pass velocity filter, uses permanent magnets to passively select the slow atoms present in the thermal atomic beam. The magnetic field $\vec{B}$ interacts with the magnetic moment $\vec{\mu}$ of the atoms giving the interaction energy $U = \vec{\mu} \cdot \vec{B} = g\mu_B m_f B$. Here $g$ is the gyromagnetic ratio, $\mu_B$ is the Bohr magneton, $m_f$ is the projection of angular momentum, and $B$ is the magnitude of the magnetic field. If the atoms are in the correct $m_f$ state, then this interaction energy will increase in regions of larger magnetic field. As a result, a force exists which will cause those atoms to be attracted to a local minimum in magnetic field. The skimmer provides a magnetic field minimum along the tube. Slow atoms are guided along a curved, conduction-limited tube by an octupole magnetic field, while fast atoms, unable to follow the curved trajectory, strike the tube wall and are removed from the beam. The details of this device were published in reference [102] and are based on work done with a quadrupole device of similar construction in a previous lab thesis [103].
The skimmer was initially tested by loading a magneto-optical trap (MOT). The number of trapped atoms was determined by observing the excited state fluorescence with a photodiode. The load rate was measured by first emptying the MOT of all atoms and then observing the increase in fluorescence during the first few seconds after the atomic beam is unblocked. A typical data set is shown in figure 4.4. Load rates of $\sim 6 \times 10^6$ atoms/s and peak numbers of $\sim 2 \times 10^8$ were obtained. The load rate dependence on the oven temperature is shown in figure 4.5. At lower oven temperatures, the number of trapped atoms rises with temperature as the number

![Figure 4.4](image1.png)

**Figure 4.4** Typical MOT fluorescence data from skimmer loading. The atomic beam is suddenly unblocked at time = 0, and the load rate is given by the increase in signal in the first few seconds.

![Figure 4.5](image2.png)

**Figure 4.5** Peak number of trapped atoms versus oven temperature for skimmer. The overall systematic uncertainty in the number of atoms is $\sim 40\%$. 
of available slow atoms increases. At the higher temperatures, however, collisions in
the beam reduce the flux of slow atoms into the skimmer. This was modelled with a
Monte Carlo calculation and found to agree with the data [102]. For the purpose of
loading the MOT and magnetic trap, we typically ran the oven at a temperature of
500° C. The performance of the traps will be discussed in chapter 6.

4.4 Electromagnetic Coils

The coils used to create the electromagnetic trap form an Ioffe-Pritchard type of
field configuration [104]. This configuration has the advantage of providing strong
confinement while maintaining a non-zero magnetic field at its minimum. Having a
non-zero minimum allows for atoms to maintain a well-defined $m_f$ angular momentum
projection at all times within the trap. If the field minimum were zero, then as atoms
pass through it they could undergo a Majorana spin flip and become unconfined [105].
Figure 4.6 shows the direction of current flow in the standard Ioffe trap. Given the

Figure 4.6 The Ioffe trap has four straight current bars which form a linear quadrupole
field. The two pinch coils on either end provide harmonic confinement along the cylindrical
axis.

...cylindrical coordinates suggested by the figure, this trap provides linear confinement
in the radial dimensions, and harmonic confinement along the axial dimension. To a
good approximation, the trapping potential is given by,

$$U(r) = \sqrt{\alpha^2 r^2 + (U_0 + \beta z^2)^2} - U_0,$$

(4.3)
in cylindrical coordinates [106]. Assuming that the atoms have a magnetic moment
$\mu$ and the magnetic field can be expanded about the minimum $B_0$ in terms of a linear
Figure 4.7 Cloverleaf magnetic trap. The various dimensions pertinent to our current trap are indicated. The separation of the coils (2.120" and 1.560"") assume that the coils are resting flat against the window glass. In reality, we find that the kovar seal of the re-entrant windows causes the coils to set further away from each other. We presently model our field assuming that the bias/curvature coils are separated by 2.36" while the quadrupole/gradient coils are separated by 1.81". We have bevelled the edges of the coil forms to avoid the kovar seals as much as possible, perhaps a future re-design could achieve the distances shown.

radial gradient $B'_r$, and an axial curvature $B''_z$, then we find that,

\begin{align}
U_o &= \mu B_o \\
\alpha &= \mu B'_r \\
\beta &= \frac{1}{2} \mu B''_z. \tag{4.6}
\end{align}

The axial confinement is usually expressed as a harmonic frequency, $\beta = \frac{1}{2} m \omega^2$. While the Ioffe trap is ideal for magnetic trapping and cooling of alkali gases, the standard electrical configuration does not lend itself to the best optical access.

The coils used to create our electromagnetic trap are based upon a planar design by the MIT group [107] and form an Ioffe potential while providing optical access. The coils consist of three distinct current paths on either side of the vacuum chamber. These current paths are shown in figure 4.7. The vacuum chamber has re-entrant windows which allow the coils to be place to within 3 cm of each other allowing for
the tightest possible field geometry while maintaining adequate space for the optical trap (MOT) beams. The bias coils are in an Helmholtz field configuration and allow us to adjust the overall bias field of the trap minimum. The curvature coils play the role of the pinch coils in the Ioffe trap, they point opposite to the bias and introduce curvature to the trapping field along the axis to provide axial, harmonic confinement. The gradient coils consist of four pairs of D-shaped anti-Helmholtz coils which sum together to give a linear field gradient which is ideally zero on axis and increases away from the center.

I should point out that these coils do not provide completely independent control of $B_0, B'_r,$ and $B''_r$. The curvature coil, while providing axial confinement, also introduces radial “anti-confinement” due to the zero-divergence property of magnetic fields. In other words, the field profile due to the curvature coil is like a saddle, the center of the trap is a local minimum axially and a local maximum radially. The atoms maintain confinement as long as the linear confinement from the gradient coils is stronger than the harmonic non-confinement created by the curvature coils. At small displacements from the trap center, the curvature coil washes out the linear confinement and causes the trap to look harmonic. As the displacement grows, the linear component increases while the curvature component decreases causing the trapping geometry to become linear. So what is a small displacement? As a general rule, the trapping field will look linear at a distance $r$ from the center once $r \cdot B'_r$ is greater than the bias field at the center of the trap. The bias field is a linear sum of the bias coil and curvature coil contributions. So in order to maintain linear confinement in the radial direction, it is important to use the bias coil to keep the field at the center of the trap to a minimum (but non-zero). Conversely, if one wants to make the overall trapping field more harmonic, then the field at the center of the trap should be increased relative to the radial gradient field. As a confined gas is cooled and occupies a smaller region within the trap, there will come a point when the gas no longer sees the linear confinement
of the radial field. At this point, the trapped gas will see a 3D harmonic potential with a radial field curvature given by [107],

\[ B''_r = \frac{B'^2}{B_0} - \frac{B''_z}{2} \]  

(4.7)

The coils must be constructed to withstand high currents (130 to 150 A) and must be mechanically stable. We have designed custom machined delrin plastic forms with channels in which copper magnet wire (18 AWG #8075 from Belden Wire and Cable) can be wrapped in the appropriate geometry for the Ioffe trap. These forms seal together with 1/32" viton gaskets. Figure 4.8 shows the delrin pieces that form the coils. Forced water flow of about 500 mL/min goes through each coil (with a backing water pressure of greater than 85 psi). A particular coil form is composed of a curvature channel, a bias channel, and a quadrupole channel. Each channel has two pipe fittings where electrical and water connections are made. The wire is brought out of the forms into copper tubing and then soldered into a small hole in the side of the tubing. Large copper lugs are then used to make electrical connections to the tubing.

The coils are mechanically attached to the chamber with 4 dual-metal rods on either side. These rods were specifically designed to minimize thermal expansion of the assembly and consequently minimize resulting magnetic field instabilities [108]. The rods are attached to the outer surface of the vacuum chamber and protrude into the re-entrant windows from either side with a separation across the chamber center of 8.55 cm. Assuming that the rods are the same material as the vacuum chamber (stainless steel 304), and assuming that the rods are firmly attached to the outside of the chamber, the net result of the chamber+rod expansion would be just the separation of the rods times the appropriate thermal coefficient. The rod ends (which support the coils) would away from each other by an amount \( \Delta x \),

\[ \Delta x = \eta_{SS304} \times x \]  

(4.8)
Figure 4.8  Delrin electromagnetic coil forms. The three pieces which comprise each form are shown. The quadrupole piece contains the radial gradient producing “D” coils with “notches” at the 9-o’clock position (as shown) to provide input/output for both the wire wrapping as well as the water flow. The next layer is the bias/curvature form which contains both the bias wrap as well as the curvature wrap. Both channels have their own input/output throughputs for the wire as well as water flow. Finally, the backing piece serves to help bolt everything together, with viton gaskets, as well as provide a sturdy connection for swage-lock fittings to copper tubing. The respective wires for each coil are brought up about 6” out of the forms and then soldered into small holes in the side of the copper tubing. Electrical connections are then made to the tubing. The six feedthroughs for water and electricity are shown on the backing piece. The backing piece also allows for four metal rods to be attached to the forms. These rods come out of the re-entrant windows and attach to a steel plate which bolts onto the side of the vacuum chamber. The metal rods are composed of a length of steel and titanium which together minimize the thermal expansion coefficient of the whole assembly. The water connections are made from three parallel sources from the wall. The two bias coils on either side of the chamber are connected in parallel with one source. Similarly, the two curvatures share a source and the two quadrupoles share the last source.
where $\eta_{SS304} = 17 \mu m/m^oC$ and $x = 8.55$ cm [108]. The bias/curvature coils sit 0.5 inches away from the rods within the delrin forms. As the delrin thermally expands, this would cause the coils to move closer by an amount $\Delta y$,

$$\Delta y = \eta_{\text{delrin}} \times y,$$

(4.9)

where $\eta_{\text{delrin}} = 70 \mu m/m^oC$ and $y = 2.54$ cm. The difference of the steel and delrin displacements gives the thermal expansion for the entire mechanical assembly. Ideally, the rod expansion and the delrin expansion should be matched in order to minimize movement of the electromagnetic coils. Dean Homan found that by making the rods a combination of SS 304 and a 2.665 inch length of titanium, this condition is satisfied. The details of this are given in reference [108].

Given the logistics of how the water connections are made, a constraint is introduced on the coil wrappings. The curvature coils are wrapped with 22 complete turns plus an extra half turn which allows the electricity to flow into one water connection and out of the other. Likewise, the bias coils are made of 23 complete turns plus an extra half turn. Figure 4.9 shows how the extra half-turns are arranged with respect to the chamber. The quadrupole coils are wrapped in a clockwise and then counterclockwise direction going around each “D” of the quadrupole form. We wrap the coil in such a way as to make 10 wraps around the inner circle of the “D” as well as along each respective bar. The outer circle of the “D” either has 9 wraps or 11 wraps and this alternates around the entire coil form. Figure 4.10 shows the alternating extra/missing wraps around the outer edge. These coils have been placed so that an 11 edge faces a 9 edge across the chamber. Post-construction, we have realized that this introduces a non-zero bias component at the center of the trap due to the quadrupole coil. While not ideal, modelling of the magnetic field has shown that a suitable choice of bias coil current can cancel this component. The exact bias current depends on the direction of current flow through the quadrupole coil. Table 4.1 shows the results of modelling the coil geometry with different currents. Once the stray bias component
Figure 4.9  Placement of half-turns within bias/curvature coil forms. The bias coils consist of 23 complete wraps and the curvature coils consist of 22 complete wraps. The extra wraps which are needed to bring the wires in/out the respective feedthroughs are shown. In each form, the half wrap of the curvature coil is on the same side as the half wrap of the bias coil. However, across the center of the trapping region, the half wraps are on opposite sides so as to minimize distortions of the Ioffe field.

<table>
<thead>
<tr>
<th>$I_B(A)$</th>
<th>$I_C(A)$</th>
<th>$I_Q(A)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>121.5</td>
<td>130</td>
<td>130</td>
</tr>
<tr>
<td>108</td>
<td>130</td>
<td>-130</td>
</tr>
</tbody>
</table>

Table 4.1  Values of current for EMTRAP which are needed to produce near-zero bias field. The bias current is given by $I_B$, the curvature by $I_C$, and the quadrupole by $I_Q$. By running the quadrupole current in different directions, a different value of $I_B$ is needed in order to cancel the bias-component of the quadrupole which results from the mis-match in extra coil wraps.
Figure 4.10 Wrapping configuration of quadrupole coil forms. Each "D" is composed of 10 wraps of wire around the inner diameter as well as along the respective bars. Since each "D" must be wrapped successively clockwise and then counter clockwise, this requires that the outer edge of the "D" must be either 9 wraps or 11. In constructing the coils, we ended up having a 9 edge face an 11 edge across the chamber as indicated by the arrows. We have since realized that this introduces a small contribution to the bias field at the center of the trap. Suitable adjusting of the bias coil can eliminate this effect.
has been suitably nulled, the resulting field geometry of either configuration looks identical. A plot of the field profile is shown in figure 4.11.

For our current trapping configuration, we use 130 A through the curvature coil to generate an axial field curvature of 88 G/cm². This corresponds to a trapping frequency of 45 Hz for ⁶Li and 42 Hz for ⁷Li. Our radial gradient of 110 G/cm is generated by running 130 A through the quadrupole coils. The bias current is experimentally adjusted to get < 5 G field at the trap center (a little over 120 A). Using currents in various coils (bias $I_B$, curvature $I_C$, and quadrupole $I_Q$) the field configuration can be computed by integrating the Biot-Savart law across the current path geometry (see description of the modelling program in appendix H). Figure 4.11 shows the calculated field for our typical 130 A trap. We have found that the electro-

ermagnet trap wants to be quite "tight". As a rule of thumb, a 1 mK cloud is contained by 15 G of magnetic field. For a radial gradient of 110 G/cm, a 1 mK

![Figure 4.11 Ioffe trap field profile. This plot shows a typical run configuration for our 130 A trap. The bias current of 120 A should roughly counteract the bias contribution of the curvature (and the mismatch in quadrupole wrappings) maintaining a bias field of around 5 G. This is the result of a computer model which is discussed in appendix H. The field geometry is tight for capturing a cold MOT, but experimentally the number of transferred atoms (and the efficiency of evaporation) appear to favor this configuration.](image-url)
cloud extends 1.4 mm (2.8 mm diameter). This is small compared to the size of our MOT (about 1 cm diameter before compression, see chapter 6) which would indicate that heating would occur during transfer. We could start with a looser trap by having a larger bias (or reducing the quadrupole current) in order to spatially mode-match the MOT. The evaporation modelling (chapter 5) favors a very tight trap and we have seen experimentally that evaporation works better in the tight configuration that is shown. Part of the work in progress involves dynamically changing the trap from "loose" to "tight" immediately following transfer in order to peak transfer efficiency.

Figure 4.12 shows the calculated field when one bias and one curvature coil are energized with 15 A while the other coils are off. This is our MOT configuration for our initial loading. I should point out that there is a slight offset to the MOT center since the two coils making the "anti-Helmholtz" field are not symmetric. We have not seen any major effect on MOT performance as a result of this although the MOT cloud does appear asymmetric when the trap is fully loaded. A series of large, rectangular coils which surround the vacuum chamber serve as a nulling cage which can be used to null Earth's magnetic field, null stray lab fields, and offset the MOT back to the center of the Ioffe trap. Offsetting the MOT to the center actually helps in maximizing the loading efficiency from MOT to the electromagnetic trap (EMTRAP). This is most likely the result of having a better spatial mode-match to the EMTRAP. We have found that about 5.5 A through the axial nulling cage is sufficient for this.

An in-depth study of these coils, as well as a future design, can be found in reference [109]. The present coils could be operated at higher currents, about 150 A, in order to peak confinement. We have been hesitant to do this for fear of stressing the coils and possibly burning them out. The system has been tested at 150 A for a period of an hour and seemed okay, but we feel the increase in confinement is not worth the increase in risk to the coils. The characteristics of the 150 A trap are shown
Figure 4.12  MOT trap field profile. Even though 15 A through the coils can produce a reasonable MOT, we find that the best MOT conditions change on a daily basis and that this current is one of many parameters which require frequent peaking. The optimal MOT field may require changing this current by a few amps. The offset of the minimum in the axial direction is due to the fact that this field is created by running the current through one curvature and one opposing bias coil. The details of this are discussed in the section concerning the electromagnetic trap switching circuit. This offset can be removed by suitable adjustment of the nulling cage surrounding the trap chamber. The minimum shown are limited by the field resolution of the magnetic trap model and do, in fact, go to zero value.
in table 4.2. A new coil design is discussed in reference [109] which increases axial confinement at the cost of radial confinement. The re-design involves using more wraps as well as changing the relative position of the bias/curvature coils versus the quadrupole coils. Our current design has the quadrupole coils as the innermost set, the new design would have the bias/curvature coils in this position. The relevant characteristics for this design are also shown in table 4.2.

<table>
<thead>
<tr>
<th></th>
<th>present (130 A)</th>
<th>present (150 A)</th>
<th>re-design</th>
</tr>
</thead>
<tbody>
<tr>
<td>$B'_r$ (G/cm)</td>
<td>110</td>
<td>138</td>
<td>114</td>
</tr>
<tr>
<td>$B''_z$ (G/cm²)</td>
<td>88</td>
<td>98</td>
<td>681</td>
</tr>
<tr>
<td>$\nu_z^{^7}$Li (Hz)</td>
<td>42</td>
<td>44</td>
<td>117</td>
</tr>
<tr>
<td>$\rho \propto (B^2 \nu_z)$</td>
<td>$5.1 \times 10^5$</td>
<td>$8.4 \times 10^5$</td>
<td>$1.5 \times 10^6$</td>
</tr>
</tbody>
</table>

Table 4.2 Characteristics of different electromagnetic traps. The characteristics for three different traps are presented: the present design with our current run condition of 130 A in the curvature and quadrupole, the same design with 150 A, and finally the new trap design by Bita Ghaffari with 150 A [109]. The characteristics reported are the radial gradient $B'_r$, the axial curvature $B''_z$, corresponding axial harmonic frequency for $^7$Li, and finally a figure-of-merit which is proportional to the phase space density $\rho$.

4.5 **High Current Switch**

The design and construction of the electromagnetic trap switch was the result of several months of work and sought to meet several requirements for effective operation. These requirements include:

- capable of handling high currents and providing a stable magnetic field
- capable of three operational modes: a MOT field configuration, an EMTRAP Ioffe field, and no field (OFF)
- capable of adjusting MOT field and EMTRAP bias field
- fast switching time compared to timescale of freely expanding cloud
Each of these items will be discussed in this section.

We have three EMI power supplies which power the complete coil configuration and which supply high currents. These power supplies can each output 165 A maximum which gives the current requirement for the switch. Two of the power supplies can run at a maximum voltage of 60 V while the third can run at 50 V. The 50 V and one of the 60 V supplies are connected in series to power the bias and curvature coils. The other 60 V supply powers the quadrupole. We designed the switch to operate at up to 150 A. Operating at higher currents will burn out the coils given the amount of water flow we can achieve through the delrin coil forms (see previous section). We typically operate at currents of 130 A to minimize thermal strain on the coils. The electrical properties of the coils have been measured and are shown in table 4.3 In our EMTRAP configuration, we typically run 130 A in the curvature and quadrupole coils, and 120 A in the bias. This gives a power drop \( I^2R \) of 
\[
130^2(0.09 + 0.09 + 0.14 + 0.14) + 120^2(0.16 + 0.16) = 12 \text{ KW}
\]
while the power supplies are capable of 
\[
165(60 + 60 + 50) = 28 \text{ KW}
\]. We certainly have more power to use if we could design coils that could handle it.

<table>
<thead>
<tr>
<th></th>
<th>resistance (( \Omega ))</th>
<th>inductance (( \mu H ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>curvature (each)</td>
<td>0.09</td>
<td>50</td>
</tr>
<tr>
<td>bias (each)</td>
<td>0.16</td>
<td>94</td>
</tr>
<tr>
<td>quadrupole (each)</td>
<td>0.14</td>
<td>33</td>
</tr>
</tbody>
</table>

**Table 4.3** Electrical characteristics of the electromagnetic trap coils.

In order to achieve bias field stability, the current which runs through the bias coils and the curvature coils should ideally come from the same power bank. Since the bias field at the center of the trap results from the difference of these two coil sets, this would ensure that any common-mode current noise on the supply would have a minimal effect on the bias field. The EMI supplies are specified to have 75 mV\text{pp}\text{pp} ripple on the output (which has been verified in measurements [108]). Operating
at 68 V (typical for the bias/curvature system), this gives a common-mode current fluctuation of 1 part-per-thousand. If the bias field was 5 G, this would indicate a field fluctuation of 5 mG or 330 nK in temperature units. Since this is roughly the energy scale of a degenerate gas, eliminating the common-mode noise is critical. Figure 4.13 shows the basic coil configuration. The bias/curvature coils are all connected in series in order to maximize field stability as required. Running the curvature at 130 A and the bias at ~ 120 A adds up to about a 62 V drop across the bias/curvature coil system (about 68 V across the whole supply once diode drops, FET on-resistances, and contact resistances are accounted for). The quadrupole coils are run at 130 A with a voltage drop of about 37 V.

The different operational modes are obtained by using transistors to control current flow. These are indicated in figure 4.13. Four of the six transistor banks operate as basic switches in an “on/off” mode. The other two banks operate in a partially open regime and regulate the amount of current that sets the MOT field and the bias field of EMTRAP. We refer to these as the “MOT shunt” and the “bias shunt” respectively; the respective current paths are indicated in the same figure. The feedback systems which control these shunts, as well as the digital control of the different modes, will be discussed later on in this section.

It is important to understand the operational modes of the EMI power supplies in order to understand how the switch was designed. The power supplies have manual/remote control of the voltage setting and the current setting. For a given load, one of these two settings will limit the power supply output. Trying to output 150 A through a 1 Ω load will not work since the supply has a maximum voltage output of less than 150 V. In this case, the supply will become voltage limited and therefore runs in voltage control mode. The amount of current through the 1 Ω load will be set by the voltage control which can be adjusted. In contrast, trying to apply 50 V across a 0.1 Ω load will cause the supply to rail at its current setting, this is called
Figure 4.13  Basic electrical configuration of EMTRAP coils. The different modes of operation are obtained by opening/closing the appropriate transistors. These modes are:

<table>
<thead>
<tr>
<th>FET</th>
<th>MOT</th>
<th>EMTRAP</th>
<th>OFF</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>on</td>
<td>off</td>
<td>off</td>
</tr>
<tr>
<td>2</td>
<td>off</td>
<td>on</td>
<td>off</td>
</tr>
<tr>
<td>3</td>
<td>off</td>
<td>on</td>
<td>on</td>
</tr>
<tr>
<td>4</td>
<td>*</td>
<td>*</td>
<td>*</td>
</tr>
<tr>
<td>5</td>
<td>*</td>
<td>off</td>
<td>off</td>
</tr>
<tr>
<td>6</td>
<td>off</td>
<td>on</td>
<td>off</td>
</tr>
</tbody>
</table>

where the '*' indicates that the transistor is partially open and is used to control the amount of current flow. Transistors #4 and #5 are shunts which are used to adjust both the EMTRAP bias field and the MOT field respectively. The MOT field is generated by one curvature and one bias coil on opposite sides of the vacuum chamber. Electrical feedback to switch '5' provides control of the MOT field. A large power resistor of 0.4 Ω is used to drop the power over switch '4' as well as provide a means of measuring the amount of current which is flowing through the bias shunt. Feedback to switch '4' controls the current through the bias shunt and so allows control of the bias current \( I_{\text{bias}} = I_{\text{curv}} - I_{\text{shunt}} \). Switch '4' is left partially on in MOT mode in order to facilitate fast mode-match operation as described in the text.
current control mode. Depending on the load and the voltage/current settings, one of these two modes will be in effect. The front face of the EMI power supply has LEDs which indicate which mode is in operation (current or voltage).

Since our MOT and EMTRAP magnetic fields are determined by current flow, we always want to operate the power supplies in current mode. If the output voltage load changes by 100% while in current mode, the output current will change by less than 0.1% [110]. While this is ideal for switching from a high impedance load to a low one, a problem occurs when one tries to do the reverse. Upon switching to a higher impedance load, the supply is forced to switch to voltage control mode, ramp the voltage up until the desired current is obtained, and then switch back to current mode. We have measured this response time for the supply to be about 50 ms (see figure 4.14). For the case of the quadrupole coil switch, this is not a problem since in MOT mode the load is infinite (transistor #6 is off). The quadrupole supply switches from voltage mode to current mode when the EMTRAP is switched on, but the voltage setting of the supply can be arbitrarily set to the exact value needed to supply 130 A to the coils when the transistor #6 bank is turned on. This eliminates any possible 50 ms switching transients for the quadrupole coils (see figure 4.15). The 50 ms power supply response is a problem when considering the bias/curvature switch. Unlike the MOT mode, the EMTRAP mode requires more current from the supply with a higher impedance load (4 coils are energized instead of 2). So what is an acceptable switching speed?

The required switching speed is determined by considering the time-of-flight expansion of a cloud of lithium. The equation which describes this expansion is derived later on in chapter 6 for the purpose of measuring temperatures. I will present the result for the waist \( w(t) \) of an expanding Gaussian cloud as a function of time \( t \) and temperature \( T \),

\[
w(t) = w_o \sqrt{1 + \frac{2k_BTt^2}{m w_o^2}},
\]  

(4.10)
Figure 4.14  EMI power supply response when switching control modes. There are two plots showing two different timescales. The measured supply voltage is taken from the bias/curvature system and shows the result of switching from the lower impedance MOT load to the higher impedance EMTRAP load (indicated by the trigger arrow). The power supplies respond on two timescales, the shorter and more important being about 50 ms (seen in the top figure and zoomed in on in the lower). The longer response is partly due to the supplies and partly to the thermal response of the coil system (changing resistances).
where \( k_B \) is the Boltzmann constant, \( m \) is the atomic mass, and \( w_0 \) is the initial waist before free expansion occurs. Once the MOT is turned off, we want to capture the atoms in the EMTRAP before any significant expansion has occurred. Figure 4.16 shows the rate of expansion for a 500 \( \mu K \) cloud with an initial waist of 3 mm. Given the physical size of the EMTRAP and the relative velocity of the cold atoms, the switch must be able to turn on fast compared to the time scale of a millisecond. The quadrupole coils are switched quickly enough provided that the voltage setting of its power supply is appropriately set during MOT mode (see previous discussion and figure 4.15). As for the bias/curvature switching, more work was involved.

Addressing the power supply response time in the bias/curvature switch involved incorporating two key elements into the design. First, the bias/curvature power supplies need to be in current mode and the value of this current must be the same between the MOT mode and the EMTRAP mode. Given that the EMTRAP requires far more current than the MOT, we set the supplies for the EMTRAP current of 130 A (as described in the previous section). Since the MOT only requires around 15 A, the excess current is shunted to ground through transistor \#5 (see figure 4.13). While
Figure 4.16  Time-of-flight expansion for a $^7$Li cloud at 500 $\mu K$ with an initial waist of 3 mm.

This eliminates the problem of the supply having to change current setting during
the switching, it still does not address the issue of the EMTRAP load impedance
causing the supply to change control mode. In MOT mode, the supply outputs 130 A
(with roughly 115 A being shunted to ground) with a voltage drop of 3.8 V across the
single bias and curvature coil making the MOT field. Going to EMTRAP, the MOT
shunt turns off and all four bias/curvature coils are energized (requiring 62 V). This
causes the supply to voltage rail (changing from current to voltage mode), making the
supply increase the output voltage until either the current setting or voltage setting
is obtained. We set the voltage setting of the supply so that it has enough voltage to
regain current mode at 130 A. To eliminate the resulting 50 ms fall off in current, we
had to bootstrap the supply voltage during this time. This was done by constructing
a large capacitor bank, which is charged to the EMTRAP operating voltage, and
which is switched in during the MOT/EMTRAP transfer. The details of this are
discussed below.

The capacitor switch is a key component of the EMTRAP which allows the bias/curvature coils to fully energize in the fastest possible time (see figure 4.18). Since the capacitor bank fully powers the coils for roughly 50 ms, and given the resistance of the coils to ground, this requires a large capacitance. A bank of 9 electrolytic capacitors with individual capacitance of 80 mF and a maximum voltage rating of 100 V are connected in parallel to give a total capacitance of about 0.7 F. A variac plus rectifier is used to charge the bank during MOT mode. In typical operation, it takes about 1-2 min to charge the bank to ~ 70 V between transfer cycles. This is limited by the maximum current which can be supplied by the rectifier; a higher power rectifier could speed this up. We cannot charge the bank higher than 70 V due to the protection zener diodes in the switch which clamp at this voltage. Since the operational voltage of the bias/curvature coils in EMTRAP is dependent on the

![Figure 4.17 Capacitor switch. The TTL signal for toggling the MOT/EMTRAP is fed into the capacitor switch and used to dump the stored charge to the top of the bias/curvature coil system.](image)
setting of the bias shunt, this will dictate to what level the capacitor bank must be charged. Given the various diode drops, contact resistances, and voltage drops across the coils, we usually charge the bank to around 68 or 69 V for a bias setting of around 5 G (about 130 A in the curvature and 120 A in the bias).

![Graph of capacitor bank switching time](image)

**Figure 4.18** Capacitor bank switching time. The measured voltage is the supply of the bias/curvature system and is identical to the measurement taken in figure 4.14 except that the capacitor switch is engaged. A comparison of the two figures shows that the capacitor switch succeeds in helping to eliminate the current droop that results from the power supply having to switch control mode. This figure also shows how the bias/curvature coils are now able to switch in a reasonable timescale compared to the time-of-flight expansion of the atom cloud.

At this point, I should point out a few safety precautions to observe while working with the capacitor switch. First, we should keep the maximum voltage charge well below the maximum amount of 100 V. Second, a bleed-off resistor is kept across the bank when it is not in use. Finally, we always monitor the voltage charge of the bank during a run. It is important to also keep in mind that when the EMTRAP is switched to OFF, the entire coil system plus switch will charge to about 70 V (this voltage is set by the zener protection of the transistors which is discussed later on). Care should be taken when moving around the apparatus while this type of switching
is being done.

In a future coil design, we hope to obtain a fourth power supply which could be used to power the MOT field from a separate set of coils. This would require redesigning the delrin coil forms so that a fourth set of coils were present in an anti-Helmholtz configuration. Despite this complication, it would greatly simplify the MOT/EMTRAP switch design. All the power supplies could then be operated in on/off current-mode, exactly how the present quadrupole coil system functions. We could eliminate the MOT shunt and the capacitor switch. This would also have the added advantage of creating a symmetric MOT magnetic field. A future coil/switch design should incorporate this feature.

So now that the power supplies, in conjunction with the capacitor bank, operate at acceptable speeds, the next step in the electromagnetic switch design was to find a way to switch the transistors as quickly as possible. The transistors that were used to handle these types of currents were the Motorola MTE215N10E. These are power field effect transistors (FETs) which are rated to 215 A, 100 V, with a total power rating of 460 W at 25°C. Since FETs of this size have a large input capacitance (about 15 nF when off), we needed to find a way to switch the gate voltage in less than 1 ms despite the large capacitance. Figure 4.19 shows the basic buffer scheme. A Darlington push-pull is used to move large currents on/off the FET gate. Since there is a large input resistance to the base of the push-pull, a CMOS push-pull buffer is used to isolate the incoming TTL type signal and the Darlington pair. This enables switching times ~ 100 µs for changing the gate-source voltage \( V_{GS} \) (see figure 4.20). While this is an excellent performance, it turns out that the overall switching time is limited by the coil inductance. Once the \( V_{GS} \) voltage is changed, there is a finite amount of time that is needed for the coil to either energize or de-energize. Since the breakdown voltage for the FET drain-source (\( V_{DS} \)) is 100 V, we must protect the FETs by clamping any inductive spikes that occur. To do this, we use banks of 75 V
Figure 4.19  Buffering scheme for driving gate voltages of high current FETs.

Figure 4.20  Gate-source voltage switching response of FET in ETRAP switch. The top trace shows the response of the gate-source voltage $V_{GS}$ of transistor #1. The lower trace shows the slower response associated with transistors #2 and #6; these transistor gates are slowed by the output capacitance of the IRFD210 which is used to drive these gates to zero volts for OFF mode (see circuit diagram in figure 4.25)
zener diodes (the highest value zeners available from Farnell with a power rating of 75 W each) [111]. Given these necessary clamps, this implies that there is a maximum voltage of about 75 V which is applied across the coils and which limits the speed for changing the current through the coils.

$$L \cdot \frac{di}{dt} = V_{\text{clamp}} ,$$  \hspace{1cm} (4.11)

where $L$ is the inductance of the coil. This equation implies that it takes about 200 $\mu$s to shut off 130 A through a 100 $\mu$H coil. It turns out that this rough estimate matches measurements of the on/off switching time quite well, we measure on/off times of about 200 to 250 $\mu$s (see figure 4.15). This is well within design specifications for capturing atoms from the MOT. This switching time could be improved by using insulated-gate bipolar transistors (IGBTs) instead of FETs. It turns out that IGBTs can sustain maximum voltages of around 900 V. This would increase the shut-off time by a factor of ten but would also require a re-design of the current switch with components which could handle those types of voltages. In particular we would need custom-designed zeners to protect the IGBTs and we would need to speed up the response of the gate buffering. Also, when the coils charge to 900V in OFF mode, there would be safety issues to consider.

Most of the transistor switches operate digitally. These include switches ‘1’, ‘2’, ‘3’, and ‘6’. These switches are comprised of 2 FETs which are connected in parallel. Since these switches either operate ‘on’ with high current and low voltage drop, or in ‘off’ with no current, their power dissipation is low. For the case of switches ‘4’ and ‘5’, these FETs operate partially open which requires a large amount of power dissipation. In order to do this, these two switches are comprised of 8 parallel FETs each. All of these FETs are mounted onto a water-cooled plate and are air-cooled as well with a muffin fan. Since these FETs are primarily designed by Motorola for digital operation, some care must be taken when requiring an array of them to operate in a partially conducting mode. The ‘on’ resistance of the various FETs can
vary substantially to the point that one FET in an array gets a disproportionate amount of current. This is called "current focusing" and can lead to a power overload of one or more FETs in the array. In order to avoid this, the ‘on’ resistance of various FETs was measured and closely matched FETs were chosen when constructing the large 8 FET arrays. Figure 4.21 shows the various ‘on’ characteristics of an assortment of such transistors.

![Figure 4.21 'On' characteristics of various MTE215N10E field effect transistors.](image)

In MOT mode, switch ‘5’ is partially open for two reasons. First, this allows a steady current of 130 A to be drawn out of the power supplies without having to supply all of that current to the coils; in this sense we refer to this as the MOT shunt. Second, by then adjusting the MOT shunt, this allows us to adjust the operating magnetic field of the MOT \( J_{\text{MOT}} = 130 - J_{\text{Shunt}} \). Figure 4.22 shows the basic feedback circuit which is used to maintain the properly chosen MOT current. The current through the MOT shunt is set by reading the voltage across a 250 \( \mu \Omega \) load. This voltage is gained up and then compared to a user-set voltage across a potentiometer. This difference voltage is integrated and applied to the push-pull buffer controlling the gate of switch
Figure 4.22 MOT feedback circuit.

'5'. When going to EMTRAP, the gate-source voltage must be brought quickly to zero in order to shut off the switch. This is done by applying the appropriate TTL signal to the gate of a smaller IRFD210 FET that opens up a channel to ground as shown in figure 4.22.

The bias feedback in EMTRAP mode is similar to the MOT feedback although it has more complexity in its design since it must switch very quickly from no feedback to a situation with precise feedback as the switch goes from MOT mode to EMTRAP mode. We found that the circuit will undergo unstable oscillations if the feedback is set to anything faster than a few ms. Since this is not fast enough for our design requirements, we circumvent this problem by setting the gate voltage to roughly the required operating level (mode match) during the MOT mode of switch operation. The idea is that once the EMTRAP mode is engaged, the current flow through the bias shunt will be close to the correct level. In this sense, the mode-match setting allows us to set the "rail" of the feedback system when no feedback is possible. After switching, a slow feedback is then used to adjust this current to bring it to the appropriately user-set "bias" amount. Figure 4.23 shows the details of this design.

The push-pull buffer of switch '4' sees the output of an op-amp summer which
Figure 4.23  Bias feedback circuit.

Figure 4.24  Feedback response of the bias shunt. The measured voltage is the error signal from the circuit in figure 4.23. Upon switching to EMTRAP (indicated by the trigger arrow), the bias shunt feedback system brings the error signal to the set value in about 20 ms. The mode-match allows for the shunt to start close to the set value as indicated by the lack of an error rail just after switching.
sums up three contributions. The first is simply an offset voltage which is equal to the voltage of the source of the FET switch. The second contribution is the user-set mode-match voltage which, together with the offset, always ideally maintains a constant gate-source voltage drop $V_{GS}$ in the absence of bias current feedback (this $V_{GS}$ is set by the mode-match to be close to the needed EMTRAP bias shunt value). The final contribution is the integrated signal of the actual current through the switch after switching to EMTRAP; this signal is used to maintain the overall $V_{GS}$ at the appropriately level determined by the bias setting of the switch. This feedback signal is formed by using an instrumentation amplifier to measure the current through a 0.4 $\Omega$ resistor in series with the shunt. Since this portion of the high current circuit operates at voltages $\sim 30$ V which exceeds the maximum common-mode input voltage of the instrumentation amplifier, a precision resistor network is used to voltage divide down the input. The output of the instrumentation amplifier is then compared with a user-set potentiometer and the difference voltage is integrated before going into the summer. A front panel switch activates/deactivates the feedback so that the mode-match potentiometer can be set independently from the feedback (and therefore allows setting of the feedback “rail”). Ideally, the mode-match setting is close to the operating gate voltage and the integrated feedback provides slow, fine adjustment of this voltage level in order to maintain a constant bias shunt current. The DG417 CMOS switch disconnects the instrumentation amplifier from the integrator during MOT mode to keep the integrator output at zero volts before switching to EMTRAP (the large 1 M potentiometer resets the integrator). Normally a FET switch across the integrator feedback could be used to zero it as long as the controlling gate voltage can be brought to $-15$ V since the integrator output can swing $\pm 15$ V (see reference [112]). The DG417 switch has the advantage of being able to switch with a positive valued TTL signal. Since the amount of current through the bias shunt is directly related to the bias field of the EMTRAP, we have modelled the field as a function of this
current and find that the bias field changes by roughly 3.5 G per amp in the shunt.

The final design consideration with the switch deals with the problem of translating a TTL type of input signal into a signal which can control all 6 FET switches. Ideally, there are two inputs into the switch box, one which toggles the MOT/EMTRAP mode, and the other which toggles the OFF mode. Since in the most general case each FET switch could require an entirely distinct gate voltage to properly open/close the switch, we designed the signal handling to be as versatile as possible. In the first

![TTL signal handling in electromagnetic trap switch](image)

**Figure 4.25** TTL signal handling in electromagnetic trap switch. The upper circuit shows how the incoming TTL MOT/EMTRAP signal is isolated and buffered into a high voltage TTL signal. Whenever the signal travels through a CMOS push-pull, its logical level is reversed. The upper circuit shows how this signal is used to drive 2 of the 6 gates in the high current switch. The lower circuit shows how the OFF TTL signal is isolated and used to drive the gate voltages of switch '2' and '6' to zero. The extra TTL signal lines which are shown connect to other gates with similar buffering schemes (see [113]).
stage, the incoming TTL signal goes through a NTE3401 optical isolator. This helps to isolate the control circuit from transients as well as prevent any possible ground loops. For the MOT/EMTRAP TTL signal, the output of the respective optical isolator is then used to drive a FET whose output is pulled up by a high-voltage (80 V, 100 mA) source. This amplifies the 0 to 5 V TTL signal into a 0 to 80 V "not TTL" signal. Since the absolute voltage of some of the transistor gates exceeds 5 V (such as transistor #3 and #4), this is necessary. This signal can then be voltage divided through 1 MΩ loads to the various gates of the FETs. Zener diodes are used to ensure that the gate-source voltages never exceed the 20 V maximum allowed by the MTE215N10E FETs. One can now see that buffering the signal going into the FETs is very important since the currents involved with the 1 MΩ loads are quite small. For the case of the OFF signal, the output of the respective isolator is used to drive the gate voltages of switches ‘2’ and ‘6’ to zero (off). The truth table for the switch is shown in table 4.4. It is important to point out that in order to completely

<table>
<thead>
<tr>
<th>MOT/EMTRAP TTL</th>
<th>OFF TTL</th>
<th>Mode</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>MOT</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>EMTRAP</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>OFF</td>
</tr>
</tbody>
</table>

**Table 4.4**  Truth table for electromagnetic trap switch.

shut off all currents in the coils, both the MOT/EMTRAP TTL and the OFF TTL signals need to be "high".

I think the overall design of the switching control circuit is a flexible system which allows for future expansion if needed. The main control circuit is air-cooled and separated from the FET bank by a shielded cable. In addition, the control circuit is contained in a shielded box to minimize transient effects from the FETs. Details concerning all of the components as well as the finer aspects of the control circuit are documented in laboratory files [113].
4.6 Optical Set-up

The laser system used to generate the necessary beams for cooling, trapping, and probing Li has undergone a variety of changes in the last year and continues to do so. What I hope to present here is an overview of the optical set-ups that were used to obtain the data discussed in chapter 6. Figure 4.26 shows a schematic of the energy levels in $^6$Li and $^7$Li which are important for laser cooling and trapping. There are two features to keep in mind in designing the optical system. First, there

![Energy Level Diagram](image)

**Figure 4.26** Energy level splittings for $^6$Li and $^7$Li [114,115].

is an isotopic difference in the transition energies which requires having different frequencies for the two isotopes. Second, the ground state hyperfine splitting requires that two frequencies are needed per atom in order to drive transitions from either ground state. For $^6$Li, in order to drive ground state transitions, we need to have two laser frequencies separated by $\sim 228 \text{ MHz}$. For $^7$Li, we need to have the frequency separation at 812 MHz which is the difference between the $f = 2 \rightarrow 3$ and the $f = 1 \rightarrow 2$ transitions. This ultimately requires 4 frequencies, 2 for $^6$Li and 2 for
$^7\text{Li}$. Since the MOT, Zeeman slower, and probing all require different frequencies, the laser system can get complicated fairly quickly.

### 4.6.1 $^6\text{Li}$

Historically, $^6\text{Li}$ was the first isotope to be magnetically trapped in our electromagnetic trap. We used an argon ion laser to pump a Coherent model 699 ring dye laser to generate the main laser frequency. This laser was locked via saturated absorption in a heat pipe cell to the $2S \ f = 3/2 \rightarrow 2P_{3/2}$ transition (discussed below). Figure 4.27 shows how the various frequencies were generated. The laser was passed through a 228 MHz AO to generate a blue sideband which was resonant with the $2S \ f = 1/2 \rightarrow 2P_{3/2}$ transition. The AO was driven such that the power in the sideband was comparable to the carrier. These two frequencies were then overlapped onto a 50/50 beam splitter. At this point, the lower frequency component was 76 MHz red of the atomic $2S \ f = 3/2 \rightarrow 2P_{3/2}$ transition due to the AO offset in the heat pipe lock. The higher frequency component was therefore 76 MHz red of the $2S \ f = 1/2 \rightarrow 2P_{3/2}$ transition. One of the dual frequency beams from the splitter was sent through a 40 MHz switching AO which could be turned on/off to generate the MOT beam (blue sideband) with a detuning of -36 MHz (-6 $\Gamma$) from both ground-state transitions. This MOT beam was spatially filtered, expanded, and collimated before being split up into 3 independent beams. These beams were appropriately polarized (circularly) and retro-reflected to make the necessary beams for the MOT. The various waveplates that are shown were used to balance the beam powers and peak the MOT performance.

The other dual frequency beam was passed through a tunable AO where the blue sideband could be tuned from 40 to 100 MHz. The sideband was set to about 70 MHz modulation frequency so that the blue sideband was near resonance to the $^6\text{Li}$ transition. This beam was then passed through another spatial filter, expanded,
3 sets of orthogonal retro-reflected MOT beams ($\sigma^+\sigma^-$)

Figure 4.27 $^6$Li laser system.
and collimated. It was then overlapped with the MOT configuration. By switching the MOT beams and the magnetic field off, and then turning this 70 MHz AO on, an optical molasses could be generated which could both cool the atoms as well as probe them (via fluorescence). We used this set-up for both testing the loading of the skimmer source as well as measuring the performance of the MOT and the magnetic trap. A Photometrics CCD camera was used to image the fluorescence image of the EMTRAP through a suitable lens system. The data describing the loading of the trap with the skimmer has been discussed in section 4.3. The data describing the number of $^6$Li atoms trapped in the EMTRAP, as well as temperature and collisional loss, is discussed in chapter 6.

In order to simultaneously trap both $^6$Li and $^7$Li, we need to develop more laser systems. Our current plan is to develop a semiconductor laser system which will be used to form the $^6$Li frequencies. Dye lasers will be used with $^7$Li. Since the D1 structure of $^7$Li is within 5 $\Gamma$ of the $f = 1/2$ D2 line of $^6$Li, we will need to trap $^6$Li using the D2 line on the $f = 3/2$ state and the D1 line on the $f = 1/2$ state. Since this frequency separation is about 10 GHz, we plan to use two diode lasers that are locked to each frequency. We have done a preliminary test of the D1D2 MOT of $^6$Li using two dye lasers and find that the MOT performs as well as the pure D2 MOT described above. The fluorescence levels were the same and the loading rate appeared the same. The lack of a suitable lock system prevented us from collecting quantitative numbers, densities, etc.

4.6.2 Tunable heat pipe lock

After our initial studies with $^6$Li, we have moved on to trapping and cooling $^7$Li. In order to obtain optimal performance with the $^7$Li trap, we had to modify the heat pipe lock so that the MOT detuning could be actively changed while transferring to the EMTRAP. This was done by introducing a double-pass AO into the heat pipe so
that the relative frequency of the main laser to the saturated absorption signal could be moved without walking the beam alignment in the heat pipe. Figure 4.28 shows the double pass AO heat pipe system. The initial AO shifts the incoming beam red by 80 MHz. This beam is then doubly passed blue through the second AO which is modulated at a frequency of 78 MHz. The double-passed beam is then used for the saturation absorption in the lock.

The absorption signal is obtained by splitting the double-passed beam into a weak probe beam and a stronger pump beam. A half-wave plate is used to make the polarizations of the two beams orthogonal so that the photodiode detector is
only sensitive to the probe beam. The probe beam is then passed through an EO which puts 10 MHz sidebands on it. Both this modulated probe beam and the pump beam are overlapped in the pipe as shown in figure 4.28. Normally these two beams are resonant with different velocity groups within the pipe since the Li vapor has a sizeable Doppler width. This results in the probe being predominantly absorbed before reaching the photodiode detector. However, for atoms with zero velocity with respect to the beams, the probe beam and the pump beam can become resonant with the same atoms. When this occurs, the pump beam saturates the atoms leaving the probe beam unabsorbed. This provides a Doppler-free signal of the resonant line of the atoms which should be limited only by the natural linewidth of the atom, about 6 MHz.

The sideband structure of the probe is of the order of this width and helps to provide an error signal which can be fed back to the laser to lock it. As the probe goes through resonance, the sidebands are absorbed by different amounts resulting in an intensity beat at the photodiode. An rf-mixer is used to detect the phase of this beat with respect to the EO modulation frequency. When the laser is on resonance, the mixer output is zero since each sideband is absorbed equally. When the laser is slightly off resonance, the mixer output will be non-zero and either negative or positive depending on whether the negative or positive sideband is absorbed more (hence this signal is a measure of the detuning of the probe from resonance). The details of this detection circuitry is discussed in reference [28]. The mixer output can be directly integrated and negatively fed back to the laser to keep it on resonance in the pipe.

When the laser is locked, the frequency of the working beam is detuned from the resonance line in the lock by an amount determined by the two AOs. We assume that the pump/probe is on the $2S \ f = 2 \rightarrow 2P_{3/2}$ resonance. The excited state hyperfine structure of the $2P_{3/2}$ state for $^7$Li is 18.1 MHz wide and is composed of $f = 0, 1, 2, 3$
states [114]. The various hyperfine lines cannot be resolved in the heat-pipe lock (see figure in appendix of reference [28]). The cycling transition, \( 2S \ f = 2 \rightarrow 2P_{3/2} \ f = 3 \), sits 6.5 MHz red of the average transition (center-of-gravity for \( 2S \ f = 2 \rightarrow 2P_{3/2} \ f = 3, 2, 1 \)). We are unable to realize a pure cycling transition in our experiments due to the low magnetic field of the trap. As a result, the center-of-gravity (\( \nu_{\text{resonance}} \)) proves to be a suitable reference for our detunings. Considering the AO offsets, this puts the laser detuning at,

\[
\nu_{\text{laser}} = \nu_{\text{resonance}} + 80 - 2 \times 78 \ \text{MHz}.
\]  
(4.12)

which implies a relative detuning of the laser to be,

\[
\nu_{\text{laser}} - \nu_{\text{resonance}} = -76 \ \text{MHz}.
\]  
(4.13)

Given that the MOT beams are switched on/off with a 40 MHz switching AO (blue band), this gives a MOT detuning of \( 40 - 76 \ \text{MHz} = -6\Gamma \) which has experimentally been the optimal detuning to run the trap at. The double pass AO has an analog voltage input which can be used to adjust the 78 MHz setting and so consequently can be used to dynamically change the trap detuning. The measured time response for moving the lock point is about 10-12 ms.

4.6.3 \( ^7\text{Li} \)

For operating the \( ^7\text{Li} \) trap, we currently use two dye lasers to generate the proper frequencies. The Coherent 699 is used to form the MOT beams, the 2D-MOT beams, and the probe beams. The Spectra-Physics dye laser provides the Zeeman slowing beam. Figure 4.29 shows the basic layout. The Coherent laser is locked to the heat pipe on the \( 2S \ f = 2 \rightarrow 2P_{3/2} \) line and the main beam passes through a 812 MHz EO which provides the needed \( f = 1 \) sideband (803.5 from the ground splitting plus the difference due to the excited state hyperfine structure). The heat pipe lock is set to 76 MHz red as explained previously. The beam continues on to a 40 MHz switching
Figure 4.29  $^7$Li laser system.
AO where the blue sideband is used for creating the MOT beams and the 2D-MOT beams; a 70/30 beam splitter is used to split off the appropriate power for each one. The MOT has been reconfigured so that the three orthogonal beams are no longer retro-reflected. Instead, 50/50 beam splitters are used to generate six independent beams whose polarizations are properly prepared for the MOT. The original spatial filter used for $^6$Li has since been replaced with an optical fiber which eliminates any walking of the beam during peaking.

The primary beam through the 40 MHz switching AO is used to generate an appropriate absorption probe. This beam passes through another AO that is operated at around 76 MHz just like the set-up with $^6$Li. The blue sideband is then fed into an optical fiber and used as an absorption beam which passes directly through the trap region and is imaged onto the CCD camera through an appropriate imaging system. In order to get fluorescence images of the EMTRAP, we can now turn off the MOT, move the heat pipe lock to change the detuning to resonance while the atoms are trapped, and then flash the MOT beams briefly. In order to help with optical cooling prior to transfer to the EMTRAP, both the MOT intensity level and the MOT detuning can now be dynamically changed with this optical set-up. We routinely peak these ramp parameters in order to optimize the temperature and the numbers of atoms which are transferred to the EMTRAP. The details of the transfer procedure and data describing the traps are presented in chapter 6.

The Zeeman slowing beam is generated with the Spectra-Physics dye laser. The beam is first passed through a 804 MHz EO in order to provide a re-pumping side-band in the beam. Normally one would think to use 812 MHz since this would take into account the excited state hyperfine structure, but we have found that 804 MHz performs slightly better (about 3%). The slower works best when the entire beam sits about 1.25 GHz red of the atomic transition. We currently peak this by hand and have no formal means of locking the frequency to the heat pipe reference. The
Zeeman slower itself is composed of a main solenoid coil and a trim coil. The details of its construction are located in references [100, 101]. We run the main at 10 A and the trim at 2 A.

As a final note, the atoms in the EMTRAP are quite sensitive to stray, near-resonant light. In order to achieve long trap lifetimes for the EMTRAP, we have found that mechanical shutters are very important for turning off the various beams. A complicated system of computer timing and digital TTL signals are used to trigger the various AOs, EOs, voltage ramps, and shutters.
Chapter 5
Evaporative Cooling

Evaporative cooling is a necessary and critical step towards achieving a quantum degenerate gas. The phase space density of the Li gas in the magneto-optical trap (MOT) is about 5 to 6 orders of magnitude away from degeneracy. After transferring to the electromagnetic trap (EMTRAP), evaporative cooling can increase the phase space density to unity. The principle of evaporative cooling is straightforward and relies on two requirements. First, one must be able to preferentially remove the "hottest" atoms in the trap, those atoms whose energy is significantly higher than the mean energy. Second, there must be some sort of interaction, typically elastic collisions, which allows the ensemble of atoms to thermalize and achieve equilibrium. Figure 5.1 shows how these two processes can reduce the mean energy, or temperature, of the gas. We are usually dealing with atoms which are confined in some type of

![Figure 5.1](image_url)

**Figure 5.1** Evaporative cooling of a distribution of atoms. In essence, one is able to remove the high-energy tail of the distribution and rely of interactions/collisions to re-thermalize the distribution. After some amount of time, the new distribution will have a lower mean energy (and so a lower temperature).
central potential \( U(r) \) which increases in value as some function of \( r \) from the trap center. In this situation, as the gas cools the remaining atoms will occupy a smaller spatial region within the trap. If the conditions are correct, even though the total number of atoms is decreasing, the peak density can increase. This in combination with the decrease in temperature can lead to an increase in phase-space density.

So how can we preferentially remove hot atoms from the EMTRAP? This is done by driving a microwave transition in the atoms. Figure 5.2 shows a harmonic trapping potential for the case of a low-field seeking atom whose spin is properly aligned. In the

![Figure 5.2](image)

**Figure 5.2** Trapping and anti-trapping potentials for RF spin-flip evaporation.

same figure, the anti-trapping potential is shown for the case where the spin has been flipped and consequently the atom is now high-field seeking. As atoms move back and forth within the potential, the most energetic atoms will climb the highest up the sides of the potential well. From the figure, one can see that there is a unique microwave transition which will only couple to those atoms. In this fashion, we can selectively remove these atoms, and then rely on elastic collisions between the remaining atoms to cool the sample.

In our apparatus, an exposed piece of coaxial cable is used to drive these transitions. This small linear antenna runs between one of the electromagnetic coil forms and the large re-entrant chamber window. The exposed section of the antenna is
about 2 cm long and runs just along the side of the central hole of the delrin coil form (see figure 4.8). Both ends of the antenna are brought out to the mounting plate of the coil and have BNC connections which allow us to connect the RF supply as well as a choice of termination. We have found that no termination (infinite resistance) gives the best coupling. Table 5.1 shows the coupling we have measured for various microwave frequencies (no termination). This antenna therefore sits between 1 to 1.5

<table>
<thead>
<tr>
<th>Frequency (MHz)</th>
<th>Power in (W)</th>
<th>Power Reflected (W)</th>
</tr>
</thead>
<tbody>
<tr>
<td>800</td>
<td>3</td>
<td>1</td>
</tr>
<tr>
<td>300</td>
<td>3</td>
<td>3/4</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>1/2</td>
</tr>
</tbody>
</table>

Table 5.1 RF antenna coupling efficiencies with no termination.

cm away from the trap region.

One of the first steps in RF evaporation is to determine how much RF power is needed. One can assume a transition rate and calculate the needed power. The Rabi frequency $\Omega$ of the M1 transition goes like,

$$\Omega = \frac{\mu B}{\hbar} = \frac{1}{100 \ \mu s}, \quad (5.1)$$

where $\mu$ is the atomic magnetic moment, $B$ is the magnetic field, and we assume to drive the transition in 100 $\mu$s. Is this a reasonable rate? There are two timescales to consider: the oscillation period of the atoms in the trap, and the collision rate. We want the RF transition to be "quick" on both these timescales. For $^7$Li, the axial trapping frequency is 42 Hz giving a period of 24 ms; the radial response is up to eight times faster ($\sim 3$ ms). As for considering the collision rate, let us assume that the atomic cloud ($^7$Li) has a density $n = 10^{12}$ cm$^{-3}$ and is at a temperature of $T = 5 \mu K$, the collision rate goes like,

$$n\sigma v = 4.2 \ s^{-1}, \quad (5.2)$$

where $\sigma = 5.4 \times 10^{-13}$ cm$^2$ is the elastic cross section and the thermal velocity for $5 \mu K$ is 7.7 cm/s. It seems that a 100 $\mu s$ M1 rate is more than reasonable.
Assuming this rate, this gives a needed magnetic field of about 1 mG at the trap. The magnetic field from the line antenna is approximately,

\[ B(r) = \frac{\mu_o I}{2\pi r} , \tag{5.3} \]

where \( \mu_o = 4\pi \times 10^{-7} \text{ Ns}^2/\text{C}^2 \) is the magnetic permeability of free space, and \( r \) is the distance from the antenna to the trap region. Assuming that \( r = 1.5 \text{ cm} \), a current of 8 mA is needed to generate the 1 mG magnetic field. If we then assume that the antenna is a 50 \( \Omega \) load (not a great assumption, but we are dealing with an order-of-magnitude argument), this gives an RF power of 3.5 mW for the antenna. Suppose we want to drive the transition 10 times faster, this gives a needed power of 350 mW. This agrees well with the experimental observation of needing a few hundred milliwatts; especially considering that we do suffer from having a non-50 \( \Omega \) antenna which does not couple well to the RF supply. Also, the finite length of the antenna would cause field fringing which would make the effective magnetic field at the trap weaker than what I have calculated here.

Given that we have enough RF power, the next step is to calculate the most efficient and quickest way of moving the RF razor (as we call it) through the trap and increasing the phase space density. This chapter is concerned with calculating the trajectory of this razor specifically for the Ioffe trap discussed in the previous chapter.

### 5.1 Boltzmann Equation

In order to model the behavior of a classical gas undergoing evaporation, we must resort to using the Boltzmann equation [2, 106]. In general, a gas such as this is described by a phase space distribution function \( f(\vec{r}, \vec{p}) \) which is normalized in such a way that,

\[ N = \frac{1}{(2\pi \hbar)^3} \int d^3r \ d^3p \ f(\vec{r}, \vec{p}) , \tag{5.4} \]
where $N$ is the total number of atoms. The dynamic evolution of this function is described by the Boltzmann equation,

$$
\left( \frac{\vec{p}}{m} \cdot \vec{\nabla}_r - \vec{\nabla}_p \cdot \vec{U} + \frac{\partial}{\partial t} \right) f(\vec{r}, \vec{p}) = I(\vec{r}, \vec{p}) - G(\vec{r}) f(\vec{r}, \vec{p}) ,
$$

(5.5)

where the term $I(\vec{r}, \vec{p})$ is the collision integral with the form,

$$
I(\vec{r}, \vec{p}_1) = \frac{\sigma}{(2\pi \hbar)^3 2\pi m} \int d^3 p_2 d^3 p_3 d^3 p_4 \delta^3(\vec{p}_1 + \vec{p}_2 - \vec{p}_3 - \vec{p}_4) \\
\times \delta(E_1 + E_2 - E_3 - E_4) [f(\vec{r}, \vec{p}_3)f(\vec{r}, \vec{p}_4) - f(\vec{r}, \vec{p}_1)f(\vec{r}, \vec{p}_2)] ,
$$

(5.6)

where $E_i = p_i^2/2m$. This collision integral describes only two-body processes. The number of atoms represented by $f(\vec{r}, \vec{p}_1) \equiv f_1$ can increase due to collisions between atoms in $f_3$ and $f_4$ which give products $f_1$ and $f_2$. Likewise, collisions between atoms in $f_1$ and $f_2$ can give products $f_3$ and $f_4$, leading to loss in the $f_1$ distribution. Both these contributions are accounted for in the collision integral as well as momentum conservation and energy conservation. The elastic cross section for the collision is given by $\sigma$.

The second term, $G(\vec{r})$, is a loss term. This has the form,

$$
G(\vec{r}) = G_1 + \frac{G_2}{(2\pi \hbar)^3} \int d^3 p f(\vec{r}, \vec{p}) ,
$$

(5.7)

where $G_1$ accounts for background loss collisions that are independent of density, and $G_2$ is the rate of density dependent dipolar loss (since a dipolar process removes 2 atoms from the trap, $G_2 = 2 \times G_{\text{dipolar}}$) [28].

In order to simplify the Boltzmann equation, one can make the assumption that the motion of the atoms is ergodic. In this sense, the behavior of a given atom is completely determined by its energy. The possible values of $\vec{r}$ and $\vec{p}$ are completely random and equally weighted. This is especially true when the degrees of freedom of the gas are allowed to mix either by anisotropy in the trap potential or by interatomic collisions. This is a good assumption for our system and it helps us to rewrite the
distribution function as,

$$f(\vec{r}, \vec{p}) = \int dE \, \delta \left( U(\vec{r}) + \frac{p^2}{2m} - E \right) f(E) ,$$  \hspace{1cm} (5.8)

where $f(E)$ is the occupation number for trap eigenstates with energy $E$. The number of atoms with energy between $E$ and $E + dE$ is,

$$\rho(E) \, f(E) \, dE ,$$  \hspace{1cm} (5.9)

where $\rho(E)$ is the density of states [2, 106]. By taking the Boltzmann equation, multiplying by $\delta(E - U(\vec{r}) - \frac{p^2}{2m})$ and integrating over $\vec{r}$ and $\vec{p}$, we find the new energy-dependent form of the Boltzmann equation to be,

$$\rho(E_1) \frac{\partial f(E_1)}{\partial t} = I(E_1) - G(E_1) \rho(E_1) f(E_1) ,$$  \hspace{1cm} (5.10)

where we have used the definition of the energy density of states,

$$\rho(E) = \frac{1}{(2\pi\hbar)^3} \int d^3r \, d^3p \, \delta \left( E - U(\vec{r}) - \frac{p^2}{2m} \right) .$$  \hspace{1cm} (5.11)

The collision integral $I(E)$ has been fully treated in both references [106] and [28]. Rather than re-work the math, I will just present the result,

$$I(E_1) = \frac{m\sigma}{\pi^2\hbar^3} \int dE_2 \, dE_3 \, dE_4 \, \rho(E_{\text{min}}) \delta(E_1 + E_2 - E_3 - E_4) \times [f_3f_4 - f_1f_2] .$$  \hspace{1cm} (5.12)

The energy $E_{\text{min}} = \min\{E_1, E_2, E_3, E_4\}$.

The two-body portion of the loss term $G_2(E)$ requires some work as well which I will outline briefly. I am interested in finding an expression for $\rho(E)G_2(E)$. This can be written out as,

$$G_2(E)\rho(E) = \frac{1}{(2\pi\hbar)^3} \int d^3r \int d^3p \, G_2(r) \delta(H(\vec{r}, \vec{p}) - E) ,$$  \hspace{1cm} (5.13)

where $H(\vec{r}, \vec{p}) = \frac{p^2}{2m} + U(\vec{r})$. Substituting in $G_2(r)$ we find,

$$G_2(E)\rho(E) = \frac{1}{(2\pi\hbar)^3} \int d^3r \int d^3p \, \delta(H(\vec{r}, \vec{p}) - E) \frac{G_2}{(2\pi\hbar)^3} \int d^3p' \, f(\vec{r}, \vec{p'}) ,$$  \hspace{1cm} (5.14)
where a substitution for the distribution function \( f(\vec{r}, \vec{p}) \) in terms of energy gives,

\[
G_2(E)\rho(E) = \frac{G_2}{(2\pi\hbar)^6} \int dE' f(E') \int d^3r \int d^3p \int d^3p' \times \delta \left( \frac{p^2}{2m} + U(\vec{r}) - E \right) \delta \left( \frac{p'^2}{2m} + U(\vec{r}) - E' \right).
\] (5.15)

Now I use the delta-function properties,

\[
\delta \left( \frac{x}{a} \right) = a\delta(x) \quad (5.16)
\]
\[
\delta(x^2 - a^2) = \frac{\delta(x - a) + \delta(x + a)}{|2a|} \quad (5.17)
\]

which enables me to arrive at the equation (with some integration),

\[
G_2(E)\rho(E) = \frac{G_2(4\pi)^22m^3}{(2\pi\hbar)^6} \int dE' f(E') \int d^3r \sqrt{E - U(\vec{r})}\sqrt{E' - U(\vec{r})}.
\] (5.18)

At this point, the specific potential and density of states for the Ioffe trap needs to be introduced.

### 5.2 Ioffe-Pritchard Trap

The method used to numerically solve the Boltzmann equation and derive the evaporation trajectories is identical to the method described previously in our lab [28]. Those techniques were developed for describing evaporation in a nearly spherical 3D harmonic trapping potential. In contrast, the electromagnetic trap is an Ioffe trap which has a significantly different potential that requires a re-working of the previous numerical procedures.

A working approximation of the Ioffe potential with regards towards calculating evaporation properties has been discussed in reference [106]. The Ioffe trapping potential is described to a good approximation by,

\[
U(\vec{r}) = \sqrt{a^2r^2 + (U_o + \beta z^2)^2 - U_o}.
\] (5.19)
where I have explicitly used cylindrical coordinates. Near the origin for energies much smaller than the bias energy $U_o$, the potential appears harmonic. At larger energies and/or further from the origin the potential appears to be linear in the radial direction and harmonic in the axial dimension. The symmetry of the potential model does not give rise to ergodic motion, but it should closely model the actual potential which will give rise to ergodic motion due to asymmetries in the actual field as well as collisional interactions. Using this model potential, Walraven and associates [106] find that the density of states for an Ioffe trap is,

$$\rho(E) = A_{1Q}(E^3 + 2U_oE^2), \quad (5.20)$$

where

$$A_{1Q} = \frac{(2m\pi^2)^{3/2}}{(2\pi\hbar)^{3/2} \alpha^2 \beta^{1/2}}. \quad (5.21)$$

Another important quantity that is needed to simplify the loss term $G_2(E)$ is the potential-energy density of states $\tilde{\rho}$ [106],

$$\tilde{\rho}(U') \equiv \int d^3r \delta(U' - U(r)) \quad (5.22)$$

where for the Ioffe potential,

$$\tilde{\rho}(U) = \frac{4\pi}{\alpha^2 \beta^{1/2}} \left(U^{3/2} + U_o U^{1/2}\right). \quad (5.23)$$

I will show how this simplifies $G_2(E)$ in a moment.

In describing the EMTRAP, we use three different quantities. The first is the axial harmonic trapping frequency $\omega_z$, where $\omega_z$ is expressed as an angular frequency ($\omega_z = 2\pi \nu_z$). This is related to $\beta$ by the relation $\beta = (1/2)m\omega_z^2$. The second quantity is the linear magnetic field gradient in the radial direction, $B'_r = \partial B/\partial r$. This is related to $\alpha$ by the relation $\alpha = \mu B'_r$ where $\mu$ is the atomic magnetic moment. The final descriptive quantity is the bias field energy given by $U_o = \mu B_o$ where $B_o$ is the magnetic field bias at the bottom of the potential well. Substituting all of this into
the above expressions for $A_{1Q}$ and $\rho(E)$ gives a density of states for the Ioffe trap which is dependent on the measurable quantities $\omega_2$, $B'_r$, and $B_o$. Table 5.2 shows the pertinent quantities for our trap assuming that atoms are trapped in the stretched state ($(f, m_f) = (2, 2)$ for $^7\text{Li}$ and $(3/2, 3/2)$ for $^6\text{Li}$).

<table>
<thead>
<tr>
<th>$\omega_2$</th>
<th>$2\pi \cdot 45\text{ Hz}$ for $^7\text{Li}$ ($2\pi \cdot 45\text{ Hz}$ for $^6\text{Li}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$B'_r$</td>
<td>110 G/cm</td>
</tr>
<tr>
<td>$B_o$</td>
<td>from 0 G to 100 G</td>
</tr>
</tbody>
</table>

**Table 5.2** Ioffe trap parameters for the EMTRAP assuming atoms are in the stretched state.

Given the form of the density of states $\rho(E)$, the potential-energy density of states $\rho(\bar{U})$, and the potential energy $U(\bar{r})$, we can now finish calculating the two-body dipolar loss term in the Boltzmann equation. In the previous section, I showed that,

$$G_2(E)\rho(E) = \frac{G_2(4\pi)^2 2m^3}{(2\pi \hbar)^6} \int dE' f(E') \int d^3r \sqrt{E - U(\bar{r})} \sqrt{E' - U(\bar{r})}.$$  \hspace{1cm} (5.24)

By using the potential-energy density of states $\rho(U)$, one can show that the three-dimension spatial integral of a function $F(U(\bar{r}))$ can be re-written into a one-dimension integral of energy $U$ only [106],

$$\int d^3r F(U(\bar{r})) = \int dU F(U) \rho(U).$$  \hspace{1cm} (5.25)

This enables me to re-write $G_2(E)\rho(E)$ as follows,

$$G_2(E)\rho(E) = \frac{2m^3(4\pi)^3G_2}{\alpha^2 \beta^{1/2}(2\pi \hbar)^6} \int dE' f(E') \sqrt{EE'} \times \left[ \int dU U^{3/2} \sqrt{1 - \frac{U}{E} \sqrt{1 - \frac{U}{E'}} + U_o \int dU U^{1/2} \sqrt{1 - \frac{U}{E} \sqrt{1 - \frac{U}{E'}}} \right].$$  \hspace{1cm} (5.26)

In order for the integration to be real-valued, the upper limit for $U$ must be $U < \min\{E, E'\}$. By letting the variable $z = U/E_<$ where $E_\prec = \min\{E, E'\}$ (and $E_\succ = \max\{E, E'\}$)
\[ G_2(E) \rho(E) = \frac{2m^3G_2}{\alpha^2 \beta^{1/2} \pi^3 \hbar^6} \int_0^\infty dE' f(E') \left[ E'^{7/2} h_1(x) + U_0 E_<^{5/2} h_2(x) \right], \quad (5.27) \]

where,

\[ h_1(x) = \int_0^1 dz \ z^{3/2} \sqrt{1 - z \sqrt{x - z}} \quad (5.28) \]
\[ h_2(x) = \int_0^1 dz \ z^{1/2} \sqrt{1 - z \sqrt{x - z}}. \quad (5.29) \]

The \( h_1 \) and \( h_2 \) functions can be numerically calculated and stored in a look-up table to use in the integration of the Boltzmann equation.

### 5.3 Numerical Procedure/Optimization

To numerically solve this problem, the distribution function \( f(E) \) is discretized. The numerical integrator which was previously developed in [28] uses a discrete energy grid of about 200 points with the highest energy corresponding to roughly \( 15k_B T \). The discretized Boltzmann equation is,

\[ \rho_i \dot{f_i} = \frac{m \sigma \Delta^2}{\pi^2 \hbar^3} \sum_{k,l} \rho_h [f_{ik} f_i - f_{ij} f_j] - \rho_i G_i, \quad (5.30) \]

where energy conservation requires that \( j = k + l - i \) and \( h = \min\{i, j, k, l\} \). The parameter \( \Delta \) is the discrete energy spacing of the grid. Evaporative cooling is modelled by setting \( f(E) = 0 \) above some cutoff energy \( E_T \). As the gas cools, the energy grid spacing \( \Delta \) is dynamically reduced. The problem of breaking the discretized Boltzmann equation into pieces which can be numerically handled is no small task. The condition on index \( h \) as well as the necessity of keeping \( j = k + l - i \) introduces singularities in the functions that must be excluded from the numerical summation.

In order to aid further refinement of the evaporation code, I will explicitly show the various expressions which exclude the singularities.
The populating terms are those terms which increase \( f_i \) and which are the various \( f_k f_l \) terms from the discrete equation. The populating terms are,

\[
\rho_1 \dot{f}_1 \bigg|_{\text{pop}} = 2A \int_{k_1/2}^{k_1} \int_{k_1 - k_3}^{k_3} \int_{k_1}^{k_4} \rho_2 \rho_3 f_4 \\
+ 2A \int_{k_1}^{n} \int_{k_1}^{k_3} \int_{k_1}^{k_4} \rho_4 f_3 f_4 + 2A \int_{k_1}^{n} \int_{k_1}^{k_3} \int_{k_1}^{k_4} \rho_1 f_3 f_4, \tag{5.31}
\]

where \( A = m\sigma \Delta^2/(\pi^2 k^3) \) and \( n \) is the grid size.

The de-populating terms decrease \( f_i \) and are the various \(-f_i f_j\) terms from the discrete equation. These terms are,

\[
\rho_1 \dot{f}_1 \bigg|_{\text{depop}} = -Af_1 \int_{0}^{k_1} \int_{0}^{k_2} \int_{0}^{k_3} df_2 \int_{0}^{k_3} \rho_3 - Af_1 \int_{0}^{k_1} \int_{0}^{k_2} \int_{0}^{k_3} \rho_4 \\
- Af_1 \int_{0}^{k_1} \int_{0}^{k_2} \int_{0}^{k_3} \rho_2 \rho_3 - Af_1 \int_{0}^{k_1} \int_{0}^{k_2} \int_{0}^{k_3} \rho_3 \\
- Af_1 \int_{0}^{k_1} \int_{0}^{k_2} \int_{0}^{k_3} \rho_4 - Af_1 \int_{0}^{k_1} \int_{0}^{k_2} \int_{0}^{k_3} \rho_1, \tag{5.32}
\]

which can be further simplified. The density of states has the form \( \rho(k) = \tilde{A}[k^3 + 2\mu B_s k^2 / \Delta] \) where \( k \) is an integer index such that the energy \( E_k = \Delta k \). Using this expression, and doing some algebra one finds that,

\[
\dot{f}_1 \bigg|_{\text{depop}} = -Af_1 \int_{0}^{k_1} \int_{0}^{k_2} \int_{0}^{k_3} \left[ \frac{k_1^2}{2 \Delta} + \frac{4\mu B_s k_1^2}{3 \Delta} \right] + \frac{\rho_2}{\rho_1} (k_1 - k_2) \\
-Af_1 \int_{0}^{k_1} \int_{0}^{k_2} \int_{0}^{k_3} \left[ \frac{k_1^2}{2 \Delta} + \frac{4\mu B_s k_1^2}{3 \Delta} \right] + (k_2 - k_1) \tag{5.33}
\]

In order to optimize the RF razor trajectory, we must dynamically move the cutoff point in the model (\( E_T \)) in such a way as to maximize the decrease in temperature while reducing the total number of atoms. The best way we have found to do this, requires optimizing the trajectory locally while the integration is being carried out \([116]\). This has been discussed and analyzed in detail in a previous thesis \([28]\) so I will only present the result. The instantaneous efficiency of evaporation is defined to be,

\[
\epsilon = -\frac{N}{\rho} \frac{d\rho}{dN}, \tag{5.34}
\]
where \( N \) is the total number of atoms in the trap and \( \rho \) is the phase space density given by \( \rho = n_o \Lambda^3 \) (\( n_o \) is the peak density and \( \Lambda \) is the de Broglie wavelength). By noting that \( \rho \propto N^4/E_{tot}^3 \) where \( E_{tot} = N\langle E \rangle \) is the total energy in the trap, we find that,

\[
\epsilon = 3 \frac{N}{E_{tot}} \frac{dE_{tot}}{dN} - 4.
\]

(5.35)

So the efficiency in the evaporation can be optimized by trying to optimize the quantity \( dE_{tot}/dN \) which is found in terms of time derivatives to be,

\[
\frac{dE_{tot}}{dN} = \frac{dE_{tot}/dt}{dN/dt},
\]

(5.36)

where the respective time derivatives can be easily calculated during the run-time of the Boltzmann equation integration.

### 5.4 Trajectories

Now that the Boltzmann equation can be numerically solved while optimizing the evaporation razor, we are now in a position to calculate various evaporation trajectories in order to find the optimal conditions for achieving a quantum degenerate gas in the EMTRAP. In the following figures, I will point out the sensitivity of evaporation to bias field, trap lifetime, initial number, and initial temperature. I have calculated these trajectories at a variety of conditions and not necessarily the ones which correspond to our current EMTRAP. This should give the reader an idea as to what initial conditions will work and which ones cannot.

Given our current trap conditions, we can now surmise what minimum number and maximum temperature are initially needed in the EMTRAP in order to achieve quantum degeneracy. Our best background pressure yields a one-body decay rate of about 400 s (see chapter 6). It seems reasonable to operate the trap around 5 G which is a small bias, and yet should be larger than any possible stray fields which could introduce a “hole” in the trap. Careful adjustment of the nulling cage and bias together
Figure 5.3  Evaporation as a function of bias field. These trajectories assume an initial number of $2 \times 10^9$ atoms, an initial temperature of 700 $\mu$K, and a background loss rate of 250 sec.
Figure 5.4  Evaporation as a function of trap lifetime (one body loss). These trajectories assume an initial number of $2 \times 10^9$ atoms, an initial temperature of 700 $\mu$K, and a bias field of 15 G.
Figure 5.5  Evaporation as a function of initial number. These trajectories assume an initial temperature of 700 $\mu$K, a background loss rate of 250 sec, and a bias field of 5 G.
Figure 5.6  Evaporation as a function of initial temperature. These trajectories assume an initial number of $2 \times 10^9$ atoms, a background loss rate of 400 sec, and a bias field of 5 G.
can yield bias fields on the order of 2 G and is the subject of current investigation. From studying the results of the evaporation modelling, it appears that having about $2 \times 10^9$ atoms in the EMTRAP at a temperature of about 700 $\mu$K should be sufficient to achieve quantum degeneracy in about 200 s of evaporation. Figure 5.7 shows a trajectory which could achieve this based upon our current EMTRAP conditions as reported in chapter 6.

5.5 Sympathetic Cooling

In order to eventually realize sympathetic cooling of $^6$Li, we will need to modify the evaporation trajectories and therefore the evaporation code. Since we will be preferentially removing $^7$Li from the dual-species EMTRAP, we will work on loading a significantly larger amount of $^7$Li compared to $^6$Li. In the initial stages of cooling, the thermodynamics of the dual-species cloud will be dominated by the dynamics and thermal properties of the $^7$Li. The cross-species scattering length for the stretched states of $^7$Li and $^6$Li is 40 Bohr (see chapter 3). This should lead to rapid thermalization of the $^6$Li cloud since this scattering amplitude is larger than the $^7$Li-$^7$Li scattering length of -27 Bohr. At least initially, the evaporation will follow the results obtained for modelling the pure $^7$Li system.

Problems will start to occur as the number of $^7$Li atoms becomes comparable to the amount of $^6$Li present. In this regime, I think the only proper way to model the evaporation will be to explicitly include the $^6$Li into the Boltzmann equation model. To do this, it seems that two coupled, distribution functions will need to be treated. There will be a distribution function $f^{(7)}(E)$ for describing the $^7$Li, and there will be a corresponding $f^{(6)}(E)$ for describing the $^6$Li. I envision two Boltzmann equations which would describe the evolution of either distribution, but there would also be additional "cross terms" which would describe the interchange of energy between the two distributions as a result of the inter-species collisions. I think the exact treatment
Figure 5.7  Trajectory for evaporating $2 \times 10^9$ atoms at 700 µK with a 5 G bias field and a background loss rate of 400 sec. The decrease in the optical density at $t > 190$ s occurs at a point where the size of the cloud radially ($r_\phi$) is decreasing faster than the increase in the peak density ($n_\phi$); $|dr_\phi/dt| > |dn_\phi/dt|$. This is a result of the evaporation having to accelerate in order to minimize two-body dipolar loss.
of this will be a non-trivial and interesting topic of future study.
Chapter 6
Experimental Data

In this chapter I will present the current information we have for characterizing the magneto-optical trap (MOT) and the electromagnetic trap (EMTRAP) for each lithium isotope. Ultimately we will need to have both isotopes simultaneously trapped in order to cool the fermion $^6$Li down to degeneracy. Historically, $^6$Li was the first isotope successfully transferred to the EMTRAP. In doing this we were able to test the performance of our magnetic guiding source (the skimmer) which was discussed in detail in chapter 4. Since that time, we have been working on trapping and cooling as much $^7$Li as possible since it will be the main component of the evaporative/sympathetic cooling. The results for both isotopes will be presented as well as our first measurements of spin-exchange decay and how it compares with the theoretical predictions discussed in chapter 2.

6.1 $^6$Li MOT

One of the first things we did with $^6$Li was to load the magneto-optical trap. We used the skimmer for this study and found it to be a suitable source for future experiments. We characterized the MOT by measuring the fluorescence level with a calibrated photodiode detector. This photodiode detector was originally built by Nicholas Ritchie and is described in his PhD thesis [117]. It has a Corion 671 nm bandpass filter (50% transmission at 670.8 nm, 11 nm FWHM) mounted on its face. Nicholas originally calibrated the photodiode with a UDT Model 61 optometer. A set of neutral density filters were calibrated to attenuate the range of powers measurable with the UDT to those measurable by the photodiode detector. I have since re-checked the calibration in a similar fashion and found it to be the same. The amplifier circuit that is part of the photodiode box has a 1 ms response time, and I have added
a divide-by-10 switch to the box in the event that the amplifier is saturated. For these studies, the original gain was used and the detector had a sensitivity rating of $S = 2.5 \pm 0.2 \times 10^7$ V/W just as Nicholas had measured it.

The fluorescence signal from the MOT was collected with a suitable lens system. This consisted of a $r = 1.25$ cm radius lens ($f = 80$ mm) located $R = 18.77$ cm away from the cloud; giving a geometric collection efficiency $C = \pi r^2 / 4 \pi R^2 = 1.1 \times 10^{-3}$. We can compute the total radiated power from the cloud as a function of photodiode output voltage $V$,

$$P(V) = \frac{V}{S \cdot C} = 3.6 \times 10^{-5} \cdot V \text{ watts} . \quad (6.1)$$

The number of radiated photons/sec, $N_\gamma$, is found by dividing this by the energy-per-photon $h\nu$,

$$N_\gamma = \frac{P(V)}{h\nu} \text{ photons/s} . \quad (6.2)$$

The number of radiated photons/sec is equal to the number of excited state atoms $N_{ee}$ (assuming steady state) times the rate of spontaneous emission $\Gamma = 2\pi \times 5.9$ MHz,

$$N_{ee} = N_\gamma / \Gamma = N_\gamma \cdot \tau , \quad (6.3)$$

where $\tau = 1/\Gamma$ is the natural lifetime of the excited state. If the fraction of atoms in the excited state is $\rho_{ee}$, then the total number of atoms present is related to the number of excited state atoms by,

$$N_{tot} = \frac{N_{ee}}{\rho_{ee}} = \frac{N_{ee}(1 + 2I + 4\Delta^2)}{I} , \quad (6.4)$$

where $\rho_{ee}$ is calculated for a steady-state 2-level Rabi flopping problem where $I$ is the intensity of the driving laser (in units of saturation intensity $I_S = \Gamma^2$) and $\Delta$ is the detuning of the laser from the atomic resonance (in units of $\Gamma$) [118]. The Li saturation intensity $I_S$ for circularly polarized light is 5.1 mW/cm². This gives us a relation between the MOT parameters $(I, \Delta)$, the voltage level of the photodiode $V$,
and the total number of atoms present \( N_{\text{tot}} \),

\[
N_{\text{tot}} = \frac{1 + 2I + 4\Delta^2}{I} \cdot (3.3 \times 10^8) \cdot V .
\]

(6.5)

By measuring the beam intensity, the detuning of the MOT, and the photodiode voltage, the total number of atoms in the MOT could be determined.

For the \(^6\)Li MOT, the laser beams have two frequencies, one for driving \( f = 3/2 \) atoms and the other for driving \( f = 1/2 \) atoms (see chapter 4). The power for each of these frequencies was roughly the same, \( I_{\text{tot}} = I_{1/2} + I_{3/2} \), so we treated the atoms in the MOT as two level systems driven by \( I = I_{\text{tot}}/2 \) which is the effective power per frequency. This is a fair treatment since the total excitation strength for each ground state is the same (see figure 6.1). Since the various MOT beams were retro-reflected, there is an extra factor of two which cancels the frequency division so that the effective \( I \) used in the number calculation is simply the measured power \( I = I_{\text{tot}} \).

We typically ran the MOT with \( I = 10I_s \) and a detuning of \( \Delta = -6 \Gamma \).

For the best \(^6\)Li MOTs, we were able to load about \( 3 \times 10^8 \) atoms based on this measurement. One of the most uncertain and sensitive parameters in this analysis is the value of the detuning, \( \Delta \). Since the MOT magnetic field gradient is \( \sim 15 \text{G/cm} \), this corresponds to a spatial shift in the detuning of \( 7.1 \Gamma/\text{cm} \). A MOT which has a waist of \( \sim 3 \text{ mm} \) would have a spatial variation in \( \Delta \) of \( 2 \Gamma \). This gives a variation of \( \Delta N/N \) of 50%. There are also complications when the MOT gets very dense and optical density issues become important; in this case not all of these atoms emit photons at the same rate. Considering all of this, I think an uncertainty of 50% for our fluorescence number measurement of \( 3 \times 10^8 \) is reasonable.

To measure the temperature we studied time-of-flight images of the atoms released from the MOT. We would turn off the MOT lasers and the magnetic field, and let the cloud expand for some amount of time before flashing on a resonant probe. This probe was in a 3D molasses configuration to minimize heating of the cloud (see optical set-up in chapter 4). The pulse time was usually set to 200 \( \mu s \) during which time the
Figure 6.1  Relative transition strengths for various hyperfine levels in the $^6\text{Li}$ D2 lines. The upper diagram is for $\pi$-polarization and the lower is for $\sigma^+$-polarization. The transition strength for $\sigma^-$ can be found by using the diagram for $\sigma^+$ and replacing all the $M$’s by $-M$. The transition strength is normalized for each line so that the strength of the weakest allowed transition becomes an integer. This figure is scanned in from reference [1].
cloud does not expand much (see figure 4.16) while giving the magnetic field ample time to shut off. The fluorescence from this probe was imaged and the size of the cloud was calculated based on the magnification of the imaging system. For these studies we used a fast Pulnix CCD camera with a telescopic lens system (D.O. Industries Zoom 7000). The magnification was determined by imaging a ruler located the same distance from the lens system as the atoms. By fitting to the waist of the cloud as a function of time from release, the mean energy (and hence the temperature) could be measured.

For obtaining temperatures from a freely expanding cloud, we need to derive the functionality of cloud waist versus time of expansion. Let us consider the following. The average \( \langle r^2 \rangle \) at time \( t = 0 \) is given by,

\[
\langle r^2 \rangle_0 = \frac{1}{N} \int d^3 r \, d^3 p \, r^2 f(\vec{r}, \vec{p}, 0),
\]

for \( N \) particles described by the usual phase space distribution function. The same expectation value at later time \( t \) is given by,

\[
\langle r^2 \rangle_t = \frac{1}{N} \int d^3 r \, d^3 p \, r^2 f(\vec{r}, \vec{p}, t).
\]

If the atoms are ballistically expanding during this time, then the momentum distribution will not change while the spatial distribution is related to the \( t = 0 \) spatial distribution by the transformation \( \vec{r} \rightarrow \vec{r} + \vec{p}t/m \). This implies that \( f(\vec{r}, \vec{p}, t) \rightarrow f(\vec{r} + \vec{p}t/m, \vec{p}, 0) \). Substituting this into the above expression yields,

\[
\langle r^2 \rangle_t = \frac{1}{N} \int d^3 r \, d^3 p \, r^2 f(\vec{r} + \vec{p}t/m, \vec{p}, 0),
\]

where a change of variables gives,

\[
\langle r^2 \rangle_t = \frac{1}{N} \int d^3 r' \, d^3 p \, (r' - \vec{p}t/m)^2 f(\vec{r}', \vec{p}, 0).
\]

One can then show that,

\[
\langle r^2 \rangle_t = \langle r^2 \rangle_0 - \left( \frac{2\vec{r} \cdot \vec{p}}{m} \right)_0 + \left( \frac{p^2 t^2}{m^2} \right)_0.
\]
Now the average of $\vec{r} \cdot \vec{p}$ will be zero over the cloud since there are no correlations between the spatial and momentum degrees of freedom. Given that the spatial distribution of the cloud looks like $n(r) = n_o \exp(-r^2/w_o^2)$, simple integration shows that $\langle r^2 \rangle_0 = 3w_o^2/2$. The square of the 3D momentum is related to the temperature by $p^2/2m = 3k_B T/2$. Putting all of this together yields,

$$w(t) = w_o \sqrt{1 + \frac{2k_B T t^2}{mw_o^2}},$$

(6.11)

where $w_o$ is the waist at $t = 0$, $T$ is the temperature, $k_B$ is the Boltzmann constant, and $m$ is the mass. As the expanding cloud gets large compared to the initial waist ($w(t) \gg w_o$), the cloud waist will be a linear function of time where the slope is related to the temperature (see figure 4.16).

Our studies of the $^6$Li MOT indicated temperatures of around 1 mK. By ramping the detuning of the MOT beams towards resonance while switching down the intensity, we had been able to cool the cloud closer to the Doppler limit before transferring to the EMTRAP. Our best obtained temperatures at this point were about 300 $\mu$K with an uncertainty of $\pm 50$ $\mu$K given the limit of how far we can spatially let the cloud expand. Assuming $N = 3 \times 10^8$ and a waist of 3 mm, this corresponds to a density of $2 \times 10^9$ cm$^{-3}$.

### 6.2 $^6$Li Electromagnetic Trap

Characterization of the $^6$Li EMTRAP was done using fluorescence imaging. Since the atoms are trapped for a significant amount of time with no light present, we had the ability to use a slower, scientific grade CCD camera from Photometrics to do the imaging. In order to analyze the CCD image, we used an analysis similar to the $^6$Li MOT studies. The major difference is that the probe light we used was near resonance, so we assumed that the atoms in the cloud were saturated and that the excited state fraction was $1/2$ [118]. We used a pulse duration of around 200-250 $\mu$s
in an optical molasses configuration to minimize heating and pushing of the cloud. We found that doubling this exposure time did not significantly alter the image. The cloud was released from the EMTRAP before imaging (about 500 $\mu$s delay) in order to eliminate any Zeeman shift effects in the fluorescence rate (the cloud did not expand appreciably in this time). We know that the magnetic fields shut off completely by this time (see chapter 4). Since the probe has frequencies resonant with both ground states (see optical set-up in chapter 4) there are no optical-pumping issues to consider.

The imaging system consisted of a simple telescope with a 300 mm lens, located the same distance from the atoms, which relayed the image to a 200 mm lens that focused the image onto the CCD. These were commercial plano-convex lenses; the quality of the lenses was not important since all the images taken were of large clouds with waists ranging from 3-5 mm (the Rayleigh length of the system was found to match this distance scale). To measure the magnification, a lens is used to focus a laser beam at the trap center before entering the imaging system. By moving the lens back and forth on a translator, the imaged spot moves the same amount allowing us to determine the scale factor. We double-binned the CCD ($256 \times 256$) and found that 20.4 binned pixels was 1 mm at the trap center. This allowed us to image cloud sizes on the order of 1 cm for these studies.

The 2D image which is seen by the camera needs to be related to both the number of atoms present as well as the temperature. Consider $N$ atoms which are fluorescing due to a short pulse of near resonant light (duration $t$). The number of photons $N_{\gamma}$ produced is,

$$N_{\gamma} = N\rho_{ee}\Gamma t = \frac{N\Gamma t}{2},$$  \hspace{1cm} (6.12)

where $\Gamma$ is the spontaneous emission rate and $\rho_{ee}$ is the excited state fraction which is assumed to be 1/2 for the case of near-resonant, saturating light. Given a geometric collection efficiency ($g = 2.2 \times 10^{-4}$) for our imaging system,

$$\text{number of photons seen} = \frac{N\Gamma tg}{2}. \hspace{1cm} (6.13)$$
The geometric collection efficiency was limited by the effective aperture of the mirror used to guide the image into the CCD lens system and not the lenses (see figure 6.2). Since the mirror is at a 45° angle with respect to the chamber, its effective collecting area is ellipsoidal with a major axis of $2a = 2 \times 11.43\text{ mm}$ and a minor axis of $2b = 2 \times 6.99\text{ mm}$ at the location of the collection lens. The geometric collection efficiency is found by taking the area of this "ellipse" ($\pi ab$) and computing the fraction of the total solid angle from the atoms at the lens ($R = 300\text{ mm}$),

$$g = \frac{\pi ab}{4\pi R^2} = 2.2 \times 10^{-4}. \tag{6.14}$$
The total joules seen given the wavelength $\lambda$ of the laser light is,

$$\text{observed joules} = \frac{hc NTtg}{\lambda}.$$  \hspace{1cm} (6.15)

So the total counts seen by the CCD given that the quantum efficiency $Q = 2 \times 1.275 \times 10^{-18}$ J/count are,

$$\text{counts} = \frac{hcNTtg}{2\lambda Q}.$$  \hspace{1cm} (6.16)

The factor of 2 multiplying $Q$ takes into account the effect of a red-filter placed in front of the camera (50\% transmission). The pixel sensitivity of $1.275 \times 10^{-18}$ J/count comes from a measurement found in references [27, 28]. This is actually a little bit better than the CCD specifications which give 45\% quantum efficiency (0.45 e\^-/\gamma) with a read-out of 1.65 e\^-/count at \times4 gain (which we usually run at).

The signal on the camera is defined to be $S(x, y)$ which has the units of counts/(pixel)$^2$. The form of $S(x, y)$ is,

$$S(x, y) = S_0 \exp \left( -\frac{x^2 + y^2}{w^2} \right),$$  \hspace{1cm} (6.17)

where the cloud is symmetric (circular) since we ran our EMTRAP for these studies at bias fields of about 90 G. The large bias washed out the linear confinement of the trap resulting in a nearly spherical 3D harmonic trap (see chapter 4).

In order to obtain the number and temperature of the cloud, we would take the 2D fluorescence image $S(x, y)$ and fit it to a 2D Gaussian function using a simplex fitting routine (see appendix H) [119]. The parameters obtained from the fit were $S_0$ and $w$. The number of atoms present was found by integrating $S(x, y)$ over the entire CCD array and equating the result to the total counts seen,

$$N = \frac{2\pi \lambda Q S_0 w^2}{hcTtg}.$$  \hspace{1cm} (6.18)

To obtain the temperature, we know that the cloud shape or density profile is Gaussian for a harmonic trap and that it has the form,

$$n(r) = n_o \exp \left( -\frac{m\omega^2 r^2}{2 k_B T} \right),$$  \hspace{1cm} (6.19)
where \( n_o \) is the peak density and \( \omega \) is the trapping frequency in radians/s. We know that the trapping frequency for \(^6\text{Li}\) in this trap is \( \omega = 2\pi \nu = 2\pi \cdot 46 \text{ Hz} \) (a little different than the 45 Hz seen at lower bias fields, this is due to the fact that the bias coils are not exactly in a perfect Helmholtz configuration). The temperature was found from the waist measurement to be,

\[
T = \frac{\omega^2 \nu^2 m}{2k_B} = \frac{2\pi^2 \omega^2 \nu^2 m}{k_B}.
\] (6.20)

Our results indicate that we can trap about \( 5 \times 10^7 \) \(^6\text{Li}\) atoms (\( \pm 10\% \)) at a temperature of \( 300 \pm 50 \) \( \mu \)K. Since this measurement is near resonance with saturated beams, it does not suffer from the sensitivity to detuning like our MOT measurements. Also, the larger EMTRAP cloud has a lower density and consequently does not suffer as much from optical density effects. These numbers give a peak density of \( 5 \times 10^8 \) \( \text{cm}^{-3} \) (\( \pm 10\% \)). Our transfer efficiency from the MOT appears to be 17\% and no appreciable heating is seen since the EMTRAP is spatially large compared with the MOT. This indicates that the process of going from a tight MOT to a loose EMTRAP quickly is irreversible and lowers the phase space density (same temperature but lower density). If one were to transfer adiabatically, this would preserve phase space density and would cool the gas at the expense of lowering the spatial density. To keep the collision rate high, it is best to spatially match the EMTRAP to the MOT [107]. Our transfer efficiency is not too surprising considering that only 2-3 of the available spin states are trappable, and these states will undergo spin-exchange loss. Our analysis of this loss, as well as attempts to optically pump, are discussed in the next section.

### 6.3 \(^6\text{Li}\) Spin-exchange

One of the first things we did when transferring \(^6\text{Li}\) atoms to the EMTRAP was to measure the lifetime. Figure 6.3 shows the decay of the atoms in the EMTRAP as a function of time. Since the fluorescence measurement is destructive, each data point was taken by loading the EMTRAP, waiting the indicated time, and then flashing
the probe. The observed lifetime was about 20 seconds. This fast decay actually is a result of spin-exchange collisions and not background loss collisions. Given the large bias of the EMTRAP (90 G) for these studies, we were likely capturing 2 or 3 different spin states in the EMTRAP. Figure 6.4 shows the possible spin states in $^6$Li that can be trapped. If only the stretched state were captured, one would

![Diagram showing possible trapped states of $^6$Li at 90 G. At this magnetic field, only the three highest lying states 4, 5, and 6 are able to be trapped within the EMTRAP.](image)

expect no collisions to occur due to Fermi statistics (see chapter 2). We attempted to spin-polarize the sample through various optical pumping techniques to eliminate collisional loss but were unsuccessful. I think the main reason for this stems from our inability to maintain a well defined quantization axis over the entire cloud. The
magnetic field seen by the atoms in the trap varies in direction across the whole trapping region.

In order to verify that this was spin-exchange, the coupled-channel equations describing the system were used to calculate the dynamics of the possible spin populations. The equation describing the density of the $\kappa$ spin state is given by [33],

$$\frac{dn_\kappa}{dt} = \sum_\lambda \sum_{\{\mu\nu\}} (1 - \delta_{\kappa\lambda}) [G_{\mu\nu}^{\kappa\lambda} n_\mu n_\nu - G_{\kappa\lambda}^{\mu\nu} n_\kappa n_\lambda] ,$$  \hspace{1cm} (6.21)

where the total density of the gas is given by $n = \sum_\kappa n_\kappa$ and the various spin-exchange rates are given by $G_{xy-ab}$ (see chapter 2). Let us number the three uppermost spin states of $^6\text{Li}$, which are trapped at 90 G, by 4, 5, and 6. Through some algebra, one finds the equations for these spin states look like,

$$\dot{n}_6 = -G_{56} n_5 n_6 - G_{46} n_4 n_6$$  \hspace{1cm} (6.22)

$$\dot{n}_5 = -G_{56} n_5 n_6 - G_{45} n_4 n_5$$  \hspace{1cm} (6.23)

$$\dot{n}_4 = -G_{46} n_4 n_6 - G_{45} n_4 n_5 .$$  \hspace{1cm} (6.24)

It turns out that things get even simpler because the coupled-channel calculations show that all the different spin exchange rates at 300 $\mu$K and 90 G are about the same. I find that $G_{56} \approx G_{46} \approx G_{45} \approx 1.0 \times 10^{-9}$ cm$^3$/s. Experimentally we observed the total density $n_{\text{tot}} = n_4 + n_5 + n_6$ and $\dot{n}_{\text{tot}} = \dot{n}_4 + \dot{n}_5 + \dot{n}_6$, I can sum up these equations to get,

$$\dot{n}_{\text{tot}} = -2G[n_5 n_6 + n_4 n_6 + n_4 n_5] .$$  \hspace{1cm} (6.25)

If I assume that the initial spin populations are the same, $n_4 = n_5 = n_6 = n_{\text{tot}}/3$, then I get the equation,

$$\dot{n}_{\text{tot}} = -\frac{2}{3} Gn_{\text{tot}}^2 .$$  \hspace{1cm} (6.26)

Even with multiple spins present, the overall system behaves as a single spin state which is decaying with a fixed two-body rate. If we go back and assume that only
spin states 5 and 6 are present, we get a similar equation,

$$\dot{n}_{\text{tot}} = -\frac{1}{2} G n_{\text{tot}}^2.$$  

(6.27)

Since we observe the total number $N$ and the total peak density $n_o$, these equations can be re-written as a function of these variables. Through some integration and algebra, we arrive at,

$$\frac{\dot{N}}{N} = -\frac{G}{4\sqrt{2}} n_o \text{ spin states 5, 6}$$  

(6.28)

$$\frac{\dot{N}}{N} = -\frac{G}{3\sqrt{2}} n_o \text{ spin states 4, 5, 6}.$$  

(6.29)

So by plotting the function $\dot{N}/N$ versus $n_o$, we should see a straight line with a slope that agrees with the coupled-channel spin exchange rate. Figure 6.5 shows the data

![Graph showing the relationship between \( \frac{\dot{N}}{N} \) and peak density \( n_o \).](image)

**Figure 6.5**  Analysis of the spin-exchange rate from the $^6$Li decay data. This particular value for $G_{\text{exc}}$ assumes that only spin states 5 and 6 are trapped. The uncertainty in the value of $G_{\text{exc}}$ is about 40% depending on whether you analyze the data assuming 2 spin states or 3 spin states.

and the fit. Our fitted value for $G_{\text{exc}}$ agrees with the coupled-channel theory shown in figure 6.6.
Figure 6.6 Coupled-channel spin-exchange rates for $^6$Li $\left\{ \begin{array}{l} \frac{1}{2} \, \frac{3}{2} \, \frac{1}{2} \\ \frac{3}{2} \end{array} \right\}$ channel as a function of temperature and magnetic field. The indicated data point is our measurement with an errorbar reflecting our uncertainty in the initial spin populations. The data matches the theory for $300 \, \mu K$ and $90 \, G$ bias.
6.4 $^7$Li MOT

We have been able to achieve much larger $^7$Li MOTs with significantly more atoms than the $^6$Li MOT. This is to be expected since our source is a Zeeman slower with much larger flux rates than the skimmer. As the $^7$Li MOT is loaded, we find that the shape distorts and becomes slightly non-Gaussian to the eye. It will appear to be almost “box-like” in shape with edges defined by the edges of the various MOT beams. Part of the reason why this occurs is that the density saturates because it becomes optically thick to the laser beams. Also, as the density gets higher, one would expect radiative pressure to become a factor as atoms start to re-absorb light emitted by neighboring atoms [1]. This makes determination of the number by fluorescence difficult since an optically thick cloud will have a spatially varying excited state population ($\rho_{ee} \rightarrow \rho_{ee}(\vec{r})$). We have had to rely on absorption measurements to ascertain the number/density of the MOT.

For our absorption measurements, the MOT is turned off momentarily while a weak probe is sent through the cloud and the amount of absorption is measured with a photomultiplier tube. The probe contains only $f = 2$ light with a waist of 0.8 mm and a power of 300 nW (intensity $I = 5.9 \times 10^{-3} I_{sat}$). This probe stays on for 10 $\mu$s scattering about 1 photon per atom. We need the probe this weak in order to avoid optically pumping to the $f = 1$ state during the measurement (this measures the number of atoms in $f = 2$) Figure 6.7 shows the transition strengths for the D2 lines of $^7$Li.

The photomultiplier tube (PMT) is a Thorn-EMI Model 9828B that has been discussed in a previous thesis [117]. The PMT was measured by Nicholas to have a sensitivity of $3.0 \times 10^4$ A/W. I measured the PMT a few years ago and found it had dropped to $1 \times 10^3$ A/W. In addition, the response appears to be non-linear making the absorption measurement difficult. Nevertheless, we have been able to use the device to estimate the optical density of our MOT as I will explain shortly.
Figure 6.7 Relative transition strengths for various hyperfine levels in the $^7\text{Li} \ D_2$ lines. The upper diagram is for $\pi$-polarization and the lower is for $\sigma^+$-polarization. The transition strength for $\sigma^-$ can be found by using the diagram for $\sigma^+$ and replacing all the $M$'s by $-M$. The transition strength is normalized for each line so that the strength of the weakest allowed transition becomes an integer. This figure is scanned in from reference [1].
The absorption $A$ is a function of the optical density $\alpha$ of the cloud,

$$A = 1 - \exp(-\alpha) = 1 - \exp \left(-\sigma \int_{-\infty}^{\infty} n(x, y, z) \, dz\right),$$

(6.30)

where $\sigma$ is the light scattering cross section and the integral is essentially the column density of the gas. We find that on resonance, the cloud is optically thick and absorbs all of the probe. By detuning the probe, this decreases the scattering cross section $\sigma \to \sigma_o/(1 + 4\Delta^2)$ Using the PMT, we can determine at what detuning the optical density has become less than one (despite the poor response). By knowing how far detuned the probe laser is, one can than ascertain what the column density must be. We have found for our best MOTs that we can detune $\pm 4.5$ $\Gamma$ before the optical density becomes less than one. This gives roughly an on-resonance optical density of about 80 (in the $f = 2$ state). The on-resonance light scattering cross section is $\sigma_o = \lambda^2/\pi = 1.4 \times 10^{-9}$ cm$^2$ since the probe beam is $\pi$-polarized. The MOT size was measured with a fast CCD camera and had a waist of about 4.4 mm (it does fit reasonably well to a Gaussian despite the flat-topping of the density). Assuming a Gaussian density distribution we can estimate the peak density. For a Gaussian cloud with waist $w$, the peak column density is,

$$\int_{-\infty}^{\infty} n(0, 0, z) \, dz = n_o w \sqrt{\pi},$$

(6.31)

where $n_o$ is the peak density. Putting all of this information together, we find an expression for the peak density $n_o$,

$$n_o = \frac{(1 + 4\Delta^2) \times \alpha_o(\Delta)}{\sigma_o w \sqrt{\pi}},$$

(6.32)

where $\alpha_o(\Delta)$ is the peak optical density at detuning $\Delta$, $\sigma_o$ is the on-resonance light scattering cross section from before, and $w$ is the waist of the cloud. From our measurements, $\alpha_o \sim 1$ at $\Delta = \pm 4.5$ $\Gamma$ which gives a peak density of about $7 \times 10^{10}$ cm$^{-3}$ ($f = 2$ state). The main uncertainties with this measurement stem from
the problems with the PMT and our ability to locate the exact detuning where the optical density is unity. The uncertainty in the peak density goes like,

$$\frac{dn_o}{n_o} = \frac{8\Delta d\Delta}{1 + 4\Delta^2},$$

(6.33)

where an uncertainty in detuning of \( d\Delta = \pm 1 \Gamma \) gives a fractional uncertainty in \( n_o \) of \( \sim 0.5 \) or 50\%. This seems to be a reasonable estimate of our uncertainty.

Since the total number of atoms for a spherically symmetric Gaussian density is given by,

$$N = n_o \pi^{3/2} w^3,$$

(6.34)

we find that \( N = 3.4 \times 10^{10} \) atoms (± 50\%). Temperature measurements are made by doing time-of-flight expansions (as discussed with the \(^6\)Li data) and we find temperatures for the \(^7\)Li MOTs of about \( 1.5 \pm 0.1 \) mK.

These \(^7\)Li MOTs operate with detunings of -6 \( \Gamma \) for both the \( f = 1 \) and \( f = 2 \) light. The frequency power balance is such that 40\% of the laser power is in the \( f = 2 \) transition while 30\% is in the \( f = 1 \) (the other 30\% is in the red sideband of the EO and does not drive any transitions, this is discussed in chapter 4). We try to run as much power as possible into the MOT, typically 180 mW total power in all six beams (only about 125 mW is useful since 30\% is in an unused frequency as described).

In order to achieve colder clouds before transferring to the EMTRAP, we change some of these MOT parameters during switching. During our “MOT compression”, the power balance between the \( f = 2 \) and \( f = 1 \) light is changed as well as the detuning. During the first stage of switching, we attenuate the \( f = 1 \) sideband by a factor of 100 for 100 \( \mu s \). Next, we ramp the detuning of both the \( f = 1 \) and the \( f = 2 \) frequencies from -6 \( \Gamma \) to \( -1.5 \Gamma \) for 10 ms. While this frequency ramp is executing, we also decrease the overall intensity by a factor of 10 and hold that for about 3 ms. This achieves a temperature of about 500 ± 50 \( \mu K \) with a compressed MOT waist of 2.7 mm. However, in doing so some atoms are lost and so the total
number of remaining atoms in the compressed MOT is about $1 \times 10^{10}$ (± 50%). This corresponds to a density of $9 \times 10^{10}$ cm$^{-3}$ (± 50%). We use an optical pump pulse to quickly transfer the atoms to the $f = 2$ spin state before transferring to the EMTRAP.

The procedure for compressing the MOT is patterned after the work of Mewes et al. with Li, and the work of Ketterle et al. with sodium [120, 121]. Table 6.1 shows the results of the work with Li and how we compare. Despite the problems with the

<table>
<thead>
<tr>
<th>Our work</th>
<th>Mewes et al.</th>
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<tbody>
<tr>
<td>$^7$Li MOT</td>
<td>$^7$Li CMOT</td>
</tr>
<tr>
<td>N</td>
<td>$3.4 \times 10^{10}$</td>
</tr>
<tr>
<td>n (cm$^{-3}$)</td>
<td>$7 \times 10^6$</td>
</tr>
<tr>
<td>T ($\mu K$)</td>
<td>1500</td>
</tr>
</tbody>
</table>

**Table 6.1** Comparison of our $^7$Li MOT and compressed MOT (CMOT) with work in the field.

PMT, we seem to agree for the most part except for the density. The most obvious difference must be the waist measurement; our clouds are significantly bigger than those seen in Mewes et al.. The lithium MOTs of Grimm et al. show that for atom numbers less than $10^8$, they see cloud waists of 1 mm. As the number is increased above $10^8$, the clouds grow rapidly in size to several mm [122]. This is in agreement with our results and disagrees with the work of Mewes et al. where they see 1 mm waists [120].

### 6.5 $^7$Li Electromagnetic Trap

In transferring $^7$Li to the EMTRAP, we have worked hard to keep the bias field of the trap low so as to maximize confinement. Currently, we try to capture the atoms with a 12 G bias which is then reduced to about 2 G for evaporation. This is done by ramping the bias field down for a period of $\sim 30$ s immediately following transfer. The axial confinement is unchanged during this procedure. We have used both fluorescence techniques as well as absorption techniques to measure distributions
in the EMTRAP. Since we run at a much lower bias field compared to $^6\text{Li}$, we find the EMTRAP is quite asymmetric with an aspect ratio of about 1 to 8 (at 2 G). We still fit a 2D Gaussian to the cloud, but the fitting program has been modified to also fit the angle of the major/minor axis and to give an appropriate waist for both axes (see appendix H). The signal has the form,

$$S(r, z) = S_0 \exp\left(-\frac{r^2}{w_r^2}\right) \exp\left(-\frac{z^2}{w_z^2}\right),$$  \hspace{1cm} (6.35)$$

where the $r$-axis is the tighter radial direction and the $z$-axis is the looser axial direction. We have gone to using an absorption probe (near resonance) in order to obtain measures of the optical density.

The Photometrics CCD camera that was discussed earlier is the basis of the new imaging system for the $^7\text{Li}$ EMTRAP. The probe has a waist of 0.8 mm with a power of 10 $\mu\text{W}$. This corresponds to 0.2 $I_{\text{sat}}$ and is flashed on for about 3 $\mu\text{s}$ resulting in scattering about 10 photons per atom. The probe is linearly polarized, but is transverse to the direction of the magnetic trap bias field. This means that the atoms see both $\sigma^+$ and $\sigma^-$ components preventing us from using a cycling transition. All of the probe light is $f = 2$, so there are problems with pumping the atoms into dark $f = 1$ states (see figure 6.7 for details on branching ratios). We have seen that increasing the light level will “bleach” the absorption signal, but we cannot go any lower without suffering signal loss. In an attempt to eliminate this, we have put $f = 1$ repumping light through the cloud along a different axis so that the CCD camera does not see it. This enables us to get better absorption signals, but it still appears that optical pumping is limiting our signals. This is mainly due to the fact that we do not have enough $f = 1$ repump light. We generate this frequency by using the 4th order sideband from a $\sim 200 \text{ MHz}$ AO. We see roughly a factor of two increase in signal as a result of this repumping light.

The imaging system has been designed for future use with an adjustment for higher magnification. Figure 6.8 shows the basic layout of the system. The initial optic is
a custom designed compound lens composed of 5 separate lenses which sits within a re-entrant window on the vacuum system [123]. This optic has a total magnification of 1.8 and simply relays an image of the cloud to a point on a mirror. We then have an infinite-conjugate microscope objective (Mitutoyo, M Plan Apo 10x) with a working distance of 20 mm which grabs the image off the mirror and relays it through a 50 mm Nikon zoom lens (variable focal length of 75 – 240 mm, set to image at infinity) which focuses the image onto the CCD array. The magnification of the objective plus zoom lens is given by \((f_{\text{zoom}} \text{mm}/20 \text{mm})\). This gives a total adjustable magnification for the entire system (compound lens + objective + zoom) of 6.75 to 21.5. Until we get very small clouds, we have been using the lower 6.75 magnification which allows us to see clouds at 15 \(\mu\)K and below. This magnification has been verified by imaging calibrated test targets.

The details of absorption imaging have already been discussed. We take a picture
of the probe with atoms present and then without. Our signal is,

\[ S = \frac{\text{noatoms} - \text{atoms}}{\text{noatoms} - \text{ref}}, \]

(6.36)

where the reference picture is just the background light without any probe (program details are discussed in appendix H). From the absorption picture and fit, we are able to get a waist (axial and radial) for the trapped cloud as well as a peak absorption coefficient. This peak absorption allows us to extract the optical density, and ultimately the peak density and number, in a similar fashion to what was described in the previous section. We start with a peaked MOT with numbers and temperatures close to what was described in the \(^7\)Li MOT section. From our measurements so far of the \(^7\)Li EMTRAP, we seem to be transferring anywhere from \(5 \times 10^8\) to \(1 \times 10^9\) atoms at a temperature of about \(700 \pm 100\) \(\mu\)K. Comparing these numbers to the work presented in chapter 5, we know this is close to the conditions we need for successful evaporation.

We appear to transfer with 5 to 10% efficiency from the compressed MOT (CMOT) where we see \(1 \times 10^{10}\) atoms in the \(f = 2\) state. This seems low and we are attempting to improve this number by optically pumping into the stretched state. If all the atoms were equally distributed among all the \(m\)-levels, you would expect 20% collection efficiency in the \((f, m_f) = (2, 2)\) state (there would not be a change in phase space density since 100% of the atoms equally distributed among 5 states has the same phase space density as 20% distributed in a single state). Some of the loss can be explained by spin-exchange decay which is discussed in the following section.

Another point to consider is the spatial mode matching of the CMOT to the EMTRAP. The observed EMTRAP temperature of 700 \(\mu\)K is higher than the CMOT temperature of 500 \(\mu\)K which indicates a spatial mismatch between the traps. The CMOT has a waist of 2.7 mm. The EMTRAP has an axial waist of 4.9 mm (at 700 \(\mu\)K); the radial waist is 1.3 mm at the initial 12 G bias (roughly 4:1 aspect ratio) which does not ideally match the CMOT dimensions. The tighter radial dimension
of the EMTRAP most likely contributes to the heating we see. We have tried transferring to larger EMTRAPs to eliminate heating, but we find that the evaporation does not work as well. Evaporation is ultimately dependent on having high collision rates leading to rapid thermalization. The collision rate, $R$, for the gas is,

$$ R = n_o \sigma v ,$$

(6.37)

where $n_o$ is the peak density, $\sigma$ is the elastic cross section (which is roughly constant at these temperatures), and $v$ is the thermal velocity of the atoms. The tighter the EMTRAP (for a given temperature and number), the higher the peak density and the corresponding collision rate. As for the temperature dependence, for a harmonic trap (characterizing a large bias field EMTRAP) the rate $R \propto n_o v \propto T^{-1}$ where $T$ is the temperature. For an Ioffe trap, $R$ will vary with bias field from the harmonic limit $R \propto T^{-1}$ to the linear (radial field) limit $R \propto T^{-2}$. This indicates that colder traps yield higher collision rates for a given number of atoms. Experimentally it seems that the higher density associated with a tightly confined EMTRAP is favored somewhat over the loss in collision rate due to heating. We expect to lose some atoms due to the mismatch and heating. Taking the peak densities and temperatures (for the stretched state), we find that the phase space density decreases by a factor of three during the transfer ($\rho_o$(CMOT) = $4.6 \times 10^{-7}$ versus $\rho_o$(EMTRAP) = $1.5 \times 10^{-7}$).

We could improve conditions by optically pumping the atoms into the stretched state thereby increasing the phase space density by as much as a factor of 5. In order to optically pump, we need two frequencies: one for repumping the $f = 1$ atoms, and another which is circularly polarized $\sigma^+$ and which is resonant with the $f = 2$ atoms. The quantization axis defined by these beams must coincide with the EMTRAP bias field, otherwise the quick turn-on of the EMTRAP could unpolarize the atoms. As a result, the $\sigma^+$ beam should travel along the axial dimension of the trap. The nulling cage can be used to provide a uniform magnetic field of a few Gauss along this dimension to maintain the polarization state of the atoms once the laser beam is
turned off and the EMTRAP is switched on. We have attempted this and achieved marginal success (factor of two improvement in transfer efficiency on a good day). The poor performance may be a manifestation of the EMTRAP switching. Over a period of $\sim 200 \, \mu s$ the EMTRAP currents are shunted through protection zeners to ground (see section 4.5). As a result of this effect, as well as inductive spikes, the magnetic field of the EMTRAP may not turn on cleanly enough to maintain adequate polarization. This certainly deserves further investigation.

6.6 $^7$Li Spin-exchange

As with $^6$Li, one of the first things we did upon transferring $^7$Li to the EMTRAP was to observe the lifetime. A plot of the peak density of trapped atoms as a function of time is shown in figure 6.9. Analyzing the decay in detail gives us a lifetime of about 400 seconds which is mainly limited by background gas collisions as shown in the lower log plot. There are deviations present at the initial times which we attribute to spin-exchange decays. We expect in the absence of optical pumping to have atoms of various populations in all the possible spin states. For the low magnetic fields we use for trapping $^7$Li, we expect that up to three different spin states are present. These are indicated in figure 6.10.

In a similar fashion to the analysis done for $^6$Li, we can write out the spin density equations for $^7$Li and try to fit it to the system. It turns out that the $^7$Li equations are a great deal more complicated than the $^6$Li equations. Numbering the possible spin states as shown in figure 6.10, and substituting actual values for the various spin-exchange coefficients, we find,

\begin{align}
\dot{n}_8 &= -9.7 \times 10^{-11} n_8 n_6 + 1.1 \times 10^{-11} n_7 n_7 - 1.1 \times 10^{-10} n_8 n_3 \quad (6.38) \\
\dot{n}_7 &= 3.2 \times 10^{-12} n_8 n_6 + 6.7 \times 10^{-12} n_8 n_3 - 1.6 \times 10^{-10} n_7 n_7 \\
&\quad - 3.2 \times 10^{-11} n_7 n_6 + 2.3 \times 10^{-11} n_8 n_6 - 1.0 \times 10^{-10} n_7 n_3 \quad (6.39) \\
\dot{n}_3 &= -1.0 \times 10^{-10} n_7 n_3 - 7.0 \times 10^{-11} n_8 n_3 - 1.1 \times 10^{-10} n_8 n_3 . \quad (6.40)
\end{align}
Figure 6.9  Decay of $^7$Li in the EMTRAP. The log plot in the lower figure indicates that the main decay process is a one-body decay due to background gas collisions. The deviations at short times are attributed to spin-exchange collisions. The solid line shows the result of modelling these decays assuming that the $(f = 2, m_f = 2)$ state initially has $1.5 \times 10^8 \text{ cm}^{-3}$ while the $(2,1)$ and the $(1,-1)$ have $1.3 \times 10^8 \text{ cm}^{-3}$.

![Diagram showing possible trapped spin states of $^7$Li](image)

Figure 6.10  Possible trapped spin states of $^7$Li. At an operating field bias of 20 G and under, only the states 3, 7, and 8 are trapped by the EMTRAP.
This does not simplify to a simple 2-body decay equation like the $^6$Li system. Instead, the system of equations is numerically integrated and the total density $n_{tot} = n_8 + n_7 + n_3$ is calculated as a function of time and plotted against the data (figure 6.9). The initial spin populations of the three states are unknown and were manually adjusted in the calculation to get the fit shown. One nice thing about $^7$Li is that the (2,2) and the (2,1) states collide along a pure triplet potential. This means that collisions between (2,2) and (2,1) cannot spin decay. For this reason, the stretched state is particularly robust to decay even in the presence of the other spin states indicated. An obvious improvement in our system could be made by optically pumping the atoms into the stretched (2,2) state before transferring. We would not only achieve higher transfer efficiency as was discussed in the previous section, but we would also eliminate this spin-decay loss.

6.7 $^7$Li Evaporation

For the bulk of the last 6 months, we have been working to evaporatively cool the trapped $^7$Li down to degeneracy. Work done with calculating optimized trajectories (see chapter 5) shows that if we have $2 \times 10^9$ atoms at 700 $\mu$K with a bias field of 5 G, we should be able to achieve degeneracy with about 200 seconds of evaporation time. The degenerate regime occurs right around 1 $\mu$K according to the modelling.

We have found on a day to day basis the bottom of the trap will drift since the EMTRAP currents and switch settings never return to exactly the same conditions each day. This may also be a sign that the high power resistor used to measure the current through the bias shunt may not be quite "burned in" yet. As a result, the trap bottom must be found to as high an accuracy as possible each day. The trap bottom is the splitting between the trap and anti-trap potentials from which the trajectories $E_T$ in chapter 5 are referenced. The trap bottom should be the ground-state hyperfine splitting plus the Zeeman shift ($\sim 3/2 \times \mu_B \times B_o$) due to the bias field $B_o$ of the trap.
(for $^{7}\text{Li}$, this is about 808 MHz for a 2 G bias). We have been experimenting with different trajectories and different ways of compressing the MOT before transfer to try and maximize the amount of $^{7}\text{Li}$ transferred to the EMTRAP. The nulling cage surrounding the apparatus can be used to spatially overlap the MOT with the center of the EMTRAP; we have found that this can help transfer efficiency. In the end, this is work in progress. We have recently been able to achieve degenerate conditions (see figure 6.12). We currently cool to around $3 \times 10^5$ atoms (±50%) at a temperature of $400 \pm 100$ nK to give a spatial density of $1.1 \times 10^{12}$ cm$^{-3}$ (±50%) with a corresponding phase space density of 1.2. Despite having thermal clouds which are in the degenerate regime, we have not been able to resolve or observe a $^{7}\text{Li}$ Bose-Einstein condensate; more work would have to be done to improve the imaging since the condensate would only be a couple pixels in size at this magnification.

![Figure 6.11](image.png)

**Figure 6.11** CCD image of an evaporated cloud of $^{7}\text{Li}$ in the EMTRAP. We started with $N = 2 \times 10^9$ atoms at $T = 700 \mu K$ and cooled to $N = 4 \times 10^8$ atoms at $T = 3 \mu K$. The image shows this final distribution which corresponds to a peak density of $2 \times 10^{11}$ cm$^{-3}$ and a phase space density of 0.01.
Figure 6.12  Current evaporation data. This was taken with absorption imaging where roughly 10 photons per atom were scattered. Each data point was destructive, so we had to stop evaporation at a particular time, take a picture, and then reload and re-evaporate for successive pictures at different points in the evaporation. In comparing these results to the calculated trajectories of chapter 5 we find qualitative agreement. The optical density peaks and then decreases as expected (figure 5.7). Meanwhile, the temperature decreases and the density increases leading to increasing phase space density. However, the quantitative numbers for optical density (and hence density and number) do not match the trajectory (figure 5.7). One reasonable systematic error may result from the bleaching of the absorption due to optical pumping to $f = 1$ as discussed in the text. We also may be starting with fewer atoms then expected ($2 \times 10^9$ for the trajectory).
Chapter 7
Conclusions

At this point I would like to summarize what we have learned so far, what the current stage of the experiment is, and where we would like to go in the future. The majority of the work presented in this thesis has dealt with increasing our understanding of collisional interactions in ultracold, magnetically trapped gases. Collisional theory describes a large variety of physical systems and the regime of ultracold atomic gases is no exception. At temperatures below 10 mK, gas collisions become much more quantum mechanical in nature while at the same time enjoy a relatively simple mathematical description due to the low energy scale and the dilute nature of these gases. One goal of trapping ultracold gases is to observe interesting aspects of quantum statistical mechanics. Achieving these conditions requires a solid foundation in collisional interactions, that is what this thesis has ultimately tried to accomplish.

The majority of the work presented has centered on understanding the specific interactions associated with ultracold lithium. In particular, since $^6$Li is a composite fermion and $^7$Li is a composite boson, this is an ideal testing ground for studying quantum statistical mechanics. In the recent past, our group at Rice University has been able to achieve quantum degeneracy and Bose-Einstein condensation (BEC) with $^7$Li [7, 95]. Part of the recipe in achieving this required understanding and measuring the collisional interactions associated with $^7$Li. This thesis describes the experiments and theory that led to that understanding. This thesis also goes beyond $^7$Li to look at $^6$Li interactions as well as interactions between the mixed isotopes. Ultimately we are trying to achieve similar quantum degenerate conditions with $^6$Li.

In order to observe quantum degenerate $^6$Li, we had to construct a new atom trap which has been discussed in detail in this work. There are two principle goals of the new trap. First, we would like to observe a quantum degenerate Fermi gas (DFG)
of $^6$Li. Second, we would like to utilize the attractive interaction that exists in the $^6$Li scattering to try and observe a superfluid, Cooper-paired $^6$Li gas [18, 19]. This attractive interaction results from a quantum mechanical resonance in the scattering that has been ascertained through experiments and theory that have been presented in this work.

We have made significant progress towards achieving these goals and there are a number of exciting experiments on the horizon. For the case of the Bose gas, $^7$Li, we now understand that the collisional interaction in the $(f, m_f) = (1, -1)$ spin state is repulsive (scattering length $= 5 \ a_0$). This would allow for the formation of a large, stable condensate in contrast to the dynamically unstable condensates that have been formed with the $(2, 2)$ state [96]. Since the $(1, -1)$ state can only be captured at magnetic fields below 127 G, the new trap design is ideal for looking at this system. We are currently working towards achieving quantum degenerate $^7$Li and have recently obtained the required phase space density. Further work is needed to peak the transfer efficiency of atoms into the electromagnetic trap. We will also have to refine the absorption probe with the possibility of moving towards phase contrast imaging.

For the case of the Fermi gas, $^6$Li, we would ultimately like to achieve quantum degeneracy and this will require sympathetically cooling the gas with $^7$Li. Since identical fermions cannot undergo low-energy collisions due to the Pauli exclusion principle, this requires us to add this extra degree of complexity to the apparatus. The electromagnetic trap has been designed with this in mind although the required laser frequencies will necessitate the development of a new laser-diode system. This is work that is currently underway. Ultimately, by cooling approximately $10^6$ $^6$Li atoms down below the Fermi temperature of $\sim 1 \ \mu$K, we should see evidence of a degenerate Fermi gas. By cooling down to around $40 \ \text{nK}$ and making the $^6$Li distinguishable (preparing two different spin states), we should be able to observe a
superfluid BCS phase transition [18, 19]. In order to achieve the required attractive collisional interaction, we will need to contain the atoms at large magnetic fields (\( \sim 900 \) G) and may need to use a dipole-force trap [1]. Alternatively, we could use the large scattering length that exists at low field for the \(|\frac{3}{2} - \frac{3}{2} \frac{1}{2} \frac{1}{2}\rangle\) channel (see appendix F).

In summary, there are a number of interesting and exciting phenomena to observe in the new apparatus discussed in this work. The experimental and theoretical work that has gone into understanding collisional physics in ultracold lithium provides a solid framework from which to refine and carry out these investigations.
Appendix A
Scattering Resolvent and Green’s Function Operator

Starting with the Lippman-Schwinger equation,

\[ |\psi\rangle = |\phi\rangle + \frac{1}{E - H_o} V |\psi\rangle, \]  \hspace{1cm} (A.1)

we need to resolve the state vectors in the position basis.

\[ \langle r |\psi\rangle = \langle r |\phi\rangle + \langle r \bigg| \frac{1}{E - H_o} V \bigg| \psi\rangle \]  \hspace{1cm} (A.2)

\[ = \langle r |\phi\rangle + \int dr' \langle r \bigg| \frac{1}{E - H_o} \bigg| r'\rangle \langle r' |V| \psi\rangle. \]  \hspace{1cm} (A.3)

The singular operator can be solved for by introducing a small, complex piece to the energy \( E \to E \pm i\epsilon \) where \( \epsilon \) goes to zero. It will become apparent later that the choice of sign will manifest itself as a choice in boundary conditions. The + sign corresponds to outgoing waves from the scatterer while the − sign corresponds to incoming. We physically pick the + sign for this derivation. To solve for the matrix element of the resolvent, we expand the expression with momentum states that diagonalize the Hamiltonian.

\[ \langle r \bigg| \frac{1}{E - H_o + i\epsilon} \bigg| r'\rangle = \int dk \, dk' \langle r |k\rangle \bigg( \frac{1}{k} \bigg| \frac{1}{E - H_o + i\epsilon} \bigg| k' \bigg\rangle \langle k' |r'\rangle, \]  \hspace{1cm} (A.4)

where,

\[ \langle k |H_o| k'\rangle = \frac{\hbar^2 k^2}{2\mu} \delta_{kk'}. \]  \hspace{1cm} (A.5)

Given that \( \langle r |k\rangle = e^{ik \cdot r}/(2\pi)^{3/2} \) we can work out that,

\[ \langle r \bigg| \frac{1}{E - H_o + i\epsilon} \bigg| r'\rangle = \int dk \, dk' \frac{1}{E - \frac{\hbar^2 k^2}{2\mu}} \langle k |k'\rangle \langle k' |r'\rangle \]  \hspace{1cm} (A.6)

\[ = \int dk \frac{\langle r |k\rangle \langle k| r'\rangle}{E - \frac{\hbar^2 k^2}{2\mu} + i\epsilon} \]  \hspace{1cm} (A.7)

\[ = \frac{1}{2\pi^3} \int d\tilde{k} \frac{e^{i\tilde{k} \cdot (r - r')}}{E - \frac{\hbar^2 k^2}{2\mu} + i\epsilon}. \]  \hspace{1cm} (A.8)
Letting \( E = \hbar^2 k_o^2 / 2\mu \) this expression becomes,
\[
\langle r \left| \frac{1}{E - H_o + i\epsilon} \right| r' \rangle = \frac{2\mu}{\hbar^2 (2\pi)^3} \int d\vec{k} \frac{e^{i\vec{k} \cdot \vec{r} - \vec{k} \cdot \vec{r}'}}{k_o^2 - k^2 + i\epsilon} .
\] (A.9)

To solve this integral, we start by defining \( \vec{R} = \vec{r} - \vec{r}' \) which will define the polar axis for which \( \vec{k} \) is expressed in spherical coordinates.
\[
\langle r \left| \frac{1}{E - H_o + i\epsilon} \right| r' \rangle = \frac{2\mu}{\hbar^2 (2\pi)^3} \int_0^\infty \int_0^{2\pi} \int_0^\pi k^2 \sin \theta \, dk \, d\theta \, d\phi \frac{e^{i k R \cos(\theta)}}{k_o^2 - k^2 + i\epsilon} \\
= \frac{2\mu}{\hbar^2 (2\pi)^3} \int_0^\infty \int_0^{\frac{k_o^2}{k_o^2 - k^2 + i\epsilon}} k^2 \frac{dk}{\sin(\theta)} e^{i k R \cos(\theta)} \\
= \frac{2\mu}{\hbar^2 (2\pi)^3} \int_0^\infty \frac{k^2 \sin(\theta)}{k_o^2 - k^2 + i\epsilon} \left( e^{i k R} - e^{-i k R} \right) \frac{dk}{i k R} \\
= \frac{2\mu}{\hbar^2 (2\pi)^3} \frac{1}{i R} \int_0^\infty \frac{k \left( e^{i k R} - e^{-i k R} \right) dk}{k_o^2 - k^2 + i\epsilon} .
\] (A.10)

Since we know that the numerator of the integrand is \( k \left( e^{i k R} - e^{-i k R} \right) = 2i k \sin(k R) \) is an even function of \( k \) as well as the denominator, we are free to let the limits of integration go to \( \pm \infty \) with an appropriate factor of 2 inserted,
\[
\langle r \left| \frac{1}{E - H_o + i\epsilon} \right| r' \rangle = \frac{2\mu}{\hbar^2 (2\pi)^2} \frac{1}{2i R} \int_{-\infty}^{\infty} \frac{k \left( e^{i k R} - e^{-i k R} \right) dk}{k_o^2 - k^2 + i\epsilon} ,
\] (A.11)

which can be rewritten as,
\[
\langle r \left| \frac{1}{E - H_o + i\epsilon} \right| r' \rangle = \frac{2\mu}{\hbar^2 (2\pi)^2} \frac{1}{2i R} \int_{-\infty}^{\infty} \frac{k e^{i k R} \, dk}{(k_o - k + i\epsilon)(k_o + k + i\epsilon)} - k e^{-i k R} \, dk}{(k_o - k + i\epsilon)(k_o + k + i\epsilon)} .
\] (A.12)

To solve for the \( k \) integrals, we make use of Cauchy’s theorem [32] which says that for a smooth function \( F(z) \) of a complex number \( z \),
\[
\oint \frac{F(z)}{z - z_o} \, dz = 2\pi i F(z_o) ,
\] (A.13)
or
\[
\oint \frac{F(z)}{z_0 - z} \, dz = -2\pi i F(z_0), \tag{A.14}
\]

where the line integral assumes a counter-clockwise direction (+\(\theta\)) around the singularity. There are two possible paths to take for each integral, we choose the appropriate path where the numerator, \(e^{\pm ikR}\), vanishes at large complex \(k\) where the path is closed. For example, since the factor \(e^{ikR}\) goes to zero for large, positive imaginary \(k\), we can say that,
\[
\int_{-\infty}^{\infty} \frac{k e^{ikR} \, dk}{(k_o - k + i\epsilon)(k_o + k + i\epsilon)} = \oint_{C_1} \frac{k e^{ikR} \, dk}{(k_o - k + i\epsilon)(k_o + k + i\epsilon)}. \tag{A.15}
\]

Likewise, the appropriate piece of the integral over \(e^{-ikR}\) is taken over the path defined by \(C_2\). The direction of integration is chosen such that the integral over the real axis of \(k\)-space goes from \(-\infty\) to \(+\infty\). By Cauchy’s theorem, since the integration over \(C_2\) is clockwise, an extra − sign is introduced to that part of the integral. So we find,
\[
\langle r \mid \frac{1}{E - H_o + i\epsilon} \mid r' \rangle = \frac{2\mu}{\hbar^2 (2\pi)^2} \frac{1}{2iR} \left[ \frac{k_o e^{ik_o R(-2\pi i)}}{k_o + k_o + i\epsilon} - \frac{-k_o e^{ik_o R(-2\pi i)}}{k_o - (-k_o) + i\epsilon} \right]
\]
\[
= \frac{2\mu}{\hbar^2 (2\pi)^2} \frac{1}{2iR} \left[ -2\pi i \left( \frac{e^{ik_o R}}{2} + \frac{e^{ik_o R}}{2} \right) \right]
\]
\[
= \frac{2\mu}{\hbar^2 4\pi} \frac{e^{ik_o R}}{R}, \tag{A.16}
\]

**Figure A.1** Poles in complex \(k\)-space for Green’s function operator.
Taking into account the arbitrary sign for the poles, we define the Green's function operator $G_o^\pm(\vec{r}, \vec{r}')$,

$$\left\langle \vec{r}' \left| \frac{1}{E - H_o \pm i\epsilon} \right| \vec{r} \right\rangle = \frac{2\mu}{\hbar^2} G_o^\pm(\vec{r}, \vec{r}') ,$$  \hfill (A.17)

where,

$$G_o^\pm(\vec{r}, \vec{r}') = -\frac{1}{4\pi} \frac{e^{\pm ik_o(|\vec{r} - \vec{r}'|)}}{|\vec{r} - \vec{r}'|} .$$  \hfill (A.18)

The ± sign in the operator corresponds to either outgoing or incoming spherical waves.

To see this boundary condition, let us return to the Lippman-Schwinger equation

$$\langle \vec{r}|\psi \rangle = \langle \vec{r}|\phi \rangle + \int d\vec{r}' \left\langle \vec{r}' \left| \frac{1}{E - H_o} \right| \vec{r}' \right\rangle \langle \vec{r}'|V|\psi \rangle .$$ \hfill (A.19)

So we can substitute in the Green's function,

$$\langle \vec{r}|\psi \rangle = \langle \vec{r}|\phi \rangle - \int d\vec{r}' \frac{e^{ik(|\vec{r} - \vec{r}'|)}}{4\pi|\vec{r} - \vec{r}'|} \hat{V}(\vec{r}') \langle \vec{r}'|\psi \rangle ,$$ \hfill (A.20)

where the reduced potential $\hat{V}$ is defined to be $\hat{V} = 2\mu V/m$. The potential term has been moved outside the matrix element $\langle \vec{r}'|\hat{V}|\psi \rangle$ since it is local and diagonal in the position basis ($\langle \vec{r}'|\hat{V}|\vec{r}' \rangle = \hat{V}(r) \langle \vec{r}'|\vec{r}' \rangle = \hat{V}(r) \delta(\vec{r}' - \vec{r}')$). Now since most scattering experiments involve looking at the scattered products far removed from the potential, we can assume that $|\vec{r}'| \gg |\vec{r}'|$, which allows us to write,

$$|\vec{r} - \vec{r}'| = \sqrt{r^2 + r'^2 - 2rr' \cos(\alpha)}$$
$$= r \sqrt{1 + \frac{r'^2}{r^2} - \frac{2r'}{r} \cos(\alpha)}$$
$$\approx r \left( 1 - \frac{r'}{r} \cos(\alpha) \right)$$
$$\approx r - \hat{r} \cdot \vec{r}' ,$$ \hfill (A.21)

where $r = |\vec{r}|$, $\hat{r}$ is the unit vector in the direction of $\vec{r}$, and $\alpha$ defines the angle between $\vec{r}$ and $\vec{r}'$. The scattering equation then takes the form,

$$\langle \vec{r}|\psi \rangle = \langle \vec{r}|\phi \rangle - \frac{e^{ikr}}{r} \int d\vec{r}' \frac{e^{-ik(|\hat{r} \cdot \vec{r}'|)}}{4\pi} \hat{V}(\vec{r}') \langle \vec{r}'|\psi \rangle ,$$
$$= A \left( e^{ikr} - \frac{e^{ikr}}{r} f \right) ,$$ \hfill (A.22)
where the overall wavefunction looks like some constant $A$ times an incident plane wave with an outgoing spherical wave with amplitude $f$. This scattering amplitude has the form,

$$ f = - \int d\vec{r}' \frac{e^{-i\vec{k}\cdot\vec{r}'}}{4\pi} \hat{V}(\vec{r}') \langle \vec{r}' | \psi \rangle , \quad (A.23) $$

where $\vec{k} = k\hat{r}$ defines the incident momentum vector. I should point out that while this is an expression for the scattering amplitude, $f$, it still contains the state vector $|\psi\rangle$ which makes it a little tricky to solve. This is discussed in chapter 2.
Appendix B
Singlet and Triplet Projection Operators

The coupled-channel scattering equation takes the form of a matrix Schrödinger equation. In the hyperfine basis characterized by two atoms in the symmetrized state \(|\{\alpha \beta\} = |\{f_1 m_1 f_2 m_2\}\rangle\) this equation looks like,

\[
\frac{d^2}{dr^2} F_{\{\alpha' \beta\},\{\alpha \beta\}}(r) = \frac{2\mu}{\hbar^2} C_{\{\alpha' \beta\},\{\alpha \beta\}}(r) F_{\{\alpha' \beta\},\{\alpha \beta\}}(r), \tag{B.1}
\]

where,

\[
C_{\{\alpha' \beta\},\{\alpha \beta\}}(r) = \left( E^{HF}_{\alpha} + E^{HF}_{\beta} - E \right) \delta_{\{\alpha' \beta\},\{\alpha \beta\}} + \\
V_T(r) \langle \{\alpha' \beta\} | P_T | \{\alpha \beta\} \rangle + \\
V_S(r) \langle \{\alpha' \beta\} | P_S | \{\alpha \beta\} \rangle. \tag{B.2}
\]

I want to show how to evaluate the triplet \(P_T\) and singlet \(P_S\) projection operators in this basis. To start with, I will use the unsymmetrized states \(|f_1 m_1 f_2 m_2\rangle\) and generalize to the symmetrized case in the end.

In order to evaluate \(P_T |f_1 m_1 f_2 m_2\rangle\) or \(P_S |f_1 m_1 f_2 m_2\rangle\) I need to expand the basis set into a linear combination of basis functions which are eigenvalues of the triplet or singlet operators. To do this, I will make use of the simple expansion,

\[
|f_1 m_1 f_2 m_2\rangle = \sum |S m_{S I m_I}\rangle \langle S m_{S I m_I}|f_1 m_1 f_2 m_2\rangle, \tag{B.3}
\]

where the coefficient \(\langle S m_{S I m_I}|f_1 m_1 f_2 m_2\rangle\) is simply the appropriate Clebsch-Gordan coefficient [124]. This coefficient can be solved for using angular algebra where the basis \(|f_1 m_1 f_2 m_2\rangle\) can be de-coupled into the basis \(|s_1 i_1 m_{s_1} m_{i_1} s_2 i_2 m_{s_2} m_{i_2}\rangle\) through the appropriate 3-j symbols [124],

\[
|f_1 m_1 f_2 m_2\rangle = (-1)^{2s_2 - 2s_1 - m_1 - m_2} \sqrt{(2f_1 + 1)(2f_2 + 1)} \times
\]

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\[
\sum_{m_{s1}m_{i1}m_{s2}m_{i2}} \left( \begin{array}{ccc}
  s_1 & i_1 & f_1 \\
  m_{s1} & m_{i1} & -m_1 \\
\end{array} \right) \left( \begin{array}{ccc}
  s_2 & i_2 & f_2 \\
  m_{s2} & m_{i2} & -m_2 \\
\end{array} \right) \times \langle (s_1i_1)m_{s1}m_{i1}(s_2i_2)m_{s2}m_{i2} \rangle .
\]

(B.4)

The uncoupled basis \( \langle (s_1i_1)m_{s1}m_{i1}(s_2i_2)m_{s2}m_{i2} \rangle \) can then be re-coupled into the basis \( |Sm_SIm_I\rangle \) [124],

\[
\langle (s_1i_1)m_{s1}m_{i1}(s_2i_2)m_{s2}m_{i2} \rangle = \sum_{Sm_SIm_I} (-1)^{-m_S-m_l} \sqrt{(2S+1)(2I+1)} \times
\left( \begin{array}{ccc}
  s_1 & s_2 & S \\
  m_{s1} & m_{s2} & -m_S \\
\end{array} \right) \left( \begin{array}{ccc}
  i_1 & i_2 & I \\
  m_{i1} & m_{i2} & -m_I \\
\end{array} \right) \times |Sm_SIm_I\rangle .
\]

(B.5)

By expanding the basis \( |f_1m_1f_2m_2\rangle \) using the previous two relations and pre-multiplying by the state \( \langle Sm_SIm_I\rangle \), we find that,

\[
\langle Sm_SIm_I|f_1m_1f_2m_2 \rangle = (-1)^{2i_2-2s_1-m_{i1}-m_{i2}-m_S-m_l} \times
\sqrt{(2f_1+1)(2f_2+1)(2S+1)(2I+1)} \times
\sum_{m_{s1}m_{i1}m_{s2}m_{i2}} \left( \begin{array}{ccc}
  s_1 & i_1 & f_1 \\
  m_{s1} & m_{i1} & -m_1 \\
\end{array} \right) \left( \begin{array}{ccc}
  s_2 & i_2 & f_2 \\
  m_{s2} & m_{i2} & -m_2 \\
\end{array} \right) \times
\left( \begin{array}{ccc}
  s_1 & s_2 & S \\
  m_{s1} & m_{s2} & -m_S \\
\end{array} \right) \left( \begin{array}{ccc}
  i_1 & i_2 & I \\
  m_{i1} & m_{i2} & -m_I \\
\end{array} \right) \times \langle Sm_SIm_I|f_1m_1f_2m_2 \rangle .
\]

(B.6)

Now we can write out what the triplet and singlet projection operators look like. Using the derived expansion, the matrix element of the projection operator looks like,

\[
\langle f_1'm_1f_2'm_2'|P_{S/T}|f_1m_1f_2m_2 \rangle = \sum_{SIm_SU'm_SU'm'_I} \langle f_1'm_1f_2'm_2'|S'm_S'I'm'_I \rangle \times
\langle S'm_S'I'm'_I|P_{S/T}|Sm_SIm_I \rangle \times
\langle Sm_SIm_I|f_1m_1f_2m_2 \rangle .
\]

(B.7)

The projection operator \( P_{S/T} \) acts on the state \( |Sm_SIm_I\rangle \) like a delta function where \( P_S = \delta_{S,0} \) and \( P_T = \delta_{S,1} \), so \( P_{(T \text{ or } S)} = \delta_{(S,1 \text{ or } 0)} \). I should also point out
that since Clebsch-Gordan coefficients are real-valued, then \( \langle Sm_SIm_I | f_1m_1 f_2m_2 \rangle = \langle f_1m_1 f_2m_2 | Sm_SIm_I \rangle \). So the matrix element becomes,

\[
\langle f'_1m'_1 f'_2m'_2 | P_{TS} | f_1m_1 f_2m_2 \rangle = \sum_{SIm_S m'_I | S'S'm'_I m'_I} \delta_{S,(1 \text{ or } 0)} \delta_{SS'} \delta_{m_S m'_S} \delta_{II'} \delta_{m_I m'_I} \times \\
\langle Sm_SIm_I | f_1m_1 f_2m_2 \rangle \langle S'm'_SIm'_I | f'_1m'_1 f'_2m'_2 \rangle \\
= \sum_{SIm_S} \delta_{S,(1 \text{ or } 0)} \langle Sm_SIm_I | f_1m_1 f_2m_2 \rangle \times \\
\langle Sm_SIm_I | f'_1m'_1 f'_2m'_2 \rangle .
\]

(B.8)

So now that \( P_{TS} \) has been expressed for an unsymmetrized basis state |\( f_1m_1f_2m_2 \rangle \), it is relatively straight-forward to extend this result to the symmetrized basis set used in the coupled-channel equations. The final result looks like,

\[
\langle \{ f'_1m'_1 f'_2m'_2 \} | P_{TS} | \{ f_1m_1 f_2m_2 \} \rangle = \frac{\langle f'_1m'_1 f'_2m'_2 | P_{TS} | f_1m_1 f_2m_2 \rangle \pm (-1)^l | f'_1m'_1 f'_2m'_2 | P_{TS} | f_2m_2 f_1m_1 \rangle}{\sqrt{2(1+\delta_{1,2})}} ,
\]

(B.10)

where the operator definitions for the unsymmetrized basis set have been defined above. The exact symmetry of the state depends on the particular partial wave one is interested in (this is labelled by the angular momentum quantum number \( l \)).
Appendix C
Numerov Routine for Solving Coupled-Channel Equations

I will outline the process by which the Numerov routine [44,45] was applied to solving the coupled-channel equations. Given that,

$$\frac{d^2}{dr^2}F = V \cdot F = F'' ,$$  \hspace{1cm} (C.1)

where $V$ and $F$ are understood to be matrices, I want to solve for $F(r \pm h)$.

$$F(r \pm h) = F(r) \pm h F'(r) + \frac{h^2}{2} F''(r) \pm \frac{h^3}{6} F'''(r) + \frac{h^4}{24} F^{(4)}(r) + O(h^5) ,$$  \hspace{1cm} (C.2)

where ‘$h$’ is some small step-size. To start with, I can write an equation relating the values of $F(r-h)$, $F(r)$, and $F(r+h)$. Using the expansion from above, I find,

$$F(r+h) - 2F(r) + F(r-h) = h^2 F'' + \frac{h^4}{12} F^{(4)}(r) + O(h^6)$$

$$= h^2 V(r) \cdot F(r) + \frac{h^4}{12} \left[ \frac{d^2}{dr^2} F''(r) \right]$$

$$= h^2 V(r) \cdot F(r) + \frac{h^4}{12} \left[ \frac{d^2}{dr^2} (V \cdot F) \right] ,$$  \hspace{1cm} (C.3)

where the final term can be written as,

$$\frac{d^2}{dr^2} (V \cdot F) = V(r+h)F(r+h) - 2V(r)F(r) + V(r-h)F(r-h) + O(h^4) .$$  \hspace{1cm} (C.4)

If I define $Y(r)$ to be,

$$Y(r) = \left( 1 - \frac{h^2}{12} V(r) \right) \cdot F(r) ,$$  \hspace{1cm} (C.5)

then I can rewrite the above equations to be,

$$Y(r+h) - 2Y(r) + Y(r-h) = h^2 V(r) \cdot F(r) + O(h^6) .$$

$$Y'(r) = \left( 1 - \frac{h^2}{12} V \right)^{-1} \cdot Y(r) ,$$  \hspace{1cm} (C.6)

Now,

$$F(r) = \left( 1 - \frac{h^2}{12} V \right)^{-1} \cdot Y(r) ,$$  \hspace{1cm} (C.7)
and I know that an inverse matrix times itself gives,

\[
\left(1 - \frac{h^2}{12} V\right)^{-1} \cdot \left(1 - \frac{h^2}{12} V\right) = 1 \text{ identity matrix} .
\]  
(C.10)

So assuming that \(h^2 V\) is small, I can expand the inverse matrix into,

\[
\left(1 - \frac{h^2}{12} V\right)^{-1} \approx 1 + \frac{h^2}{12} V + \frac{h^4}{144} V \cdot V ,
\]  
(C.11)

which is good to order \(h^6\) as shown by,

\[
\left(1 + \frac{h^2}{12} V + \frac{h^4}{144} V \cdot V\right) \left(1 - \frac{h^2}{12} V\right) = 1 - \frac{h^2}{12} V + \frac{h^2}{12} V - \frac{h^4}{144} V \cdot V \\
+ \frac{h^4}{144} V \cdot V - \frac{h^6}{12^3} V \cdot V \cdot V \\
\approx 1 + O(h^6) .
\]  
(C.12)

So now I can write the expression for \(F(r)\) as a function of \(Y(r)\) which is good to order \(h^6\),

\[
F(r) = \left(1 - \frac{h^2}{12} V\right)^{-1} Y(r) \approx \left(1 + \frac{h^2}{12} V + \frac{h^4}{144} V \cdot V\right) Y(r) \\
= \left[1 + \frac{h^2}{12} \left(V + \frac{h^2}{12} V \cdot V\right)\right] Y(r) .
\]  
(C.13)

This can then be substituted back into the recursive equation to get,

\[
Y(r + h) - 2Y(r) + Y(r - h) = h^2 V(r) \left[1 + \frac{h^2}{12} \left(V(r) + \frac{h^2}{12} V(r) \cdot V(r)\right)\right] Y(r) \\
+ O(h^6) \\
= \left[h^2 V(r) + \frac{h^4}{12} V(r) \cdot V(r)\right] Y(r) + O(h^6) .
\]  
(C.14)

So the final Numerov equations can be written in terms of \(W(r)\) where,

\[
W(r) \equiv h^2 V(r) + \frac{h^4}{12} V(r) \cdot V(r) ,
\]  
(C.15)

and

\[
Y(r + h) - 2Y(r) + Y(r - h) = W(r) \cdot Y(r) ,
\]  
(C.16)
given the following transforms,

\[ F(r) = \left[ 1 + \frac{1}{12} W(r) \right] Y(r) \]  \hspace{1cm} (C.17)

\[ Y(r) = \left[ 1 - \frac{h^2}{12} V(R) \right] F(r) . \]  \hspace{1cm} (C.18)

This recursive equation can be used to integrate the coupled-channel equations and should converge to the proper answer with an error proportional to \( h^6 \).
Appendix D
Long Range Form of Scattering Wavefunctions, $I(r)$ and $O(r)$

The scattering theory of chapter 2 shows that the long range form of the scattering wavefunctions in the coupled-channel equation should have the appearance of incoming and outgoing spherical waves. The singlet and triplet potentials will introduce phase shifts between these incoming and outgoing pieces which completely characterizes the scattering process (as compared to the “free” case where there is no potential). In order to solve for these phase shifts we need to fit our solution from the coupled-channel equations, $F(r)$, to a linear combination of incoming and outgoing wavefunctions which satisfy the zero-potential Schrödinger equation. In other words,

$$F(r) = [I(r) + O(r) \cdot S] \cdot A,$$

where $S$ is the S-matrix of chapter 2 and contains the phase shift information, and the diagonal matrices $I$ and $O$ are the respective incoming and outgoing wavefunctions that solve the zero-potential scattering equation and are the topic of this appendix.

For the case of no potential interaction, the solution to Schrödinger’s equation looks like,

$$\Psi(r, \theta, \phi) = R_i(r)Y_{lm}(\theta, \phi),$$

a radial function times a spherical harmonic. The radial function is related to the solution of the coupled-channel equations, $F(r)/r = R_i(r)$. Since the zero-potential radial wavefunction looks like,

$$R_i(r) = c_1 h_i^{(1)}(kr) + c_2 h_i^{(2)}(kr),$$

where $h_i^{(1)}$ and $h_i^{(2)}$ are spherical Hankel functions, we know that $F(r)$ for the case of no potential scattering looks like,

$$F(r) = c_1 r h_i^{(1)}(kr) + c_2 r h_i^{(2)}(kr) = O(r) + I(r).$$
The two types of spherical Hankel functions can be identified directly with either \( I(r) \) or \( O(r) \). In the formalism of Henk Stoof's paper on coupled-channel calculations [33], I choose the coefficients \( c_1 \) and \( c_2 \) such that,

\[
I(r) = -\sqrt{kr}h^{(2)}_i(kr) \tag{D.5}
\]
\[
O(r) = I^*(r) = -\sqrt{kr}h^{(1)}_i(kr) , \tag{D.6}
\]

if \( k \) is real. There is an extra factor of \( 'i' \) in Henk's paper which I ignore, it seems to do nothing more than add an overall phase factor that does not affect the S-matrix results.

Now I need to derive expressions for \( I(r) \) and \( O(r) \) which are computer friendly and applicable to either open channels (\( k \) real), or closed channels (\( k \) imaginary). Numerical recipes has routines for calculating Bessel functions \( (J_n(x)) \), Neumann functions \( (N_n(x)) \), as well as Modified Bessel functions \( (I_n(x) \) and \( K_n(x)) \)[119]. I will now show how to re-write the functions \( I(r) \) and \( O(r) \) in terms of these functions and taking into account whether \( k \) is real or imaginary. For the case of open channels, where \( k = \sqrt{E - E_{\alpha}^{HF} - E_{\beta}^{HF}} \) is real, the wavefunctions \( I(r) \) and \( O(r) \) can be found in terms of Bessel and Neumann functions to be,

\[
I_{mn}(r) = -\delta_{mn}\sqrt{\frac{kr}{2\pi}}\bigg[ J_{l+1/2}(kr) - iN_{l+1/2}(kr) \bigg] \tag{D.7}
\]
\[
O_{mn}(r) = I^*_{mn}(r) \tag{D.8}
\]

For the case of closed channels, the momentum \( k \) becomes purely imaginary and looks like,

\[
k = \sqrt{E - E_{\alpha}^{HF} - E_{\beta}^{HF}} = \sqrt{E_{\alpha}^{HF} + E_{\beta}^{HF} - E} \cdot \sqrt{-1} = |k|i . \tag{D.10}
\]

Taking the function \( I(r) \) and substituting the imaginary dependence explicitly, we
\[
I_{mn}(r) = -\delta_{mn}\sqrt{|k_m|}\sqrt{ir}h_1^{(2)}(|k|ir) .
\] (D.11)

So two parts of this expression must be carefully treated, first the \(\sqrt{i}\) and then the Hankel function of an imaginary argument. Considering the first part, taking the square root of an imaginary number is best thought of in the complex-plane representation. If \(z\) is a complex number, then \(z\) looks like \(z = |z|e^{i\theta}\) in polar notation (magnitude and phase). Therefore, taking the square root of \(z\) looks like,

\[
\sqrt{z} = \sqrt{|z|}e^{i\theta/2} = \sqrt{|z|} \cdot e^{i\theta/2} .
\] (D.12)

So following this, it is easy to see that,

\[
\sqrt{i} = \frac{1}{\sqrt{2}}(1 + i) .
\] (D.13)

Finding the Hankel function of a complex argument takes a little more work. First I need to make use of some of the properties and relations concerning Bessel functions and Modified Bessel functions. Using a reference such as Arfken [32], I find,

\[
J_n(ix) = i^n I_n(x) ,
\] (D.14)

where \(x\) is real and \(I_n(x)\) is one type of modified Bessel function. Another important relation exists between the spherical Neumann function and the Bessel function,

\[
n_n(x) = (-1)^{n+1}\sqrt{\frac{\pi}{2x}}J_{n-1/2}(x) ,
\] (D.15)

which allows me to rewrite the Neumann part of the Hankel function as a Bessel function. Once I do that, I can use the relation between the Bessel function of an imaginary argument and the Modified Bessel function to find,

\[
h_n^{(2)}(xi) = i^n \sqrt{\frac{\pi}{2x}}I_{n+1/2}(x) - (-1)^{n+1}i^{-n} \sqrt{\frac{\pi}{2x}}I_{-n-1/2}(x) .
\] (D.16)

Unfortunately, numerical routines found in references such as Numerical Recipes [119] cannot deal with Modified Bessel functions of negative type \(I_{-n}(x)\). To get around
this, I need to use another relation that exists between the two types of Modified Bessel functions,

\[ I_{-n}(x) = I_n(x) + \frac{2}{\pi} \sin(n\pi) K_n(x) \]. \tag{D.17}

Using this final piece of information, I can write,

\[ I_{mn}(r) = -\delta_{mn} \sqrt{\frac{\pi r}{4}} (1 + i)^i \left[ 2 I_{l+1/2}(kr) + \frac{2}{\pi} \sin \left[ (l + 1/2)\pi \right] K_{l+1/2}(kr) \right] \]. \tag{D.18}

for the case where \( k = |k|i \).

To find the form of \( O(r) \) for imaginary \( k \) is a little tricky because the complex conjugate which relates \( O(r) = I^*(r) \) must be taken at the beginning of the calculation. Starting with \( I(r) \),

\[ I_{mn}(r) = -\delta_{mn} \sqrt{|k|} \sqrt{i} r h_n^{(2)}(|k|i r) \] \tag{D.19}

\[ = -\delta_{mn} \sqrt{|k|} \sqrt{i} r \sqrt{\frac{\pi}{2i|kr|}} H_{l+1/2}^{(2)}(|k|i r) \], \tag{D.20}

where I have used the definition of the spherical Hankel function,

\[ h_n^{(2)}(x) = \sqrt{\frac{\pi}{2x}} H_{n+1/2}^{(2)}(x). \] \tag{D.21}

Taking the complex conjugate to find \( O(r) \),

\[ O_{mn}(r) = -\delta_{mn} \sqrt{|k|} \sqrt{-i} r \sqrt{\frac{\pi}{-2i|kr|}} H_{l+1/2}^{(1)}(-|k|i r) \], \tag{D.22}

and using the relation,

\[ H_n^{(1)}(ix) = \frac{2}{\pi} (-i)^n K_n(x) \], \tag{D.23}

I find that,

\[ O_{mn}(r) = -\delta_{mn} \sqrt{\frac{r}{\pi}} (1 + i)(-i)^l K_{l+1/2}(-|k|r) \]. \tag{D.24}

Since the numerical routines for the Modified Bessel function \( K_n(x) \) cannot handle negative values of \( x \), I can use the relation,

\[ K_{n+1/2}(-|k|r) = (-1)^{n+1/2} K_{n+1/2}(|k|r) \], \tag{D.25}
to rewrite this expression. In the end, I find that for closed channels and imaginary \( k \), the expression for the outgoing wavefunction is,

\[
O_{mn}(r) = +\delta_{mn}\sqrt{\frac{r}{\pi}}(1 - i)\frac{1}{t}K_{i+1/2}(|k|r). 
\]

(D.26)
Appendix E
Zeeman and Hyperfine Interactions

In this appendix, I want to show the derivations for the various matrix elements that are needed to take into account hyperfine and Zeeman energy shifts in the coupled-channel equations. I will also outline how to calculate molecular hyperfine and Zeeman structure so as to approximate the location of Feshbach resonances.

I will begin by considering the hyperfine and Zeeman energy of a single atom. The Hamiltonian describing this is,

\[ H^{HZ} = A^{HF} \vec{s} \cdot \vec{i} + g_s \mu_B m_s B + g_i \mu_N m_i B, \]  

(E.1)

where \( \vec{s} \) is the electronic spin (with projection \( m_s \)), \( \vec{i} \) is the nuclear spin (with projection \( m_i \)), \( \mu_B \) is the Bohr magneton, \( \mu_N \) is the nuclear magneton, \( A^{HF} \) is the atomic hyperfine constant, \( B \) is the external magnetic field, \( g_s \) is the electronic g-factor, and \( g_i \) is the nuclear g-factor. Table E.1 gives the appropriate constants for lithium. In

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<th>( ^7\text{Li} )</th>
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Table E.1 Hyperfine constants and g-factors for \( ^6\text{Li} \) and \( ^7\text{Li} \) [114, 115, 125, 126].

the atomic hyperfine basis, the hyperfine interaction \( \vec{s} \cdot \vec{i} \) is diagonal and characterized by \( \vec{s} \cdot \vec{i} = \frac{f^2 - s^2 - i^2}{2} \) where \( f = s + i \). The Zeeman terms are off-diagonal and can be expressed through 3-j symbols,

\[ \langle si'f'm'|H^{HZ}|sifm\rangle = \frac{A^{HF}}{2} [f(f + 1) - i(i + 1) - s(s + 1)] \delta_{ff'}\delta_{mm'} \]  

(E.2)

\[ + g_s \mu_B B \sqrt{(2f' + 1)(2f + 1)} \sum m_s m_i \begin{pmatrix} s & i & f' \\ m_s & m_i & -m' \end{pmatrix} \begin{pmatrix} s & i & f \\ m_s & m_i & -m \end{pmatrix} \delta_{mm'} \]

\[ + g_i \mu_N B \sqrt{(2f' + 1)(2f + 1)} \sum m_i \begin{pmatrix} s & i & f' \\ m_s & m_i & -m' \end{pmatrix} \begin{pmatrix} s & i & f \\ m_s & m_i & -m \end{pmatrix} \delta_{mm'} \]
So this constitutes the hyperfine/Zeeman interaction for a single atom and can be
diagonalized to give the appropriate Breit-Rabi energies [46]. The hyperfine and
Zeeman structure of $^6$Li and $^7$Li is given in figures E.1 and E.2.

![Graph showing hyperfine/Zeeman structure](image)

**Figure E.1** Zeeman structure of $^6$Li.

For the case of the coupled-channel code, we need to figure out the appropriate
matrix element,

$$\langle \{f'_1 m'_1 f'_2 m'_2\} | H_1^{HZ} + H_2^{HZ} | \{f_1 m_1 f_2 m_2\} \rangle .$$  \hspace{1cm} (E.3)

The symmetrized state is defined by,

$$|\{\alpha \beta\}\rangle = \frac{|\alpha \beta\rangle \pm (-1)^i |\beta \alpha\rangle}{\sqrt{2(1 + \delta_{\alpha \beta})}} ,$$  \hspace{1cm} (E.4)

where $|\alpha \beta\rangle$ means atom ‘1’ in state $\alpha$ and atom ‘2’ in state $\beta$. Since the hyperfine/Zeeman Hamiltonian has one part ($H_1^{HZ}$) which operates only on atom ‘1’ and
another part ($H_2^{HZ}$) which operates only on atom ‘2’, I can write out the two-atom
Figure E.2  Zeeman structure of $^7$Li.

matrix element as a sum of single atom matrix elements keeping the proper symmetries,

$$
\langle \{\alpha' \beta'\}|H_1^{HZ} + H_2^{HZ}|\{\alpha \beta\} \rangle = \frac{1}{\sqrt{(1 + \delta_{\alpha'\beta'})(1 + \delta_{\alpha\beta})}} \left[ \langle \alpha'|H^{HZ}|\alpha\rangle \delta_{\beta \beta'} 
+ \langle \beta'|H^{HZ}|\beta\rangle \delta_{\alpha \alpha'} \pm (-1)^{l} \langle \alpha'|H^{HZ}|\beta\rangle \delta_{\beta \alpha} \pm (-1)^{l} \langle \beta'|H^{HZ}|\alpha\rangle \delta_{\alpha' \beta} \right], \text{(E.5)}
$$

where each single atom matrix element is identical to the one derived earlier in the hyperfine basis characterized by $|\alpha\rangle = |fm\rangle$. This is the expression that is substituted into the coupled-channel calculation to include the effects of magnetic field.

Finally, in order to find the approximate location of Feshbach resonances, I needed to solve for the Zeeman structure of bound molecular states and compare these energies to those calculated for the scattering state. The molecular basis state is given by $|S_{m_s}I_{m_I}\rangle$ where $S = s_1 + s_2$ and $I = i_1 + i_2$. The Zeeman structure for a molecular
state is then given by diagonalizing,

$$(S'm'_S I'm'_I | H_1^{HZ} + H_2^{HZ} | S m_S I m_I ) .$$

(E.6)

I can solve for these matrix elements by expanding the molecular basis into an atomic basis and using the results I have already presented for the hyperfine basis,

$$|S m_S I m_I ) = \sqrt{(2S + 1)(2I + 1)} \sum_{m_{s1} m_{s2} m_{i1} m_{i2} f_1 f_2} (-1)^{-m_S - m_I - m_1 - m_2 - 2s_1 + 2i_2} \times \sqrt{(2f_1 + 1)(2f_2 + 1)} \begin{pmatrix} s_1 & s_2 & S \\ m_{s1} & m_{s2} & -m_S \end{pmatrix} \begin{pmatrix} i_1 & i_2 & I \\ m_{i1} & m_{i2} & -m_I \end{pmatrix} \times \begin{pmatrix} s_1 & i_1 & f_1 \\ m_{s1} & m_{i1} & -m_1 \end{pmatrix} \begin{pmatrix} s_2 & i_2 & f_2 \\ m_{s2} & m_{i2} & -m_2 \end{pmatrix} |f_1 m_1 f_2 m_2) .$$

(E.7)

This expansion enables me to describe the energy shift of a molecular state in terms of shifted atomic states,

$$\langle S'm'_S I'm'_I | H_1^{HZ} + H_2^{HZ} | S m_S I m_I ) = \sum_i C_i \langle f'_1 m'_1 | H^{HZ} | f_1 m_1 \rangle + D_i \langle f'_2 m'_2 | H^{HZ} | f_2 m_2 \rangle .$$

(E.8)

To find Feshbach resonances at experimentally obtainable magnetic fields, I only have to consider the Zeeman structure of the highest lying singlet and triplet molecular states. The scattering state will only couple to those molecular states which have the same total spin projection, so $m_S + m_I = m_1 + m_2$. The energies of the highest lying states are given in table E.2. The singlet levels will not shift much with magnetic

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Table E.2  Binding energies of the highest lying vibrational levels of the ground state potentials for lithium.

field since $\vec{S} = 0$ so $\vec{S} \cdot \vec{B} = 0$. The triplet levels have $\vec{S} = 1$, so I can expect to see Zeeman splittings corresponding to $m_S = -1, 0, 1$. Figure E.3 shows level crossings
for the $^6\text{Li} \left\{ \frac{1}{2} \frac{1}{2} - \frac{1}{2} \right\}$ scattering state and where Feshbach resonances should occur. These types of curve crossings were calculated and used to help isolate those values.

![Diagram showing energy levels as a function of magnetic field.](image)

**Figure E.3** Zeeman energy of $\left\{ \frac{1}{2} \frac{1}{2} - \frac{1}{2} \right\}$ scattering state compared with the molecular Zeeman structure of the highest lying triplet and singlet bound states. The states shown are those states which have the same total spin projection and are thus coupled through the coupled-channel equations.

of magnetic field where Feshbach resonances can occur.
Appendix F
Coupled-Channel Results: s-wave

In this appendix, I will present only those coupled-channel results involving channels which are experimentally relevant to magnetic traps and optical traps. Most of these are calculated in the zero-energy limit ($T = 0.1$ nK) and consider only s-wave collisions (exceptions are appropriately labelled). I use the $|f m_f\rangle$ basis which are the good quantum numbers in the zero-magnetic field regime. The notation $|f_1 m_1, f_2 m_2\rangle$ labels the symmetric/anti-symmetric collision between two atoms, one in state $|f_1 m_1\rangle$ and the other in $|f_2 m_2\rangle$.

F.1 $^6\text{Li} + ^6\text{Li}$

For the case of $^6\text{Li} + ^6\text{Li}$, I should point out that Fermi statistics prevent s-wave collisions between atoms in the same states. The following experimentally interesting channels have zero collisional amplitude.

\[
\begin{align*}
|\{\frac{1}{2} - \frac{1}{2} \frac{1}{2} - \frac{1}{2}\}\rangle &= 0 \\
|\{\frac{3}{2} \frac{3}{2} \frac{3}{2} \frac{3}{2}\}\rangle &= 0 \\
|\{\frac{3}{2} \frac{3}{2} \frac{3}{2} \frac{3}{2}\}\rangle &= 0
\end{align*}
\]
Figure F.1  Coupled-channel calculation for s-wave, $T = 0 \left\{ \frac{3}{2} \frac{3}{2} \frac{3}{2} \right\}$.

Figure F.2  Coupled-channel calculation for s-wave, $T = 0 \left[ \frac{1}{2} \frac{1}{2} \frac{1}{2} - \frac{1}{2} \right]$.
Figure F.3  Coupled-channel calculation for $\left|\left(\frac{1}{2}\frac{1}{2}\frac{1}{2} - \frac{1}{2}\right)\right|$ as a function of temperature. The elastic cross section is also shown; one can see the effect of the collisional resonance (at $B > 600$ G) in the cross section as the temperature is reduced. Only when the collisional resonance has been "frozen out" at low temperatures does the Feshbach resonance become pronounced in the cross section. The scattering length remains undefined in the vicinity of the Feshbach resonance despite the flat cross section at higher temperatures.
Figure F.4 Coupled-channel calculation for s-wave, $T = 0 \left\{ \frac{3}{2} - \frac{3}{2} \frac{1}{2} \right\}$. 
Figure F.5  Coupled-channel calculation for $\left\{ \left\{ \frac{3}{2} - \frac{3}{2} \right\} \frac{1}{2} \right\}$ as a function of temperature. The elastic cross section is also shown and the effect of the collisional resonance can be seen both at low field and high field. Only when the collisional resonance has been “frozen out” at low temperatures does the Feshbach resonance become pronounced in the cross section.
F.2 \(^7\text{Li} + ^7\text{Li}\)

For the case of \(^7\text{Li} + ^7\text{Li}\) the following magnetically low-field seeking channels are pure triplets.

\[
\begin{align*}
|\{22 22\}\rangle &= \text{triplet} \\
|\{22 21\}\rangle &= \text{triplet}
\end{align*}
\]

These channels do not undergo spin-exchange decay and have a scattering length of \(a = -27 \ a_0\) at all values of magnetic field.

Figure F.6 Coupled-channel calculation for s-wave, \(T = 0 \ |\{21 21\}\rangle\).
Figure F.7  Coupled-channel calculation for s-wave, $T = 0 \{1 - 1 1 - 1\}$.

Figure F.8  Coupled-channel calculation for s-wave, $T = 0 \{11 11\}$. 
Figure F.9  Coupled-channel calculation for \( |\{22 1 1\} \) as a function of temperature. The scattering length, elastic cross section, and spin-exchange rate are shown. The 10 nK and 1 \( \mu \)K curves sit on top of one another.
F.3 $^6\text{Li} + ^7\text{Li}$

For the case of $^6\text{Li} + ^7\text{Li}$ collisions, there is only one pure triplet channel. The $\left| \begin{array}{c} 22 \\ 3/2 \\ 2/2 \end{array} \right\rangle$ channel, which is important for sympathetic cooling, has a scattering length of 40.9 $a_o$ at all magnetic fields and does not undergo spin-exchange decay. The properties of other experimentally interesting channels are shown in the following figures.

![Graph showing scattering length and total exchange rate as functions of magnetic field](image)

**Figure F.10** Coupled-channel calculation for s-wave, $T = 0$ $\left| \begin{array}{c} 21 \\ 3/2 \\ 2/2 \end{array} \right\rangle$. 


Figure F.11  Coupled-channel calculation for s-wave, $T = 0 \left\{ \frac{1}{2}, \frac{1}{2} \right\}$. 

Figure F.12  Coupled-channel calculation for s-wave, $T = 0 \left\{ \frac{3}{2}, \frac{1}{2} \right\}$. 
Figure F.13  Coupled-channel calculation for s-wave, $T = 0 \left| \left( \begin{array}{c} 1 - 1/2 - 1/3 \end{array} \right) \right\rangle$. The spin-exchange decay is zero at low field and becomes non-zero at the field value where the $\left| \left( \begin{array}{c} 10 \ 3/2 - 3/2 \end{array} \right) \right\rangle$ channel becomes lower in energy than the initial channel.
Figure F.14  Coupled-channel calculation for $|\{1 - 1 \frac{1}{2} - \frac{1}{2}\}|$ as a function of temperature. The scattering length, elastic cross section, and spin-exchange rate are shown. The Feshbach resonances have complicated behavior because of the imaginary component to the phase shift (spin-exchange). The resonance on the far left is bounded and does not extend to $\pm\infty$. The resonance structure on the right is actually two resonances on top of one another, one of which is bounded and the other goes $\pm\infty$ (see reference [127] for a detailed discussion). The magnetic field resolution of this calculation does not show this structure for all the temperatures indicated, but it is there.
Figure F.15  Coupled-channel calculation for \( \left\{ 1 - 1 \frac{1}{2} \right\} \) as a function of temperature. The scattering length, elastic cross section, and spin-exchange rate are shown. The Feshbach resonances have complicated behavior because of the imaginary component to the phase shift (spin-exchange). The 10 nK and 1 \( \mu \)K curves sit on top of one another.
Appendix G
Molecular Potentials

G.1 \( a^3\Sigma_u^+ \) Potential

The \( a^3\Sigma_u^+ \) potential was adjusted to fit to two-photon photoassociation data. The various multipolar terms, \( C_6, C_8, \) and \( C_{10} \) are obtained from reference [90],

\[
C_6 = 1393.39 \ \text{atomic units} \quad \quad (G.1)
\]
\[
C_8 = 83425.8 \quad \quad (G.2)
\]
\[
C_{10} = 7372100. \quad \quad (G.3)
\]

The exchange portion of the analytic region has the form [91],

\[
V_{\text{exc}} = r^\alpha \exp(-\beta r) \quad . \quad (G.4)
\]

where

\[
\alpha = 4.558 \quad \quad (G.5)
\]
\[
\beta = 1.259 \quad \quad (G.6)
\]
\[
\gamma = 0.01288 \quad , \quad (G.7)
\]

so that the entire long-range portion of the \( a^3\Sigma_u^+ \) state looks like,

\[
V(r) = -\frac{C_6}{r^6} - \frac{C_8}{r^8} - \frac{C_{10}}{r^{10}} + V_{\text{exc}} \quad . \quad (G.8)
\]

The RKR region of the potential comes from the dense RKR curve found in reference [89] and covers the range from \( r = 6.3 \ a_o \) to \( r = 17.5 \ a_o \). The \( D_e \) value that was used to fit the model to the two-photon data is indicated in the tables. The innerwall from \( r = 3.0 \ a_o \) to \( r = 6.0 \ a_o \) was constructed from the OVC \textit{ab initio} calculation found in reference [71].

226
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**Table G.1** $^6$Li$_2$ ($N=0$) eigenstates in $a^3\Sigma_u^+$ potential. The value of $D_e$ needed to fit $v = 9$ was 333.742 cm$^{-1}$

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**Table G.2** $^7$Li$_2$ ($N=0$) eigenstates in $a^3\Sigma_u^+$ potential. The value of $D_e$ needed to fit $v = 10$ was 333.777 cm$^{-1}$
G.2 $X^1\Sigma_g^+$ Potential

The $X^1\Sigma_g^+$ potential was adjusted to fit to the one-photon photoassociation node seen in the singlet spectra. The various multipolar terms, $C_6$, $C_8$, and $C_{10}$ are obtained from reference [90],

\begin{align*}
C_6 & = 1393.39 \text{ atomic units} \quad (G.9) \\
C_8 & = 83425.8 \quad (G.10) \\
C_{10} & = 7372100. \quad (G.11)
\end{align*}

The exchange portion of the analytic region has the form [91],

\[ V_{\text{exc}} = \gamma r^\alpha \exp(-\beta r) , \quad (G.12) \]

where

\begin{align*}
\alpha & = 4.558 \quad (G.13) \\
\beta & = 1.259 \quad (G.14) \\
\gamma & = 0.01288 , \quad (G.15)
\end{align*}

so that the entire long-range portion of the $X^1\Sigma_g^+$ state looks like,

\[ V(r) = -\frac{C_6}{r^6} - \frac{C_8}{r^8} - \frac{C_{10}}{r^{10}} - V_{\text{exc}} . \quad (G.16) \]

The RKR region of the potential comes from Barakat et al. and covers the range from $r = 3.4 \ a_0$ to $r = 23.9 \ a_0$ [94]. The $D_e$ value that was used to fit the model to the one-photon transition node is indicated in the tables. The inner wall of the model is made up of three \textit{ab initio} points, two at $r = 2.75 \ a_0$ and $r = 3.00 \ a_0$ from reference [69], and one at $r = 3.25 \ a_0$ from reference [67].
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Table G.3 $^6\text{Li}_2$ (N=0) eigenstates in $X^1\Sigma^+_g$ potential. The fitted value for $D_e$ was found to be 8516.70 cm$^{-1}$. 
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**Table G.4** \(^7\text{Li}_2\) (N=0) eigenstates in \(X^1\Sigma^+_g\) potential. The fitted value for \(D_e\) was found to be 8516.75 cm\(^{-1}\).
G.3 $1^3\Sigma_g^+$ Potential

The $1^3\Sigma_g^+$ potential is the least well-known of the four major potentials discussed in this thesis. I use the same $D_\circ$ for both isotopes and use various multipolar terms found from previous fits [52, 56] and theory [128, 129]. These values are,

\[ C_3 = 11.0022 \text{ atomic units} \]  
\[ C_6 = 2300 \]  
\[ C_8 = 2.705 \times 10^5 \text{,} \]  

where some of these numbers have been adjusted simultaneously while adjusting the middle ab initio region of the potential in order to fit as best as possible with the observed photoassociation data [51, 58]. The RKR data comes from reference [66] and covers the range $r = 4.6 \ a_\circ$ to $r = 7.8 \ a_\circ$ where this data is reference to the long-range asymptote using,

\[ D_\circ = 7092.0 \text{ cm}^{-1} \]  

The ab initio data used from $r = 3.25 \ a_\circ$ to $r = 4.5 \ a_\circ$ and from $r = 8.0 \ a_\circ$ to $r = 20.0 \ a_\circ$ comes from a composite potential constructed from references [68–71]. The middle ab initio region was adjusted by a fit where,

\[ V(r) \to V(r) \times \left(1 + A + \frac{B}{r} + \frac{C}{r^3}\right) \]  

and the fitted constants used are,

\[ A = 0.0080144 \]  
\[ B = 0.000621279 \]  
\[ C = 0.000548877 \text{.} \]  

This model presented here assumes a $0_g^-$ long range Hund’s case (c) state [72]. There are some problems matching this model spectrum with the very high-lying photoassociation data since the observed features will be a mixture of $0_g^-$ and $1_s$ states and this
is not accounted for in the model. Since the observed one-photon photoassociation spectra was primarily $N = 1$ rotationally excited, that effect is included as well as the Born-Oppenheimer rotation correction, $P(R)$, which is discussed in chapter 3.

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**Table G.6** $^7\text{Li}_2$ (N=1) eigenstates in $1^3\Sigma_g^+$ potential.
G.4 1\(^1\Sigma^+_u\) Potential

The 1\(^1\Sigma^+_u\) potential is one of the best known potentials and consequently can be modelled to high accuracy. This results from the large amount of experimental data, essentially every vibrational level has been measured. We used the RKR from Linton et al. [73] which covers a range from \(r = 3.8 \ a_o\) to \(r = 97.3 \ a_o\). We only use this data up to \(r = 25.4 \ a_o\) since this covers the energy range from the inner part of the well out to where our observed photoassociation data overlaps [52]. Two ab initio points are used for the inner wall at \(r = 3.25 \ a_o\) and \(r = 3.50 \ a_o\) [67]. These tables show eigenvalues for the two isotopes assuming \(N = 1\) rotational excitation, and taking into account Born-Oppenheimer corrections as well as radiation retardation in the \(C_3\) coefficient (see chapter 3). The long-range analytic form approaches a Hund’s case (c) \(O^+_u\) state [72]. The \(C_8\) coefficient is assumed constant with a value of \(2.705 \times 10^5\) atomic units [128, 129]. The \(C_3\), \(C_6\), and \(D_e\) values are fitted for each isotope and are given in the respective table.
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Table G.7 $^6$Li$_2$ (N=1) eigenstates in 1$^1$Σ$^+_u$ potential. The fitted potential parameters are $C_3 = 11.0032$ a.u., $C_6 = 2140$ a.u., and $D_8 = 9352.18$ cm$^{-1}$. 


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<td>-196.889</td>
<td>3.7</td>
</tr>
<tr>
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<td>3.7</td>
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<td>-105.533</td>
<td>3.7</td>
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<td>3.7</td>
<td>91</td>
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<td>3.7</td>
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Table G.8: $^7\text{Li}_2$ ($N=1$) eigenstates in $1^1\Sigma_u^+$ potential. The fitted potential parameters are $C_3 = 11.0022$ a.u., $C_6 = 2350$ a.u., and $D_e = 9352.10$ cm$^{-1}$. 
Appendix H

Computer Programs

The work presented in this thesis relies on several computer programs which I would like to discuss here. All of this code is written in C and compiled under the Unix based AIX operating system on an IBM workstation. I have tried to make the various pieces of code as readable as possible with comments within the code listings. The code discussed here was originally developed in my personal directories and now has been transferred to "/lab/source/iancode”. Some of the data files presented in this thesis can be found in either location. With the exception of the evaporation code, most of the programs are compiled with the syntax “cc -O filename.c -o filename -lm”. The evaporation program is compiled with the “makefile” utility. I have tried to write “readme” files where appropriate to further explain the code compilation and execution. Most of the programs require command-line inputs. If a program is executed without the proper inputs, a short description of the required input is given.

H.1 Coupled-channel Code

This program is the largest and most complicated of the various programs presented. As a result, I have tried to make its execution as straightforward and user-friendly as possible. The code is compiled with the command “cc -O coupled.c -o coupled -lm”. The syntax is,

\[
\text{couple [atom(6,7,67)] [r}_{\text{start}}(a_o)] [r}_{\text{end}}(a_o)] [\text{step}(a_o)] \\
[\text{E(mK)}] [f_1] [m_1] [f_2] [m_2] [\text{B(G)}] [N] \{\text{wave outfile}\}
\]

Required command line inputs are indicated with square brackets “[]” while optional inputs are in braces “{}”. The first input specifies whether the collision is pure $^6\text{Li}$, pure $^7\text{Li}$, or mixed $^6\text{Li} + ^7\text{Li}$.
The next four inputs specify the starting and ending points for the integrated wavefunctions as well as the step size used and the collision energy. The starting point must be located within the classically forbidden region of the innerwall. Typically a value of 1 Bohr is used. The integration is then carried out to \( r_{\text{end}} \) as entered by the user. In order to get accurate scattering information, the user must make sure that this point is reasonably far into the asymptotic region. Typically a value of 1500 Bohr will work for collision energies of 1 nK or higher. The asymptotic region is defined to be where the two-body potential energy is much less than the kinetic energy in the channel; therefore as the energy is reduced the integration must be carried out to further values of interatomic separation. If the value of the potential at \( r_{\text{end}} \) is greater than the entered collision energy, the program will warn the user and roughly estimate what \( r_{\text{end}} \) should be. The required step size should be small and a typical value is 0.01 Bohr. Once the integration is beyond 25 Bohr, the step size is increased by the code in order to speed up the run time.

The channel spin states are specified by the next four inputs. These are the atomic angular momentum \( f_1 \) and \( f_2 \) for each respective atom as well as the corresponding projection \( m_1 \) and \( m_2 \). For \(^6\text{Li} \), these values are \( f = 1.5 \) with \( m = 1.5, 0.5, -0.5, -1.5 \) and \( f = 0.5 \) with \( m = 0.5, -0.5 \). For \(^7\text{Li} \), these values are \( f = 2 \) with \( m = 2, 1, 0, -1, -2 \) and \( f = 1 \) with \( m = 1, 0, -1 \). For the case of \(^6\text{Li} + ^7\text{Li} \), the \( f_1, m_1 \) pair must be \(^6\text{Li} \) and the \( f_2, m_2 \) pair must be \(^7\text{Li} \). Even though multiple channels are calculated simultaneously, the asymptotic channel which defines \( E = 0 \) is specified by these inputs.

The final two required inputs specify the magnetic field (in Gauss) and the rotational quantum number \( N \) of the collision. An s-wave collision has \( N = 0 \), a p-wave has \( N = 1 \), etc. If a given collision is not allowed by symmetry, this is indicated. The last optional input specifies a file into which the wavefunction, \( \Psi(r) \), of the input channel is written. The format for this file is
\[ r(\text{Bohr}) \, \text{Re}(\Psi) \, \text{Im}(\Psi) \, \text{Re}(P_S \Psi) \, \text{Im}(P_S \Psi) \, \text{Re}(P_T \Psi) \, \text{Im}(P_T \Psi), \]

where \( P_S \) and \( P_T \) are the corresponding singlet and triplet projection operators.

Depending on the number of channels involved, the runtime of the code can vary by quite a bit. Scattering problems requiring only a few channels can run in less than a minute on the computer. For large problems, such as \(^6\text{Li}\) colliding with \(^7\text{Li}\), this can require up to 11 channels and may take many minutes. The S-matrix is written to a file called “S_matrix.out” along with other information such as the magnetic field, collision energy, and scattering length of the input channel. Most of this information is also mirrored to the screen and is self-explanatory.

In order to facilitate running large batch files, I have written addition code which aids in this endeavor. The programs “chout” and “chout2” analyze the “S_matrix.out” file and output the relevant information in a single line. The syntax is,

```
chout(or chout2) [s-matrix file] \textit{[f1]} \textit{[m1]} \textit{[f2]} \textit{[m2]}
```

The output for “chout” is,

\[
\text{B(G) E(mK) N [cross section (cm\(^2\)] [Re(phase)] [Im(phase)]} \\
\text{[scattering length (a\(_o\))] [G\(_1\)…G\(_n\) (cm\(^3/s\))] [G\(_\text{total}\) (cm\(^3/s\))],}
\]

where \( G_1…G_n \) specify the spin-exchange rate for decay into channels 1...n and \( G_{\text{total}} \) is the sum. The output for “chout2” is similar,

\[
\text{B(G) E(mK) N [momentum k (atomic units)] [cross section (cm\(^2\)]} \\
\text{[Re(phase)] [Im(phase)] [scattering length (a\(_o\)]} \\
\text{[k cot(phase)] [G\(_1\)…G\(_n\) (cm\(^3/s\))] [G_{total} (cm\(^3/s\))].}
\]

The program “getrate” specifies the information regarding spin-exchange in more detail. The syntax is,

```
getrate [s-matrix file]
```
and it outputs all the explicit $G_1...G_n$ as described above.

Finally, the program "bat" is a batch code which runs the "chout" program for a specified range of magnetic field. The syntax is,

\[
\text{bat [atom(6,7,67)] [f_1] [m_1] [f_2] [m_2] [B_{\text{min}}(G)] [B_{\text{max}}(G)] [E{(\text{mK})}] [N]
\]

and the output is appended to a file called "dat..f_1..m_1..f_2..m_2..E". These files contain a list of "chout" outputs making them easy to import into a graphing program for plotting scattering properties as a function of magnetic field. This program stores the file in "../data/ch(atom)" based on the type of collision (6, 7, or 67). The step-size for changing the magnetic field from $B_{\text{min}}$ to $B_{\text{max}}$ is hardwired in "bat.c" and can be altered before compiling the code.

All of these programs can be found in "../lab/source/iancode/cc_code". The original code was developed in a number of stages which can be found in "../wim/models/cc_calc", "../wim/models/cc_calc2", and "../wim/models/cc_calc3". The scattering calculations presented in the majority of this thesis can be found in "../cc_calc2", "../cc_calc3", and the new directory "../lab/source/iancode/cc_code".

H.2 Calculation of Bound States and Frank-Condon Overlap

The main program used to analyze bound states of the various potentials is a Numerov-Cooley integration routine [44, 45]. This program can be found in "../lab/source/iancode/cooley" and is entitled "cooley.c". The source listing has definitions which specify the particular lithium potential to use as well as the appropriate mass. Once these have been selected, the code is compiled with the usual "cc -O cooley.c -o cooley -lm". The Numerov-Cooley routine constructs the wavefunction in two pieces, one from an inner point and the other from an outer point both of which should be in the classically forbidden regions of the potential. At some intermediate matching point, the slopes of the inner and outer wavefunctions are compared and a
correction to the energy is made before restarting the integration process. This is discussed in my previous thesis [56]. The eigenvalue/wavefunction correction converges to the actual answer rapidly and with a tolerance indicated by the user. The input is parsed with the following flags,

```
cooley [e X] { n X } { h X } { i X } { o X } { t X } { ep X } { w Y } ,
```

where “X” is a number and “Y” is a file name. The flags are defined:

- “e” initial guess to energy in GHz (or Hartrees)
- “n” rotational quantum number
- “h” step size of integration in Bohr
- “o” outer starting point of integration in Bohr
- “i” inner starting point of integration in Bohr
- “t” tolerance of integration
- “ep” value of wavefunction at starting points (should be small)
- “w” write wavefunction to file with name “Y” given

The default values of these parameters are indicated by running “cooley” without any inputs.

When the program completes running, the converged eigenvalue is reported. Since the particular eigenvalue which it converges to is dependent on the various inputs, it is important to have reasonably close “first guesses” for the inputs. This program is used to generate eigenvalue spectra for all the potentials discussed in this thesis. These spectra, with their corresponding run codes, are found in “/lab/source/iancode/cooley”.

I have a number of different versions of “cooley”; the versions used to generate the
spectra also report classical turning points in addition to the converged eigenvalue. As an additional note, some of these versions require the initial energy guess to be in Hartrees instead of GHz.

Another important application of this bound-state integration program is to generate wavefunctions for calculating Frank-Condon overlaps. This is particularly useful for estimating photoassociation transition strengths. In addition, this was needed in order to fit the observed transition nodes in the single photoassociation data and consequently extract information about the ground state singlet potentials (see chapter 3). The singlet extraction code has been documented in "/lab/source/iancode/cc_code/singlet". The "cooley" integrator was used to generate excited bound-state singlet wavefunctions while the coupled-channel "couple" code was used to generate various ground state scattering wavefunctions. The observed singlet spectra is a measure of the overlap between the singlet component of the scattering wavefunction and the excited singlet state into which the atoms are photoassociating. This overlap calculation is done with "aveoverlap.c" which is found in "../singlet/six" and "../singlet/seven" depending on the isotope in question. The various ground-state scattering wavefunctions are located in my personal directories and are calculated at various values of singlet dissociation energy as described in chapter 3. All of this is discussed in the appropriate "readme" files.

I have also calculated overlaps for $^7$Li free-bound and bound-bound transitions. The bound-bound transitions are found using only "cooley" wavefunctions and these are documented in "/lab/source/iancode/cooley/bndexc". The free-bound transitions are found using the coupled-channel code and the cooley code. These transitions are documented in "/lab/source/iancode/cooley/gndexc".
H.3 Optimization of Evaporation for Ioffe Trap

This program is a modification of Cass Sackett’s original program as described in his PhD thesis. The program is found in the directory “/lab/source/iancode/evap/ioffe” and is run using the syntax,

\[
\text{opt2} \ [N_{\text{start}}] \ [N_{\text{stop}}] \ [T_{\text{start}}(\mu K)] \ [n_{\text{grid}}] \ [\text{fileroof}] \ \{ -b \ G_1^{-1}(s) \} \ \{ -t \ 2G_2 \ (\text{cm}^3/\text{s}) \} ,
\]

where \( N_{\text{start}} \) is the initial number of atoms in the trap, \( N_{\text{stop}} \) is the number of atoms at which the simulation halts, \( T_{\text{start}} \) is the initial temperature, \( n_{\text{grid}} \) is the number of energy grid points to use, and “fileroof” is an identifier used in the data files created by the run. The optional inputs \( G_1 \) and \( G_2 \) are the background loss rate and two-body dipolar loss rate respectively. Typically, \( n_{\text{grid}} = 200 \), and “fileroof” has the form “opt2_{N_{\text{start}}-T_{\text{start}}-G_1-B}” where the magnetic bias field \( B \) must be hardwired into the source code header file “evap.h”. In fact, all of the Ioffe trap parameters such as the radial gradient, the axial harmonic frequency, as well as the bias field are in “evap.h” which is located in the directory “/lab/source/iancode/evap/ioffe/source2”.

To change these parameters, one must edit the “evap.h” file and then recompile “opt2” using the “makefile -f” command as described in Cass’ thesis. The two-body dipolar rate \( G_2 \) is hardwired within the code to be the accepted value of \( 1 \times 10^{-14} \ \text{cm}^3/\text{s} \) (for \( ^7\text{Li} \)).

When “opt2” is run, it produces four files named “fileroof” with the extensions “.dat”, “.log”, “.dist”, and “.eta”. The “.dat” file is the most important as it contains all of the information pertaining to the evaporation trajectory. It reports, as a function of time, the number of atoms remaining, their average energy, the peak density, the energy position of the evaporation razor, and the log of the peak phase space density normalized to the critical quantum degenerate phase space density. This file is used to generate the evaporation trajectory for the experiment. The “.log” file records various, self-explanatory aspects of the program execution. The “.dist” file records the energy distribution of the cloud at the end of the simulation. Finally, the
".eta" file lists the value of the evaporation razor \((\eta_{\text{cut}} = E_{\text{cut}}/(E))\) as a function of time.

In order to create an evaporation trajectory for use in the experiment, two steps are involved. First, "opt2" must be executed as described above to generate the necessary ".dat" file. These files have been stored in "/lab/source/iancode/evap/ioffe/traj2" and "/lab/source/iancode/evap/ioffe/traj3". Once a trajectory ".dat" file is created, the next step is to convert the energy razor to frequency units and time steps using the program "evaptraj". This program is located in the source listings with "opt2" and has the syntax,

\[
\text{evaptraj [ infile ] [ outfile ] [ } T_{\text{start}}(\mu K) \text{ ] ,}
\]

where \(\text{infile}\) is the full name of the ".dat" file, \(\text{outfile}\) is the name of the file produced which I usually designate "fileroot.in", and \(T_{\text{start}}\) is the temperature at which the cooling trajectory is to begin. This allows us to extract a trajectory from a ".dat" file which may have been started with a higher initial temperature than the one which we wish to use. The format of the \(\text{outfile}\) from "evaptraj" has two columns, the first column is the duration (in ms) at which the microwave frequency (the second column) is applied. The various ".in" files which are used for experimental evaporation are found in the directories "/lab/source/iancode/evap/ioffe/traj2" and "/lab/source/iancode/evap/ioffe/traj3".

### H.4 Spin-Exchange Decay

The programs used to calculate spin-exchange decay for both \(^6\text{Li}\) and \(^7\text{Li}\) data can be found in "/lab/source/iancode/exchange". In this directory, various files with the ending ".dat" contain actual data taken from electromagnetic trap measurements. The files are indexed in the "readme" file and their format consists of three columns: time (s), number, and peak density (cm\(^{-3}\)).
The program for analyzing $^6\text{Li}$ data is called “excfit”. The syntax for execution is,

\[ \text{excfit [filename(.dat)]}, \]

where the appropriate data file, with the format described above, is used. It uses a Levenberg-Marquardt non-linear fitting method [119] to fit the change in the number of atoms,

\[ \frac{dN}{dt} = N_0(1 + kt)^\gamma, \]  

(H.1)

where $N_0$ is the initial number, and $(k, \gamma)$ are fit parameters. If the decay is primarily a constant two-body effect (as is the case for $^6\text{Li}$) then a plot of $dN/dt \times 1/N$ versus $n_0$ (peak density) should be a straight line. This has been discussed in chapter 6. The program “excfit” outputs five columns: the time, number of atoms $N$, $dN/dt$, peak density $n_0$, $dN/dt \times 1/N$, and the fitted $dN/dt \times 1/N$. The slope of the line $dN/dt \times 1/N$ versus $n_0$ is related to the spin-exchange decay of the $^6\text{Li}$ system subject to assumptions about the initial spin populations (see chapter 6). At the end of the output, “excfit” outputs two different rate constants depending on whether two or three spin states are initially present.

The program for analyzing $^7\text{Li}$ decay is substantially more complicated since the $^7\text{Li}$ gas is not expected to spin-decay with a constant two-body rate (see chapter 6). Instead, the entire system must be modelled as a set of coupled differential equations which govern the decay of the various spin populations. The programs “model” and “model2” both describe this decay; the “model2” version has the added feature of also taking into account one-body background loss effects. There are no inputs for the “model” or “model2” programs, the initial spin populations and the various decay rates must be hardwired into the code. I never had time to develop a non-linear fitting routine for these parameters, instead I just adjust the initial spin populations within the code and compare the output to the data. The output of
“model” and “model2” consists of seven columns: \( t \text{ime(s)}, \) total peak density \( n_{\text{tot}}, \) peak density of \((f, m) = (1, -1), \) density \((2, 0), \) density \((2, 1), \) density \((2, 2), \) and \( dn_{\text{tot}}/dt \times 1/n_{\text{tot}}. \) The \((2, 0)\) state should not be trapped at low magnetic field so I usually set its spin population to zero. The results of these program runs are stored in “/lab/source/iancode/exchange”.

### H.5 Constants and Library Functions

Many of the programs described in this appendix rely on a number of physical constants and conversions. Rather than having multiple definitions of these constants scattered throughout different programs, I have elected to construct a single library which most of these codes have access to. This library is named “constants.h” and is located in the directory “/lab/source/iancode/lib”. Among the defined constants are: hyperfine constants for \(^6\text{Li}\) and \(^7\text{Li}\), nuclear g-ratios for both isotopes, atomic masses for both isotopes, the speed of light, Planck’s constant, Rydberg’s constant, \(\pi\), etc. These are all explained clearly in the file along with references where needed. The library also includes conversion functions for Angstroms to Bohr, wavenumbers to Hartrees, and frequency to Hartrees. These constants are seen by the coupled-channel program, the potential files, and a number of other programs I have written. This system eliminates variations of physical constants between programs helping to reduce numerical errors.

### H.6 Calculation of Magnetic Field

The directory “/lab/source/iancode/magfield” contains all the versions of the program used to calculate the magnetic field distribution of the electromagnetic trap. The original code is “/lab/source/iancode/magfield/mag.c” and models what we took to be our ideal coil geometry. Since installing the coils and making a number of measurements, we feel that the coils do not sit flush against the re-entrant windows, so we had to modify the assumed geometry. These modifications were made by Bita.
Ghaffari and are located in the directory "/lab/source/iancode/magfield/bita". The various dimensions which define the coil geometry are defined at the beginning of the respective program source code.

The modified program is "/lab/source/iancode/magfield/bita/mag0_fr.c" and has the syntax,

\[ \text{mag0}_{.}\text{fr} [x(\text{cm})] [y(\text{cm})] [z(\text{cm})] [\text{range(\text{cm})}] [I_B(A)] [I_C(A)] [I_Q(A)] , \]

where the coordinate (x,y,z) specifies the point in 3-space where the cross sections of the field are calculated (the point (0,0,0) is the trap center), the range specifies how far the cross sections are calculated, and the current in the bias, curvature, and quadrupole coils are specified by \( I_B \), \( I_C \), and \( I_Q \) respectively. The program outputs four different cross sections to four different files. These files are “xout.dat”, “yout.dat”, “xyout.dat”, and “zout.dat”. Each file has a five column format: coordinate (cm), \( B_x \) (G), \( B_y \) (G), \( B_z \) (G), and \( |B| \) (G). The coordinate system assumes that the ‘z’ direction is defined by the cylindrical axis of the Ioffe field. The “xout.dat” file shows the field at (x±range,y,z) where the coordinate ranges from x-range to x+range. Similarly, the “yout.dat” file shows the field at (x,y±range,z), the “zout.dat” file shows the field at (x,y,z±range), and the “xyout.dat” files shows the field at (x±range,y±range,z). In order to look at these various cross sections, the Gnuplot file “b.gnu” can be used. As a final note, the program “magmot” allows one to look at the MOT configuration of the coils. It only energizes one bias and one curvature coil in its modelling and has the same syntax as “mag0_fr” (one needs to set \( I_Q = 0 \)).

### H.7 Photometrics CCD Image Fitting

The programs used to fit to both fluorescence and absorption images taken with the Photometrics CCD camera can be found within the directory “/lab/source/iancode/pmisp”. There are a couple of versions which are explained
in the “readme” files found within this directory. The most up-to-date version of the fluorescence image fitter is located in "/lab/source/iancode/pmis/asym_fit". This program, “cfit.c”, is compiled under the name “cf” and uses a simplex fitting routine (described in chapter 6) to fit the fluorescence image with a 2D Gaussian. The major/minor axes of this fit are at an angle with respect to the CCD array and this angle is a fit parameter as well. The syntax is,

\[ \text{cf [atom (6/7)] [atom/natom file#] [pulsetime (\mu s)]}, \]

where the first input indicates whether the image is \(^6\text{Li}\) or \(^7\text{Li}\), the second input indicates the file number to analyze, and the pulsetime is the amount of time the fluorescence pulse is applied.

The fluorescence image is calculated from two different images. During the measurement, a picture is taken with the atoms present and is named “atomsX.pmi” where “X” is a number. Immediately afterwards, another picture is taken under similar conditions without the atoms and is named “natomX.pmi”. The “cf” program takes the fluorescence picture to be (atomsX.pmi − natomX.pmi) where “X” is the file number input. The program assumes that the axial and radial frequencies are known; these are defined constants within “cfit.c” and can be changed. In addition to these constants, the horizontal scaling, vertical scaling, and geometric collection efficiency must also be properly set. The output of “cf” gives the fit parameters as well as the number of atoms present, the peak density, and the effective temperatures seen in both the radial and axial axes. The radial frequency is bias field dependent (see chapter 4) and is usually not known well. Consequently, we usually read the axial temperature as the “proper measurement”. In fact, since we assume that the axial and radial temperatures are the same (the ergodic approximation ensures this) one can use the fit to ascertain what the effective radial frequency is. This has been done in the absorption analysis program “afit.c” discussed in the following paragraph.
The absorption analysis program is located with “cf” in the sub-directory “abs” and is called “afit.c”. The executable is “af” and has the syntax,

\[ \text{af [atom (6/7)] [atom/natom file#] [magnification] \{ x y centerguess \}} \]

where the isotope number is the first input, the file number is the second, the magnification for the imaging is the third, and an optional CCD array coordinate (x,y) can be entered to aid in finding the center of the image. The absorption data discussed in this thesis was primarily taken with a much faster, less sensitive, Electrum CCD with its own software. The “af” program will eventually be used for analysis with the better Photometrics CCD once evaporative cooling achieves dense enough clouds. I have found that the program fitting routine does not always make accurate enough guesses for the fitting parameters and consequently gets “stuck” in local minimum in the \( \chi^2 \)-space of the fit. This program will need further development. The absorption image is calculated from “atomsX.pmi” and “natomX.pmi” images as discussed with “cf”, but it also uses a reference picture “ref.pmi” which is essentially a background picture without any probe light present. So,

\[
\text{absorption} = \frac{\text{noatom} - \text{atom}}{\text{noatom} - \text{ref}}.
\]  

(\( H.2 \))

**H.8 Molecular Potentials**

The various molecular potentials described and used in this thesis can be found in “/lab/source/iancode/potentials”. The potentials are constructed out of a variety of \textit{ab initio} points, RKR points, and analytic points which are encoded in various “.c” files. There are four different files corresponding to the ground and excited state potentials. These are “ssigg.c” and “tsigu.c” for the ground state singlet and triplet respectively. The excited state singlet and triplet are “ssigu.c” and “tsigg.c”. The various data points and analytic forms of each potential are described within these files. Where appropriate, I use data in the original form; the \textit{ab initio} and RKR are
encoded in the exact units in which they are reported in the respective literature. This makes a direct comparison with the references easy. When the code is executed, the various pieces are converted to atomic units (using “constants.h” from the common library routines) before splining everything together.

The program “plpot” is used to select one potential and output data pairs ‘r’ and ‘V(r)’ over a given range. This program has no inputs, the code listing must be modified to select both the potential and the range of points to output. For the case of the ground state potentials, the dissociation energy varies between isotopes and must be properly selected in the appropriate potential “.c” file. The listings are well commented and this should be straightforward. The output of “plpot” is in atomic units: Bohr versus Hartrees. I have run “plpot” for each potential and these files are the “.DAT” files in the “../potentials” directory. These files represent our most current potential models to date. I should point out that the bound-state integrator “cooley.c” uses these routines when it is compiled. In contrast, the coupled-channel code “couple.c” has its own definition of the singlet and triplet ground state potential which is located with its source listing.
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