

Chapter 1

Introduction

The study of particle collisions has a long and storied history in the annals of scientific exploration. Much of our understanding of the fundamental nature of particles and their underlying microscopic interactions has been derived from scattering experiments. A famous example is the work of Ernest Rutherford, who in 1911 scattered alpha particles off thin gold foil. He quickly realized that the only explanation for the observed distribution of backscattered particles was the presence of a charged massive core concentrated within a tiny spatial region. He thus discovered the nucleus and proposed a celestial model for the atom, with electrons orbiting a massive central nucleus. Soon thereafter, Neils Bohr combined his quantum theory of light with Rutherford's model to build a theory of the hydrogen atom and with it modern atomic physics was born.

The existence of atoms (or at least something called atoms) had been accepted in some scientific circles hundreds of years earlier. One of the first gas dynamics experiment was performed by Robert Boyle who discovered in 1662 the inverse relationship between the volume and pressure of a gas. This relationship was independently verified by Mariotte[1] five years later. However, it was probably Bernoulli (1739) who first recognized that the pressure of a gas is a result of collisions between the particles and the container. The development of the kinetic theory of gases by Maxwell, Boltzmann, Krönig, and Clausius, among others, was begun in the mid-1800's to combat the hopeless task of evaluating each individual particle's contribution to the bulk properties of the gas. Kinetic theory replaces the individual particle motion with average quantities based on the statistics of the sample. From these considerations, Maxwell developed his theory of velocity distributions (1860). A key concept in kinetic theory is that any disturbance in one part of the gas is transmitted throughout by particle collisions. In this manner, energy (thermal conductivity), momentum (viscosity), and mass (diffusion) can be moved around within the gas. Boltzmann (1872) (improving on an earlier result of Maxwell's) derived a nonlinear integrodifferential equation that describes the evolution of an initially non-uniform gas and, from which, these transport properties can be calculated. Treating the gas particles as tiny classical "billiard balls" bouncing off one another, Maxwell found that the viscosity of a gas is independent of its density. His

subsequent experiments validated this surprising result, which proved to be one of the first successes for the classical kinetic theory of gases and thus for the underlying mechanism of particle collisions. (Later measurements showed that this result is not exact for real gases but it is a good approximation at moderate densities).

With the development of quantum mechanics and a better understanding of the structure of atoms, it became clear that atomic collisions are a much more complicated process than envisioned by Maxwell and his fellow 19th century scientists. However, classical kinetic theory continues to provide a reliable method for determining the macroscopic properties of a gas, provided quantum mechanical collision cross sections are used in place of the corresponding classical scattering cross sections. In the particular case of dilute monatomic gases, Chapman (1916) and Enskog (1917) were able to show that classically, the bulk transport properties are related to integrals over the interatomic potential energy surfaces. This provided the first direct link between macroscopic properties of the gas and the underlying microscopic forces that atoms exert on one another. With it came the obvious question: can a study of the bulk properties of a gas be used to understand the underlying atomic interactions? Given the complexity of the relationship, the answer was far from obvious, but over the last half-century great strides have been made (see for example Ref.[2]). (Transport measurements are not the only avenue to obtain this information but they are the most relevant for this particular work). In particular, the temperature dependence of the viscosity of a gas has yielded useful information about the interatomic potential. This is due in large part to the fact that viscosity can be measured much more accurately than other transport properties. Measurements over the temperature ranges from tens of degrees Kelvin to several thousand degrees Kelvin have been made for both pure and binary mixtures of dilute gases, primarily by the groups of Smith[3], Guevara[4], and Kestin[5].

Further departures from the classical physics of Maxwell's day arose with the development of laser cooling and trapping of neutral atoms (1985, see Ref.[6, 7]). The translational motion of the atoms can now be slowed to the point where the effects of quantum statistics begin to affect the overall behavior of the gas. Probably the biggest single achievement in this regard has been the realization of a Bose-Einstein condensate (BEC), first seen here at JILA (1995) in a dilute gas of ^{87}Rb [8] atoms and quickly followed by observations in gases of ^7Li [9] and ^{23}Na [10] atoms. It has since been observed by nearly twenty groups (see <http://amo.phy.gasou.edu/bec.html> for the latest BEC developments). Bose-Einstein condensation is a macroscopic quantum mechanical phase transition in which a large fraction of bosons spontaneously occupies the quantum mechanical ground state as its temperature approaches absolute zero. A condensate thus exhibits purely quantum mechanical properties on a macroscopic scale, which makes it unique.

Collisions play an important role both in the road to condensation and in the behavior of the condensate itself. Cooling atoms with laser light has thus far proven insufficient to produce BEC. Instead, it has proven necessary to use evapo-

rative cooling techniques to maintain the phase space density required for condensation. With evaporative cooling, the atoms are loaded into a magnetic trap that is approximately harmonic. A radio-frequency field is then applied, lowering the trapping potential so that only the “hottest” (i.e., most energetic) atoms are removed from the trap. The remaining atoms are left to re-thermalize to a colder temperature via elastic collisions. These elastic collisions are loosely termed “good” collisions, since they are an essential part of the cooling process. On the other hand, magnetic traps are extremely weak, with depths on the order of few milliKelvin. If a pair of atoms should collide and “flip” a spin, they may end up in untrapped spin states or the collision may release enough energy to eject the pair from the trap. Either outcome constitutes a “bad” inelastic collision. A general rule of thumb devised by experimentalists is that about 100 good elastic collisions are needed for every bad inelastic collision if the cloud is to re-thermalize sufficiently quickly to condense the gas before too many atoms are lost.

Once a condensate is produced, its properties are almost wholly determined by the s -wave two body scattering length a (which is related to the elastic scattering cross section in the $T \rightarrow 0$ limit). In fact, the sign (positive or negative) of the scattering length determines whether condensates comprised of large numbers of atoms can even be produced[11]. A variety of mean-field and Hartree-Fock approaches have been introduced for evaluating condensate properties, all of which adequately approximate the strength of atom-atom interactions using a mean-field interaction term that is proportional to a . (A good review of current BEC theories is provided in Ref[12].) In addition, modern kinetic theories that describe condensate formation[13] require atomic scattering input.

Another intriguing aspect of collisions in this cold regime is the prospect of using external fields to influence the outcome. One method proposed by Stwalley[14] is to induce a Feshbach resonance using a magnetic bias field. The resonance would in principle allow control over the s -wave scattering length. This was recently realized in ^{23}Na condensates[15] and in thermal Rb[16, 17] and Cs[18] clouds. In terms of condensates, the appeal of this idea is two-fold: 1) it provides a mechanism for enhancing the elastic collision rate, which could allow condensation of isotopes that are hard to cool otherwise (this is somewhat of a fine line since generally the inelastic collision rate is also increased near the resonance), and more importantly 2) it provides for “tunable” condensate properties. (Tunability was not achieved in the Na experiment because of a large increase in the three-body recombination rate. Whether this an inherent problem or instead is isolated to this particular Na experiment is still unresolved.) Magnetic-field tuning of the scattering length is possible only because the average collision energy of the atoms is much less than the atomic hyperfine splitting.

Extremely low collision energies also imply that the atoms interact with one another for a long time during a collision event. This makes the study of cold collisions an ideal method for understanding the weak long-range forces that atoms

exert on one another. Photoassociation spectroscopy is a tool that has been successfully applied in this regard. The idea was first proposed by Thorsheim, *et al.*[19]. In photoassociation, an excited molecular bound state is resonantly formed through photoexcitation during the collision of two atoms, (e.g. with a CW laser). The low collision energies lead to well-resolved rotational (and in some cases hyperfine) spectra with linewidths approaching the natural linewidth. In particular, this technique has been extremely useful for measuring nodes and antinodes of the ground state colliding wave function (via the Franck-Condon overlap). In this way, accurate values for the *s*-wave scattering lengths have been derived for most of the alkalis. In addition, retardation effects[20] have been observed in excited Na₂ bound states[21], and accurate values of atomic lifetimes for ²³Na[21] and ³⁹K[22] have been derived from these bound state measurements.

This dissertation has developed and extended the theoretical tools necessary to calculate and understand two-body and three-body collisions of trapped alkali atoms. In brief, ground state two-body collisions comprise Chapters 2-5, while photoassociation spectroscopy is the subject of Chapters 6-7, and three-body collisions of ground state atoms are treated in Chapter 8.

The chapters are broken down as follows: the coupled Schrödinger equations for two-body ground state alkali collisions are derived in Chapter 2. Here, definitions for cross sections, scattering event rates, and scattering lengths are provided in terms of the scattering matrix. The interactions and the corresponding Hamiltonian for the colliding atom pair are also discussed in this chapter. Numerical techniques for obtaining the scattering matrix by solving the coupled Schrödinger equations are presented in Chapter 3. Chapter 4 develops a powerful alternative approach for evaluating the scattering matrix. Here, the ideas of multichannel spectroscopy[23] are applied to the two-body collision problem. The outcome is a short-range reaction matrix that incorporates the bulk of the scattering physics, yet remains essentially energy-independent over nearly a degree Kelvin. Simple algebraic manipulations allow the scattering matrix to be evaluated in terms of this reaction matrix and a set of long-range parameters. Moreover, these long-range parameters are “standardized” in a form that makes them nearly atom-independent. In addition it is shown that the reaction matrix can be approximated, with reasonable accuracy sufficient for survey calculation in most systems, entirely in terms of single channel parameters and a recoupling matrix.

The theory developed in the previous chapters is then applied to a set of collision experiments conducted here at JILA. These results are discussed in Chapter 5. The new experimental information permitted us to refine the Rb interatomic interaction potentials. Based on these state-of-the art potentials, predictions of scattering observables are then provided for other Rb isotopes. The theory of photoassociation lineshapes is presented in Chapter 6. This theory is then applied in Chapter 7 to analyze measured rovibrational spectra of the ³⁹K 0_g⁻ state. This analysis extracted the first accurate values of the ³⁹K scattering lengths. Finally, Chapter 8 presents a

theory of three-body recombination, a process in which two atoms recombine into a molecule along with the conversion of the excess binding energy into kinetic energy. Three-body recombination is an extremely difficult problem and Chapter 8 will only scratch its surface. However, from our investigation of doubly-spin-polarized atoms using model potentials, we have been able to uncover universal systematics of the recombination process.