Efimov

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Contents

1 Background

1.1 The Three-body Problem

The n-body problem is a class of problems in physics which, in a highly general sense, consists of modelling the motion of n objects, interacting through some physical force. In classical mechanics the equations of motion for n point particles can be derived from Newton's second law of motion, which states that the rate of change in momentum for an object equals the force acting on it, or from analytical formulations such as Lagrangian and Hamiltonian mechanics, which consider scalar properties of motion like kinetic and potential energies. In the quantum regime, where the wave-like property of matter has to be taken into account, the state of an n-body system of is described by a total wave function, where the Hamiltonian operator generates the time evolution of the state as given by Schrödinger's differential equation.

The core of the n-body problem is that the classical equations of motion and the Schrödinger equation are not analytically solvable for more than two interacting particles. Consider the case where $n = 3$. Albeit apparently simple, the configuration space for the three-body problem is six dimensional after separating out the center of mass motion. Three additional constants of motion can be provided by conservation of total angular momentum, which effectively reduces the problem to that of three coupled second order non-linear differential equations in the classical case and a three dimensional Schrödinger equation for the quantum problem. The quest for a general solution to the classical three-body problem is renowned. As a recurrent muse to a number of great mathematicians during the past centuries, dating back to Newton himself, the three-body problem has been a catalysator for the development of analysis and the modern theory of dynamical systems [**Chenciner2015**]. Although there are a number of special cases that have explicit solutions, nonlinear dynamical systems often display highly unpredictable behavoir due to sensitive dependence on initial conditions, i.e. they are chaotic. Different numerical approaches are used to solve this kind of problems nowadays but the computational load can be substantial. However, the quantum three-body problem is amenable to an analytic solution.

Within the quantum realm of few-body systems the Faddeev and the Faddeev-Yakubovsky equations, which are equivalent formulations of the Schrödinger equation for three- and four-body systems repectively, can be solved analytically by iteration for a few special cases [**Faddeev:1960su**, **Zubarev:1994**]. For the three-body scattering problem, bound state solutions can exist in cases where all three two-body subsystems have short-ranged interactions, if at least two of these interactions are close to resonance. This is called the Efimov effect.

1.2 The Birth of Efimov Physics

In 1970, Vitaly Efimov predicted that resonant two-body forces could give rise to a series of bound energy levels in three-particle systems [**Efimov:1970zz**]. When the short-ranged two-body forces approached resonance, he found a universal long-range three-body attraction emerging, giving rise to an infinite number of trimer states with binding energies obeying a discrete scaling law at resonance.

Efimov proposed that attractive three-body interaction appearing in systems with resonant short-ranged interactions and repulsive Coulomb forces could explain the binding of three particle nuclei such as the three nucleon triton ^{3}H and the triple-alpha Hoyl state of ^{12}C.

The notion of Efimov physics comprise a range of universal phenomena that occurs in few-body systems exibiting the Efimov effect. Short-ranged forces are commonly occuring in nature and few-body effects are expected to appear in a broad range of physical sytems. Developments in the theory of few-body quantum systems is important since it would bridge existing well developed models of treating one- and two-body sytems with the statistical methods used to describe many-body systems, and it may give insight...

2 Introduction

2.1 Three-body Theory

A short reveiw concerning some important aspects of quantum mechanical systems and two-body scattering will follow in order to set the stage for a discussion of quantum effects in few-body systems in general and Efimov states in three-body systems in particular.

Entering the quantum regime All particles of matter exhibit wave-like properties. The wave length of a particle with momentum p is given by the de Broglie equation

$$\lambda = \frac{h}{p} = \frac{h}{mv} \tag{1}$$

where h is the Planck constant. The wave characteristics of matter grows with increasing de Broglie wave length. When the wave length is sufficently large, classical physics no longer applies and the system has reached the quantum regime. From (10) it is evident that this is true for particles that are either very small or very slow.

Scattering theory In the low energy limit two In the ultracold regime, the behavoir of atoms are governed by quantum mechanics.

2.1.1 Two-body interactions

When atoms are cooled down to a point where the uncertainty In an ultracold quantum gas atoms move so slowly that the uncertainty in position becomes so large overlap behave as matter waves and quantum mechanics governs their behavoir

vad r spridningslngd: Consider a system consisting of a few particles such as dilute gas At sufficently low energies In low energy scattering processes where the particle wave length is larger than

The scattering length a is defined as

$$\lim_{k\to 0} k \cot \delta(k) = -\frac{1}{a} \tag{2}$$

2.2 Experimental Evidence

2.2.1 Efimov Trimers in Atomic Systems

Ultracold atomic clouds provided the first staging ground for exploring Efimov physics and related few-body phenomena because of the ability to control atom-atom interactions by an external field. In experiments with trapped ultracold atomic and molecular gases of alkali atoms with tunable two-body interactions, the existance of Efimov trimers have been inferred from resonantly enhanced loss rates

^{133}Cs 1) Efimov states have been observed in ultracold atomic and molecular gases of cesiumatoms

2) in three-component Fermi gases of6Li

3) Bose gas of39K atoms

4) mixturesof41K and87Rb atoms

5) In all these experiments, Efimovstates manifest themselves as resonantly enhanced losses,ei-ther in atomic three-body recombination or in atom-dimer re-laxation processes.

Indirect signatures:

The first observations of an Efimov state was reported in 2006 by the Innsbruck-group of Grimm and coworkers, [**Grimm:2006**]. In experiments with ultracold gases of caesium atoms, with magnetically tunable two-body interactions, they found the first signatures of the exotic three-body state consisting of three-body recombination resonances emerging when an Efi- mov state couples to the triatomic threshold at distinct negative s-wave scattering lengths a.

Direct approach: a prime candidate to study Efimov physics the ground state of the helium trimer is not an Efimov state Coulomb explosion imaging Helium [**Kunitski:2015qth**]

2.2.2 Four-body Recombination connected to Efimov Trimers

6) four-body recombination in the particu-lar region of interest near a triatomic Efimov resonance [**Grimm:2009**].

"Our resultsobtained with an ultracold sample of cesium atoms at negative scattering lengths show a resonant enhancementof losses and provide strong evidence for the existence of a pair of four-body states, which is strictly con-nectedto Efimov trimers via universal relations. Our findings confirm recent theoretical predictions and demonstratethe enrichment of the Efimov scenario when a fourth particle is added to the generic three-body problem "

2.2.3 Efimov States in Nuclei

2.3 Normalized Center-of-Mass Coordinates

The spatial position of three particles are fixed by nine coordinates x^i_α, where $i(=1,2,3)$, and $\alpha(=1,2,3)$ labels the particles, and their Cartesian space coordinates, respectively. Let $\mathbf{x}^i$ and m_i be the position vector and mass of the ith particle. If the total mass M, the three particle reduced mass μ_3, and the normalizing constants d_k $(k = 1, 2, 3)$ are defined as

$$M = \sum_{i=1}^{3} m_i, \tag{3}$$

$$\mu_3^2 = \prod_{i=1}^{3} m_i/M, \tag{4}$$

$$d_k^2 = \frac{m_k}{\mu_3}\frac{(m_i + m_j)}{M}, \tag{5}$$

then the set of mass normalized Jacobi coordinates are defined by

$$\mathbf{r}^k = d_k^{-1}(\mathbf{x}^j - \mathbf{x}^i), \tag{6}$$

$$\mathbf{R}^k = d_k\Big[\mathbf{x}^k - \frac{(m_i\mathbf{x}^i + m_i\mathbf{x}^j)}{m_i + m_j}\Big], \tag{7}$$

$$\mathbf{X} = \frac{1}{M}\sum_{i=1}^{3} m_i\mathbf{x}^i, \tag{8}$$

where, the indices i, j, k are cyclic permutations of $(1, 2, 3)$. The kinetic energy for three particles is given by

$$T = -\frac{\hbar^2}{2}\sum_{i=1}^{3} m_i^{-1}\nabla^2_{\mathbf{x}^i} \tag{9}$$

2.4 The Hyperspherical Method

The theoretical framework to describe systems of three particles

2.5 Coordinate Transformations

2.5.1 Delves Coordinates

Blabla labframe coordinates

Jacobi vectors:

$$\vec{x} = \vec{r}_2 - \vec{r}_1 \tag{10a}$$

$$\vec{y} = \vec{r}_3 - \frac{1}{2}(\vec{r}_1 + \vec{r}_2) \tag{10b}$$

$$\vec{X}_{cm} = \frac{1}{3}(\vec{r}_1 + \vec{r}_2 + \vec{r}_3) \tag{10c}$$

Exchange of particles

$$\hat{P}_{13} = \begin{cases} \vec{x}\,' = \vec{r}_2 - \vec{r}_3 & = \frac{1}{2}\vec{x} - \vec{y} \\ \vec{y}\,' = \vec{r}_1 - \frac{1}{2}(\vec{r}_3 + \vec{r}_2) & = -\frac{1}{2}(\frac{3}{2}\vec{x} + \vec{y}) \end{cases} \tag{11}$$

$$\hat{P}_{23} = \begin{cases} \vec{x}\,'' = \vec{r}_3 - \vec{r}_1 & = \frac{1}{2}\vec{x} + \vec{y} \\ \vec{y}\,'' = \vec{r}_2 - \frac{1}{2}(\vec{r}_1 + \vec{r}_3) & = -\frac{1}{2}(\frac{3}{2}\vec{x} - \vec{y}) \end{cases} \tag{12}$$

Introducing hyperspherical coordinates:

$$x = \sqrt{2}\rho\sin(\alpha) \tag{13a}$$

$$y = \sqrt{\frac{3}{2}}\rho\cos(\alpha) \tag{13b}$$

$$\tag{13c}$$

Hyperspherical coordinates:

$$\begin{aligned} \rho &= \Big(\frac{1}{2}x^2 + \frac{2}{3}y^2\Big)^{1/2} &&, 0 \leq \rho < \infty \\ \tan\alpha &= \frac{\sqrt{3}}{2}\frac{x}{y} &&, 0 \leq \alpha < \tfrac{\pi}{2} \\ \cos\theta &= \frac{\vec{x}\cdot\vec{y}}{xy} &&, 0 \leq \theta < \pi \end{aligned}$$

Jacobi vectors:

$$x' = \Big(\frac{1}{4}x^2 + y^2 - \vec{x}\cdot\vec{y}\Big)^{1/2} = \frac{\rho}{\sqrt{2}}\big(\sin^2(\alpha) + 3\cos^2(\alpha) - \sqrt{3}\sin(2\alpha)\cos\theta\big)^{1/2} \tag{14a}$$

$$x'' = \Big(\frac{1}{4}x^2 + y^2 + \vec{x}\cdot\vec{y}\Big)^{1/2} = \frac{\rho}{\sqrt{2}}\big(\sin^2(\alpha) + 3\cos^2(\alpha) + \sqrt{3}\sin(2\alpha)\cos\theta\big)^{1/2} \tag{14b}$$

Volume element from the transformation is $dr_1 dr_2 dr_3 = 3/2 dx dy dX_{cm}$.

(The massweighted Schrödinger equation of a N-body system with position vectors $\mathbf{r}_k$ and masses m_k, $(k = 1, ..., N)$, is given by)

$$\Big(-\frac{\hbar^2}{2}\sum_{k=1}^{N} m_k^{-1}\nabla^2_{\mathbf{r}_k}\Psi + V\Psi = E\Psi\Big) \tag{15}$$

where the Laplacian is

$$\nabla^2 = \Big(\frac{1}{r^2}\partial_r\big(r^2\partial_r\big) - \frac{1}{\sin(\theta)}\partial_\theta\big(\sin(\theta)\partial_\theta\big) + \frac{1}{\sin^2\theta}\partial_\phi^2\Big) = \Big(\frac{1}{r^2}\partial_r\big(r^2\partial_r\big) + \frac{L^2}{\hbar^2}\Big) \tag{16}$$

The kinetic energy for three particles with identical masses is given by

$$\hat{T} = -\frac{\hbar^2}{2m}(\nabla_{r_1}^2 + \nabla_{r_2}^2 + \nabla_{r_3}^2) \tag{17}$$

in hyperspherical coordinates this becomes

$$\hat{T} = -\frac{\hbar^2}{2m}(2\nabla_x^2 + \frac{3}{2}\nabla_y^2 + \frac{1}{3}\nabla_{X_{cm}}^2), \tag{18}$$

where

$$\nabla_x^2 = \frac{1}{x^2}\frac{\partial}{\partial x}\Big(x^2\frac{\partial}{\partial x}\Big) - \frac{\hat{l}_x^2}{x^2} = \frac{2}{x}\frac{\partial}{\partial x} + \frac{\partial^2}{\partial x^2} - \frac{\hat{l}_x^2}{x^2} \tag{19a}$$

$$\nabla_y^2 = \frac{1}{y^2}\frac{\partial}{\partial y}\Big(y^2\frac{\partial}{\partial y}\Big) - \frac{\hat{l}_y^2}{y^2} = \frac{2}{y}\frac{\partial}{\partial y} + \frac{\partial^2}{\partial y^2} - \frac{\hat{l}_y^2}{y^2} \tag{19b}$$

If spin interactions are excluded the total orbital angular momentum is zero and we have

$$\hat{l}_x^2 = \hat{l}_y^2 = -\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\Big(\sin(\theta)\frac{\partial}{\partial\theta}\Big) \tag{20a}$$

$$\begin{aligned}
\frac{\partial\alpha}{\partial x} &= \frac{1}{\sqrt{2}\rho}\cos(\alpha), \quad & \frac{\partial\rho}{\partial x} &= \frac{1}{\sqrt{2}}\sin(\alpha)\\
\frac{\partial\alpha}{\partial y} &= -\frac{\sqrt{6}}{3\rho}\sin(\alpha), \quad & \frac{\partial\rho}{\partial y} &= \sqrt{\frac{2}{3}}\cos(\alpha)
\end{aligned}$$

$$\begin{aligned}
\frac{\partial}{\partial x} &= \frac{\partial\alpha}{\partial x}\frac{\partial}{\partial\alpha} + \frac{\partial\rho}{\partial x}\frac{\partial}{\partial\rho}\\
\frac{\partial^2}{\partial x^2} &= \frac{1}{2}\Big(\frac{1}{\rho}\cos(\alpha)\frac{\partial}{\partial\alpha} + \sin(\alpha)\frac{\partial}{\partial\rho}\Big)\Big(\frac{1}{\rho}\cos(\alpha)\frac{\partial}{\partial\alpha} + \sin(\alpha)\frac{\partial}{\partial\rho}\Big)\\
&= \frac{1}{2}\Big[\frac{1}{\rho^2}\cos(\alpha)\frac{\partial}{\partial\alpha}\Big(\cos(\alpha)\frac{\partial}{\partial\alpha}\Big) + \frac{1}{\rho}\cos(\alpha)\frac{\partial}{\partial\alpha}\Big(\sin(\alpha)\frac{\partial}{\partial\rho}\Big) + \sin(\alpha)\frac{\partial}{\partial\rho}\Big(\frac{1}{\rho}\cos(\alpha)\frac{\partial}{\partial\alpha} + \sin(\alpha)\frac{\partial}{\partial\rho}\Big)\Big]\\
&= \frac{1}{2}\Big[-\frac{2}{\rho^2}\cos(\alpha)\sin(\alpha)\frac{\partial}{\partial\alpha} + \frac{1}{\rho^2}\cos^2(\alpha)\frac{\partial^2}{\partial\alpha^2} + \frac{1}{\rho}\cos^2(\alpha)\frac{\partial}{\partial\rho} + \frac{2}{\rho}\cos(\alpha)\sin(\alpha)\frac{\partial^2}{\partial\alpha\partial\rho} + \sin^2(\alpha)\frac{\partial^2}{\partial\rho^2}\Big]\\
&= \frac{1}{2}\Big[\frac{1}{\rho^2}\cos^2(\alpha)\frac{\partial^2}{\partial\alpha^2} - \frac{1}{\rho^2}\sin(2\alpha)\frac{\partial}{\partial\alpha} + \sin^2(\alpha)\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\cos^2(\alpha)\frac{\partial}{\partial\rho} + \frac{1}{\rho}\sin(2\alpha)\frac{\partial^2}{\partial\alpha\partial\rho}\Big]
\end{aligned}$$

$$
\begin{aligned}
\frac{\partial}{\partial y} &= \frac{\partial \alpha}{\partial y}\frac{\partial}{\partial \alpha} + \frac{\partial \rho}{\partial y}\frac{\partial}{\partial \rho} \\
\frac{\partial^2}{\partial y^2} &= \Big(-\frac{\sqrt{6}}{3\rho}\sin(\alpha)\frac{\partial}{\partial \alpha} + \sqrt{\frac{2}{3}}\cos(\alpha)\frac{\partial}{\partial \rho}\Big)\Big(-\frac{\sqrt{6}}{3}\sin(\alpha)\frac{\partial}{\partial \alpha} + \sqrt{\frac{2}{3}}\cos(\alpha)\frac{\partial}{\partial \rho}\Big) \\
&= \frac{2}{3}\Big[\frac{1}{\rho^2}\sin(\alpha)\frac{\partial}{\partial \alpha}\Big(\sin(\alpha)\frac{\partial}{\partial \alpha}\Big) - \frac{1}{\rho}\sin(\alpha)\frac{\partial}{\partial \alpha}\Big(\cos(\alpha)\frac{\partial}{\partial \rho}\Big) - \cos(\alpha)\frac{\partial}{\partial \rho}\Big(\frac{1}{\rho}\sin(\alpha)\frac{\partial}{\partial \alpha}\Big) + \cos^2(\alpha)\frac{\partial^2}{\partial \rho^2}\Big] \\
&= \frac{2}{3}\Big[\frac{2}{\rho^2}\sin(\alpha)\cos(\alpha)\frac{\partial}{\partial \alpha} + \frac{1}{\rho^2}\sin^2(\alpha)\frac{\partial^2}{\partial \alpha^2} + \frac{1}{\rho}\sin^2(\alpha)\frac{\partial}{\partial \rho} - \frac{2}{\rho}\sin(\alpha)\cos(\alpha)\frac{\partial^2}{\partial \alpha \partial \rho} + \cos^2(\alpha)\frac{\partial^2}{\partial \rho^2}\Big] \\
&= \frac{2}{3}\Big[\frac{1}{\rho^2}\sin^2(\alpha)\frac{\partial^2}{\partial \alpha^2} + \frac{1}{\rho^2}\sin(2\alpha)\frac{\partial}{\partial \alpha} + \cos^2(\alpha)\frac{\partial^2}{\rho^2} - \frac{1}{\rho}\sin(2\alpha)\frac{\partial^2}{\partial \alpha \partial \rho}\Big]
\end{aligned}
$$

$$
\begin{aligned}
2\nabla_x^2 + \frac{3}{2}\nabla_y^2 &= \frac{4}{x}\frac{\partial}{\partial x} + \frac{3}{y}\frac{\partial}{\partial y} + 2\frac{\partial^2}{\partial x^2} + \frac{3}{2}\frac{\partial^2}{\partial y^2} - 2\frac{\hat{l}_x^2}{x^2} - \frac{3}{2}\frac{\hat{l}_y^2}{y^2} \\
&= \frac{4}{\rho^2}\cot(2\alpha)\frac{\partial}{\partial \alpha} + \frac{5}{\rho}\frac{\partial}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial \alpha^2} + \frac{\partial^2}{\partial \rho^2} + \frac{4}{\rho^2\sin^2(2\alpha)\sin(\theta)}\frac{\partial}{\partial \theta}\Big(\sin(\theta)\frac{\partial}{\partial \theta}\Big) \\
&= \frac{1}{\rho^5}\frac{\partial}{\partial \rho}\Big(\rho^5\frac{\partial}{\partial \rho}\Big) + \frac{1}{\rho^2\sin^2(2\alpha)}\Big(\frac{\partial}{\partial \alpha}\sin^2(2\alpha)\frac{\partial}{\partial \alpha} + \frac{4}{\sin(\theta)}\frac{\partial}{\partial \theta}\Big)
\end{aligned}
$$

The kinetic energy operators expressed in Delves hypershericical coordinates is thus

$$
\hat{T} = \hat{T}_\rho + \hat{T}_\alpha + \hat{T}_\theta \qquad (25)
$$

where

$$\begin{aligned}
\hat{T}_\rho &= -\frac{\hbar^2}{2m}\Big[\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\Big(\rho^5\frac{\partial}{\partial\rho}\Big)\Big] \\
&= -\frac{\hbar^2}{2m}\Big[\rho^{-5/2}\Big(\rho^{5/2}\frac{5}{\rho}\frac{\partial}{\partial\rho} + \rho^{5/2}\frac{\partial^2}{\partial\rho^2}\Big)\rho^{-5/2}\rho^{5/2}\Big] \\
&= -\frac{\hbar^2}{2m}\rho^{-5/2}\Big[-\frac{15}{4}\frac{1}{\rho^2} + \frac{\partial^2}{\partial\rho^2}\Big]\rho^{5/2}
\end{aligned}$$

$$\begin{aligned}
\hat{T}_\alpha &= -\frac{\hbar^2}{2m}\frac{1}{\rho^2\sin^2(2\alpha)}\Big[\frac{\partial}{\partial\alpha}\sin^2(2\alpha)\frac{\partial}{\partial\alpha}\Big] \\
&= -\frac{\hbar^2}{2m}\frac{1}{\rho^2}\Big[\frac{\partial^2}{\partial\alpha^2} + 4\cot(2\alpha)\frac{\partial}{\partial\alpha}\Big] \\
&= -\frac{\hbar^2}{2m}\frac{1}{\rho^2}\Big[\sin^{-1}(2\alpha)\Big(\sin(2\alpha)\frac{\partial^2}{\partial\alpha^2} + 4\cos(2\alpha)\frac{\partial}{\partial\alpha}\Big)\sin^{-1}(2\alpha)\sin(2\alpha)\Big] \\
&= -\frac{\hbar^2}{2m}\frac{1}{\rho^2}\sin^{-1}(2\alpha)\Big[\frac{\partial^2}{\partial\alpha^2} + 4\Big]\sin(2\alpha) \\
&= -\frac{\hbar^2}{2m}\frac{1}{\rho^2}(\sin(\alpha)\cos(\alpha))^{-1}\Big[\frac{\partial^2}{\partial\alpha^2} + 4\Big]\sin(\alpha)\cos(\alpha)
\end{aligned}$$

$$\begin{aligned}
\hat{T}_\theta &= -\frac{\hbar^2}{2m}\Big[\frac{4}{\rho^2\sin^2(2\alpha)\sin(\theta)}\frac{\partial}{\partial\theta}\Big(\sin(\theta)\frac{\partial}{\partial\theta}\Big)\Big] \\
&= -\frac{\hbar^2}{2m}\Big[\frac{1}{\rho^2\sin^2(\alpha)\cos^2(\alpha)\sin(\theta)}\frac{\partial}{\partial\theta}\Big(\sin(\theta)\frac{\partial}{\partial\theta}\Big)\Big]
\end{aligned}$$

And we get the Hamiltonian

$$H_0 = \hat{T}_\rho + \hat{T}_\alpha + \hat{T}_\theta + V(\rho,\alpha,\theta) \tag{27}$$

From now on $\hbar = 1$. To remove first derivatives with respect to ρ and α we make the following transformation $\Psi = \rho^{-5/2}(\sin(\alpha)\cos(\alpha))^{-1}\psi$. This corresponds to the following transformation of the Hamiltonian

$$\begin{aligned}
H &= \rho^{5/2}\sin(\alpha)\cos(\alpha)H_0\rho^{-5/2}(\sin(\alpha)\cos(\alpha))^{-1} \\
&= -\frac{1}{2m}\Big[\frac{\partial^2}{\partial\rho^2} - \frac{15}{4\rho^2} + \frac{1}{\rho^2}\Big(\frac{\partial^2}{\partial\alpha^2} + 4 + \frac{1}{\sin^2(\alpha)\cos^2(\alpha)\sin(\theta)}\frac{\partial}{\partial\theta}\Big(\sin(\theta)\frac{\partial}{\partial\theta}\Big)\Big)\Big] \\
&= -\frac{1}{2m}\Big[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho^2}\Big(\frac{\partial^2}{\partial\alpha^2} + \frac{1}{\sin^2(\alpha)\cos^2(\alpha)\sin(\theta)}\frac{\partial}{\partial\theta}\Big(\sin(\theta)\frac{\partial}{\partial\theta}\Big)\Big) + \frac{1}{4\rho^2}\Big] \\
&= -\frac{1}{2m}\frac{\partial^2}{\partial\rho^2} + \frac{\Lambda^2 - 1/4}{2m\rho^2}
\end{aligned}$$

Where the Grand angular momentum operator is

$$\Lambda^2 = -\frac{\partial^2}{\partial\alpha^2} - \frac{1}{\sin^2(\alpha)\cos^2(\alpha)\sin(\theta)}\frac{\partial}{\partial\theta}\Big(\sin(\theta)\frac{\partial}{\partial\theta}\Big) \tag{29}$$

The volume element is proportional to $\rho^5 \sin^2(\alpha)\cos^2(\alpha)\sin(\theta)d\rho d\alpha d\theta$. Boundary conditions: The wavefunction needs to be square-integrable, so $\Psi = 0$ at $\rho = 0$ and $\alpha = 0$ or π. Further,

$$\begin{aligned}
&\psi(0,\alpha,\theta) = 0\\
&\psi(\rho,0,\theta) = \psi(\rho,\frac{\pi}{2},\theta) = 0\\
&\frac{\partial\psi}{\partial\theta}\Big|_{\theta=0} = \frac{\partial\psi}{\partial\theta}\Big|_{\theta=\pi} = 0
\end{aligned}$$

2.5.2 Modified Smith-Whitten Coordinates

In this section, we show how the three-body system can be represented in a symmetric way. The derivation of the Hamiltonian for this representation is described using a modified set of Smith-Whitten (democratic) coordinates.

For a system of three particles, let $\mathbf{r}^i$ and m_i be the position vector and mass of the ith particle. The set of Jacobi coordinates for the system is given by

$$\mathbf{x}^k = \mathbf{r}_0^j - \mathbf{r}_0^i, \tag{31a}$$

$$\vec{y}_k = \vec{r}_k - \frac{1}{2}(\vec{r}_i + \vec{r}_j), \tag{31b}$$

$$\vec{X}_{cm} = \frac{1}{3}\sum_{i=1}^{3}\vec{r}_i. \tag{31c}$$

The center of mass coordinate separates from the equations of motion and we will not consider it further. We can define a new set of mass normalized Jacobi coordinates. If the total mass M, the three particle reduced mass μ_3, and the normalizing constants $d_k (k = 1,2,3)$ are defined as

$$M = \sum_{i=1}^{3} m_i, \tag{32}$$

$$\mu_3^2 = \prod_{i=1}^{3} m_i/M, \tag{33}$$

$$d_k^2 = \frac{m_k}{\mu_3}\frac{(m_i + m_j)}{M}. \tag{34}$$

The set of mass normalized Jacobi coordinates are defined by

$$
\begin{aligned}
\mathbf{r}_k &= d_k^{-1}\mathbf{x}_k, && (35)\\
\mathbf{R}_k &= d_k\mathbf{y}_k. && (36)
\end{aligned}
$$

The masses of the particles define angles that are useful to describe permutations of the system. If we consider an even permutation (ijk) of the set (123), then the obtuse angle β_{ij} has the properties

$$
\begin{aligned}
&\beta_{ij} = -\beta_{ji}, \quad \beta_{ii} = 0, && (37a)\\
&\tan\beta_{ij} = -m_k/\mu, && (37b)\\
&d_i d_j \sin\beta_{ij} = 1, && (37c)\\
&d_i d_j m_k \cos\beta_{ij} = -\mu, && (37d)\\
&\beta_{12} + \beta_{23} + \beta_{31} = 2\pi && (37e)
\end{aligned}
$$

Orthogonal transformations within the coordinate set are then given by

$$
\begin{pmatrix} \mathbf{r}_j \\ \mathbf{R}_j \end{pmatrix} = \begin{pmatrix} \cos\beta_{ij} & \sin\beta_{ij} \\ -\sin\beta_{ij} & \cos\beta_{ij} \end{pmatrix} \begin{pmatrix} \mathbf{r}_i \\ \mathbf{R}_i \end{pmatrix} \tag{38}
$$

From hereon we choose one set to work in and suppress all vector indices. In six dimensional space, the components of the two vectors $\mathbf{r}$ and $\mathbf{R}$ can be regarded as the Cartesian components of a point that space. The kinetic energy is then given by

$$
\hat{T} = -\frac{1}{2m}\Big(\Delta_{\mathbf{r}} + \Delta_{\mathbf{R}}\Big). \tag{39}
$$

At any instant, three particles form a plane in $\mathbb{R}^3$. If we consider this plane to be the x-y plane, and define the internal motion of the particles within this plane in terms of hyperspherical coordinates, our coordinate system must rotate in this plane. That is, we use a body-fixed coordinate system XYZ, which rotates with respect to the space fixed axis $X'Y'Z'$. [Details](spatial rotation). The internal coordinates ρ, Θ, and Φ determine the size and shape of the triangle formed by the three particle system. With the z-axis perpendicular to the plane, Smith and Whitten [ref] defined these as

$$
\begin{aligned}
r_x &= \rho\cos(\Theta)\cos(\Phi),\\
r_y &= -\rho\sin(\Theta)\sin(\Phi),\\
r_z &= 0\\
R_x &= \rho\cos(\Theta)\sin(\Phi),\\
R_y &= \rho\sin(\Theta)\cos(\Phi),\\
R_z &= 0.
\end{aligned}
$$

The distance between the particles are given by

$$x_3 = d_3 \mid \mathbf{r}_3 \mid = \frac{\rho d_3}{2^{1/2}}\big[1+\cos(2\Theta)\cos(2\Phi_3)\big]^{1/2} \tag{41}$$

$$\begin{aligned} x_1 = d_1 \mid \mathbf{r}_1 \mid &= d_1\big[\cos^2\beta_{31}\mathbf{r}_3^2 + \sin^2\beta_{31}\mathbf{R}_3^2 + 2\sin\beta_{31}\cos\beta_{31}\mathbf{r}_3\cdot\mathbf{R}_3\big]^{1/2} \qquad (42)\\ &= \frac{d_1\rho}{2^{1/2}}\big[\cos^2\beta_{31}(1+\cos(2\Theta)\cos(2\Phi_3))\\ &+ \sin^2\beta_{31}(1-\cos(2\Theta)\cos(2\Phi_3))\\ &+ 2\sin\beta_{31}\cos\beta_{31}\cos(2\Theta)\sin(2\Phi_3)\big]^{1/2}\\ &= \frac{d_1\rho}{2^{1/2}}\big[1+\cos(2\Theta)\big(\cos(\Phi_3)\cos(2\beta_{31})+\sin(2\Phi_3)\sin(2\beta_{31})\big)\big]^{1/2}\\ &= \frac{d_1\rho}{2^{1/2}}\big[1+\cos(2\Theta)\cos(2\Phi_3-2\beta_{31})\big]^{1/2}\\ &= \frac{d_1\rho}{2^{1/2}}\big[1+\cos(2\Theta)\cos(2\Phi_1)\big]^{1/2}\\ x_2 = d_2 \mid \mathbf{r}_2 \mid &= d_2\big[\cos^2\beta_{23}\mathbf{r}_3^2 + \sin^2\beta_{23}\mathbf{R}_3^2 - 2\sin\beta_{23}\cos\beta_{23}\mathbf{r}_3\cdot\mathbf{R}_3\big]^{1/2}\\ &= \frac{d_2\rho}{2^{1/2}}\big[1+\cos(2\Theta)\big(\cos(\Phi_3)\cos(2\beta_{23})-\sin(2\Phi_3)\sin(2\beta_{23})\big)\big]^{1/2}\\ &= \frac{d_1\rho}{2^{1/2}}\big[1+\cos(2\Theta)\cos(2\Phi_3+2\beta_{23})\big]^{1/2}\\ &= \frac{d_1\rho}{2^{1/2}}\big[1+\cos(2\Theta)\cos(2\Phi_2)\big]^{1/2} \end{aligned}$$

Thus, $\Phi_j = \Phi_i - \beta_{ij}$ and

$$x_k = \frac{d_k\rho}{2^{1/2}}\big[1+\cos(2\Theta)\cos(2\Phi_k)\big]^{1/2}. \tag{43}$$

Now we choose $\Phi_3 = \Phi$

$$x_3 = \frac{\rho d_3}{2^{1/2}}\big[1+\cos(2\Theta)\cos(2\Phi)\big]^{1/2} \tag{44}$$

$$x_1 = \frac{d_1\rho}{2^{1/2}}\big[1+\cos(2\Theta)\cos(2\Phi+\epsilon_1)\big]^{1/2} \tag{45}$$

$$x_2 = \frac{d_1\rho}{2^{1/2}}\big[1+\cos(2\Theta)\cos(2\Phi+\epsilon_2)\big]^{1/2} \tag{46}$$

where

$$\epsilon_1 = -2\tan^{-1}(-m_2/\mu) \tag{47}$$

$$\epsilon_2 = 2\tan^{-1}(-m_1/\mu) \tag{48}$$

Now for three identical particles we get

$$x_3 = \frac{\rho}{3^{1/4}}\big[1+\cos(2\Theta)\cos(2\Phi)\big]^{1/2} \tag{49}$$

$$x_1 = \frac{\rho}{3^{1/4}}\big[1+\cos(2\Theta)\cos(2\Phi-4\pi/3)\big]^{1/2} \tag{50}$$

$$x_2 = \frac{\rho}{3^{1/4}}\big[1+\cos(2\Theta)\cos(2\Phi+4\pi/3)\big]^{1/2} \tag{51}$$

Now, with $\phi_k = \pi/2 - 2\Phi_k$, we get $\phi_j = \phi_i + 2\beta_{ij}$, where $(-7\pi/2 \le \phi_k < \pi/2)$. Now with $2\beta_{ij} = -2\eta_{ij}$ and

$$\eta_{ij} = -\eta_{ji}, \quad \eta_{ii} = 0, \tag{52}$$

$$\tan\eta_{ij} = m_k/\mu, \tag{53}$$

$$\eta_{12}+\eta_{23}+\eta_{31} = \pi \tag{54}$$

We get

$$x_k = \frac{d_k\rho}{2^{1/2}}\big[1+\sin\theta\sin\phi_k\big]^{1/2}. \tag{55}$$

$$x_3 = \frac{d_3\rho}{2^{1/2}}\big[1+\sin\theta\sin\phi\big]^{1/2} \tag{56}$$

$$x_1 = \frac{d_1\rho}{2^{1/2}}\big[1+\sin\theta\sin(\phi-\varphi_1)\big]^{1/2} \tag{57}$$

$$x_2 = \frac{d_1\rho}{2^{1/2}}\big[1+\sin\theta\sin(\phi+\varphi_2)\big]^{1/2} \tag{58}$$

$$\varphi_1 = 2\tan^{-1}(m_2/\mu) \tag{59}$$

$$\varphi_2 = 2\tan^{-1}(m_1/\mu) \tag{60}$$

Now we redefine $\phi'_k = \phi_k + 7\pi/2$, so that the range is $0 \le \phi'_k < 4\pi$. Then $\sin\phi_k = \cos\phi'_k$. We finally get $(2\Phi = 4\pi - \phi')$

$$x_3 = \frac{d_3\rho}{2^{1/2}}\big[1+\sin\theta\cos\phi'\big]^{1/2} \tag{61}$$

$$x_1 = \frac{d_1\rho}{2^{1/2}}\big[1+\sin\theta\cos(\phi'-\varphi_1)\big]^{1/2} \tag{62}$$

$$x_2 = \frac{d_1\rho}{2^{1/2}}\big[1+\sin\theta\cos(\phi'+\varphi_2)\big]^{1/2}. \tag{63}$$

This is the same expression as Blume and Wang get, however the define there angles slightly different. Our interval is two times Blumes interval

The area of the triangle formed by the three particles is the length of the vector given by

$$\mathbf{A} = \frac{1}{2}(\mathbf{r} \times \mathbf{R}) \tag{64}$$

$$A = \frac{1}{2}(r_x R_y - r_y R_x) = \frac{1}{4}\rho^2 \sin(2\Theta) \tag{65}$$
$$\sin 2\Theta = 4A/\rho^2 \tag{66}$$

Since both the area and the hyperradius are positive quantities the angle must be in the range, $0 \leq \Theta \leq \pi/4$. For some reason $0 \leq \Phi < 2\pi$. The transformed coordinates then have the range $0 \leq \theta \leq \pi/2$ and

To describe how rotations of the BF system affects the derivatives in the SF system, introduce the infinitesimal rotations ω. The velocities of the SF system vectors are given by

$$\dot{\mathbf{r}}' = \dot{\mathbf{r}} + \omega \times \mathbf{r}$$
$$\dot{\mathbf{R}}' = \dot{\mathbf{R}} + \omega \times \mathbf{R}$$

which is given explicitly by

$$\begin{pmatrix} \dot{r}'_x \\ \dot{r}'_y \\ \dot{r}'_z \\ \dot{R}'_x \\ \dot{R}'_y \\ \dot{R}'_z \end{pmatrix} = \begin{pmatrix} \partial_\rho r_x & \partial_\Theta r_x & \partial_\Theta r_x & 0 & r_z & -r_y \\ \partial_\rho r_y & \partial_\Theta r_y & \partial_\Theta r_y & -r_z & 0 & r_x \\ \partial_\rho r_z & \partial_\Theta r_z & \partial_\Theta r_z & r_y & -r_x & 0 \\ \partial_\rho R_x & \partial_\Theta R_x & \partial_\Theta R_x & 0 & R_z & -R_y \\ \partial_\rho R_y & \partial_\Theta R_y & \partial_\Theta R_y & -R_z & 0 & R_x \\ \partial_\rho R_z & \partial_\Theta R_z & \partial_\Theta R_z & R_y & -R_x & 0 \end{pmatrix} \begin{pmatrix} \dot{\rho} \\ \dot{\Theta} \\ \dot{\Phi} \\ \omega_x \\ \omega_y \\ \omega_z \end{pmatrix}$$
$$= \begin{pmatrix} cc & -sc & -cs & 0 & 0 & ss \\ -ss & -cs & -sc & 0 & 0 & cc \\ 0 & 0 & 0 & -ss & -cc & 0 \\ cs & -ss & cc & 0 & 0 & -sc \\ sc & cc & -ss & 0 & 0 & cs \\ 0 & 0 & 0 & sc & -cs & 0 \end{pmatrix} \begin{pmatrix} \dot{\rho} \\ \rho\dot{\Theta} \\ \rho\dot{\Phi} \\ \rho\omega_x \\ \rho\omega_y \\ \rho\omega_z \end{pmatrix} \tag{68}$$

(69)

In matrix notation:

$$\dot{\mathbf{q}}' = \hat{A}\dot{\mathbf{q}}, \tag{70}$$

where

$$\dot{\mathbf{q}}' = \begin{pmatrix} \dot{r}'_x \\ \dot{r}'_y \\ \dot{r}'_z \\ \dot{R}'_x \\ \dot{R}'_y \\ \dot{R}'_z \end{pmatrix}, \dot{\mathbf{q}} = \begin{pmatrix} \dot{\rho} \\ \dot{\Theta} \\ \dot{\Phi} \\ \omega_x \\ \omega_y \\ \omega_z \end{pmatrix}$$

The arclength is given by

$$s = \int_a^b \|\dot{\mathbf{q}}'\| dt = \int_a^b \sqrt{\dot{\mathbf{q}}'^T \dot{\mathbf{q}}'} dt \tag{71}$$

and

$$(ds)^2 = (d\mathbf{q}')^T (d\mathbf{q}') = d\mathbf{q}^T \hat{A}^T \hat{A} d\mathbf{q} = d\mathbf{q}^T \mathbf{g} d\mathbf{q}, \tag{72}$$

where $\mathbf{g}$ is the metric tensor

$$\mathbf{g} = \begin{pmatrix} \mathbf{G} & \mathbf{C} \\ \mathbf{C}^T & \mathbf{K} \end{pmatrix} \tag{73}$$

where the submatrices $\mathbf{G}$, $\mathbf{K}$ and $\mathbf{C}$ are

$$\mathbf{G} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \rho^2 & 0 \\ 0 & 0 & \rho^2 \end{pmatrix} \tag{74}$$

$$\mathbf{K} = \rho^2 \begin{pmatrix} \sin^2\Theta & 0 & 0 \\ 0 & \cos^2\Theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{75}$$

$$\mathbf{C} = -\rho^2 \sin^2(2\Theta) \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{76}$$

the inverse of the metric tensor $\mathbf{g}^{-1}$

$$\mathbf{g}^{-1} = \begin{pmatrix} \mathbf{V} & \mathbf{W} \\ \mathbf{W}^T & \mathbf{U} \end{pmatrix} \tag{77}$$

where the submatrices $\mathbf{V}$, $\mathbf{W}$ and $\mathbf{U}$ are

$$\mathbf{V} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/\rho^2 & 0 \\ 0 & 0 & 1/\rho^2 \cos^2(2\Theta) \end{pmatrix} \tag{78}$$

$$\mathbf{U} = \frac{1}{\rho^2} \begin{pmatrix} 1/\sin^2\Theta & 0 & 0 \\ 0 & 1/\cos^2\Theta & 0 \\ 0 & 0 & 1/\cos^2(2\Theta) \end{pmatrix} \tag{79}$$

$$\mathbf{W} = \frac{\sin(2\Theta)}{\rho^2 \cos^2(2\Theta)} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{80}$$

The determinant of the metric tensor is given by

$$g = \mid \mathbf{g} \mid = \begin{vmatrix} \mathbf{G} & \mathbf{C} \\ \mathbf{C}^T & \mathbf{K} \end{vmatrix} = \begin{vmatrix} \mathbf{G} & \mathbf{C} \\ 0 & \mathbf{K} - \mathbf{C}^T\mathbf{G}^{-1}\mathbf{C} \end{vmatrix} \tag{81}$$

$$= \mid \mathbf{G} \mid \cdot \mid \mathbf{K} - \mathbf{C}^T\mathbf{G}^{-1}\mathbf{C} \mid = \frac{\rho^{10}}{16} \sin^2(4\Theta) \tag{82}$$

$$\sqrt{g} = \frac{\rho^5}{4} \sin(4\Theta) \tag{83}$$

The kinetic energy operator of a particle with mass μ in a curvilinear coordinate system of N dimensions is given by

$$T = -\frac{\hbar^2}{2\mu} \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{1}{\sqrt{g}} \frac{\partial}{\partial q_i} \left(\sqrt{g} g^{ij} \frac{\partial}{\partial q_j} \right) \tag{84}$$

where g^{ij} is the inverse metric tensor. The momentum vector is given by

$$\mathbf{p} = i\hbar \begin{pmatrix} \partial/\partial q_1 \\ \vdots \\ \partial/\partial q_N \end{pmatrix} \tag{85}$$

With ω expressed in Euler angles

$$\omega = \begin{pmatrix} d\Omega_x \\ d\Omega_y \\ d\Omega_z \end{pmatrix} \tag{86}$$

we get the kinetic energy

$$
\begin{aligned}
-\frac{1}{\hbar^2}\hat{T} &= -\frac{1}{2\mu\rho^5\sin(4\Theta)}\mathbf{p}^T\left(\rho^5\sin(4\Theta)\mathbf{g}^{-1}\right)\mathbf{p} \\
&= \frac{1}{2\mu\rho^5\sin(4\Theta)}\left[\frac{\partial}{\partial\rho}\left(\rho^5\sin(4\Theta)\frac{\partial}{\partial\rho}\right)+\frac{\partial}{\partial\Theta}\left(\rho^3\sin(4\Theta)\frac{\partial}{\partial\Theta}\right)\right. \\
&+\frac{\partial}{\partial\Phi}\left(2\rho^3\tan(2\Theta)\frac{\partial}{\partial\Phi}+2\tan^2(2\Theta)\cos(2\Theta)\frac{\partial}{\partial\Omega_z}\right) \\
&+\frac{\partial}{\partial\Omega_x}\left(4\rho^3\cot(\Theta)\cos(2\Theta)\frac{\partial}{\partial\Omega_x}\right) \\
&+\frac{\partial}{\partial\Omega_y}\left(4\rho^3\tan(2\Theta)\cos(2\Theta)\frac{\partial}{\partial\Omega_y}\right) \\
&\left.+\frac{\partial}{\partial\Omega_z}\left(2\rho^3\tan^2(2\Theta)\frac{\partial}{\partial\Phi}+2\rho^3\tan(2\Theta)\frac{\partial}{\partial\Omega_z}\right)\right] \\
&= \frac{1}{2\mu}\left[\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\left(\rho^5\frac{\partial}{\partial\rho}\right)+\frac{1}{\rho^2\sin(4\Theta)}\frac{\partial}{\partial\Theta}\left(\sin(4\Theta)\frac{\partial}{\partial\Theta}\right)\right. \\
&+\frac{1}{\rho^2\cos^2(2\Theta)}\frac{\partial^2}{\partial\Phi^2}+\frac{\sin(2\Theta)}{\rho^2\cos^2(2\Theta)}\frac{\partial}{\partial\Phi}\frac{\partial}{\partial\Omega_z} \\
&+\frac{1}{\rho^2\sin^2(\Theta)}\frac{\partial^2}{\partial\Omega_x^2}+\frac{1}{\rho^2\cos^2(\Theta)}\frac{\partial^2}{\partial\Omega_y^2}+\frac{\sin(2\Theta)}{\rho^2\cos^2(2\Theta)}\frac{\partial}{\partial\Omega_z}\frac{\partial}{\partial\Phi} \\
&\left.+\frac{1}{\rho^2\cos^2(2\Theta)}\frac{\partial^2}{\partial\Omega_z^2}\right] \\
&= \frac{1}{2\mu\rho^5}\frac{\partial}{\partial\rho}\left(\rho^5\frac{\partial}{\partial\rho}\right)+\frac{1}{2\mu\rho^2}\left[\frac{1}{\sin(4\Theta)}\frac{\partial}{\partial\Theta}\left(\sin(4\Theta)\frac{\partial}{\partial\Theta}\right)\right. \\
&\left.+\frac{1}{\cos^2(2\Theta)}\frac{\partial^2}{\partial\Phi^2}\right]+\frac{1}{2\mu\rho^2}\left[\frac{1}{\sin^2(\Theta)}\frac{\partial^2}{\partial\Omega_x^2}+\frac{1}{\cos^2(\Theta)}\frac{\partial^2}{\partial\Omega_y^2}+\frac{1}{\cos^2(2\Theta)}\frac{\partial^2}{\partial\Omega_z^2}\right. \\
&\left.+\frac{2\sin(2\Theta)}{\cos^2(2\Theta)}\frac{\partial}{\partial\Phi}\frac{\partial}{\partial\Omega_z}\right].
\end{aligned}
$$

The volume element in a general coordinate system of N dimensions is given by

$$
d^N v = g^{1/2}\prod_{i=1}^{N} dq_i \tag{87}
$$

The Euler angles are given by

$$\begin{pmatrix} d\Omega_x \\ d\Omega_y \\ d\Omega_z \end{pmatrix} = \mathbf{A} \begin{pmatrix} d\alpha \\ d\beta \\ d\gamma \end{pmatrix} \tag{88}$$

where

$$\mathbf{A} = \begin{pmatrix} -\sin\beta\cos\gamma & \sin\gamma & 0 \\ \sin\beta\sin\gamma & \cos\gamma & 0 \\ \cos\beta & 0 & 1 \end{pmatrix} \tag{89}$$

$$d\mathbf{q} = \begin{pmatrix} d\rho \\ d\Theta \\ d\Phi \\ d\Omega_x \\ d\Omega_y \\ d\Omega_z \end{pmatrix}, d\mathbf{q}' = \begin{pmatrix} d\rho \\ d\Theta \\ d\Phi \\ d\alpha \\ d\beta \\ d\gamma \end{pmatrix}$$

$$ds^2 = (d\mathbf{q})^T \mathbf{g} d\mathbf{q} = (d\mathbf{q}')^T \mathbf{g}' d\mathbf{q}' \tag{90}$$

with

$$\mathbf{B} = \begin{pmatrix} \mathbf{I} & 0 \\ 0 & \mathbf{A} \end{pmatrix} \tag{91}$$

$$\mathbf{g}' = \mathbf{B}^T \mathbf{g} \mathbf{B} \tag{92}$$

and the determinant is then

$$g'^{1/2} = (\mid \mathbf{B} \mid^2 \mid \mathbf{g} \mid)^{1/2} = (\mid \mathbf{A} \mid^2 \mid \mathbf{g} \mid)^{1/2} = \frac{\rho^5}{4}\sin(4\Theta)\sin\beta \tag{93}$$

In our set up we thus get

$$d^6 v = g^{1/2} \prod_{i=1}^{6} dq_i = \frac{\rho^5}{4}\sin(4\Theta)\sin\beta d\rho d\Theta d\Phi d\alpha d\beta d\gamma \tag{94}$$

Now, we make a transformation of the angles (Kuppermann)

$$\Theta = \pi/4 - \theta/2$$
$$\Phi = \pi/4 - \phi/2$$

and

$$\frac{\partial}{\partial\Theta} = -2\frac{\partial}{\partial\theta}$$
$$\frac{\partial}{\partial\Phi} = -2\frac{\partial}{\partial\phi}$$

$$\begin{aligned}
\sin(4\Theta) &= \sin(2\theta) \\
\cos^2(2\Theta) &= \sin^2(\theta) \\
\sin^2(2\Theta) &= \cos^2(\theta) \\
\cos^2\Theta &= \frac{1}{2}(1+\sin\theta) \\
\sin^2\Theta &= \frac{1}{2}(1-\sin\theta)
\end{aligned}$$

The corresponding volume element is then

$$d^6v = \frac{1}{8}\rho^5 \sin\theta\cos\theta\sin\beta d\rho d\theta d\phi d\alpha d\beta d\gamma \tag{95}$$

Now with

$$\mathbf{P} = -i\hbar \begin{pmatrix} \partial/\partial\rho \\ \partial/\partial\theta \\ \partial/\partial\phi \end{pmatrix} = \begin{pmatrix} P_\rho \\ P_\theta \\ P_\phi \end{pmatrix} \tag{96}$$

and

$$\mathbf{J} = -i\hbar \begin{pmatrix} \partial/\partial\Omega_x \\ \partial/\partial\Omega_y \\ \partial/\partial\Omega_z \end{pmatrix} = \begin{pmatrix} J_x \\ J_y \\ J_z \end{pmatrix} \tag{97}$$

The kinetic energy operator then becomes

$$\begin{aligned}
\hat{T} = -\frac{\hbar^2}{2\mu}\Bigg[\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\rho^5\frac{\partial}{\partial\rho} + \frac{4}{\rho^2}\Bigg(\frac{1}{\sin(2\theta)}\frac{\partial}{\partial\theta}\sin(2\theta)\frac{\partial}{\partial\theta} \\
+ \frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}\Bigg)\Bigg] - \frac{1}{\mu\rho^2}\Bigg[\frac{J_x^2}{(1-\sin\theta)} + \frac{J_y^2}{(1+\sin\theta)} + \frac{J_z^2}{2\sin^2\theta}\Bigg] \\
+ \frac{4i\hbar\cos\theta J_z}{2\mu\rho^2\sin^2\theta}\frac{\partial}{\partial\phi}
\end{aligned}$$

If we only consider $J=0$ states, the Hamiltonian reduces to

$$H_0 = -\frac{\hbar^2}{2\mu}\left[\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\rho^5\frac{\partial}{\partial\rho} + \frac{4}{\rho^2}\left(\frac{1}{\sin(2\theta)}\frac{\partial}{\partial\theta}\sin(2\theta)\frac{\partial}{\partial\theta} + \frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}\right)\right] + V(\rho,\theta,\phi) \tag{98}$$

By making the following transformation of the wave function

$$\psi = \rho^{5/2}\Psi, \tag{99}$$

the Schrödinger equation becomes

$$H\psi = E\psi. \tag{100}$$

Where the transformed Hamiltonian operator is given by

$$H = \rho^{5/2} H_0 \rho^{-5/2}. \tag{101}$$

This transformation removes the first derivative in the hyper radial kinetic-energy operator since

$$T_\rho = \rho^{5/2} T_{\rho_0} \rho^{-5/2} = \rho^{5/2} \frac{1}{\rho^5} \frac{\partial}{\partial \rho} \rho^5 \frac{\partial}{\partial \rho} \Big(\rho^{-5/2}\Big) = -\frac{15}{4} \frac{1}{\rho^2} + \frac{\partial^2}{\partial \rho^2} \tag{102}$$

and we get the final expression for the Hamiltonian

$$H = -\frac{\hbar^2}{2\mu} \Bigg[-\frac{15}{4} \frac{1}{\rho^2} + \frac{\partial^2}{\partial \rho^2} + \frac{4}{\rho^2} \Big(\frac{1}{\sin(2\theta)} \frac{\partial}{\partial \theta} \sin(2\theta) \frac{\partial}{\partial \theta} + \frac{1}{\sin^2(\theta)} \frac{\partial^2}{\partial \phi^2} \Big) \Bigg] + V(\rho, \theta, \phi) \tag{103}$$

$$= -\frac{\hbar^2}{2\mu\rho^2} \frac{\partial^2}{\partial \rho^2} + \frac{\hbar^2}{2\mu\rho^2} \left(\Lambda^2 + \frac{15}{4} \right) + V(\rho, \theta, \phi), \tag{104}$$

where Λ^2 is the grand angular momentum operator.

2.5.3 Symmetries

The Smith-Whitten coordinates θ and ϕ are connected to the geometry of the triangle formed by the three particles. If the three particles represent the vertecis of a triangle, θ will determine its shape, while ϕ determines the arrangement of the particles at its vertecis. Now lets determine the eigenvalues and eigenfunctions of the grand angular momentum operator. For the ϕ equation we have

$$\frac{\partial^2}{\partial \phi^2} \mathrm{e}^{i\nu\phi} = -\nu^2 \mathrm{e}^{i\nu\phi}, \tag{105}$$

so the total eigenfunction can be written

$$f_{\nu n}(\theta, \phi) = g_{n\nu}(\theta) \mathrm{e}^{i\nu\phi}. \tag{106}$$

For a general system we have the symmetry

$$f_{\nu n}(\theta, \phi = 0) = \Pi f_{\nu n}(\theta, \phi = 2\pi), \qquad \text{for} \qquad \Pi = \pm 1, \tag{107}$$

the symmetry of a three identical particle system will reduce the interval of ϕ to $[0, 2\pi/3]$. (symmetry group C_{3v} with irreducible representations A_1, A_2, and E), we will consider bosons and states with $J = 0$ so this leads to vibrational wave functions of A_1 symmetry and this will reduce the interval of ϕ further to $[0, \pi/3]$, so

$$f_{\nu n}(\theta, \phi = 0) = \Pi f_{\nu n}(\theta, \phi = 2\pi/3), \qquad \text{for} \qquad \Pi = \pm 1, \tag{108}$$

where the parity $\Pi = 1$ for bosons. Thus

$$\mathrm{e}^{i\nu 2\pi/3} = 1 \quad \Leftrightarrow \quad \nu = 3n \quad \text{for} \quad n = 0, 1, 2, ... \tag{109}$$

so we get

$$\Lambda^2 g_{n\nu}(\theta) = -4\left(\frac{1}{\sin(2\theta)}\frac{\partial}{\partial\theta}\sin(2\theta)\frac{\partial}{\partial\theta} - \frac{\nu^2}{\sin^2(\theta)}\right)g_{n\nu}(\theta) = \lambda_{n\nu}g_{n\nu}(\theta). \tag{110}$$

The interval for θ is $[0, \pi/2]$. Lets look at the boundary as $\theta \to 0$. The small angle approximation leads to

$$\Lambda^2 \to -4\left(\frac{1}{\theta}\frac{\partial}{\partial\theta} + \frac{\partial^2}{\partial\theta^2} - \frac{\nu^2}{\theta^2}\right)g_{n\nu}(\theta) = \lambda_{n\nu}g_{n\nu}(\theta). \tag{111}$$

we thus need to solve a differential equation of the form

$$g''_{n\nu}(\theta) + \frac{P(\theta)}{\theta}g'_{n\nu}(\theta) + \frac{Q(\theta)}{\theta^2}g_{n\nu}(\theta) = 0, \tag{112}$$

with

$$P(\theta) = 1 \quad \text{and} \quad Q(\theta) = \frac{\lambda_{n\nu}\theta^2 - 4\nu^2}{4}. \tag{113}$$

Since ref[the differential equation] has a regular singular point at $\theta = 0$ and both $P(\theta)$ and $Q(\theta)$ are analytic functions, we seek a power series solution of the form

$$g_{n\nu}(\theta) = \sum_{k=0}^{\infty} A_k\theta^{k+s}, \quad (A_0 \neq 0). \tag{114}$$

differentiating

$$g'_{n\nu}(\theta) = \sum_{k=0}^{\infty}(k+s)A_k\theta^{k+s-1}, \tag{115}$$

$$g''_{n\nu}(\theta) = \sum_{k=0}^{\infty}(k+s)(k+s-1)A_k\theta^{k+s-2}, \tag{116}$$

and substituting into [ref] we get

$$\sum_{k=0}^{\infty}\Bigg((k+s)(k+s-1)+(k+s)-\nu^2\Bigg)A_k\theta^{k+s-2}+\Bigg(\frac{\lambda_{n\nu}}{4}\Bigg)A_k\theta^{k+s}=$$

$$\big[s(s-1)+s-\nu^2\big]A_0\theta^{s-2}+\sum_{k=1}^{\infty}\Bigg(\big[(k+s)(k+s-1)+(k+s)-\nu^2\big]A_k+\frac{\lambda_{n\nu}}{4}A_{k-2}\Bigg)\theta^{k+s-2}$$

From $s^2-\nu^2=0$ we get the two roots $s=\pm\nu$. Using these roots, we set the coefficients of θ^{k+s-2} to be zero, and we get the equations

$$\big(k^2\pm 2k\nu\big)A_k=\frac{\lambda_{n\nu}}{4}A_{k-2} \tag{117}$$

2.6 Hyperangular and hyperradial equations

The hyperradius is given by

$$\rho=(\mathbf{R}^2+\mathbf{r}^2)^{1/2} \tag{118}$$

In hyperspherical coordinates the three-body Schrödiner equation becomes

$$\Bigg(-\frac{1}{2\mu}\frac{\partial^2}{\partial\rho^2}+\frac{\Lambda^2+15/4}{2\mu\rho^2}+V\Bigg)\psi(\rho,\Omega)=E\psi(\rho,\Omega). \tag{119}$$

To solve (make ref) we expand $\psi(\rho,\theta,\phi)$ into radial wave functions $F_{\nu n}(\rho)$ and a set of complete, orthonormal channel functions $\Phi_\nu(\rho;\theta,\phi)$ that depend parametrically on ρ. The channel functions Φ_ν are solutions of the hyperangular part of the Hamiltonian

$$H(\rho,\Omega)=T(\rho)+H_{ad}(\rho,\Omega) \tag{120}$$

$$H_{ad}(\rho,\Omega)=\frac{\Lambda^2}{2\mu_3\rho^2}+\sum_{i<j}V(r_{ij}) \tag{121}$$

$$H_{ad}\Phi_\nu(\rho;\Omega)=U_\nu(\rho)\Phi_\nu(\rho;\Omega) \tag{122}$$

$$\psi_n=\sum_{\nu}\frac{F_{\nu n}(\rho)}{\rho^{5/2}}\Phi_\nu(\rho;\theta,\phi) \tag{123}$$

Smith-Whitten (democratic) hyperangles

$$r_{ij}=\frac{d_{ij}\rho}{\sqrt{2}}\Big[1+\sin(\theta)\cos\left(\varphi+\varphi_{ij}\right)\Big]^{1/2} \tag{124}$$

$$\varphi_{12} = 2 \arctan\left(m_3/\mu_3\right)$$
$$\varphi_{23} = 0$$
$$\varphi_{31} = -2 \arctan\left(m_2/\mu_3\right)$$

$$d_{ij}^2 = \frac{m_k}{\mu_3} \frac{m_i + m_j}{m_i + m_j + m_k} \tag{125}$$

$$\Lambda^2 = T_\theta + T_\phi + T_{rot} \tag{126}$$

$$T_\theta = -\frac{4}{\sin(2\theta)} \frac{\partial}{\partial\theta} \sin(2\theta) \frac{\partial}{\partial\theta} \tag{127}$$

$$T_\phi = \frac{2}{\sin^2(2\theta)} \Big(i \frac{\partial}{\partial\phi} - \frac{\cos\theta}{2} J_z \Big)^2 \tag{128}$$

$$T_{rot} = \frac{2}{1 - \sin(\theta)} J_x^2 + \frac{2}{1 + \sin(\theta)} J_y^2 + J_z^2 \tag{129}$$

2.7 Three identical particles

2.7.1 Permutation symmetries in Smith-Whitten coordinates

2.8 Effective three-body interaction

The two-body interaction

$$V(r) = d \cosh\left(r/r_0\right) \tag{130}$$