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DEVELOPMENT OF THEORETICAL AND COMPUTATIONAL METHODS FOR FEW-BODY PROCESSES IN ULTRACOLD QUANTUM GASES

by

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B.S. University of Florida, 2004

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in the Department of Physics in the College of Sciences at the University of Central Florida Orlando, FL

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ABSTRACT

We are developing theoretical and computational methods to study two related three-body processes in ultracold quantum gases: three-body resonances and three-body recombination. Three-body recombination causes the ultracold gas to heat up and atoms to leave the trap where they are confined. Therefore, it is an undesirable effect in the process of forming ultracold quantum gases. Metastable three-body states (resonances) are formed in the ultracold gas. When decaying they also give additional kinetic energy to the gas, that leads to the heating too. In addition, a reliable method to obtain three-body resonances would be useful in a number of problems in other fields of physics, for example, in models of metastable nuclei or to study dissociative recombination of $\text{H}_3^+$. 

Our project consists of employing computer modeling to develop a method to obtain three-body resonances. The method uses a novel two-step diagonalization approach to solve the three-body Schrödinger equation. The approach employs the SVD method of Tolstikhin et al. [Tol96] coupled with a complex absorbing potential. We tested this method on a model system of three identical bosons with nucleon mass and compared it to the results of a previous study. This model can be employed to understand the $^3\text{He}$ nucleus [Fed03]. We found one three-body bound state and four resonances.

We are also studying Efimov resonances using a $^4\text{He}$-based model. In a system of identical spinless bosons, Efimov states are a series of loosely bound three-body states which begin to appear as the energy of the two-body bound state approaches zero [Efi71]. Although they were predicted 35 years ago, recent evidence of Efimov states found by Kraemer et al. [Kra06] in a gas of ultracold Cs atoms has sparked great interest by theorists and experimentalists. Efimov resonances are a kind of pre-dissociated Efimov trimer. To search for
Efimov resonances we tune the diatom interaction potential, $V(r) \rightarrow \lambda V(r)$ as Esry \textit{et al.} did [Esr06]. We calculated the first two values of $\lambda$ for which there is a “condensation” (infinite number) of Efimov states. They are $\lambda_{Efimov1} = 0.9765$ and $\lambda_{Efimov2} = 6.834$. We performed calculations for $\lambda = 2.4$, but found no evidence of Efimov resonances. For future work we plan to work with $\lambda \approx 4$ and $\lambda \approx \lambda_{Efimov2}$ where we might see $d$-wave and higher $l$-wave Efimov resonances.

There is also a many-body project that forms part of this thesis and consists of a direct diagonalization of the Bogolyubov Hamiltonian, which describes elementary excitations of a gas of bosons interacting through a pairwise interaction. We would like to reproduce the corresponding energy spectrum. So far we have performed several convergence tests, but have not observed the desired energy spectrum. We show preliminary results.
Dedicated to my family.
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# LIST OF SYMBOLS, ABBREVIATIONS AND ACRONYMS

\(a\) or \(A\)  
scattering length

\(\rho\) or \(R\)  
hyper-radius

\((\theta, \varphi)\)  
hyperangles

\(\psi_a(\rho)\)  
hyper-radial wave function

\(\phi_a(\rho, \theta, \varphi)\)  
hyperangular wave function

**BEC**  
Bose-Einstein Condensate

**CAP**  
Complex Absorbing Potential

**DFG**  
Degenerate Fermi Gas

**DFT**  
Density Functional Theory

**DVR**  
Discrete Variable Representation

**ET**  
Efimov Trimer

**FR**  
Feshbach Resonance

**MOT**  
Magneto-Optical Trap

**NCSA**  
National Center for Supercomputer Applications

**NERSC**  
National Energy Research Scientific Computing Center
CHAPTER I: INTRODUCTION

The thesis consists of two related but independent studies into (1) few-body and (2) many-body interactions. Therefore, throughout the thesis each chapter will be divided into two main sections, which consist of many-body interactions in ultracold quantum gases (BECs, DFGs) and three-body resonances (not necessarily in this order). Under each of these two sections we go into more specific topics and details, which are separated by further sub-divisions.

For convenience, atomic units are used throughout most of the thesis; see the Appendix for conversion factors.

1.1 Bose-Einstein Condensates and Degenerate Fermi Gases

1.1.1. Many-Body Problem: Brief Background and Motivation

The study of many-body systems is notoriously difficult and has a long history. One of the motivations for employing computer modeling to study many-body processes in ultracold quantum gases is to, perhaps, shed some light into this difficult problem. Modeling ultracold quantum gases is in itself also important due to their importance, reflected in the abundance of research and interest that exists since the realization of Bose-Einstein condensation in the 1990s. Today, there is a plethora of areas of interest with respect to BECs and DFGs including atom optics, atom chips, quantum information processing, superconductivity, superfluidity, improved precision measurements of physical quantities, and basic research into fundamental physical concepts. See, for instance, a review by Dalfovo et al. [Dal99] or Refs. [Gre03], [Gre05], [Hol00], [Reg03], [Nai03], or Ph.D. thesis by Naidon [Nai04].

Being able to tune the two-body interaction in BECs offers a remarkable opportunity to experimentally study many-body systems with unprecedented control. Independently determining
the two-body interaction by new spectroscopies eliminates the uncertainty in the nature of the interaction that can otherwise plague the theory of many-body systems. Therefore, theoretical calculations on these systems can be done from first principles and with accurate, predetermined parameters [Bur02].

Bose-Einstein condensation was observed in 1995 in a series of experiments involving vapors of rubidium and sodium [Dal99]. A trademark feature of a BEC is a tendency for all the bosons (integer multiple of $\hbar$ spin particles) in a system to occupy the same ground state of a given external potential, or “condense,” at extremely low temperatures, thus having the same energy and momentum [Sak94]. This can be seen in the velocity distributions of an ultracold quantum gas as the BEC forms, as shown by E. A. Cornell in Figure 1 [Cor96].

The BEC was made possible by the advent of laser- and evaporative-cooling. And with new spectroscopy techniques, such as photoassociation, atomic interactions can now be controlled with remarkable accuracy, making a quantitative many-body theory for BECs possible [Bur02]. BECs are created and held in magnetic and optical traps such as the magneto-optical trap (MOT) shown in Figure 2. These traps confine the atoms into ultracold clouds of different shapes using optical potentials. MOTs typically hold hundreds of thousands to millions of atoms. Atomic pairwise interactions can be tuned using an external magnetic field. This tuning of the interaction, which effectively translates to a tuning of the two-body scattering length (scattering length is discussed in detail later), is achieved through the use of so-called Feshbach resonances (FR) [Bur02].
Figure 1: Bose-Einstein condensation observed by Cornell et al. in 1996: snapshots of velocity distribution of trapped atoms as the BEC is formed. Starting from left frame BEC is not yet formed, center frame shows formation of BEC. As more atoms evaporate from the trap a purer sample of BEC is left (right frame) [Cor96].

Figure 2: Example of modern magneto-optical trap and magnetic trap [Cor02].
Superfluids and BECs are believed to be inextricably linked. London (1938) considered superfluidity in helium as a possible manifestation of Bose-Einstein condensation [Dal99]. Penrose and Onsager (1956) made an argument on first principles indicating that liquid helium II in equilibrium shows Bose-Einstein condensation [Pen56]. So, in fact, BEC was first experimentally observed in superfluid $^4$He in the early 1900s. However, a theory to explain it was not developed until the mid-1920s by Satyendranath Bose and Albert Einstein. At that time, it was realized that a system of bosons can all condense to the lowest single particle state at low enough temperatures so long as the kinetic energy of the particles is much greater than the interaction energy. This happens because bosons are not restricted by the Pauli exclusion principle. For a gas of bosons, however, the kinetic energy can drop without limit as the temperature drops, and so interactions become important [Bow99]. In this regime, one can no longer consider single particle states. Instead, one speaks of states and energies of the entire system as a whole. What these energies are under specific circumstances, how these states form, and how they can be described are issues which have provided challenges to theorists and experimentalists for decades. In the many-body part of the current project, we aim to employ computer modeling to explore these issues starting from the Bogolyubov Hamiltonian. This part of the project is still in its beginning stages.

A degenerate Fermi gas (DFG) consists of fermions (half-integer multiple of $\hbar$ spin particles) which, when cooled to ultracold temperatures, can form BECs through mechanisms like Cooper pairing. A Cooper pair is a boson which is composed of two interacting fermions. These pairs may form a degenerate Fermi gas, which can be considered as a BEC. In recent BEC and DFG experiments one can adjust the coupling leading to the superfluidity (see Refs. [Gre03], [Gre05], [Hol00], and [Reg03]). Thus, studying the adjustable Cooper pairing in DFG may help
to understand high-temperature superconductivity.

1.1.2. Originality of Approach

There are many ways to approach many-body problems, such as density functional theory (DFT) and mean-field approximations. Our approach is a direct diagonalization of the Bogolyubov Hamiltonian, which may now be possible using parallel computations with supercomputers. The Bogolyubov Hamiltonian, our model, and results are discussed in the second main part of Chapter II.

With respect to three-body resonances, this project is the first time a mapped DVR basis in the hyper-radius is employed. It's originality relies on the employment of the SVD method of Tolstikhin et al. coupled with a complex absorbing potential.

1.2 Three-Body Recombination

1.2.1. Brief Background and Motivation

At ultracold temperatures, the quantum nature of atomic interactions in degenerate fermionic and bosonic gases becomes prominent, providing a new challenge to theorists and experimentalists in the field of collision dynamics [Bur02]. An example of this is the so-called three-body recombination, which is a type of collision that can cause these gases to heat up. During this process, three free atoms collide, which results in the formation of a dimer and a third atom. The dimer and free atom carry away the excess energy and momentum, which leads to the loss of atoms from the confining trap. The process places a fundamental limit on the lifetimes of trapped atomic BECs. Hence, this process is of special interest in the study of ultracold quantum gases. For instance, see references [Bor03] and [Sea04].
1.2.2. Three-Body Bound States and Resonances

In general, a true three-body bound state is the one which has an infinite lifetime whereas a three-body resonance is a three-body quasi-bound state that decays in time with a lifetime $\Gamma^{-1}$. It can decay into either three free atoms or a dimer plus a free atom. In this section we expand on some concepts and nomenclature germane to three-body resonances and which will be used throughout the thesis.

1. Shape versus Feshbach Resonances

We will discuss two general mechanisms by which a three-body bound state dissociates, i.e. two types of resonances: shape resonances and Feshbach resonances. We will deal with these kinds of resonances throughout the thesis. A shape resonance arises from the shape of the interaction potential. This is the case when the potential has a barrier through which bound states can tunnel out of the bound region and dissociate. In Figure 3, bottom, we see an interaction potential that illustrates this point: for a state with energy greater than the dissociation energy of the system, $E_{\text{diss}}$, as we move along the dissociation coordinate $x$ there is a finite probability that the state can tunnel through the barrier and into the dissociation region. In the case of a three-body interaction potential, like the one we are studying in this thesis, the dissociation would correspond to a final state of a dimer plus a free atom since $E_{\text{diss}} < 0$ (more on this in Chapter II).
A Feshbach resonance can be thought of as a pre-dissociated state. Consider the potential adiabatic energy curves $U_1$ and $U_2$ for two given rotational states of the molecule (Figure 3, top). There can exist some vibrational level in state 2 with energy $E_{\text{bound}}$ which is above the dissociation energy of state 1, $E_{\text{diss}} < 0$. Then, if the non-adiabatic coupling between states 1 and 2 is not negligible, the vibrational level is not bound, strictly speaking. It decays in time to state 1 and the molecule automatically dissociates [Lan77]. If we consider these potentials to correspond to a three-body system, then this dissociation process would correspond to a disintegration into a

---

**Figure 3:** Shape resonance versus Feshbach resonance. $E = 0$ represents the threshold energy for three free atoms.
dimer plus a free atom. Figure 4 in section 2.1.1 describes different mechanisms by which three-body recombination occurs.

1.2.3. Efimov Bound States and Resonances

Thirty-five years ago an exotic three-body state was predicted by Vitali Efimov. In his 1971 paper, Efimov theorized the existence of an infinite family of loosely-bound trimer states which formed even though the two-body attraction cannot hold a bound pair [Efi71]. This counterintuitive state is called an Efimov bound state. Experimentally proving the existence of Efimov states has been facilitated by the ability to tune the two-body interaction in ultracold quantum gases through Feshbach resonances, as has recently been the case with the work of Kraemer et al. with an ultracold gas of Cesium atoms [Kra06]. These experimental results confirm key predictions and open up few-body quantum systems to further experiment [Esr06].

Efimov states are discussed in more detail in Chapter II. There, we also present our results for calculations of Efimov resonances in a system of three helium atoms.
CHAPTER II: METHODS AND RESULTS

2.1 Three-Body Recombination

The calculations of bound states and resonances in three-body recombination were performed by formulating the problem in hyperspherical coordinates \((\rho, \theta, \varphi)\) and implementing a novel two-step diagonalization procedure. This means employing the hyperspherical adiabatic approximation [Kok06] and slow variable discretization procedure of Tolstikhin et al. [Tol96] to solve the three-body system's Schrödinger equation. The two-step diagonalization procedure consists of (1) fixing the hyper-radius and obtaining adiabatic eigenenergies \(U_a (\rho)\) and corresponding eigenfunctions in the two-dimensional space of hyperangles and (2) using these adiabatic eigenenergies and eigenfunctions to solve the one-dimensional (in terms of \(\rho\)) one-channel Schrödinger equation. This method is described in the following sections, in which we present a detailed description of three-body recombination, the quantum formalism necessary to formulate our problem, and our results on three-body resonances.

For this part of the thesis, I was provided with Fortran code that calculated three-body states. The program was not quite stable; we modified it to calculate three-body resonances. The next step was to perform convergence tests which would prove the validity of the program. We made several adjustments to the code as required by the specific problem at hand. The different numerical methods employed are discussed in this chapter.

2.1.1. *Introduction to Three-Body Recombination*

Three-body recombination (Figure 4) occurs when three free atoms collide to form a predissociated “temporary” three-body state which goes on to decay into a dimer and a free atom:

\[ X + X + X \rightarrow X_2 + X, \]
for some atom X. There are several mechanisms by which three-body recombination occurs depending on the sign of the two-body scattering length $a$ (Figure 4). The scattering length determines the two-body interaction in ultracold quantum gases (see section 2.1.2).

Figure 4: Graphic depiction of three-body recombination for Cs atoms: three atoms collide to form a pre-dissociated three-body state which consequently decays into a dimer plus a free atom. There are two recombination mechanisms for negative (left frame) and positive (right frame) scattering length [Esr06]. $R$ is hyper-radius in this figure.

Figure 4 shows three-body potentials as a function of hyper-radius $\rho$ of the three-body system. The hyper-radius is a measure of the size of the triangular configuration of a three-body system: a larger hyper-radius means a larger triangle (of whatever shape); see top frame of Figure 11. Hence, as one moves along the hyper-radial coordinate, the triangular shape dissociates into either three free atoms or a free atom plus a dimer. Hyper-radius is discussed in more detail in section 2.1.4-1.

The red potentials in Figure 4 are those of the three-body system before recombination takes place, while the black potentials are for the system after recombination. The blue line gives the energy of the three incident atoms. If $a > 0$, right frame Figure 4, we see the transition from the red potential to the black one at some hyper-radius $\rho \sim a$. There are two mechanisms for this transition. In the first mechanism, the system jumps from the red to the black potential when still
decreasing in size to $\rho \sim a$ (blue pathway). The hyper-radius decreases as the free atom rebounds off the dimer at which point $\rho$ increases (still in the recombined state), eventually leading to dissociation. Note that the size of the triangle decreases before the system dissociates. In the second mechanism (yellow path), the three atoms initially rebound elastically (in the red potential) to then recombine (and enter the black potential) when they cross $\rho \sim a$. The green arrow represents the outgoing channel where quantum-mechanical interference between these two paths may occur [Esr06].

For $a < 0$ there is just one mechanism for the transition, which occurs at $\rho \ll |a|$. To recombine, the system must first quantum-mechanically tunnel into the small-$\rho$ region of the red potential. The existence of resonances (as indicated by the red line) in this small-$\rho$ potential well enhances the tunneling probability. The resonance positions change with the scattering length (red arrow). This tunes the system in and out of resonance, yielding a series of peaks in the recombination length, for instance [Esr06]. The behavior of the recombination length as a function of $a$ is one of the predicted features which were observed by Kraemer et al in their experiments on Cesium recombination; see Ref. [Kra06] for details.

In the recombination process the binding energy of the dimer is approximately taken by the dimer and free atom as kinetic energy. This dimer and/or free atom may then cause additional collisions, escape of atoms from the trap, and heating of the trap. This process places a fundamental restriction on the lifetime of atomic BECs [Sea04]. To clarify how the kinetic energies of the dimer plus free atom approximately equal the dimer binding energy, we begin by considering the diagram shown in Figure 5.
We consider the system of the center of mass of three bodies. We choose the origin $E_{\text{threshold}} = 0$ of the energy when the atoms are at infinity from each other. Therefore, for a two-body system, $E_{\text{threshold}} = 0$ corresponds to two-body dissociation, for a three-body system the origin is when all three atoms are at infinity with zero kinetic energy. In total there are five relevant energies: $E_{\text{threshold}}$, a two-body binding energy ($E_{\text{dimer}}$), the energy of the three-body resonance ($E_{\text{res}}$), the three-body dissociation energy (essentially the threshold for a dimer plus a free atom, $E_{\text{diss}}$) and the kinetic energy of the dimer plus free atom ($E_{\text{kin}}$).

Figure 5 shows that any three-body resonance has to dissociate into a dimer with binding energy equal to the dissociation energy of the lowest three-body channel, i.e. $E_{\text{diss}} \rightarrow E_{\text{dimer}}$ as $\rho \rightarrow \infty$. As the resonant three-body state dissociates into a dimer and a free atom, we must have conservation of energy: $|E_{\text{diss}}| = |E_{\text{res}}| + |E_{\text{kin}}|$. But $E_{\text{diss}} = E_{\text{dimer}}$ and so if we assume that $|E_{\text{res}}| \ll |E_{\text{kin}}|$ then we have $E_{\text{kin}} \approx E_{\text{dimer}}$. We use this estimation to calculate the CAP parameters.

Figure 5: Sketch of two- and three-body potentials and relevant energies.
2.1.2. About the Elastic Scattering of Slow Particles

When considering few-body and many-body interactions in ultracold quantum gases there is one parameter which characterizes the net effect attributable to complex, short-range atomic interactions: the scattering length $a$ [Bur02]. Therefore, in this section we review some aspects of the elastic scattering of slow particles, focusing on the two-body scattering length and its relevance to ultracold quantum gases.

For slow elastic collisions, $kd \ll 1$ (where $d$ is the effective range of the two-body potential), the scattering wave function is determined by the equation

$$
\left( \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2 \right) R_l(r) = \frac{2\mu}{\hbar^2} V(r) R_l(r),
$$

for $l = 0$, where $k$ is the wave number of the scattering wave function, $r$ is the inter-particle distance, and $\mu$ the reduced mass. The boundary conditions are

$$R_o(0) = 0$$

and for large $r$,

$$R_o(r) = C \sin(kr + \delta_o).$$

where $\delta_o$ is the scattering phase shift [Dav76].

For a rectangular spherical potential well,

$$V(r) = -V_o \text{ if } r \leq d.$$  

$$= 0 \text{ if } r > d.$$  

Eq. (1) becomes

$$\left( \frac{d^2}{dr^2} + K^2 \right) R_{01}(r) = 0,$$

inside the well, where
\[ K^2 = k^2 + K_o^2; \quad K_o^2 = \frac{2\mu V_o}{\hbar^2}. \] (4)

Equation (3) is satisfied by
\[ R_{01} = C_1 \sin Kr. \] (5)

Equating the logarithmic derivatives of Eq. (2) and Eq. (5) at \( r = d \) yields the scattering phase shift \( \delta_o \):
\[ k \cot (kd + \delta_o) = K \cot Kd \]
and if we let \( D^{-1} \equiv K \cot Kd \), then we have
\[ \tan \delta_o = \frac{kD - \tan kd}{1 + kD \tan kd}, \]
where \(-\pi/2 \leq \delta_o \leq \pi/2\) [Dav76].

For small values of the energy of the relative motion, \( kd \ll 1 \), then
\[ \tan \delta_o \approx k (D - d - \frac{(kd)^3}{3k}). \]

Assuming that also \( k^2 Dd \ll 1 \), then
\[ \tan \delta_o \approx k (D - d) \approx kd \left[ \frac{\tan Kd}{Kd} - 1 \right]. \]

Therefore, the cross-section is given by
\[ \sigma = \frac{4\pi}{k^2} \sin^2 \delta_o \approx 4\pi (D - d)^2 = 4\pi d^2 \left[ 1 - \frac{\tan Kd}{Kd} \right]^2 = 4\pi a^2 \quad [Lan77]. \]

For elastic scattering by a deep rectangular spherical well and for small energies of the relative motion we have
\[ K^2 = k^2 + K_o^2 \approx K_o^2. \]
and consequently the scattering length is given by

$$a = d \left[ 1 - \frac{\tan K_o d}{K_o d} \right]$$

(6)

The condition for the presence of an \( s \)-level with zero energy in the well is \( \cot K_o d = 0 \) [Dav76]. Note that this is precisely where \( a \) reaches its maximum. If \( K_o d = \pi/2 \) then there is exactly one \( s \)-level with \( E = 0 \). If \( K_o d = 3\pi/2 \) then there are two \( s \)-levels, one with \( E = 0 \). If \( K_o d = 5\pi/2 \) then there are three \( s \)-levels, one with \( E = 0 \), and so on...

Another way to obtain the scattering length is by extrapolating the scattering wave function, Eq. (2), into the region of small \( r \) and normalizing to 1 at \( r = 0 \) gives [Dav76]:

$$g(r) = \cos kr + \cot \delta_0 \sin kr$$

For small energies and small \( r \), \( kr \ll 1 \), we can write

$$g(r) = 1 - \frac{r}{a}$$

where \( a \) is given in terms of the phase shift,

$$a = -[k \cot \delta_0]^{-1}$$

If \( \delta_0 > 0 \), then \( a < 0 \), and vice-versa. Hence \( a \) can be either positive or negative for an attractive two-body interaction, depending on \( \delta_0 \). If the depth of the potential well is not very large, then a different equation must be used [Dav76].

If, instead, we consider a spherical potential barrier,

$$V(r) = V_o \quad \text{if} \quad r < d$$

$$= 0 \quad \text{if} \quad r > d$$

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then $K$ in Eq. (4) is instead given by

$$K^2 = k^2 - K_o^2, ~ K_o^2 = \frac{2\mu V_o}{\hbar^2}. \tag{4}$$

Outside the barrier the solution is still given by Eq. (2), inside it is given by

$$R_{01} = C_1 \sin Kr, \text{ if } k \geq K_o,$$

$$R_{01} = C_1 \sin Qr, \text{ if } k \leq K_o,$$

where $Q = \sqrt{K_o^2 - k^2}$. For small energies, $Q \approx K_o$ and by equating the logarithmic derivatives as before we obtain, as before,

$$\tan \delta_o = \frac{kD - \tan kd}{1 + kD \tan kd},$$

except that now $D^{-1} = Q \coth Qd \approx K_o \coth (K_od)$ [Dav76]. Similarly as before, the $s$-wave scattering cross-section for small energies and high barriers is given by

$$\sigma_o = \frac{4\pi}{k^2} \sin^2 \delta_o \approx 4\pi d^2 \left[ \frac{\tanh K_od}{K_od} - 1 \right]^2,$$

and so the corresponding scattering length is

$$a = d \left[ 1 - \frac{\tanh K_od}{K_od} \right]. \tag{7}$$

So, for a repulsive two-body interaction, $a$ is positive.

One can visualize the scattering length as changing the boundary conditions near $r = 0$ of the scattering wave function [Bur02]. Figure 6 illustrates this concept for two particles of mass $m$ confined to a one-dimensional infinite square potential well of length $L$. 

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The node at the origin is moved by $\pm |a|$ (or 'A' in Figure 6). Consequently, the energy of the scattering wave function is also changed by an amount proportional to

$$\pm \frac{|a|}{mL^3}.$$  

For $N$ pairs of particles the energy change would be proportional to

$$\pm \frac{|a|}{m} n$$  

where $n$ is the particle number density. More sophisticated theories show that the particle interactions result in a

$$4\pi a \hbar^2 \frac{n}{m}$$
energy term.

This explains why the scattering length determines the collective interaction energy of a system of many particles at low temperature, $a < 0$ means an attractive collective interaction while for $a > 0$ the collective interaction is repulsive [Bur02]. Stable BECs can exist in an infinite homogeneous gas with repulsive collective interactions ($a > 0$), but not with attractive interactions ($a < 0$). Collapse of the BEC can be avoided in small finite-size trap because of the zero-point motion in the trap [Bur02]. In ultracold quantum gases it is possible to tune the scattering length through the use of an external magnetic field $\mathbf{B}$ near a Feshbach resonance. This tuning of $a$ is illustrated in Figure 7.

![Figure 7: Scattering length versus external magnetic field taken from [Cor00].](image)

The magnetic Feshbach resonance is located at the vertical line in the $a$ vs $\mathbf{B}$ plot (Figure 7). When the magnetic field is adiabatically increased across the FR, $a$ goes from negative infinity to positive infinity.

Feshbach resonances are used in photoassociation and other experiments. Magnetic Feshbach resonances come about as a result of an applied external magnetic field, which couples...
two channels through hyperfine interaction, Figure 8.

\[ E_{\text{bound}} \quad U_{hc} \quad E_{\phi} + E_{\epsilon} \quad \hbar \Delta \quad E_{\phi} + E_{a} \quad \]

**Figure 8:** Feshbach resonance, an external magnetic field couples two channels by hyperfine interaction [Nai03].

Here, $\Delta$ is the so-called detuning. Optical Feshbach resonances involve electronically excited states. For a detailed explanation of Feshbach resonances see Ref. [Ino98].

2.1.3. $C_{3v}$ Symmetry and Irreducible Representations $^{[\text{Lan77}]}$

A study of a system of three bodies can be greatly simplified by considering the different symmetries of such a system. We only consider systems of identical particles, which are described by the $S_3$ symmetry group. Some of the wave functions of the system (namely, the hyperangular wave functions) will therefore possess symmetries described by the $C_{3v}$ symmetry group, which is isomorphic to $S_3$. $C_{3v}$ is a point group, meaning that at least one point of the system must remain fixed when any transformations are applied. This means all axes and planes of symmetry must have at least one common point as shown in Figure 9 $^{[\text{Lan77}]}$. The $C_{3v}$ group has a single axis of symmetry (see Figure 9).
2π/3 rotations about this axis leaves the system unchanged. There are three planes of symmetry which pass through this axis, intersecting along the axis at angles of π/3 [Lan77]. The system then remains unchanged after reflections σv through the vertical planes. In total, this group has 6 elements (i.e. its order = 6), including the identity element.

Let us now discuss the irreducible representations of C3v. Each element of a symmetry group can be considered to be a matrix which acts like an operator on a set of linearly independent functions ψk like

\[ \hat{G} \psi_k = \sum_{i=1}^f G_{ki} \psi_i, \]

where \( f \leq g \) and g is the order of the group (f is called the dimension of the representation). The functions ψk are single-valued functions of the coordinates in the configuration space of the physical system [Lan77]. For example, in our system these would be the hyperangular coordinates. A representation of a group is the set of matrices of all elements in a group and ψk are called the basis of the representation [Lan77]. If we make some linear transformation \( \hat{S} \) of the base functions

\[ \psi_k' = \hat{S} \psi_k \quad (8) \]
then the matrix of the operator $\hat{G}$ in the new primed representation is the matrix of the operator

$$\hat{G}' = \hat{S}^{-1}\hat{G}\hat{S},$$

in the old unprimed representation [Lan77].

If $\hat{S}$ in Eq. (8) is a suitable transformation such that the base functions divide into sets of $f_1, f_2, \ldots (f_1 + f_2 + \ldots = f)$ functions so that, when any element of the group acts on them, the functions in each set are transformed only into combinations of themselves then the representation in question is called reducible [Lan77].

A representation is called irreducible if the number of base functions that are transformed only into combinations of themselves cannot be reduced by any linear transformation of them. Irreducible representations play an important role in quantum mechanical applications of group theory [Lan77].

Any reducible representation can be decomposed into irreducible ones. There are three irreducible representations of the $C_{3V}$ group: $E$, $A_1$ and $A_2$. The $A$ representations are one-dimensional.

<table>
<thead>
<tr>
<th>$C_{1v}$</th>
<th>$E$ $2C_3$ $3\sigma_v$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_1$</td>
<td>$E$ $2C_3$ $3\sigma_v$</td>
</tr>
<tr>
<td>$A_1$</td>
<td>$A_1$ 1 1 1</td>
</tr>
<tr>
<td>$A_2$</td>
<td>$A_2$ 1 1 -1</td>
</tr>
<tr>
<td>$E;x,y$</td>
<td>$E;x,y$ 2 -1 0</td>
</tr>
</tbody>
</table>

**Figure 10:** Characters of irreducible representations of $C_{3V}$ and its isomorphous group $D_1$.

Their base functions are symmetric with respect to rotations about the principal axis, $z$ in Figure 10, of the $n^{th}$ order (here, $n = 3$). However, these base functions may be either symmetric or anti-
symmetric with respect to $\sigma_v$ reflections. When one makes a reflection about one of the vertical planes the $A_1$ irreducible representation leaves the system unaltered while the $A_2$ representation introduces a negative sign. The $E$ representation is two-dimensional. Base functions of the complex conjugate representations $E$ change into each other on reflection. The letters $x$, $y$, and $z$ label the representations by which the coordinates themselves are transformed.

The quantum mechanical applications of group theory are based on the fact that the Schrödinger equation for the physical system is invariant with respect to symmetry transformations of the system [Lan77]. This implies that under a symmetry transformation, the wave functions of the stationary states of the system belonging to a given energy level transform into linear combinations of one another. This forms a representation of the group, which is in fact irreducible. Hence, to each energy level of the system there corresponds some irreducible representation of its symmetry group. The dimension of the representation equals the degeneracy of the level. Fixing the irreducible representation determines the behavior of the given state with respect to the various symmetry transformations. These applications are discussed in extensive detail by Landau in Ref. [Lan77].

2.1.4. Three-Body Quantum Formalism

1. Hyperspherical Coordinates [Kok06]

We use Smith-Whitten hyperspherical coordinates to describe the three-dimensional inter-particle motion of the three-body system. But before we can define the hyper-radius $\rho$ and hyperangles ($\theta$, $\phi$), we have to define some preliminary quantities. If $x^{(i)}$ with $i = 1, 2, 3$ represent the radius vectors of the three particles in the laboratory reference frame, with corresponding masses $m_i$, then we can define the following:

$$M = m_1 + m_2 + m_3,$$
\[
\mu = \sqrt{\frac{m_1 m_2 m_3}{M}},
\]
\[
d_i = \sqrt{\frac{m_i}{\mu} \left(1 - \frac{m_i}{M}\right)},
\]
\[
\tilde{r}^{(k)} = \frac{1}{d_k} (\vec{x}^{(j)} - \vec{x}^{(i)}), \quad i, j, k \text{ are different}
\]
\[
\tilde{R}^{(k)} = d_k \left[ \vec{x}^{(k)} - \frac{m_j \vec{x}^{(j)} + m_i \vec{x}^{(i)}}{m_j + m_i} \right], \quad i, j, k \text{ are different}
\]
\[
\epsilon_2 = 2 \arctan \left( \frac{m_3}{\mu} \right),
\]
\[
\epsilon_3 = 2 \arctan \left( \frac{m_2}{\mu} \right),
\]
such that we can now define \((\rho, \theta, \phi)\) as follows:
\[
\rho^2 = |\tilde{r}^{(k)}|^2 + |\tilde{R}^{(k)}|^2,
\]
\[
|\tilde{r}^{(1)}| = \frac{\rho}{\sqrt{2}} \sqrt{1 + \sin \theta \sin \phi},
\]
\[
|\tilde{r}^{(2)}| = \frac{\rho}{\sqrt{2}} \sqrt{1 + \sin \theta \sin (\phi - \epsilon_2)},
\]
\[
|\tilde{r}^{(3)}| = \frac{\rho}{\sqrt{2}} \sqrt{1 + \sin \theta \sin (\phi + \epsilon_3)},
\]
where \(0 \leq \rho < \infty, \ 0 \leq \theta \leq \pi/2\) and \(0 \leq \phi < 2\pi\). Even though the hyper-radius is defined through \(\tilde{r}^k\) and \(\tilde{R}^k\) it is independent of the index \(k = 1, 2, 3\).
One can visualize hyperspherical coordinates as shown in the two diagrams in Figure 11.

First, for a fixed hyper-radius one has an infinite number of triangular configurations for the three-body system. Each configuration is described by a set of hyperangles \((\theta, \phi)\) which are plotted analogously to polar coordinates, that is, \(\theta\) runs outward from the origin in the 'radial' direction while \(\phi\) runs in the 'angular' direction. Above: for given hyperangular coordinates \((\theta', \phi')\), as we increase the hyper-radius \(R\) the size of the triangle increases while the shape remains the same.
direction' while $\phi$ runs in the 'angular' direction from 0 to $2\pi$. Note that the triangles become less equilateral as $\theta$ increases and, instead, we have two atoms very close to one another as the third atom gets further and further away and the configuration becomes collinear.

If instead one fixes the hyperangles $(\theta, \phi)$ and varies the hyper-radius ($\rho$), then, as the hyper-radius increases, one sees the size of the triangle increase, making the hyper-radius the dissociation coordinate. Large hyper-radius (i.e. $\rho \to \infty$) corresponds to the dissociation of the three-body system. Depending of the hyperangular configuration at large $\rho$, it could be three-free-atom dissociation of diatom plus atom dissociation.

2. Hyperspherical Adiabatic Approach $^{[Kok06]}$

The hyperspherical adiabatic approach consists of (1) formulating the three-body problem in hyperspherical coordinates as defined in the previous section and (2) obtaining the vibrational eigenenergies ($E_n^{\text{vib}}$) and eigenfunctions ($\Phi_n$) in a two-step procedure. It is analogous to the Born-Oppenheimer approximation in diatomic molecules. It involves solving the three-body Schrödinger equation

$$\left[ T(\rho, \theta, \phi) + V(\rho, \theta, \phi) \right] \Phi_n(\rho, \theta, \phi) = E_n^{\text{vib}} \Phi_n(\rho, \theta, \phi), \quad (9)$$

by fixing $\rho$ at $\rho_i$ and diagonalizing the adiabatic Hamiltonian $H_{\rho_i}^{\text{ad}}$ in a two-dimensional space of hyperangles $(\theta, \phi)$

$$H_{\rho_i}^{\text{ad}} \Phi_n(\rho_i, \theta, \phi) = U_a(\rho_i) \Phi_n(\rho_i, \theta, \phi), \quad (10)$$

where $a$ labels eigenenergies and eigenfunctions at fixed $\rho_i$. The Hamiltonian in the above equation is
\[ H_{\rho}^{ad} = \frac{\Lambda_0^2 + \frac{15}{4}}{2 \mu \rho_i^2} + V(\rho_i; \theta, \varphi), \]  

where

\[ \Lambda_0^2 = -4 \left[ \frac{1}{\sin(2\theta)} \frac{\partial}{\partial \theta} \sin(2\theta) \frac{\partial}{\partial \theta} + \frac{1}{\sin^2(\theta)} \frac{\partial^2}{\partial \phi^2} \right], \]

is the square of the grand angular momentum operator associated with the hyperspherical coordinates. Here and everywhere below, we assume that the total angular momentum of the system is 0.

This procedure produces the hyperangular wave functions \( \phi_a(\rho_i, \theta, \varphi) \) and the adiabatic energies \( U_a(\rho) \), which define a set of adiabatic channels. We obtain the hyper-radial wave functions \( \psi_a(\rho) \) and the vibrational eigenenergies \( E_n^{\text{vib}} \) by solving a set of multi-channel hyper-radial coupled Schrödinger equations with the adiabatic energies \( U_a(\rho) \) taking the place of one-dimensional three-body potentials,

\[
[K(\rho) + U_a(\rho)]\psi_{a,n}(\rho) + \sum_{a'} [W_{a,a'} \psi_{a',n}(\rho)] = E_n^{\text{vib}} \psi_{a,n}(\rho),
\]

where \( K(\rho) = -\frac{1}{2\mu} \frac{d^2}{d \rho^2} \) is the kinetic energy operator, \( n \) labels the vibrational level of the trimer, \( \psi_{a,n}(\rho) \) is the \( a^{\text{th}} \) component of the hyper-radial eigenfunction \( \psi_n(\rho) \), and

\[
W_{a,a'} = -\frac{1}{2\mu} \langle \phi_{a}(\rho_i, \theta, \varphi) | \frac{d^2}{d \rho^2} | \phi_{a}(\rho_i, \theta, \varphi) \rangle + \frac{1}{\mu} \langle \phi_{a}(\rho_i, \theta, \varphi) | \frac{d}{d \rho} | \phi_{a}(\rho_i, \theta, \varphi) \rangle \frac{d}{d \rho},
\]

represents the non-adiabatic coupling elements. Solving equation (13) numerically would yield a numerically exact solution for the original Schrödinger equation, Eq. (9), assuming all \( a \)-channels are taken into account. However, if the non-adiabatic couplings have a spiky dependence on \( \rho \)
then a numerical solution becomes very difficult. Therefore, in most applications these coupling terms are ignored. This is called the adiabatic approximation. The procedure relies on separating the total wave function into a product of hyperangular and a hyper-radial components for each channel \( a \), and it makes the following approximation for the total three-body vibrational wave functions and eigenenergies:

\[
\Phi_n(\rho, \theta, \varphi) \approx \Phi_{a,v}(\rho, \theta, \varphi) = \phi_a(\rho, \theta, \varphi) \psi_{a,v}(\rho)
\]  

(15)

i.e. only the main component of \( \psi_{a,v}(\rho) \) is considered as a hyper-radial part of the eigenfunction in the adiabatic approximation, and

\[
E_n^{\text{vib}} \approx \epsilon_{a,v}.
\]

where \( \epsilon_{a,v} \) is vibrational energy obtained if we ignore the coupling elements in Eq. (13), i.e. when we solve Eq. (17).

For numerical calculations, we expand \( \psi_{a,v}(\rho) \) in a basis set \( \pi_j(\rho) \):

\[
\psi_{a,v}(\rho) = \sum_{j=1}^{N} c_{j,a,v} \pi_j(\rho).
\]  

(16)

The computer code which calculates the three-body resonances has used \( B \)-spline basis and the discrete variable representation (DVR) basis set. These are commonly used basis functions, for example, like sines or Legendre polynomials. The numerical method through which the DVR basis is applied, mapped DVR basis, is discussed later in this chapter in the section with the same name. Since this method does not account for non-adiabatic couplings between the different channels, say, \( a \) and \( a' \), then we are essentially solving the following eigenvalue problem:

\[
[K(\rho) + U_a(\rho)]\psi_{a,v}(\rho) = \epsilon_{a,v} \psi_{a,v}(\rho).
\]  

(17)

In order to account for non-adiabatic couplings between different channels, we use the slow
variable discretization method of Tolstikhin et al., which is described in the next section.

3. Slow Variable Discretization\textsuperscript{[Tol96]}

In this section we will abbreviate slow variable discretization by SVD (not to be confused with 'single value decomposition', an unrelated mathematical procedure). Solving equation (13) would solve the three-body problem exactly. SVD offers an opportunity to keep the hyper-radius as the dissociation coordinate and to obtain essentially exact vibrational eigenfunctions, $\Phi_n(\rho, \theta, \phi)$ \textsuperscript{[Kok06]}. The SVD method applied here is slightly modified from \textsuperscript{Tol96} in order to be able to apply the DVR basis.

We begin, just like in the adiabatic approach, by solving for the adiabatic eigenenergies $U_a(\rho)$ and eigenfunctions $\phi_a(\rho, \theta, \phi)$ at a fixed hyper-radius $\rho_i$. However, instead of approximating the vibrational eigenfunction $\Phi_n(\rho, \theta, \phi)$ by equation (15), we now expand in the $\phi_a(\rho, \theta, \phi)$ basis with hyper-radial eigenfunctions $\psi_a(\rho)$ as the expansion coefficients

$$\Phi_n(\rho, \theta, \phi) = \sum_a \psi_a(\rho) \phi_a(\rho, \theta, \phi). \quad (18)$$

The sum is over the adiabatic channels. Next, the hyper-radial eigenfunctions are expanded in a basis (DVR, B-splines, Legendre polynomials...) as in equation (16)

$$\psi_a(\rho) = \sum_{j=1}^N c_{j,a} \pi_j(\rho). \quad (19)$$

By putting equations (18) and (19) into the Schrödinger equation, $H\Phi_n(\rho, \theta, \phi) = E\Phi_n(\rho, \theta, \phi)$, we obtain

$$\sum_{i',a'} \left[ \langle \pi_{i'}|K(\rho)|\pi_i\rangle O_{i'\cdot a',ia} + \langle \pi_{i'}|U_a(\rho_i)|\pi_i\rangle \delta_{a',a}\right] c_{i',a'} = E \sum_{i',a'} O_{i'\cdot a',ia} c_{i,a'}, \quad (20)$$

where
\[ O_{i',a',ia} = \langle \phi_{a'}(\rho_{i'}, \theta, \varphi) | \phi_{a}(\rho_{i}, \theta, \varphi) \rangle, \]

represent overlapping matrix elements between hyperangular adiabatic states \( \phi_{a}(\rho_{i}, \theta, \varphi) \) at different hyper-radii. When we use the DVR basis representation, Eq. (20) becomes

\[
\sum_{i',a'} \left[ \langle \pi_{i'} | K(\rho) | \pi_{i} \rangle O_{i',a',ia} + U_{a}(\rho) \delta_{i',i} \delta_{a',a} \right] c_{i',a'} = E \sum_{a} O_{i'a',ia} c_{i,a'}.
\]

Equation (21) has the form of a generalized eigenvalue problem, which can be solved through commonly known methods. If we take \( M \) to be the number of adiabatic channels taken into account and \( N \) to be the number of basis functions (Eq. (19)) then \( H \) and \( O \) are \( NM \times NM \) matrices.

In the SVD method, then, the non-adiabatic coupling terms \( W_{a,a'} \) in equation (13) are replaced by the overlapping matrix elements \( O_{i'a',ia} \). Therefore, there is no need to calculate first and second derivatives of \( \phi_{a}(\rho_{i}, \theta, \varphi) \) (see Eq. (14)) and it becomes easier to implement a computer solution to the Schrödinger equation [Kok06].

4. Complex Absorbing Potential

Complex absorbing potentials (CAPs) are needed to absorb wave packets near the edges of grids in time-dependent quantum dynamical calculations [Vib92]. In the absence of a CAP, the outgoing flux would be bounced back from the right side of the grid. Such a behavior is unphysical. The presence of a CAP simulates the infinite grid: the outgoing flux is never coming back.

CAPs are placed on the grid itself and they come in different forms: linear, quadratic, cubic, quartic, and exponential. The extent to which the different potentials transmit or reflect the wave packet can be quantified. Optimal potential parameters (strength \( A \), and length \( L \)) to minimize both reflection (\( R \)) and transmission (\( T \)) for each type of potential are derived for use.
with any chosen mass or kinetic energy in Ref. [Vib92]. In this reference, which also explains CAP theory in more detail, tables (see Figure 12) are presented which show optimal parameters for a particular CAP so as to allow us to obtain preselected (and very small) $R + T$ values [Vib92].

One would always like to devote a minimal region to the CAP, while at the same time absorbing all the wave packet and neither transmitting nor reflecting any of it [Vib92].

The CAP which we decided to use has the quadratic form (see lower inset in Figure 14)

$$V(x) = -iA \left[ \frac{3}{2} x^2 \right]$$

where $x = \frac{r}{L}$

and $r$ can be the hyper-radius or some other inter-atomic distance, and $L$ is the 'optical length' of the potential. Therefore $0 \leq x \leq 1$. Other possible CAPs used in other studies are linear, cubic, quartic and exponential with respect to $x$. We picked the quadratic form because it works best.
when the length of the grid is not too much bigger than the length of the CAP.

In order to determine $L$ and $A$ for some value of $R + T$ we must first know the deBroglie wavelength $\lambda_{dB}$ of the dissociating flux in the asymptotic region; this is equivalent to the deBroglie wavelength $\lambda_{dB}$ of the dissociating particles.

From section 2.1.1 we already know that $|E_{kin}| = |E_{dimer}| - |E_{res}|$. And since,

$$|E_{kin}| = \left(\frac{2\pi}{2\mu}\right)^2$$

where $\mu$ is the reduced mass of the dissociating products, then right away we can determine $\lambda_{dB}$. This is how we incorporate CAPs into our model.

5. Calculation of Linewidths

The introduction of a CAP, -$iV$, changes the Hamiltonian, $H \rightarrow H - iV$, to a non-Hermitian one. There are some instances where this non-Hermitian Hamiltonian can be solved analytically; see for instance, Ref. [Ris93]. The solutions produce resonance energies and widths; for a detailed description see Ref. [Ris93].

Numerically solving the eigenvalue equation (13) in the presence of CAP, $iV(\rho)$,

$$[K(\rho) + U_a(\rho) + iV(\rho)]\psi_{a,n}(\rho) + \sum_{a'} [W_{a,a'} \psi_{a',n}(\rho)] = E_{a,n}^{vib} \psi_{a,n}(\rho).$$

produces complex eigenenergies $E_{a,n}^{vib}$ and eigenfunctions $\psi_{a,n}$,

$$E_{n}^{vib} = E' - i \frac{\Gamma}{2}.$$

The imaginary part $\Gamma/2$ of the energy determines the linewidth of the resonance, the real part $E'$ gives the position of the resonance. $\Gamma$ is the linewidth, the inverse of the resonance lifetime.

6. Hyper-Radial and Hyperangular Wave Functions

Hyper-radial wave functions may have nonzero components in each adiabatic channel due
to coupling between channels (see Eq. (13)). Therefore, for a given energy level \( n \), the sum of the probabilities over all channels should total 1

\[
\sum_a |\psi_{a,n}|^2 = 1.
\]

This is not so with hyperangular wave functions, which are solved independently for each channel and the total probability for each channel totals 1

\[
|\phi_a(\rho, \theta, \varphi)|^2 = 1.
\]

Hyperangular and hyper-radial wave functions have real and imaginary components because of the presence of the CAP, as stated in the previous section. For detailed information see Ref. [Ris93]. If the state is a true bound state, the wave function (both, hyperangular and hyper-radial parts) can be made real by appropriate choice of the phase.

2.1.5. Numerical Methods

The program that calculated the three-body resonances was divided into two parts. The first part calculated the adiabatic curves. The second part, which takes significantly less time, uses these curves to calculate wave functions and vibrational eigenenergies for some CAP parameters.

1. Parallel Computers

The way the three-body dissociation problem is formulated allows us to take advantage of parallel computations on supercomputers. For each hyper-radial point a separate and independent calculation is made. Therefore for a grid which contains \( N \) hyper-radial points we can simultaneously employ \( N \) processors. The computers we used allowed us to submit jobs to be carried out in “nodes”. In our case a node consisted of 16 processors and therefore the number of hyper-radial points in our grid had to be a multiple of 16. The more nodes we used the faster a
given job will be done for the same total computational cost.

We changed the parameters of the problem through the use of input files, which allowed changing of variables such as number of states, number of basis functions, interaction strength, or CAP parameters without compiling the program each time.

We used National Center for Supercomputer Applications (NCSA) and National Energy Research Scientific Computer Center (NERSC) supercomputer resources which were allocated through different grants. We submitted interactive and regular jobs through the use of an SSH (Secure Shell) console. This was done through executable and batch files. For parallel calculations we use MPI (Message Passing Interface) software. The program itself is written in Fortran.

Let us label the number of hyperangular basis functions in the $\phi$ direction by $n_\phi$, and the number in the $\theta$ direction by $n_\theta$. In a typical run for the three identical bosons with nucleon mass model, for instance, for 256 hyper-radial points we observed convergence for $n_\phi \approx 170$ and $n_\theta \approx 40$. Calculation times generally increase more with $n_\theta$ than with $n_\phi$. The number of hyper-radial points we used was 256, the maximum. Typical runs may last around two hours (for these we used 16 or 32 processors), but for the Efimov resonance problem some runs have lasted up to 6 to 7 hours due to the large number of hyperangular basis functions required (see section 2.1.7) and we used up to 64 processors. It was more than double the number required for the first model. However, due to long queues, especially at NCSA, it may be a day or more before your program runs. We were also able to change the number of requested adiabatic states. There was no restriction on the number of requested states (channels), but sometimes if the number was 4 or less we did not observe convergence. So far all that has been discussed applies to the first part of the program, the second part took at most 30 minutes and most of the time we ran this part
interactively. The second part relies on the results of the first part (adiabatic curves). In the second part of the program we specified the CAP parameters and obtained the vibrational eigenfunctions and eigenenergies.

2. Mapped Fourier Grid and Mapped DVR Basis

This method aims to avoid the implementation of very large grids. One of the purposes of using a mapping procedure is to reduce the calculation time while improving the accuracy of the calculations. For instance, when considering a system like the loosely bound helium trimer one must take into large distances between the particles (large $\rho$). This necessitates the use of a large number $N$ of basis functions $\pi_j(\rho)$ the expansion of the hyper-radial wave function (Eq. (16)) and thus to the diagonalization of a large $N \times N$ Hamiltonian matrix [Kok06]. However, computation time can be reduced by using a mapping procedure that defines a new set of basis functions by performing a change of variable in hyper-radius: $\rho \rightarrow x(\rho)$. The mapping is made such that a relatively small number of basis functions $\pi_j(x)$ are needed to represent the required eigenfunctions of the Hamiltonian. In our method, we used the DVR basis in this mapping.

By doing this we can accurately represent wave functions for which the deBroglie wavelength varies by more than one order of magnitude from small to large inter-nuclear distances, for instance. When the deBroglie wavelength is small a smaller grid step is required than when the deBroglie wavelength is large. This means that in the momentum representation the wave function is not localized. To represent the wave function using a constant grid step, therefore, makes the DVR basis unnecessarily large [Kok06]. The solution is to make the change in variable such that in the new variable $x$ the wave function $\psi_{\alpha,\nu}$ has a local deBroglie wavelength that is approximately constant. In practice, this mapping of $\rho(x)$ can be done by estimating the local deBroglie wavelength [Kok06]. Since the eigenfunction in the conjugated
momentum space is much more localized, then a smaller number of \( \pi_j(x) \) basis functions is needed for accurate representation. Hence, in the \( \rho \) representation this procedure produces a non-uniform DVR grid along \( \rho \). For example, for wave functions of weakly bound two-body states, which may oscillate much more at short internuclear distances than at larger ones, the grid would be more dense at small internuclear distances where the wave function oscillates more.

We apply this mapping procedure to the hyper-radius. This is the first time a mapped DVR basis is applied in hyper-radius [Kok06]. The grid steps \( \Delta \rho \) and \( \Delta x \) are related by

\[
\Delta \rho = J(x) \Delta x, \text{ where } J(x) = \frac{d \rho}{dx}.
\]

We can write Eq. (17) as

\[
[K(x) + U_a(\rho(x))] \theta_{a,v}(x) = \epsilon_{a,v} \theta_{a,v}(x),
\]

where \( \theta_{a,v}(x) \) is given by

\[
\theta_{a,v}(x) = \sqrt{J(x)} \psi_{a,v}(x),
\]

such that it is normalized to 1,

\[
\int |\theta_{a,v}(x)|^2 dx = \int J(x) |\psi_{a,v}(x)|^2 \frac{d \rho}{J(x)} = \int |\psi_{a,v}(x)|^2 d \rho = 1.
\]

In the \( x \) coordinate we can rewrite the kinetic energy operator as

\[
K(x) = K(\rho(x)) = -\frac{1}{2\mu} \frac{d^2}{d\rho(x)^2} = \frac{1}{4 \mu} \left[ -\frac{1}{J^2} \frac{d^2}{dx^2} - \frac{1}{J^2} \frac{d^2}{dx^2} \frac{J'}{J} + \frac{7}{2} \frac{(J')^2}{J^3} - \frac{J'''}{J^3} \right],
\]

where \( J \) is a function of \( x \). The primes represent derivatives with respect to \( x \). Eq. (22) is solved to determine all levels up to a maximum energy \( E_{\text{max}} \).

In practice, \( J(x), \rho(x), \) and the step sizes \( \Delta \rho \) and \( \Delta x \) are determined in the following way. We know that \( \Delta x \) is constant, and can be chosen to equal 1 for simplicity. \( \Delta \rho \) is variable and chosen according to the desirable density in a given region of \( \rho \). So we have \( J(x) = \Delta \rho(x) \) and

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determining $\Delta \rho$ is sufficient to determine $J(x)$ and $\rho(x)$. We begin with the smallest value of $\rho$, $\rho_1$, and determine the step size $\Delta \rho_1$ according to the required accuracy. The next point in the grid is given by $\rho_2 = \rho_1 + \Delta \rho_1$. We determine $\Delta \rho_2$ according to the required accuracy, and the next point will be given by $\rho_3 = \rho_2 + \Delta \rho_2$. This is repeated until we reach the end of the grid. The corresponding values of $x$ are $x_i = i$ [Kok06].

To determine $\Delta \rho_i$ at a given $\rho_i$ we must consider how dense the grid must be at that particular region. For instance, if $\psi_{a,v}(\rho(x))$ in the neighborhood of $\rho_i$ can be effectively represented by just a few $\pi_i(x)$ basis functions, then the step size $\Delta \rho_i = J(x)$ can be relatively large. Kokoouline et al. showed in Ref. [Kok99] that wave functions of excited levels, which have many oscillations, are well represented using the mapped DVR basis with the grid step given by

$$
\Delta \rho_i = \beta \frac{\pi}{\sqrt{2 \mu E_{\text{kin}}(\rho_i)}}.
$$

The kinetic energy in the above equation is calculated using the semi-classical approximation that at a given point $\rho_i$, it is the difference, $E_{\text{kin}}(\rho_i) = E_{\text{max}} - U_a(\rho_i)$, between the maximum energy considered in the calculation ($E_{\text{max}}$ constant for all $\rho_i$) and the value of the three-body potential $U_a(\rho)$ at $\rho_i$. The constant $\beta < 1$ is introduced to uniformly control the accuracy of the calculations by uniformly reducing the step size, which would produce more accurate eigenenergies and wave functions. When several channels $a$ are involved the same grid can be used for all channels, in view of calculations involving non-adiabatic couplings. In that case, $E_{\text{kin}}$ becomes $E_{\text{kin}}(\rho_i) = E_{\text{max}} - \min[U_a(\rho_i)]$, where $\min[U_a(\rho_i)]$ is the lowest potential curve at $\rho_i$.

The approach for determining $\Delta \rho$ using $E_{\text{kin}}(\rho_i)$ is only efficient for excited states having many nodes. If only the ground state and/or a few weakly excited states are considered then the
step size should be adapted to the local variation of the states [Kok06].

3. Gaussian Quadrature and Legendre Points

We used the Gaussian quadrature method to numerically evaluate integrals throughout all of our calculations. This method employs the so-called Legendre points $x_k$ and Legendre coefficients $A_k$ to evaluate integrals. For instance, the integral of $f(x)$ from $a$ to $b$,

\[ \int_a^b f(x) \, dx = \int_{-1}^{1} f(y) \, dy = \sum_{k=1}^{n} A_k \cdot f(y_k) \]

is evaluated by first changing the limits from -1 to 1. The new integral can now be evaluated by summing $A_k \cdot f(x_k)$ over $k$ for $n$ Legendre points $-1 \leq x_k \leq 1$ and Legendre coefficients. Larger $n$ means better accuracy. Our integrals were mainly products of sine and cosine functions and so we did not have to use a large $n$. For the many-body model we used $n = 48$, for the three-body problem we used $n = 10$. The Legendre points and coefficients have been previously calculated for some given $n$ and were given in a separate file. This is a widely used and very accurate method for a small cost in calculation times. For a detailed description see Ref. [Arf01].

2.1.6. Model Problem: Three Identical Bosons with Nucleon Mass

1. Description and Formulation of Problem

This is a model of a system consisting of three identical bosons with nucleon mass. The particles interact through the model pairwise interaction given by

\[ V(r) = -55 \text{MeV} \exp[-0.2 \text{ fm}^{-2} r^2] + 1.5 \text{MeV} \exp[-0.01 \text{ fm}^{-2} (r-5 \text{ fm})^2]. \tag{23} \]

This interaction potential is taken from Fedorov et al [Fed03]. It only acts on the $s$-waves and consists of a Gaussian attractive pocket and a repulsive barrier [Fed03]. This two-body interaction is plugged into the formalism, beginning with Eq. (10), to solve the three-body system. This barrier in turn produces a barrier in the three-body adiabatic curves (Figure 14). The
barrier in the adiabatic curves will give rise to three-body shape resonances.

![Two-Body Potential](image)

**Figure 13:** Model two-body interaction for identical bosons with nucleon mass given by potential $V(r)$ in equation (23). Note the barrier in the interaction. The inter-particle distance is plotted in logarithmic scale.

We studied this model, in part, to test a simple method to find three-body resonances with a simple model, after which, different applications may come along (such as Efimov resonances). This model may also have some applications for the $^4$He nucleus [Fed03].

2. Convergence Tests

One way to test the validity of a model and the physical accuracy of its results is to perform convergence tests on the results. This consists of optimizing the different available parameters (such $n_\phi$, $n_\theta$, the size of the hyper-radial grid, $A$, and $L$) to obtain maximum accuracy. For us, satisfactory convergence meant achieving convergence within 5%. This means that we can significantly change one of our parameters but the quantity for which we want convergence does not change by more than 5%. For the three bosons with nucleon mass model we performed
several convergence tests on the dissociation energies, as well as the lifetimes and eigenenergies of the resonances.

The first set of tests consisted of checking the convergence of the dissociation limit of the adiabatic curves. From section 2.1.1, we must have $E_{\text{diss}} \to E_{\text{dimer}}$ as $\rho \to \infty$. We know what $E_{\text{dimer}}$ should be. According to Fedorov et al. $E_{\text{dimer}} = -6.76$ MeV (this simply amounts to solving the Schrödinger equation for $V(r)$) [Fed03]. In order to get the dissociation limit to converge to $E_{\text{dimer}}$, we increased the number of hyperangular basis states as well as the number of hyper-radial points until we obtained an acceptable value. However, since we are only interested in the value of the adiabatic energy at one point (the last point in the grid) then we can run the program interactively for only this hyper-radial point, saving calculation and waiting times. Using this method we obtained $E_{\text{diss}} = -6.753$ MeV. This amounts to a percent difference of 0.1%.

Next we tested the convergence of the resonance linewidths and eigenenergies with respect to the CAP. As discussed in section 2.1.4, the CAP introduces two important parameters which affect the results of the model: the strength $A$ and the length $L$. In order to determine which parameters to use we first had to determine the $\lambda_{\text{dB}}$ of the dissociating products (as discussed in section 2.1.4). We did this by estimating the kinetic energy $E_{\text{kin}} \approx E_{\text{dimer}}$ as a first approximation (see section 2.1.1). Usually, CAP works (i.e. absorbs the flux) for an interval of energies $E_{\text{kin}}$. If the actual complete calculation of $E_{\text{res}}$ shows that $E_{\text{kin}}$ is too different from $E_{\text{dimer}}$, one can correspondingly change the CAP and do the calculation one more time until we get a better approximation for $E_{\text{kin}}$. Once the optimal $A$ and $L$ parameters are chosen, one must check that the resonance widths and energies converge with respect to variations of these parameters. Therefore, we varied $A$ and $L$ by 30% and checked for convergence (see Figure 15). Our model was very sensitive to the values of $A$ and $L$ due to the small hyper-radial grid size. These set of
convergence tests were performed in the second part of the program, which relies on the convergence of the dissociation energy in the first part of the program, as already mentioned.

There are additional convergence tests which we could apply in the future to further confirm our results. These include convergence tests with respect to the form of the CAP, with respect to the number of requested adiabatic channels, and with respect to the size of the hyper-radial grid.

3. Results

Figure 14 shows the $A_1$ symmetry adiabatic channels produced from equation (10). We only consider $A_1$ symmetry states because, first, we are dealing with a system of bosons, which should have symmetrized wave functions, and, second, because all the $A_2$ and $E$ symmetry adiabatic curves are repulsive and cannot hold bound or resonant states. For future reference, let us call the channels 1, 2, 3 and 4 beginning with the lowest channel (blue curve) and working our way up to the brown curve (channel 4); see Figure 14.

Of the channels we consider, only the lowest channel can hold bound states, while the three other channels are repulsive everywhere and therefore only correspond to continuum states. The upper inset of Figure 14 shows the energy range of interest for shape resonances, which runs from $\sim -7$ MeV to $\sim -5$ MeV. This corresponds to the range of energies for which we would expect shape resonances. We consider this energy range in Figure 15, where we look at the linewidths of states. The CAP begins at about the middle of the grid but it's still sufficiently far away from the short-range interaction region so that, essentially, the physics of the problem remains unaltered.
Once we obtain the linewidths and vibrational energies of the three-body states, we can make a plot to check for convergence against the CAP parameters $A$ and $L$, as discussed above. The number of continuum states is determined by the grid length and grows as the grid becomes longer. The widths and energies of the continuum states don't converge with respect to $A$ and $L$ whereas the resonances do converge. The reason is that changing $A$ and $L$ changes the boundary conditions at the end of the grid, which has little effect on the short-range physics – which is where most of the resonance physics occurs. However, the change in boundary conditions does

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{three_body_potentials.png}
\caption{Three-body adiabatic energy curves. The lowest channel has the possibility of producing shape resonances due to the small potential barrier (shown magnified in upper inset). Lower inset shows complex absorbing potential (imaginary part) which is placed at the end of the grid to absorb the outgoing flux of atoms.}
\end{figure}
affect the *continuum* states since the amplitudes of their hyper-radial wave functions are large at long distances. From Figure 15 we see, then, that there are four good candidates for resonant states.

We tested convergence with respect to two different sets of optimal CAP parameters $L/\lambda_{dB} = 4$ and $L/\lambda_{dB} = 6$ where $\lambda_{dB}$ is the deBroglie wavelength of the dissociating products. Again, for a larger or smaller CAP (larger or smaller $L/\lambda_{dB}$) the convergence is not as good. Clearly, if we increase the size of the CAP even by one deBroglie wavelength ($\sim 1.7 \times 10^{-4} a_o$) then it would begin to interfere with the short-range physics. On the other hand, if the CAP is made shorter the $R + T$ factor will be larger.

![Figure 15: This plot shows linewidths versus eigenenergies of continuum and resonant vibrational states for the region of interest -7 MeV to -4.5 MeV. A minimum in the linewidth separates resonances from continuum states. Here, there are four possible resonances.*Optimal parameters for $L/\lambda_{dB} = 4$.**Optimal parameters for $L/\lambda_{dB} = 6$.](image)
Let us arbitrarily number the calculated eigenstates by counting the number of states starting from the ground state as number 1. Then the possible resonances are the $3^{\text{rd}}$, $8^{\text{th}}$, $11^{\text{th}}$, and $13^{\text{th}}$ states. The next step is to look at the hyper-radial wave functions. If the hyper-radial wave function is of a resonant state then it should have some component at short distance of the three-body potential and some component in the continuum. Continuum states have essentially no probability of being in the bound region. From Figure 14 we can say that the bound region extends to $\rho \sim 2.5 \times 10^{-4} a_0$. The probability density of bound states decays exponentially at large distances (see Figure 16). In the next five figures we show the hyper-radial wave functions for the ground and resonant states. The ground state is shown for comparison (Figure 16).

![Figure 16: Ground state hyper-radial wave function shown for comparison with resonance wave functions. Hyper-radius is shown in logarithmic scale. Note that most of the wave function is inside the bound region of the three-body potentials. Only the real components of $\psi_{a,n}$ corresponding to the first two adiabatic hyperspherical channels $a = 1$ and 2 are shown.](image)
The hyper-radial (as well as hyperangular) wave functions can have real and imaginary components in each channel (see section 2.1.4). So in this instance, where we consider four channels (see Figure 14), each hyper-radial wave function can have up to four complex and four real components.

The five plots shown in Figure 16 through Figure 20 only show the real and imaginary components in the two lowest channels ($a = 1$ and $2$ for $\psi_a(\rho)$). This is because the wave function components in the other two channels ($a = 3$ and $4$ for $\psi_a(\rho)$) are essentially zero. For the ground state, (Figure 16) the imaginary component in channels 1 and 2 is essentially zero. The wave function of a bound state can always be made real.

![Figure 17: Hyper-radial wave function for first resonance. Note logarithmic scale for hyper-radius.](image)

Figure 17 shows that for the first resonance candidate, at the 3rd position, the hyper-radial wave
function exhibits characteristics of a resonance: there is a significant probability for the wave function to be inside and outside the bound region. Note that the probability to be in channel two is much smaller, though nonzero, than the probability to be in the lower channel. This is a recurring theme because shape resonances have to obviously occur in channel 1.

Again, the function has a much higher probability to be in channel 1 than in channel 2. The same is true for the next three resonance candidates, as seen in Figure 17 through Figure 20. The probability to be in the bound region becomes more pronounced as we look at the last two hyper-radial wave functions.

Figure 18: Hyper-radial wave function for second resonance.
One point to note here is that in the wave function component in channel 2, \( \psi_2(\rho) \), lower part of Figure 19, there is a cusp in the real part. This is an undesired effect of the program, which sometimes artificially switches the sign of \( \psi_2(\rho) \) at some points of the hyper-radial wave function. So all the points beyond the cusp should be multiplied by -1 in order to see the correct, smooth-flowing wave function. This happens because the hyper-angular functions \( \phi_a(\rho, \theta, \varphi) \) at two different values \( \rho_i \) and \( \rho_{i+1} \) of hyper-radius are calculated independently. Therefore, the phases of \( \phi_a(\rho_i, \theta, \varphi) \) and \( \phi_a(\rho_{i+1}, \theta, \varphi) \) are independent. Because the wave functions \( \phi_a(\rho, \theta, \varphi) \) are real, the phase must be either 1 or -1. Since the the product \( \phi_a(\rho, \theta, \varphi) \psi_a(\rho) \) should have the same phase, the change of sign in \( \phi_a(\rho, \theta, \varphi) \) makes \( \psi_a(\rho) \) change sign too.

\[ \text{Figure 19: Hyper-radial wave function for third resonance.} \]
So, to get the smooth function $\psi_a(\rho)$ we have to multiply $\psi_a(\rho)$ with -1 on certain points $\rho_i$. We corrected this problem as we plotted the hyper-radial wave functions by reversing the sign-switch, but we were unable to fix it for this particular cusp in Figure 19...

![Hyper-radial wave function for fourth resonance.](image)

**Figure 20:** Hyper-radial wave function for fourth resonance.

Next we look at the contour plots of hyperangular wave functions and see what they tell us about the resonances. Hyperangular wave functions are solved separately for each channel $U_a$ after we have fixed hyper-radius $\rho$. What we show in Figure 21 and Figure 22 are sets of hyperangular wave functions for two different values of $\rho$: $\rho = 0.0001 \ a_o$ (inside bound region) and $\rho = 0.001 \ a_o$ (outside bound region). Each figure shows the wave functions for four channels, three with $A_1$ symmetry, and the last one for $A_2$ symmetry, for comparison. Counting from the upper left corner clockwise, the wave functions shown are for channels 1, 2, 3 and 4. The
coordinates of the plot are the same \((\theta, \varphi)\) as represented in Figure 11.

The wave functions display \(C_{3v}\) symmetry (the \(C_{3v}\) symmetry group is discussed in section 2.1.3). So, for example, we can rotate the wave functions by 120° and they remain unchanged. If we reflect them across vertical planes \(\sigma_v\) then the \(A_1\) representation leaves the wave function unchanged while the \(A_2\) representation multiplies the wave function by a negative sign (see lower-right frames in Figure 21 and Figure 22). In addition to \(A_1\) and \(A_2\) states, states of the \(E\) irreducible representation can also be obtained. They are not shown in our plots. To see examples of the \(E\) states, though for a different system, see Ref. [Hua06].

As can be seen in Figure 21, the hyperangular wave functions inside the bound region have a higher probability of possessing an equilateral-like configuration, even though there is a smooth probability distribution which is not necessarily concentrated in any one region of the space of hyperangles.
In Figure 22 we see that channel 1 has the most probability in a region of hyperangles which is essentially a dimer + free atom. This channel 1 wave function should display $C_{3v}$ symmetry but it

\textbf{Figure 21:} Hyperangular wave functions inside bound region, 
$\phi_a(0.0001, \theta, \phi)$ for $a = 1, 2, \text{ and } 3$, and $\phi_A(0.0001, \theta, \phi)$. 

\[ \begin{align*} 
\text{Figure 21: Hyperangular wave functions inside bound region,} \\
\phi_a(0.0001, \theta, \phi) \text{ for } a = 1, 2, \text{ and } 3, \text{ and } \phi_A(0.0001, \theta, \phi). \\
\end{align*} \]
is a technicality of the program which causes it to only show one corner of the wave function and not show the full symmetry.

**Figure 22:** Hyperangular wave functions far away from bound region, $\phi_{a}(0.001, \theta, \varphi)$ for $a = 1, 2, \text{ and } 3$, and $\phi_{A_1}(0.001, \theta, \varphi)$. 
4. Comparison to Fedorov et al.

Fedorov [Fed03] used a so-called complex scaling method of hyperspherical coordinates and the Faddeev equations to make three-body bound state and resonance calculations for the three identical bosons with nucleon mass model. He found the two-body bound state to be at $E^{(2)} = -6.76$ MeV, a three-body bound state at $E_0 = -37.22$ MeV, and a resonance at $E_1 = -5.96 - 0.40i$ MeV. Our calculations yielded the three-body bound state to be located at $E_0 = -37.24$ MeV. We found four resonances at $E_1 = -6.58 - 0.0060i$ MeV, $E_2 = -6.07 - 0.038i$ MeV, $E_3 = -5.44 - 0.040i$ MeV, and $E_4 = -5.09 - 0.054i$ MeV. Also, as discussed earlier, our dissociation energy was within 1% of the dimer binding energy calculated by Fedorov et al. Fedorov's values for the bound state and the resonance are close to the values that we found, except for the linewidth of the resonance, which is different from ours by one or two orders of magnitude. Fedorov mentions that his calculations were for illustrative purposes only and therefore he was not particularly interested in maximum accuracy [Fed03]. This may explain smaller discrepancies in the energies, but not those in the linewidths.

2.1.7. Efimov Bound States and Resonances

1. Description and Formulation of Problem

Efimov states are a family of three-body bound states that appear when the two-body scattering length $a$ is much larger than the radius of the forces $r_0$, or equivalently, if there exists a very shallow two-body bound or virtual state [Efi71]. Efimov (1971) studied a system of three particles that interact only within a vanishingly small range and derived a three-body potential-energy curve in terms of $\rho$ [Esr06], [Efi71]. The three-body potential turns out to be of the form $s_i^2 / \rho^2$. The constants $s_i$ are roots of a transcendental equation and may be real and imaginary. There is one imaginary root $s_0 \approx 1$, such that the three-body potential has a universal, negative
coefficient of proportionality and Efimov states appear [Efi71]. The properties of this potential are well-known since it resembles the potential of a charged particle in the field of a dipole.

$$\left(-\frac{d^2}{d\rho^2} - \frac{1}{\rho} \frac{d}{d\rho} + \frac{s_i^2}{\rho^2}\right) F_{s_i}(\rho) = E F_{s_i}(\rho)$$

Solving the time-independent Schrödinger equation yields that the energy levels condense to zero exponentially, with an exponent

$$E_n = E_{n+1} \exp \left( \frac{2\pi |s_0|}{s_0} \right) \approx 500 E_{n+1},$$

where $s_0$ is related to the strength of the so-called effective dipole moment [Esr06]. The most favorable conditions for the formation of Efimov states are for identical, spinless, neutral bosons with zero relative angular momentum $l$ [Efi71].

Figure 23 from [Kra06] gives a visual explanation of Efimov states. In this figure, we are looking at a plot of inverse scattering length $a^{-1}$ versus the three-body energy for a region where $a >> r_0$. For $a < 0$ the gray region corresponds to the dissociation of the system to three free atoms, while for $a > 0$ the gray area corresponds to the dimer + free atom dissociation. The first Efimov state is predicted to appear at $a_i \approx 22r_0$ [Efi71]. At this point, the three-body energy $E$ becomes negative. As we increase $a$, we find the second Efimov state at $a_2 \approx 22a_i$, the third Efimov state can be found at $a_3 \approx 22a_2$, and so on... The $n + 1$ state appears at [Efi71]

$$a_{n+1} \approx 22a_n.$$  \hspace{1cm} (24)

For a given $a > 0$ the number of levels is [Efi71] (with logarithmic accuracy)

$$N(a) = \left[ \frac{|s_0|}{2\pi} \ln \left( \frac{a}{r_0} \right) \right].$$

As $a \to \infty$, i.e. as the energy of the two-body bound state approaches zero, there is a
“condensation” of three-body bound states and an infinite number of bound states, Efimov trimers (ETs), appear.

Figure 23 Description of Efimov states (Kraemer et al.) [Kra06].

The ability to manipulate the interactions between atoms, i.e. to tune $a$, in ultracold quantum gases using Feshbach resonances has facilitated the possibility of observing Efimov physics.

There has been recent experimental evidence for the existence of Efimov bound states from Kraemer et al. [Kra06], making a study of Efimov resonances specially relevant. An Efimov resonance occurs when a pre-dissociated ET dissociates into a dimer and a free atom. This can occur when the three free atoms threshold or the dimer + free atom threshold meets the Efimov trimer, i.e. near those values of the scattering length (given by Eq. (24)) where ETs meet continuum states. In principle, at these respective junctures one may observe a dissociation of an ET into three free atoms or a dimer + free atom. We are interested in investigating the latter case in our $^4$He-based model.
2. $^4\text{He}$ Efimov Resonances

Model three-body systems of $^4\text{He}$ are known to posses Efimov physics [Esr96]. There are several reasons why this is true and why we chose to study this system. First, the $^4\text{He}$ dimer potential, Figure 24, has a very shallow bound state at around 1mK. Second, since the helium atom is neutral there is a rapid decrease in diatom Coulomb interaction with internuclear distance. Third, accurate helium dimer potentials have become available which are consistent with each other as well as with experimental measurements [Esr96].

For $^4\text{He}$, \( r_0 = 14 \ a_0 \) and \( a = 220 \ a_0 \), so \( r_0 << a \). However, in our calculations we do not observe any Efimov resonances in this situation. This is because the conditions are not favorable for the resonances we are interested in obtaining. For us, the most favorable conditions correspond to when the two-body bound state is deeper than some bound three-body state. This would allow
the possibility for this three-body state to dissociate into the dimer state plus a free atom. To produce these conditions, we have to artificially tune the two-body interaction, $V(r)$, by multiplying it by a constant: $V(r) \rightarrow \lambda V(r)$ just as Esry et al. did ($r$ is the inter-atomic distance) [Esr96]. This is equivalent to tuning $a$. Although it is currently not possible to tune the scattering length in ultracold $^4$He (unlike with ultracold alkali atoms), we decided to explore this unphysical possibility with $^4$He as opposed, say, to Cs, since Cs$_2$ and Cs$_3$ have many more bound states, which would make our calculations longer.

There are special values of $\lambda$ at which there is a zero energy two-body $s$-wave bound state (i.e. where we find an infinite number of Efimov states and the two-body scattering length is infinite). Let us call this value $\lambda_{\text{Efimov}}$. Obviously, there are multiple values of $\lambda_{\text{Efimov}}$ since, as we increase $\lambda$ from $\lambda_{\text{Efimov}}$, at some point, we will find the energy of the first excited two-body bound state to be zero and hence we will again find an infinite number of Efimov bound states. This argument carries on for higher excited two-body states. Let us call the first two values of $\lambda_{\text{Efimov}}$ (for the ground state and the first excited state) $\lambda_{\text{Efimov1}}$ and $\lambda_{\text{Efimov2}}$.

Increasing $\lambda$ will cause the two-body and three-body bound states to become deeper, but the two-body bound state becomes deeper more quickly than the three-body bound state. Also, the second channel in the three-body adiabatic curves develops a minimum which means it may be able to hold bound states (Figure 25). This creates favorable conditions for a pre-dissociated three-body state to exist, which will eventually decay into a dimer + free atom. However, by increasing $\lambda$ ($\lambda_{\text{Efimov1}} < \lambda < \lambda_{\text{Efimov2}}$) we are also decreasing $a$ and so Efimov physics becomes less likely, and any pre-dissociated states which may appear could be regular three-body resonances instead of Efimov resonances (we discuss this in more detail in the Results section).
We increase $\lambda$ up to $\lambda = 2.4$. If we increase $\lambda$ any further then two-body rotational states in the asymptotic region of $\rho$ appear, increasing the number of thresholds at $\rho = \infty$. The rotational energies are given by

$$E_l = B_v I(l+1)$$

where $B_v = \langle \frac{1}{2I} \rangle$ is the rotational constant, and $I$ is the inertia of the two-body system. For the dimer relative angular momentum $l = 1$ at $\rho = \infty$, we approximated $E_l \approx 3K$. Therefore, in order to avoid introducing rotational energies into the system, we would have to restrict the energies of the system to less than 3K.

**Figure 25:** Increasing $\lambda$ can allow excited channel to hold bound states.
3. Variable-Grid Mapping in Space of Hyperangles ($\theta, \varphi$)

We decided to extend the hyper-radial grid of the three-body potential to 1000 $a_o$ (Figure 30). One reason is that a longer grid would allow us to better distinguish resonances from other states. This is because longer grids allow us to see the long-range behavior of the wave functions. Another reason is that as we increased $\lambda$ then we had to increase the size of the grid of hyper-radius in order to accurately represent the dissociation energy. Increasing the grid requires increasing the number basis functions in the $\theta$ and $\varphi$ directions ($n_\theta$ and $n_\varphi$). This is due to the fact that a longer hyper-radius means that in the dissociation limit two of the particles are closer to each other with respect to the third. This translates to a smaller region represented in the two-dimensional space of hyperangles, namely the areas representing a dimer + free atom configuration (that is, $\theta \approx \pi/2$ and $\varphi \approx \pi/6$ or $5\pi/6$, see Figure 11).

In order to get around the problem of using more basis functions we (1) only considered a portion of the two-dimensional space of hyperangles $\pi/6 \leq \varphi \leq 5\pi/6$ and (2) implemented a variable-grid scheme where the step sizes $\Delta \theta$ and $\Delta \varphi$ varied according to Figure 26.

![Variable step-sizes of grid in hyperangles $\theta$ and $\varphi$.](image)

We decrease the step size $\Delta \theta$ as $\theta \to \pi/2$ and $\Delta \varphi$ as $\varphi \to \pi/6$ or $5\pi/6$. The above limitations of
the domain of variation of the hyperangles don't allow us to represent states with \( E \) symmetry. One would need at least \( \varphi \) from 0 to \( \pi \) or to represent the \( E \) states.

4. Convergence Tests

Just like in the model of three bosons with identical mass, we performed convergence tests with respect to the dissociation energy of the three-body potentials, and with respect to the CAP parameters \( A \) and \( L \).

Observing convergence of the three-body potentials with respect to the dissociation energy was more difficult in this case than in the three boson with identical mass model. This model required a much larger number of hyperangular basis states due to the large size of the grid. This is the reason for the variable-grid mapping discussed above. The computation times are consequently much longer. This is a reason why originally we did not work with larger \( \lambda \), such as \( \lambda = 6.9 \). For the same reason (the large hyper-radial grid size), we expect to see good convergence of the CAP parameters with respect to resonances.

One of the convergence tests we plan to do in the future is with respect to the form of the CAP. Since the length of the hyper-radial grid is much longer than the length \( L \) of the CAP, then we may use other types of CAPs, such as the exponential or linear (where larger \( L \) is required), to check the convergence of the resonances.
5. Results

Our calculations yielded $\lambda_{\text{Efimov}1} \approx 0.9765$ and $\lambda_{\text{Efimov}2} \approx 6.834$. For a $^4\text{He}$, Esry et al. found $\lambda_{\text{Efimov}1} = 0.9741$ and $\lambda_{\text{Efimov}2} = 6.823$ [Esr96]. We concentrated on the range $\lambda_{\text{Efimov}1} < \lambda \leq 2.4$ since for $\lambda > 2.4$ rotational energies enter the problem (as discussed in 2.1.7-2) and also a large number of hyperangular basis functions would be required to observe convergence of the dissociation energy. Further advantages and disadvantages to the restriction $\lambda_{\text{Efimov}1} < \lambda \leq 2.4$ are discussed later in this section.

These results are for $\lambda = 2.4$. Figure 27 shows the three-body potentials with $A_1$ symmetry for the three-body $^4\text{He}$ model. For future reference, let us label the adiabatic channels by 1, 2, 3, and 4 beginning from the lowest (blue) channel and moving up (see Figure 27). As discussed earlier, we introduced a large grid ($1000 \ a_0$) because we think this will help us better identify resonances whose hyper-radial wave functions could have extended tails. Also, as we increase $\lambda$, we require a larger grid to observe convergence of the dissociation energy. Note that the hyper-radius is plotted in logarithmic scale.

We can see from Figure 27 that there is the possibility of having Feshbach resonances between the two lowest channels since the first excited channel (black) may be able to hold a bound state whose energy is higher than the dissociation energy of the ground state (blue) channel. If this were the case, we would still have to distinguish Efimov resonances from normal resonances.
Note, however, that as it is a defining property of Efimov states, the number of Efimov states decreases as the interaction strength $\lambda$, increases. So as we increase $\lambda$ from $\lambda_{\text{Efimov}}$ the states which disappear are Efimov while the states that remain are normal states [Esr96]. We expect this to be true for bound states as well as resonances since resonances are quasi-bound states. So we can use this fact to distinguish Efimov from regular three-body resonances.

We needed a high value of $\lambda$ such that the second channel could hold bound states, but at the same time increasing $\lambda$ would also decrease $a$, diminishing the possibility of Efimov physics. With that in mind, we first searched for evidence of resonances in the linewidth versus energy plot, Figure 28.

Figure 27: $^4\text{He}$ three-body adiabatic curves for $\lambda = 2.4$. 

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{three-body_potentials.png}
\caption{\textbf{$^4\text{He}$ Three-body Potentials (A$_1$ symmetry)}

\begin{center}
\begin{tabular}{c}
\hline
Hyper-radius $p$ (a.u.) \\
\hline
\end{tabular}
\end{center}

\begin{center}
\begin{tabular}{c}
\hline
Energy (K) \\
\hline
\end{tabular}
\end{center}

\begin{center}
\begin{tabular}{c}
\hline
1 & 2 & 3 & 4 \\
\hline
\end{tabular}
\end{center}

\textbf{Figure 27: $^4\text{He}$ three-body adiabatic curves for $\lambda = 2.4$.}
\end{figure}
From the figure, we see that there are several continuum states in the region of interest and some possible resonances where there is a minimum in linewidth. However, we looked at the hyper-radial wave functions of these states and determined that they were not resonances, but discretized-continuum states created due to the finite length of the grid. Therefore, we found no evidence of Efimov resonances for $\lambda = 2.4$.

We also considered the hyperangular wave functions at two different values of hyper-radius and for $\pi/6 \leq \phi \leq 5\pi/6$. Figure 29 and Figure 30 are for values of hyper-radius inside the bound region ($\rho = 10 \, a_0$) and in the dissociation region ($\rho = 100 \, a_0$), respectively. Each figure has four wave functions, each for a different adiabatic channel. Besides channels 1 through 4 shown in Figure 27, in Figure 30 we also include a wave function for an $A_2$ symmetry channel not shown in Figure 27.

*Figure 28:* $^4$He linewidth versus energy for $\lambda = 2.4$. 
Beginning from the upper-left frame, we show $\phi_a(10, \theta, \phi)$ for the four $A_1$ symmetry channels from Figure 27. The upper-left and upper-right frames are for $a = 1$ and 2, respectively, while the

Figure 29: Hyperangular wave functions for $\rho = 10 \text{ a}_0 (\pi/6 \leq \phi \leq 5\pi/6)$, $\phi_a(10, \theta, \phi)$ for $a = 1$, 2, 3 and 4.
lower-left and lower-right frames are for $a = 3$ and 4, respectively. In the bound region, $\rho = 10\ a_o$, we see that there is an even distribution of probabilities, but mostly concentrated around the center.

**Figure 30:** Hyperangular wave functions for $\rho = 100\ a_o\ (\pi/6 \leq \varphi \leq 5\pi/6)$, $\phi_a(100, \theta, \varphi)$ for $a = 1, 2, \text{and } 3$, and $\phi_{A_2}(100, \theta, \varphi)$. 

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In Figure 30 we see $\phi_{a}(100, \theta, \varphi)$ for $a = 1, 2$ and $3$ and we also see the hyperangular wave function $\phi_{A_2}(100, \theta, \varphi)$ for an $A_2$ symmetry channel not shown in Figure 27. The upper-left frame is for $a = 1$. Upper-right frame is $\phi_{A_2}(100, \theta, \varphi)$. Lower-left and lower-right frames are for $a = 2$ and $3$, respectively. For $\rho = 100 \, a_0$, Figure 30, the higher probabilities lie in the outer regions which represent dimer + free atom configurations. Hence, although there were no Efimov resonances discovered for $\lambda = 2.4$, we still observe the expected physics for large and small hyper-radii and for the variable grid mapping in the space of hyperangles.

Currently, we are considering several possibilities for observing Efimov resonances. The first is one to look at $\lambda \approx 4$ and see if $U_{l=2}$ has bound states which would open the possibility for $d$-wave Efimov physics, something not previously considered. We can then take the energy of the three-body state to threshold so that there could be a possibility of decay into the lower energy two-body bound state. A second option would be to consider $\lambda \approx \lambda_{\text{Efimov2}}$, which would of course require more hyperangular basis functions and perhaps a larger grid, and hence more computation time.
2.2 Bose-Einstein Condensates and Degenerate Fermi Gases

Our ultimate goal is to model many-body processes in superfluids and provide a general model of the Bose-Einstein condensate and degenerate Fermi gas phenomena which can be useful for theoretical understanding and prediction of BEC/DFG behavior under different experimental conditions. We want to begin with the many-body processes in superfluids and bosonic ultracold quantum gases (BECs). Once we obtain some satisfactory results we would like to expand into ultracold fermionic quantum gases (DFGs). So far we are still working on superfluidity and BECs, and have not entered into the latter part of the plan. Therefore, this project is not yet complete. All the programming for this part of the thesis has been done in the Python language (see Appendix). In this section, we formulate the ultracold quantum gas many-body problem, present its quantum formalism, describe our model and preliminary results.

The initial stages of the project consist of writing and debugging python code that would produce the energy spectrum, \( E(k) \), of \( N_{tot} \) bosons trapped in a one-dimensional box. In order to verify that any results we obtained were valid, we performed various different convergence tests.

2.2.1. BEC Quantum Formalism

1. Second Quantization

We present here a quick review of second quantization, which we will use in the formulation of the many-body problem. Second quantization is a convenient way of studying systems of identical indistinguishable particles because it automatically chooses functions of the required symmetry (under the permutation of two particles). It uses the occupation number, or Fock, representation. In such a representation, the states of the whole system, or Fock states, tell you the number of particles in each single-particle state and are represented by

\[ |n_1, n_2, \ldots, n_N \rangle, \]
where \( n_k \) is the number of particles in the single-particle state \( k, k = 1, 2, \ldots N_s \) [Dav76]. Such Fock states are eigenstates of the system if the particles do not interact. A note to avoid confusion, when talking about the Fock states of the many-body system, the subscript labels the single-particle energy level while the letter \( (n) \) labels the number of particles in that level.

In the usual coordinate representation, the wave functions of a system of \( N \) particles with \( q \) degrees of freedom depends on \( Nq \) variables. In the second quantization representation, all operators are expressed in terms of creation and annihilation operators \( (\hat{a}_k^\dagger \text{ and } \hat{a}_k, \text{ respectively}) \) of single-particle states \( |k> \) with the number of degrees of freedom of only one particle [Dav76]. The operators \( \hat{a}_k^\dagger \) and \( \hat{a}_k \) operate on the \( k^{th} \) single-particle state. So, if there are \( n_k \) particles in state \( k \) then the number of particles is either decreased or increased by one,

\[
\hat{a}_k |n_k> = \sqrt{n_k} |n_k - 1>,
\]
\[
\hat{a}_k^\dagger |n_k> = \sqrt{n_k + 1} |n_k + 1>.
\]

Therefore, the total number of particles \( n_k \) in a given energy level \( k \) is given by

\[
<n_k|\hat{a}_k^\dagger \hat{a}_k |n_k> = n_k
\]

when the single-particle Fock states \( |k> \) are orthogonal.

The second quantization method is practically irreplaceable for studying a system with variable number of particles, that is, a system in which particles are converted into one another [Dav76].

2. Bogolyubov Hamiltonian

In the second quantization, a system of weakly-interacting identical bosons can be approximated by the Bogolyubov Hamiltonian [Dav76]. Bogolyubov gave a microscopic theory of the superfluidity of helium [Dav76]. This Hamiltonian, Eq. (27), describes elementary
excitations in such a system. This method is of considerable interest not just for the theory of superfluidity, but also for other applications where perturbation theory cannot be applied [Dav76]. The link between superfluidity and Bose-Einstein condensation is not yet clear. As early as 1938, London considered superfluidity in helium as a possible manifestation of BEC [Dal99]. A first principles argument was made by Penrose and Onsager in 1957, indicating that helium II in equilibrium shows Bose-Einstein condensation [Pen56]. It is still widely believed that superfluids and BEC are inextricably linked, with the main difference lying in the strength of the particle interactions.

To describe the Bogolyubov Hamiltonian, let’s call the pairwise interaction $\hat{W}$, so the Bogolyubov Hamiltonian is given by

$$H = \sum_k \epsilon_k \hat{a}_k^\dagger \hat{a}_k + \frac{1}{2} \sum_{k_1, k_2, k_{1}', k_{2}'} \hat{a}_{k_1} \hat{a}_{k_2} \hat{a}_{k_{1}'} \hat{a}_{k_{2}'} \langle k_1 k_2 | \hat{W} | k_{1}' k_{2}' \rangle,$$  \hspace{1cm} (27)

where the first sum is over the non-interacting single-particle energy eigenstates labeled by $k = 1, 2, ..., \infty$, and the second sum is over all single-particle momenta $0 \leq k_1, k_2, k_{1}', k_{2}' \leq \infty$. The first term in the Hamiltonian accounts for the kinetic energy of the non-interacting particles $\epsilon_k = \frac{k^2}{2m}$, while the second term accounts for the inter-particle interactions. So if $\hat{W} = 0$, we would have an ideal gas of bosons and the spectrum would be described by the first term of the Hamiltonian only. In our model $\hat{W}$ is given by a square potential well, $W(x)$ in Figure 33 (more on this in the next section). To evaluate the $\langle k_1 k_2 | \hat{W} | k_{1}' k_{2}' \rangle$ terms in Eq. (27), the $|k_1 k_2\rangle$ states are written as a product of two non-interacting single-particle eigenstates, $|k_1\rangle$ and $|k_2\rangle$, with momenta $k_1$ and $k_2$,

$$|k_1 k_2\rangle \equiv |k_1\rangle |k_2\rangle .$$  \hspace{1cm} (28)
One point to note here is that Eq. (28) comes about as a result of formulating the problem in the second quantization representation and does not need to be symmetrized with respect to exchange of bosons; see [Dav76].

The first sum in Eq. (27), the non-interacting particle energy term, is a simple sum over each energy level that multiplies the energy $\epsilon_k$ of a given state $k$, by the number of particles $n_k$ in that level. The number of particles is given by the creation and annihilation operators, $\hat{a}_k^\dagger$ and $\hat{a}_k$, as described in the preceding section, see Eq. (26). If we construct the Hamiltonian as a matrix, then this sum contributes only to the diagonal elements (more on this in section 2.2.3).

The total number of particles in the system, $N_{tot}$, is given by the number operator

$$N_{tot} = \sum_k \hat{a}_k^\dagger \hat{a}_k.$$  

Since this operator commutes with the Bogolyubov Hamiltonian then the total number of particles in the system is conserved. Hence, when the number of particles is some state $k$ is decreased by one, then the number of particles in another state is increased by one [Dav76].

If the bosons are confined to a large volume $V$, then the transition term in the second sum of Eq. (27) is given by

$$\langle k_1 k_2 | \hat{W} | k'_1 k'_2 \rangle = \frac{\nu(||k'_1 - k_1||)}{V} \Delta(k'_2 + k'_1 - k_2 - k_1), \quad \text{(29)}$$

where,

$$\Delta(k'_2 + k'_1 - k_2 - k_1) = 1, \text{ if } k'_2 + k'_1 = k_2 + k_1. \quad \text{(30)}$$

Here, $\nu(k)$ is the Fourier transform of the interaction energy, $\hat{W}$, of a pair of bosons. Equation (29) represents a pair of particles with momenta $k'_1$ and $k'_2$ which interact through the two-body
potential $\hat{W}$. The interaction corresponds to the disappearance of a pair of particles in states with momenta $k'_1$ and $k'_2$, and their simultaneous appearance in states with momenta $k_1$ and $k_2$, respectively [Dav76]. This transition is taken into account by the creation and annihilation operators $\hat{a}_{k'_1}$, $\hat{a}_{k'_2}$, $\hat{a}_{k_1}$, and $\hat{a}_{k_2}$. Equation (29), gives the probability of this transition. This term connects low-energy single particle states to high-energy single-particle states.

Bogolyubov suggested an approximate way to find the spectrum of the Hamiltonian given by Eq. (27) [Dav76]. Basically, in the Bogolyubov approximation, the energy $E(k)$ of the eigenstates of the Hamiltonian (such states are called elementary excitations or quasi-particles in this theory) is given by

$$E(k) = \frac{\hbar^2 k^2}{2m} + n \nu(k)$$  \hspace{1cm} (31)

where $n$ is the number density of bosons, and $\nu(k)$ is the same as defined above. This gives the energy versus momentum ($p = \hbar k$) relation sketched in Figure 31. Clearly, if there is no interaction between the bosons, i.e. $\hat{W} = 0$, only the first term in Eq. (31), the kinetic energy of the non-interacting bosons, contributes to the energy spectrum, and $E(k)$ is parabolic. The dip in the spectrum occurs at some $k_0$.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure31.png}
\caption{Momentum dependence of the energy of elementary excitations in a BEC system (interacting bosons). When there is no interaction, the curve is a simple parabola.}
\end{figure}
Landau showed that such an energy spectrum leads to superfluidity of the gas or liquid [Dav76], [Lan77].

2.2.2. Description of Model

Our current model of the gas in the BEC phase consists of \( N = N_{\text{tot}} \) identical bosons of mass \( m \) trapped in a one-dimensional infinite square well potential, as sketched in Figure 32.

Each non-interacting boson in the infinite square potential well is labeled by \( i \), and is in the corresponding single-particle level with momentum \( k_i \). The single-particle eigenfunctions and eigenenergies are given by

\[
\Phi_{k_i} = |k_i> = \sqrt{\frac{2}{L}} \sin(k_i x_i),
\]

\[
\epsilon_{k_i} = \frac{k_i^2}{2m} = \frac{\pi^2 m_i^2}{2mL^2}, \text{ where } k_i = \frac{\pi m_i}{L},
\]

where \( i = 1, 2, ..., N_{\text{tot}} \) labels the \( i^{th} \) boson in the state with momentum \( k_i \) and energy level labeled by \( m_i = 1, 2, ..., N_s \). Note that this labeling, \( |k_i> \) (where the subscript labels the boson), of the
single-particle eigenstates has a different meaning from the labeling of the Fock states, $|n_1 n_2 ... n_{Ns}>$, in which the subscript refers to the single-particle energy level. For numerical calculations, we restrict all the bosons to $N_s$ energy levels. We have performed calculations for $N_s = 2, 3$ and $4$. Given the single-particle eigenstates and eigenenergies, Eq. (32), we can now rewrite Eq. (28) as

$$|k_1 k_2> = \frac{2}{L} \sin (k_1 x_1) \sin (k_2 x_2),$$

for all single-particle levels $k_1$ and $k_2$.

We would like to start with the simplest situation to see how far it takes us and then make more realistic assumptions. We begin by modeling the two-body interaction, $\hat{W}$ in Eq. (27), by a simple one-dimensional square well interaction (Figure 33).
1. Rectangular Spherical Potential Well

![Diagram of a rectangular spherical potential well]

Figure 33: Top: Pair interaction potential $W(x)$ acts between the $i^{th}$ and $j^{th}$ pair of bosons in the infinite well potential. Bottom: The interaction potential $W(x)$ depends only on the distance ($x = |x_i - x_j|$) between the $i^{th}$ and $j^{th}$ bosons. If the separation between the pair of bosons is greater than $d$, then there is no interaction between that pair.

In Figure 33, we display our pairwise interaction $W(x)$, $\hat{W}$ Eq. (27), which is given by a one-dimensional rectangular spherical potential well. The cut-off distance for the interaction is given by $d$. Obviously $d$ cannot exceed $L$. Note that the diatom interaction, $W$, is given in terms of separation distance, $x$, while the single-particle states $|k_i>$, Eq. (32), are written in terms of the position of the bosons, $x_i$. 
Since we can substitute $\hat{W} = W(x)$ in Eq. (27), and combining this with Eq. (33), we can now write the transition term (more on this term in the next section) in the second sum of the Hamiltonian as

$$\langle k_1 k_2 | \hat{W} | k'_2 k'_1 \rangle =$$

$$= \int \int \left( \frac{2}{L} \right)^2 \sin (k_1 x_1) \sin (k_2 x_2) W(x) \sin (k'_1 x_1) \sin (k'_2 x_2) dx_1 dx_2,$$

(34)

where we have substituted $i$ and $j$ by 1 and 2. Since the eigenstates are in terms of boson “position” $x$, while the interaction is in terms of the separation distance $x = |x_1 - x_2|$, then we have to perform a substitution in order to evaluate these integrals. Equation (34) is simplified before it is evaluated numerically (more on this in section 2.2.3).

2. Number of Single-Particle Energy Levels

From considerations of Eq. (27), we can calculate the dimensions of the Hamiltonian matrix in terms of $N_s$ and $N_{tot}$. For a given number of single-particle levels $N_s$ and for a total number of particles $N_{tot}$, the number of rows and columns of the $M \times M$ Hamiltonian matrix is given by

$$M = \frac{(N_{tot} + N_s - 1)!}{(N_s - 1)! \cdot N_{tot}!}.$$

One can get this result by considering $N_{tot}$ particles and the total number of ways which one can arrange them into $N_s$ cells (or energy levels), with each cell being able to hold anywhere from 0 to $N_{tot}$ balls (Figure 34).
This number can easily get out of hand for computations involving a relatively small number of bosons. For instance, for 1,000 bosons each being a four-level system \( (N_s = 4) \), we obtain \( M = 167,668,501 \) and \( H \) would have \( M^2 \approx 3 \times 10^{16} \) elements! This is one reason why we have so far restricted ourselves to four-level atoms or less.

Obviously, a one level system is not very interesting if studying excitations of a many-body system. A two level system is more interesting but perhaps not very realistic. We consider three level and four level \( (N_s = 3, 4) \) systems more realistic and interesting, while still computationally feasible. Using such a low number of single-particle states may be an obstacle to observing convergence in our model. This can be seen from Eq. (34), which, as mentioned earlier, connects low-energy and high-energy single-particle states (i.e. \( \langle k_1k_2|\hat{W}|k'_1k'_2 \rangle \), for \( k_i \) and \( k'_i \) very different). In our construction, this corresponds to matrix elements far from the diagonal. If there is a strong connection between low-energy and high-energy states, i.e. if these matrix elements are significant, then we must increase the number of single-particle states, \( N_s \), before we can observe convergence in our results. We would like to check if these matrix elements do in fact decay to zero for large \( N_s \). Looking at Eq. (34), we suspect that such matrix elements are in fact negligible since the sine functions in the integral should become more and more orthogonal as the difference between \( k_i \) and \( k'_i \) increases. However, since our two-body

\[ Figure 34: Arrangement of N_{tot} particles into N_s states. \]
potential $W(x)$ has sharp corners, which are difficult to represent in a Fourier expansion with a low number of basis functions (that is, small $N_s$), then for the Fourier transform of $W(x)$, Eq. (34), we will need to perform more tests of convergence.

We propose getting around the problem of the size of the Hamiltonian by reducing the size of it as follows. We restrict the number of bosons that can be excited from the ground state. Let's label this number $N_{ex}$. If we label the number of bosons restricted to remain in the ground state to $N_{gd}$, then clearly the total number of bosons is given by $N_{tot} = N_{gd} + N_{ex}$. Consequently, the dimension of the Hamiltonian is now given by

$$M = \frac{(N_{ex} + N_s - 1)!}{(N_s - 1)! N_{ex}!}. \quad (35)$$

This restriction drastically reduces the size of $H$. For example, for 1,000 bosons and $N_s = 4$, with 10 of them allowed to be excited, we get $M = 286$. This is a computation which can easily be done in a few minutes using a desktop. If, instead, we allow 50 bosons to be excited, then $M = 23,426$. This calculation is probably no longer manageable with a desktop, but may still be manageable with a supercomputer.

3. Scattering Length

As already mentioned, the scattering length is an important parameter which determines the inter-particle interaction in ultracold quantum gases. Therefore, it is important to keep track of the scattering length in our model since it would give us a good indication of the physics behind our calculations. In our model, the two-body interaction is modeled by a rectangular spherical potential well, $U_o > 0$ in Figure 33, or barrier, $U_o < 0$. For an attractive interaction, $U_o > 0$, the scattering length $a$ can be negative or positive. It was previously obtained analytically (Eq. (6), section 2.1.2), and is given by
\[ a = d \left[ 1 - \frac{\tan K_0 d}{K_0 d} \right], \]  

(36)

where \( K_0 \) is defined as in section 2.1.2. For a repulsive interaction \((U_0 < 0)\) \(a\) is positive and given by (see Eq. (7), section 2.1.2)

\[ a = d \left[ 1 - \frac{\tanh K_0 d}{K_0 d} \right]. \]  

(37)

In our model, as we tune the two-body interaction we are automatically tuning the scattering length, as is obvious from Eqs. (36) and (37).

As discussed in section 2.1.2, the scattering lengths can be viewed as changing the boundary conditions at \( r = 0 \) of the scattering wave function. This idea is sketched for our model potentials in Figure 35.

![Figure 35: Sketch of scattering wave function and scattering length.](image-url)
2.2.3. **Numerical Details**

1. **Diagonalization Procedure**

   We use a direct diagonalization procedure of the Bogolyubov Hamiltonian, Eq. (27). We construct the Hamiltonian as an $M \times M$ matrix where $M$ is given by Eq. (35). The columns and rows of $H$ are labeled by a corresponding Fock state. Each matrix element in the Hamiltonian is given by

   $$
   \langle n_1 n_2 ... n_N | H | m_1 m_2 ... m_N \rangle
   $$

   for all the Fock states $|n_1 n_2 ... n_N \rangle$ of the system. As before, $N_s$ is the number of available single-particle states. For instance, for $N_s = 3$ we construct the Hamiltonian matrix as depicted in Figure 36.

   ![Figure 36](image)

   **Figure 36**: Example of construction of Hamiltonian matrix for $N_s = 3$. 

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This construction is achieved through the use of multiple loops. Afterwards, we rearrange the matrix so that the diagonal elements go in increasing strength (the same must be done for the corresponding momenta).

There are two terms to evaluate in the diagonalization of the Bogolyubov Hamiltonian (Eq. (27)). The first term, a sum over non-interacting particle energies, is a simple sum which only contributes to the diagonal elements of $H$. Each term in the sum can thus be calculated using a delta function,

$$
\langle n_1 n_2 ... n_{N_s} | e_j \hat{a}_j^\dagger \hat{a}_j | m_1 m_2 ... m_{N_s} \rangle = \epsilon_j \delta_{n_1 n_2 ... n_{N_s}; m_1 m_2 ... m_{N_s}},
$$

where $\epsilon_j = \frac{f^2 \pi^2}{2mL^2}$ is the $j^{th}$ non-interacting energy level, and $n_j$ is the number of particles in this level.

The second term of the Hamiltonian,

$$
\langle n_1 n_2 ... n_{N_s} \left| \frac{1}{2} \sum_{k_1, k_2, k_1', k_2'} \hat{a}_{k_1}^\dagger \hat{a}_{k_2}^\dagger \hat{a}_{k_1'} \hat{a}_{k_2'} \langle k_1 k_2 | \hat{W} | k_1' k_2' \rangle \right| m_1 m_2 ... m_{N_s} \rangle. \tag{38}
$$

is a little more difficult to evaluate. We evaluate it in two separate calculations. First, we evaluate the transition term,

$$
\langle k_1 k_2 | \hat{W} | k_1' k_2' \rangle,
$$

which is given by the integrals in Eq. (34). It is evaluated numerically for all possible $|k_1 k_2>$ and $<k_1 k_2|$ states as given by Eq. (33). This forms an $N_s^2 \times N_s^2$ matrix. It's a very quick calculation. The numerical evaluation is done by substituting $x_1 = x + x_2$ in Eq. (34) and changing the integration limits accordingly. Then Eq. (34) becomes

$$
\int_0^L dx_2 \int_a^{b=\min[L, x_2 + d]} dx \left( \frac{2 \pi}{L} \right)^2 \sin[k_1(x + x_2)] \sin[k_2 x_2] U(x) \sin[k_1'(x + x_2)] \sin[k_2' x_2] dx.
$$
The limits over $dx$, $a = \max[0, x_2 - d]$ and $b = \min[L, x_2 + d]$, depend on $x_2$. Therefore, the integral over $dx$ is a function of $x_2$, which we can write as

$$I(x_2) = \int_a^b \sin[k_1(x + x_2)] \sin[k'_1(x + x_2)] dx.$$ 

Then we can rewrite the transition term as

$$\langle k_1 k_2 | U | k'_1 k'_2 \rangle = -\frac{4U_o}{L^2} \int_0^L \sin(k_2 x_2) \sin(k'_2 x_2) I(x_2) dx_2 = \beta,$$

where $\beta$ is a constant. Equation (39) can then be evaluated using commonly known procedures such as Gaussian quadrature. In fact, all numerical evaluations of integrals in this model are done using Gaussian quadrature. Now, Eq. (38) becomes

$$\frac{\beta}{2} \sum_{k_1, k_2, k'_1, k'_2} \langle n_1 n_2 ... n_N | (\hat{a}_{k_1}^\dagger \hat{a}_{k_2}^\dagger \hat{a}_{k_1'} \hat{a}_{k_2'}) | m_1 m_2 ... m_{N_S} \rangle.$$ 

We evaluate these raising and lowering operators acting on all Fock states $|m_1 m_2 ... m_{N_S}\rangle$, and sum over all single-particle energy levels $k_1, k_2, k'_1,$ and $k'_2$. When doing this we must also keep in mind the momentum conservation criterion exemplified by Eq. (30). Once we obtain the entire Hamiltonian matrix, we find the eigenenergies of the system using a standard Python module that find the eigenvalues of matrices. These energies are matched to their corresponding momentum $k$ and an energy spectrum $E(k)$ is consequently produced. Our Hamiltonian matrix, Figure 36, turns out to be a bent matrix, i.e. most of the non-diagonal elements are zero, this is expected from the fact that the creation and annihilation operators in Eq. (38) do not move more than two particles at a time.

2.2.4. Convergence Tests

In the initial stages of writing the code, we compared calculation times and accuracy for
two procedures for evaluating integrals (rectangular vs Gaussian approximations). We chose to use Gaussian quadrature.

Later on, we performed convergence tests of the energy spectrum with respect to (1) the number of states of the system, (2) the number of total particles in the system, $N_{tots}$, (3) the number of particles allowed to be excited, and (4) the two-body interaction strength (both sign and magnitude). We have not observed the desired energy spectrum, but below we show preliminary results. We are continually debugging and rewriting the code.

2.2.5. Analysis of Results

1. Energy Spectrum

We would like to reproduce the energy spectrum predicted by the Bogolyubov Hamiltonian, which is illustrated in Figure 31. The results shown in this section are preliminary and are shown to illustrate the current status of the project and, perhaps, the direction which it will take. Figure 37 shows the many-body energy density spectrum (energy per particle versus momentum per particle, $k/N_{tot}$) when we tune the diatom interaction to zero, $U_o = 0$ (i.e. an ideal gas).
The spectrum shows the parabolic behavior expected from Eq. (31). The calculation is for \( N_s = 4 \), \( N_{\text{tot}} = 400 \), \( N_{\text{ex}} = 4 \). We can calculate the ground state of the system as the first element of the matrix, 

\[
\begin{pmatrix}
  400 & 0 & 0 \\
  0 & 0 & 0 \\
  0 & 0 & 0 
\end{pmatrix}
\]

\( \pi^2/2L^2 \) = \( \frac{1}{2} \), since we chose \( L = \pi \) and \( m = 1 \), for simplicity. Likewise, ground state momentum is given by \( k = \pi/L = 1 \). So far this energy per particle spectrum seems to give correct results.

For the same parameters, however, when we turn on the diatom interaction, the analysis is not as straight-forward. Figure 38 shows the energy per particle spectrum when the two-body interaction is turned on, \( U_o = 1 \). This represents an attractive interaction. The spectrum now goes into negative energies and the momentum is shifted to slightly greater than 1. In general, we expect the energies to become negative since the contribution from the interaction term in the

Figure 37: Energy spectrum when there is no interaction between the particles (\( U_o = 0 \)).
Hamiltonian will be a negative one for an attractive diatom interaction. The opposite, then, should occur for a repulsive interaction; see Figure 40, for example.

Another test to perform is to check the convergence of the energy per particle spectrum with respect to the total number of particles \( N_{\text{tot}} \). The energy per particle of interacting bosons should have some dependence on the total number of particles, for a fixed trap length. For instance, if the diatom interaction energy is negative, we might expect a decrease (more negative value) in the energy per particle when we increase the total number of particles. On the other hand, we do not expect the energy per particle of a system of non-interacting bosons to be affected by a change in the total number of bosons in the trap. In Figure 39, we plot the energy per particle

**Figure 38:** Energy spectrum when the two-body interaction between the particles is turned on \((U_o = 1)\).
spectra for two values of $N_{tot}$, 400 and 500, with all other parameters being the same ($N_s = 4$, $N_{ex} = 4$ and $U_o = 1$). There, we see that the energy per particle is shifted down when we increase the total number of particles, which seems reasonable in a system of attractively interacting bosons.

![Energy per particle spectra for two values of $N_{tot}$ (400 and 500); all other parameters being equal.](image)

**Figure 39:** Energy per particle spectra for two values of $N_{tot}$ (400 and 500); all other parameters being equal.

However, we still do not see the desired spectrum. One reason could be that some parameters (such as $m$, $L$, $U_o$, etc...) are out of proportion with each other and do not represent physically realistic conditions. Another reason could be the way we incorporate the momentum conservation condition into the code, Eq. (30), is not correct (I have had some issues with this point). Yet another reason could be related to some problem with the code which requires debugging. I believe this last reason is less likely since the other results are generally consistent.
with what we would expect or show good convergence (see Figure 37, Figure 38, Figure 40, and Figure 41), and so the first two seem more likely to be the problem. We still have yet to estimate $k_0$, to compare with our results.

In Figure 40, we see that switching the interaction between repulsive and attractive shifts the energy per particle spectrum either shifted up or down, respectively. The shift up or down from the zero interaction spectrum (Figure 38) is approximately equal in magnitude. The spectra also have similar shapes. This should be expected since the only change in the calculations is by a constant: $U_o \rightarrow -U_o$.

**Figure 40:** Energy spectrum for $U_o = +1$ and $U_o = -1$.

Lastly, we look at the convergence with respect to number of single-particle states, $N_s = 3$ and 4
(Figure 41). The other parameters are \( U_0 = 1 \), \( N_{\text{tot}} = 100 \) and \( N_{ex} = 4 \) These results show good convergence. As we can see from the figure, the lowest part of the spectra match very closely, with the \( N_s = 4 \) spectrum having more and higher energies and momenta.

These preliminary results highlight several obstacles we have to overcome before we obtain the expected energy spectrum. We are looking at the issues raised by these preliminary results and believe that we are not far from obtaining desirable results.

![Figure 41: Energy per particle spectra for two different values of \( N_s \) (3 and 4); all other parameters being equal.](image)

2. Introduction of Additional Parameters

There are some additional parameters we would like to introduce into our model after we observed the desired energy spectrum. We want to introduce parameters that reflect more
realistic experimental conditions. These include a more realistic diatom interaction (and hence a more realistic scattering length), using plane waves for the single-particle eigenstates instead of sine functions, the effects of an external magnetic field, the chemical potential for DFG (see below), a more realistic trap potential (for example, finite, harmonic oscillator trap, etc..), the temperature, time evolution, and increasing the dimensions of the problem. Of course, all this depends on first achieving the desired preliminary results from the simple model we are now using.

2.2.6. DFG Quantum Formalism

For a system of identical fermions interacting through pair forces and where the total number of particles is conserved, the Bogolyubov Hamiltonian is given by [Dav76]

$$H = \sum_s (\epsilon_s - \mu) \hat{\sigma}_s^\dagger \hat{\sigma}_s + \frac{1}{2} \sum_{s, l, p, q} \hat{\sigma}_s^\dagger \hat{\sigma}_l^\dagger \hat{\sigma}_p \hat{\sigma}_q \langle s l | \hat{W} | p q \rangle.$$  \hfill (40)

In Eq. (40), $\mu$ is the chemical potential and $\hat{\sigma}_s^\dagger$ and $\hat{\sigma}_s$ are the creation and annihilation operators for fermions. This Hamiltonian looks similar to that of a system of bosons (Eq. (27)), but the physics of the two systems are fundamentally different due to the fundamental difference between fermions and bosons. For instance, since fermions must obey the Pauli Exclusion principle, number of particles in any state is either 0 or 1. Therefore, once a state is occupied it becomes inaccessible to all other fermions. This Hamiltonian can be used to describe a system of electrons or protons, for instance.
CHAPTER III: CONCLUSION

3.1 Three-Body Problem

We are developing a method to obtain three-body resonances [Kok06]. The method (1) describes the internuclear motion in terms of Smith-Whitten hyperspherical coordinates and (2) employs a novel two-step diagonalization approach to solve the Schrödinger equation of the three-body system. It combines the SVD method of Tolstikhin et al. with a complex absorbing potential. The two-step diagonalization procedure consists of first fixing the hyper-radius and solving the Schrödinger equation in the two-dimensional space of hyperangles. This produces adiabatic curves and adiabatic hyperangular states, which are then used in the second step to solve the one-channel one-dimensional (in hyper-radius) Schrödinger equation. We also applied a mapped Fourier grid and a mapped DVR basis in the hyper-radius.

We applied the method to a model problem of three identical bosons with nucleon mass. This model may be used to study the $^4$He nucleus [Fed03]. This simple model also allowed us to test our approach to obtaining three-body resonances, which opened the door to other applications. The results were compared to those of Fedorov et al. We found evidence for resonances and a bound state by considering hyper-radial and hyperangular wave functions and analyzing the energy versus linewidth plot for the model. We found one three-body bound state at $E_0 = -37.24$ MeV. We found four resonances at $E_1 = -6.58 - 0.0060i$ MeV, $E_2 = -6.07 - 0.038i$ MeV, $E_3 = -5.44 - 0.040i$ MeV, and $E_4 = -5.09 - 0.054i$ MeV. Fedorov et al. found a three-body bound state at $E_0 = -37.22$ MeV, and a resonance at $E_1 = -5.96 - 0.40i$ MeV.

We are also applying the method to find Efimov resonances in a $^4$He-based model. We do this by tuning the diatom interaction $V(r)$, as Esry et al. did, by multiplying it by a constant $\lambda$:
We calculated the first two values of $\lambda$ for which an infinite number of Efimov bound states are predicted to exist, $\lambda_{\text{Efimov1}} = 0.9765$ and $\lambda_{\text{Efimov2}} = 6.834$. These values are similar to those found by Esry et al., $\lambda_{\text{Efimov1}} = 0.9741$ and $\lambda_{\text{Efimov2}} = 6.823$. We were also able to represent hyperangular states with $A_1$ and $A_2$ symmetries, but not states with $E$ symmetry. To reduce calculation times we applied an additional variable-grid mapping in the space of hyperangles.

We obtained results for $\lambda = 2.4$. We looked at hyper-radial and hyperangular wave functions, as well as the linewidth versus energy plot for the system. However, these results did not produce evidence for Efimov resonances. We are currently looking into several options which we believe would be more favorable for the existence of Efimov resonances in our model problem. One option is to look at $\lambda \approx 4$, where we expect that the second adiabatic channel will hold some bound states that will decay into the first channel. Increasing $\lambda$ for $\lambda_{\text{Efimov1}} \leq \lambda \leq \lambda_{\text{Efimov2}}$, however, decreases the two-body scattering length $a$ and any three-body resonances we find are more likely to be regular resonances and not Efimov resonances.

Our current method to find three-body resonances may be modified to study three-body systems of different particles, such as mixtures of fermions and bosons which may be useful in studying three-body recombination in recently achieved triple MOTs; see Ref. [Tag06] for a description of a triple MOT. We may also be able to use this model to study other nuclear systems besides the one studied here. Another future application, which we are closely looking at, is the study of dissociative recombination of $\text{H}_3^+$. $\text{H}_3^+$ is an important molecular ion to the chemistry of interstellar clouds since it initiates a network of chemical reactions that produce many molecules. The dissociative recombination of $\text{H}_3^+$ affects the abundance of $\text{H}_3^+$ in the cloud. $\text{H}_3^+$ also plays significant roles in other astronomical systems and serves as a benchmark molecular ion to quantum chemists.
3.2 BEC

We are conducting an ongoing investigation of small excitations of a system of \(N_{\text{tot}}\) identical bosons that interact through a pairwise interaction. This model can be used to carry out simulations of small excitations in superfluids and BECs. We begin by looking at the Bogolyubov Hamiltonian, which describes the small excitations of such a system. Our current model consists of three and four level single-particle systems. We control the number of particles which can be excited so as to reduce computation time. This restriction also makes for a more physically accurate description. Our model has not yet reproduced the expected energy spectrum. We have identified several possible reasons why this is the case. For example, it could be that the parameters we are using (trap size, interaction strength and range, etc...) are unphysically out of proportion with each other.

After overcoming these obstacles and obtaining reliable results for our simple model, we would like to include a more realistic interaction potential and generalize to more dimensions. This is with the aim of having a model that more closely resembles experimental conditions. Some of these parameters could include: a more realistic diatom interaction, an external magnetic field, the chemical potential for DFG, and a more realistic trap potential. We will probably transfer the problem to Fortran code before we move it forward. Perhaps we will then be able to use parallel computations with supercomputers to carry out large computations.

After we obtain the corresponding energy spectrum we would like to move on to model degenerate Fermi gases. There, we would have to include the chemical potential (a standard procedure) along with other new parameters to account for the fundamental difference in the physics of bosons and fermions.
APPENDIX A ON PYTHON LANGUAGE
Python is an object-oriented programming language. It has been very useful as an introduction to programming to solve physical problems. However, it has several limitations (some of which are listed here), but also several advantages. Up until now we have used Python to carry out calculations of the many-body problem, but perhaps in the near future we will switch most of the programming to Fortran. Python can be downloaded from  http://www.python.org/. For a written tutorial by the creator of Python, visit  www.python.org/doc/current. The numerical and scientific packages are documented at  http://www.numpy.org/ and  http://www.scipy.org/, respectively. There are some advantages and disadvantages to using python programming language for the many-body part of the thesis. Here we briefly discuss highlight some aspects of the Python language.

Features of Python:

- No declaration of variable types
- Only defined operations allowed
- No separate compilation process
- Errors caught at runtime
- Object-oriented programming
- Procedural programming
- Functional programming
- Runs on Unix/Linux, Windows, Mac and Sun
- Rich set of modules in standard library (i.e. Gaussian quadrature, ODE modules)
- Can import both pure Python code and “extension modules” written in compiled languages; hence, large set of third-party libraries available: numerics, graphics/visualizations, databases, web servers
Pros:

- Very expressive, easy to learn and get things done
- Makes good introduction to programming to solve physical problems
- Wide variety of third-party modules
- Tools for wrapping C++/C, Fortran
- Large, enthusiastic, and diverse community of developers
- Innumerable *free* sources of help available
- Can be easily adapted to formulate and solve physical problems
- User-friendly, easy to do quick programming
- Monetarily, intellectually and legally free
- Can be used with most operating systems

Cons:

- Not a single unified package (like Matlab or Maple)
- Can be significantly slower than compiled code
- Not many options to modify and play around with plots
- May not lend itself to some long, sophisticated calculations when working with physical problems as other languages do, like Fortran, for example.

You may start an interactive Python session using one of:

- **Idle** - Windows or Unix
- **Pythonwin** - Windows
Python IDE - MacPython under MacOS X

Sources: [Mye04], and ©M.D. Johnson, September 26, 2002; Revised August 19, 2003
Atomic units are used throughout most of the thesis since they have proved to be the most convenient. This is the reason why, for example, we did not explicitly write $\hbar$ in most equations throughout most of the thesis. Here we give a brief reminder of atomic units and relevant conversion factors for this thesis. For instance, in atomic units (au), the unit of angular momentum is $1.055 \times 10^{-34}$ J s in SI units, i.e. $\hbar=1$. The unit for mass is the electron mass $m_e$, while the unit for length is the Bohr radius $a_o$, etc...

Conversion to units used in the thesis:

1 au unit of angular momentum,

$\hbar=1.054572 \times 10^{-34}$ J s.

1 au of energy (Hartree),

$1 \text{Eh} = 3.1577465 \times 10^5 K$,

$1 \text{Eh} = 27.2113845 \text{eV}$.

1 au of length (Bohr radius),

$a_o=0.5291772108 \, \text{Å}$.

1 au of mass (electron mass),

$m_e=9.1093826 \times 10^{-31} \text{Kg}$.

LIST OF REFERENCES


