

Theoretical and Numerical Studies of Efimov States

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September 2, 2019

1. Hi, my name is Kajsa-My Blomdahl, I study Efimov Physics, which is encapsulate a number of effects that appear in the quantum 3BP.

- 1 Introduction
- 2 Theoretical Approach
- 3 Effective Potentials
- 4 Numerical Approach
- 5 Scattering Model
- 6 Results

1. To understand important features of the quantum 3BP I will start by introduce a few concepts from quantum scattering of 2 particles.

Two-body (2-b) Interactions

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Introduction

Two-body
Interactions

Scattering
Length

Universality

The Efimov
Effect

Theoretical
Approach

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

• Atomic collisions in the ultra cold regime

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- Scattering Length
- Universality
- The Efimov Effect

Results

- Atomic collisions in the ultra cold regime
1. Atomic interactions are, essentially, pair-wise and short-ranged, which means that they interact when they are close to each other.

- └ Introduction
 - └ Two-body Interactions
 - └ Two-body (2-b) Interactions

- Atomic collisions in the ultra cold regime

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Two-body (2-b) Interactions

Kajsa-My
Blomdahl

Introduction

Two-body
Interactions

Scattering
Length

Universality

The Efimov
Effect

Theoretical
Approach

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

- Atomic collisions in the ultra cold regime
- Quantized orbital angular momenta $l = 0, 1, 2$, are referred to as s -waves, p -waves and d -waves etc.

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Results

- 2019-09-02

Introduction

Two-body (2-b) Interactions

Two-body Interactions

Two-body (2-b) Interactions

Two-body (2-b) Interactions

Two-body (2-b) Interactions

 - Atomic collisions in the ultra cold regime
 - Quantized orbital angular momenta $l = 0, 1, 2$, are referred to as s-waves, p-waves and d-waves etc.

1. At very low energies, atoms behave like point particles and have quantized orbital angular momenta l . The quantum numbers $l = 0, 1, 2$, associated with an atom, are referred to as s-waves, p-waves and d-waves, and so on

2019-09-02

- └ Introduction
- └ Two-body Interactions
 - └ Two-body (2-b) Interactions

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Two-body (2-b) Interactions

Kajsa-My
Blomdahl

Introduction

Two-body
Interactions

Scattering
Length

Universality

The Efimov
Effect

Theoretical
Approach

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

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◀ ≡ ▶

◀ ≡ ▶

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↺ 🔍 ↻

Results

- 2019-09-02

└ Introduction

└ Two-body Interactions

└ Two-body (2-b) Interactions

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- Atomic collisions in the ultra cold regime
 - Quantized orbital angular momenta $l = 0, 1, 2, \dots$ are referred to as *s-waves*, *p-waves* and *d-waves* etc.

1. In the ultracold regime s-wave collisions dominate (because higher partial waves are reflected by the centrifugal barrier in the SE)

2019-09-02

- └ Introduction
- └ Two-body Interactions
 - └ Two-body (2-b) Interactions

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- Atomic collisions in the ultra cold regime
- Quantized orbital angular momenta $l = 0, 1, 2, \dots$ are referred to as *s-waves*, *p-waves* and *d-waves* etc.

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Two-body (2-b) Interactions

- Atomic collisions in the ultra cold regime
- Quantized orbital angular momenta $l = 0, 1, 2$, are referred to as s -waves, p -waves and d -waves etc.
- 2-b scattering in this regime is governed by a parameter called the **s -wave scattering length a**

Results

- 2019-09-02

└ Introduction

└ Two-body Interactions

└ Two-body (2-b) Interactions

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- Atomic collisions in the ultra cold regime
 - Quantized orbital angular momenta $l = 0, 1, 2$, are referred to as s-waves, p-waves and d-waves etc.
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1. Two-body scattering in this regime is solely governed by a single parameter called the s-wave scattering length a , or just scattering length for short

2019-09-02

- └ Introduction
 - └ Two-body Interactions
 - └ Two-body (2-b) Interactions

Two-body (2-b) Interactions

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Scattering Length

Kajsa-My
Blomdahl

Introduction

Two-body
Interactions

Scattering Length

Universality
The Efimov
Effect

Theoretical Approach

Effective Potentials

Numerical Approach

Scattering Model

Results

- Definition:

$$a = \lim_{k \rightarrow 0} -\frac{\tan \delta_0(k)}{k}$$

2019-09-02

└ Introduction
└ Scattering Length
└ Scattering Length

Scattering Length

• Definition:

$$a = \lim_{k \rightarrow 0} -\frac{\tan \delta_0(k)}{k}$$

1. The s-wave scattering length is defined in the low-energy limit as

Scattering Length

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Blomdahl

Introduction

Two-body
Interactions

**Scattering
Length**

Universality
The Efimov
Effect

Theoretical
Approach

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

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$$a = \lim_{k \rightarrow 0} -\frac{\tan \delta_0(k)}{k}$$

2019-09-02

└ Introduction
└ Scattering Length
└ Scattering Length

Scattering Length

• Definition:

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1. where δ is the s-wave phase shift of the outgoing wave (and k is the wave number $= \sqrt{2\mu E}/\hbar$)

Scattering Length

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IntroductionTwo-body InteractionsScattering LengthUniversalityThe Efimov EffectTheoretical ApproachEffective PotentialsNumerical ApproachScattering ModelResults

- Definition:
$$a = \lim_{k \rightarrow 0} -\frac{\tan \delta_0(k)}{k}$$
- Characterizes the strength of the interparticle interaction
- The sign of a and the effective interaction

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↺ 🔍 ↻

Results

- $$a = \lim_{k \rightarrow 0} -\frac{\tan \delta_0(k)}{k}$$

- └ Introduction
- └ Scattering Length
- └ Scattering Length

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$$a = \lim_{k \rightarrow 0} -\frac{\tan \delta_0(k)}{k}$$
- Characterizes the strength of the interparticle interaction
- The sign of a and the effective interaction

1. The sign of a carries information about whether the effective interaction is attractive or repulsive. If the two-body interaction has no bound states a is negative. However if the interaction has one or more bound state a can be both positive and negative.

Scattering Length

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Introduction

Two-body
Interactions

Scattering
Length

Universality
The Efimov
Effect

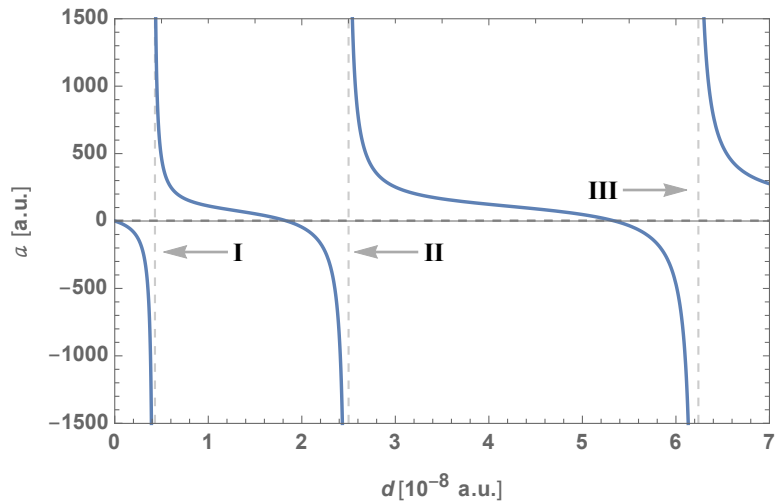
Theoretical
Approach

Effective
Potentials

Numerical
Approach

Scattering
Model

Results



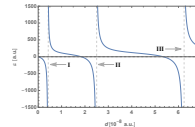
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Introduction

Scattering Length

Scattering Length

Scattering Length



1. To illustrate this I have finetuned a model two body potential by changing the depth of the potential. Here we have a on the y-axis and the depth d of the attractive 2b-potential on the x-axis.

Scattering Length

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Introduction

Two-body
Interactions

Scattering
Length

Universality

The Efimov
Effect

Theoretical
Approach

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

- Definition:
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- Negative $a \rightarrow$ attractive effective interactions

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2019-09-02

- └ Introduction
- └ Scattering Length
- └ Scattering Length

- └ Introduction
 - └ Scattering Length
 - └ Scattering Length

Scattering Length

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- Negative $a \rightarrow$ attractive effective interactions

1. Negative scattering lengths correspond to attractive effective interactions, meaning the scattered wave is being pulled in by the potential

Scattering Length

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Introduction

- Two-body Interactions
- Scattering Length**
- Universality
- The Efimov Effect

Theoretical Approach

Effective Potentials

Numerical Approach

Scattering Model

Results

- Definition:

$$a = \lim_{k \rightarrow 0} -\frac{\tan \delta_0(k)}{k}$$

- Characterizes the strength of the interparticle interaction
- The sign of a and the effective interaction
- Negative $a \rightarrow$ attractive effective interactions
- Positive $a \rightarrow$ repulsive effective interactions

2019-09-02

└ Introduction

Scattering Length

Scattering Length

Scattering Length

- Definition:

$$a = \lim_{k \rightarrow 0} -\frac{\tan \delta_0(k)}{k}$$
- Characterizes the strength of the interparticle interaction
- The sign of a and the effective interaction
 - Negative $a \rightarrow$ attractive effective interactions
 - Positive $a \rightarrow$ repulsive effective interactions

1. Positive scattering lengths correspond to repulsive effective interactions, meaning the scattered wave is being pushed out by the potential

Scattering Length

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Blomdahl

Introduction

Two-body
Interactions

Scattering
Length

Universality
The Efimov
Effect

Theoretical
Approach

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

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$$a = \lim_{k \rightarrow 0} -\frac{\tan \delta_0(k)}{k}$$

- Characterizes the strength of the interparticle interaction
- The sign of a and the effective interaction
- Negative $a \rightarrow$ attractive effective interactions
- Positive $a \rightarrow$ repulsive effective interactions
- For $|a| \rightarrow \infty$ the interaction is called **resonant**

2019-09-02

Introduction

Scattering Length

Scattering Length

Scattering Length

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$$a = \lim_{k \rightarrow 0} -\frac{\tan \delta_0(k)}{k}$$
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- For $|a| \rightarrow \infty$ the interaction is called **resonant**

1. When the magnitude of $a \rightarrow \infty$ we say that the interaction is resonant. In this case the interaction is fully characterized by the scattering length, which is much larger than the interaction range of the particles.

Universality in 2-b systems

The image shows a presentation slide with a light blue sidebar on the left containing navigation links: Kajsa-My Blomdahl, Introduction, Two-body Interactions, Scattering Length, Universality, The Efimov Effect, Theoretical Approach, Effective Potentials, Numerical Approach, Scattering Model, and Results. The main area has a dark blue header bar with the title "2-b scattering". Below it, a white box contains the text: "Particles with large $|a|$ in the low-energy regime have universal properties". At the bottom right are several small navigation icons.

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Introduction

Two-body
Interactions

Scattering
Length

Universality

The Efimov
Effect

Theoretical
Approach

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

2-b scattering

Particles with large $|a|$ in the low-energy regime have universal properties

Navigation icons: back, forward, search, etc.

Results

Particles with large $|a|$ in the low-energy regime have universal properties

- └ Introduction
- └ Universality
- └ Universality in 2-b systems

Universality in 2-b systems

2-b scattering

Particles with large $|a|$ in the low-energy regime have universal properties

Universality in 2-b systems

Rajsa-Miy Blomdahl Introduction

Two-body Interactions
Scattering Length
2-b scattering
Particles with large $|a|$ in the low energy regime have universal

Universality
The Efimov Effect

Particles with large $|a|$ in the low-energy regime have universal properties

properties

Theoretical Approach

Universal properties ... In what sense?

Numerical Approach Depend on the scattering length alone and not on the details of the short-range interaction

Scattering
Model

- 2019-09-02
 - └ Introduction
 - └ Universality
 - └ Universality in 2-b systems

- └ Introduction
- └ Universality

- └ Universality
 - └ Universality in 2-b systems

- └ Universality in 2-b systems

Universality in 2-b systems

2-b scattering
Particles with large $|a|$ in the low-energy regime have universal properties

Universal properties ... In what sense?
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 Particles with large $|a|$ in the low-energy regime have universal properties

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Universal properties ... In what sense?

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Universal properties ... In what sense?
Depend on the scattering length alone and not on the details of the short-range interaction

Universal properties ... In what sense?
Depend on the scattering length alone and not on the details of the short-range interaction

1. What do we mean by universal? It means that they depend on the scattering alone and not on the details of the short-range interaction, which means all bosons behave in the same way it does not matter what atomic species we look at

Universality in 2-b systems

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Blomdahl

Introduction

Two-body
Interactions
Scattering
Length

Universality
The Efimov
Effect

Theoretical
Approach

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

2-b scattering

Particles with large $|a|$ in the low-energy regime have universal properties

Universal properties ... In what sense?

Depend on the scattering length alone and not on the details of the short-range interaction

Example: 2-b binding energy for 2 identical bosons

$$E_D = \frac{\hbar^2}{ma^2}$$

2019-09-02

└ Introduction
└└ Universality
└└└ Universality in 2-b systems

1. For example:

Universality in 2-b systems

2-b scattering

Particles with large $|a|$ in the low-energy regime have universal properties

Universal properties ... In what sense?

Depend on the scattering length alone and not on the details of the short-range interaction

Example: 2-b binding energy for 2 identical bosons

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Efimov's Prediction

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Blomdahl

Introduction

Two-body
Interactions
Scattering
Length
Universality

The Efimov Effect

Theoretical Approach

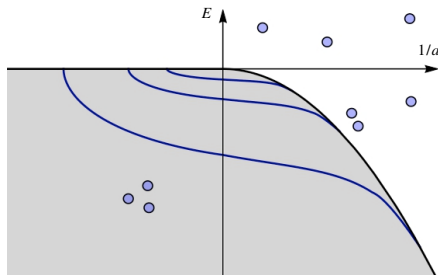
Effective Potentials

Numerical Approach

Scattering Model

Results

- Resonant 2-b forces give rise to bound energy levels in 3-particle systems



2019-09-02

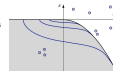
Introduction

The Efimov Effect

Efimov's Prediction

Efimov's Prediction

Resonant 2-b forces give rise to bound energy levels in 3-particle systems



- In the 1970 Vitaly Efimov predicted that resonant can give rise to a series of bound energy levels in 3-particle systems, which we now call Efimov states

Efimov's Prediction

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Blomdahl

Introduction

Two-body
Interactions
Scattering
Length
Universality
The Efimov
Effect

Theoretical
Approach

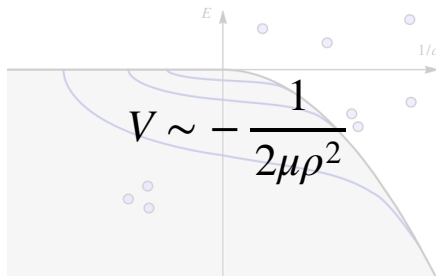
Effective
Potentials

Numerical
Approach

Scattering
Model

Results

- When $|a| \rightarrow \infty$ a universal long-range 3-body attraction emerge

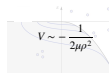


2019-09-02

└ Introduction
└ The Efimov Effect
└ Efimov's Prediction

Efimov's Prediction

• When $|a| \rightarrow \infty$ a universal long-range 3-body attraction emerge



1. 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's Prediction

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Blomdahl

Introduction

Two-body
Interactions
Scattering
Length
Universality

The Efimov Effect

Theoretical Approach

Effective Potentials

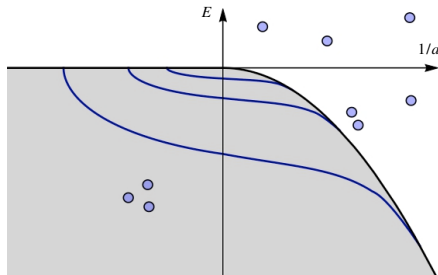
Numerical Approach

Scattering Model

Results

- Scale transformation constant

$$\lambda = e^{\pi/s_0} \approx 22.7$$



2019-09-02

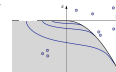
Introduction

- └ The Efimov Effect
 - └ Efimov's Prediction

Efimov's Prediction

- Scale transformation constant

$$\lambda = e^{\pi/s_0} \approx 22.7$$



1. The Efimov states have universal properties. For three identical bosons are that the size and energy of successive trimer states in the resonant limit are related by a scale transformation with a constant $\lambda = e^{\pi/s_0} \approx 22.7$

Efimov's Prediction

Kajsa-My
Blomdahl

Introduction

Two-body
Interactions
Scattering
Length
Universality

The Efimov Effect

Theoretical Approach

Effective Potentials

Numerical Approach

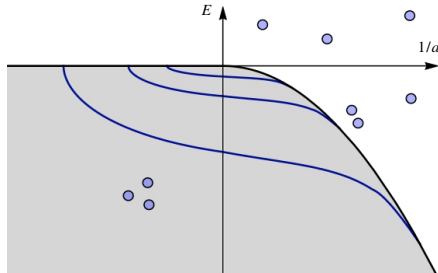
Scattering Model

Results

- Scale transformation constant

$$\lambda = e^{\pi/s_0} \approx 22.7$$

- $s_0 \approx 1.00624$



2019-09-02

Introduction

The Efimov Effect

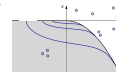
Efimov's Prediction

Efimov's Prediction

- Scale transformation constant

$$\lambda = e^{\pi/s_0} \approx 22.7$$

- $s_0 \approx 1.00624$



1. Is a universal constant in Efimov physics, which I will return to later

Efimov's Prediction

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Blomdahl

Introduction

Two-body
Interactions
Scattering
Length
Universality

The Efimov Effect

Theoretical Approach

Effective Potentials

Numerical Approach

Scattering Model

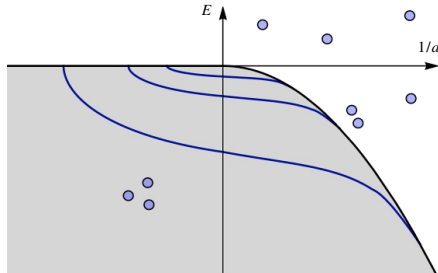
Results

- Scale transformation constant

$$\lambda = e^{\pi/s_0} \approx 22.7$$

- $s_0 \approx 1.00624$
- Size scaling:

$$\rho^{n+1}/\rho^n \approx \lambda$$



2019-09-02

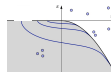
Introduction

The Efimov Effect

Efimov's Prediction

Efimov's Prediction

- Scale transformation constant
 $\lambda = e^{\pi/s_0} \approx 22.7$
- $s_0 \approx 1.00624$
- Size scaling:
 $\rho^{n+1}/\rho^n \approx \lambda$



1. The ratio of the size of two successive Efimov states is given by the constant lambda

Efimov's Prediction

Kajsa-My
Blomdahl

Introduction

Two-body
Interactions
Scattering
Length
Universality

The Efimov Effect

Theoretical Approach

Effective Potentials

Numerical Approach

Scattering Model

Results

- Scale transformation constant

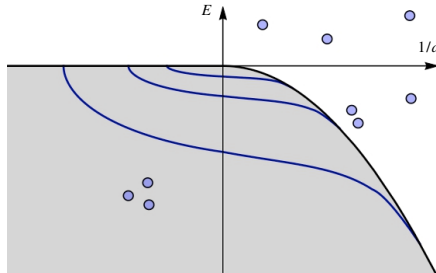
$$\lambda = e^{\pi/s_0} \approx 22.7$$

- $s_0 \approx 1.00624$
- Size scaling:

$$\rho^{n+1}/\rho^n \approx \lambda$$

- Energy scaling:

$$E_T^{n+1}/E_T^n \approx \lambda^2 \approx 515$$



2019-09-02

Introduction

The Efimov Effect

Efimov's Prediction

Efimov's Prediction

- Scale transformation constant

$$\lambda = e^{\pi/s_0} \approx 22.7$$

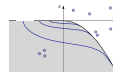
- $s_0 \approx 1.00624$

- Size scaling:

$$\rho^{n+1}/\rho^n \approx \lambda$$

- Energy scaling:

$$E_T^{n+1}/E_T^n \approx \lambda^2 \approx 515$$



1. while the ratio of the energy of two successive Efimov states scale geometrically with lambda

The Peculiar Efimov Effect

- 2019-09-02
 - └ Introduction
 - └ The Efimov Effect
 - └ The Peculiar Efimov Effect

1. The Efimov effect is remarkable in many ways

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The Peculiar Efimov Effect

1. The Efimov effect is remarkable in many ways

2019

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The Peculiar Efimov Effect

Kajsa-My Blomdahl

Introduction

- Two-body Interactions
- Scattering Length
- Universality
- The Efimov Effect**

Theoretical Approach

Effective Potentials

Numerical Approach

Scattering Model

Results

- Two-body Interactions
- Scattering Length
- Universality
- The Efimov Effect**

Results

- The size of each Efimov state (ES) \gg the interaction range (r_0) between the individual particle pairs \rightarrow QM effect

- 2019-09-02
 - └ Introduction
 - └ The Efimov Effect
 - └ The Peculiar Efimov Effect

└ The Peculiar Efimov Effect

1. Because the size of each Efimov state is much larger than the force-range between the individual pairs it means we are dealing with a pure quantum mechanical effect

- The size of each Efimov state (ES) \gg the interaction range (r_0) between the individual particle pairs \rightarrow QM effect

The Peculiar Efimov Effect

- The size of each Efimov state (ES) \gg the interaction range (r_0) between the individual particle pairs \rightarrow QM effect
- When $a \rightarrow \pm\infty$ the # of ES $\rightarrow \infty$

- Two-body Interactions
- Scattering Length
- Universality
- The Efimov Effect**

Effective Potentials

Scattering Model

- The size of each Efimov state (ES) \gg the interaction range (r_0) between the individual particle pairs \rightarrow QM effect
- When $a \rightarrow \pm\infty$ the # of ES $\rightarrow \infty$

- 2019-09-02
 - └ Introduction
 - └ The Efimov Effect
 - └ The Peculiar Efimov Effect

└ The Peculiar Efimov Effect

1. When the magnitude of scattering length approach infity, there is an infinite number of Efimov states

- The size of each Efimov state (ES) \gg the interaction range (r_0) between the individual particle pairs \rightarrow QM effect
- When $a \rightarrow \pm\infty$ the # of ES $\rightarrow \infty$

The Peculiar Efimov Effect

- The size of each Efimov state (ES) \gg the interaction range (r_0) between the individual particle pairs \rightarrow QM effect
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- The # of ES is **reduced** as the 2-b interaction is made more attractive

- Two-body Interactions
- Scattering Length
- Universality
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Effective Potentials

Scattering Model

- The size of each Efimov state (ES) \gg the interaction range (r_0) between the individual particle pairs \rightarrow QM effect
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- 2019-09-02
 - └ Introduction
 - └ The Efimov Effect
 - └ The Peculiar Efimov Effect

— The Efimov Effect

└ The Peculiar Efimov Effect

The Peculiar Efimov Effect

- The size of each Efimov state (ES) \gg the interaction range (n_0) between the individual particle pairs \rightarrow QM effect
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- When $a \rightarrow \pm\infty$ the # of ES $\rightarrow \infty$
- The # of ES is **reduced** as the 2-b interaction is made **more attractive**

1. # of 3-b bound states is *reduced* as the 2-b interaction is made more attractive.

The Peculiar Efimov Effect

- The size of each Efimov state (ES) \gg the interaction range (r_0) between the individual particle pairs \rightarrow QM effect
- When $a \rightarrow \pm\infty$ the # of ES $\rightarrow \infty$
- The # of ES is reduced as the 2-b interaction is made more attractive
- The effect is universal and can *in principle* be observed in any QM system

- Two-body Interactions
- Scattering Length
- Universality
- The Efimov Effect**

Effective Potentials

Scattering Model

- The size of each Efimov state (ES) \gg the interaction range (r_0) between the individual particle pairs \rightarrow QM effect
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- 2019-09-02
 - └ Introduction
 - └ The Efimov Effect
 - └ The Peculiar Efimov Effect

└ The Efimov Effect

└ The Peculiar Efimov Effect

The Peculiar Efimov Effect

- The size of each Efimov state (ES) \gg the interaction range (n_0) between the individual particle pairs \rightarrow QM effect
- When $a \rightarrow \pm\infty$ the $\#$ of ES $\rightarrow \infty$
- The $\#$ of ES is reduced as the 2-b interaction is made more attractive
- The effect is universal and can in principle be observed in any QM system

- merge
principle

1. The effect is universal, which means that the states emerge irrespective of the nature of the 2-b forces and can in principle be observed in all quantum mechanical systems

Theoretical Approach

Kajsa-My Blomdahl	
Introduction	
Theoretical Approach	
Step 1	
Step 2	
Step 3	
Effective Potentials	
Numerical Approach	
Scattering Model	
Results	

Introduction

Theoretical Approach

Step 1
Step 2
Step 3

Effective Potentials

Numerical Approach

Scattering Model

Results

2019-09-02

- └ Theoretical Approach
- └ Theoretical Approach

└ Theoretical Approach

- └ Theoretical Approach

1. The 3BP is famous for being hard to solve

Theoretical Approach

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Introduction

**Theoretical
Approach**

Step 1

Step 2

Step 3

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

Q: 3-Particles, What Is The Problem?

2019-09-02

└ Theoretical Approach

└ Theoretical Approach

1. So why is the problem of 3 so complex?

Theoretical Approach

Q: 3-Particles, What Is The Problem?

Theoretical Approach

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Step 1
Step 2
Step 3

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

Q: 3-Particles, What Is The Problem?

A: The configuration space (CS) for the 3BP is 9D and highly non-trivial ...

2019-09-02

└ Theoretical Approach

└ Theoretical Approach

1. Well, the configuration space for the 3BP is 9D and highly non-trivial ...

Theoretical Approach

Q: 3-Particles, What Is The Problem?
A: The configuration space (CS) for the 3BP is 9D and highly non-trivial ...

Theoretical Approach

Kajsa-My Blomdahl	
Introduction	
Theoretical Approach	
Step 1	
Step 2	
Step 3	
Effective Potentials	
Numerical Approach	
Scattering Model	
Results	
	<p>Q: 3-Particles, What Is The Problem?</p> <p>A: The configuration space (CS) for the 3BP is 9D and highly non-trivial ...</p> <p>Solution: Reduce the number of dimensions!</p>

Q: 3-Particles, What Is The Problem?

A: The configuration space (CS) for the 3BP is 9D and highly non-trivial ...

Solution: Reduce the number of dimensions!

A: The configuration space (CS) for the 3BP is 9D and highly non-trivial ...

Solution: Reduce the number of dimensions!

Solution: Reduce the number of dimensions!

2019-09-02

- └ Theoretical Approach
- └ Theoretical Approach

- └ Theoretical Approach

1. So what we want to do is to reduce the dimensionality of the problem

Theoretical Approach

Q: 3-Particles, What Is The Problem?

A: The configuration space (CS) for the 3BP is 9D and highly non-trivial ...

Solution: Reduce the number of dimensions!

Step 1: Relative Coordinates

Kajsa-My Blomdahl

Introduction

Theoretical Approach

Step 1

Step 2

Step 3

Effective Potentials

Numerical Approach

Scattering Model

Results

Introduction

Theoretical Approach

Step 1
Step 2
Step 3

Effective Potentials

Numerical Approach

Scattering Model

Results

- Separate out CoM by introducing relative coordinates

- 2019-09-02
 - └ Theoretical Approach
 - └ Step 1
 - └ Step 1: Relative Coordinates

└ Theoretical Approach

Step 1

└ Step 1: Relative Coordinates

Step 1: Relative Coordinates

- Separate out CoM by introducing relative coordinates

- Separate out CoM by introducing relative coordinates

1. The first step to reduce the number of D is to separate out the CoM by introducing relative coordinates.

Step 1: Relative Coordinates

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- Introduction
- Theoretical Approach
 - Step 1
 - Step 2
 - Step 3
- Effective Potentials
- Numerical Approach
- Scattering Model
- Results

- Separate out CoM by introducing relative coordinates
- CS → 6D

Navigation icons at the bottom right.

Results

- 2019-09-02

Theoretical Approach

Step 1

Step 1: Relative Coordinates

Step 1: Relative Coordinates

Separate out CoM by introducing relative coordinates

CS \rightarrow 6D

1. CoM motion decouples from the internal motion in the SE the configuration space is effectively reduced to 6D

Step 1: Relative Coordinates

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Introduction

Theoretical
Approach

Step 1

Step 2

Step 3

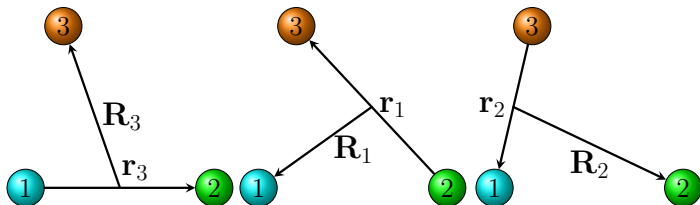
Effective
Potentials

Numerical
Approach

Scattering
Model

Results

- Separate out CoM by introducing relative coordinates
- Choice: Mass-normalized **Jacobi coordinates**
- CS \rightarrow 6D



2019-09-02

Theoretical Approach

Step 1

Step 1: Relative Coordinates

Step 1: Relative Coordinates

- Separate out CoM by introducing relative coordinates
- Choice: Mass-normalized **Jacobi coordinates**
- CS \rightarrow 6D



1. \mathbf{r} is the vector that connects two of the particles and \mathbf{R} connects the CoM of these two particles with the third particle
2. Particle permutations are easily performed using these coord.

Step 2: Hyperspherical Coordinates

2019-09-02

└ Theoretical Approach

└ Step 2

└ Step 2: Hyperspherical Coordinates

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Blomdahl

Introduction

Theoretical
Approach

Step 1

Step 2

Step 3

Effective
PotentialsNumerical
ApproachScattering
Model

Results

1. Step 2 in simplifying the problem of three particles is to introduce hyperspherical coordinates

Step 2: Hyperspherical Coordinates

Kajsa-My Blomdahl

Introduction

Theoretical Approach

- Step 1
- Step 2**
- Step 3

Effective Potentials

Numerical Approach

Scattering Model

Results

Theoretical Approach

Step 2

Effective Potentials

Numerical Approach

Scattering Model

Results

- Combine \mathbf{r}_k and \mathbf{R}_k into a 6D position vector in \mathbb{R}^6

- 2019-09-02
 - └ Theoretical Approach
 - └ Step 2
 - └ Step 2: Hyperspherical Coordinates

Step 2

- Combine \mathbf{r}_k and \mathbf{R}_k into a 6D position vector in \mathbb{R}^6

1. The general idea is to combine the components of the two Jacobi vectors into a single six-dimensional position vector \mathbf{q} , which represents a point in \mathbb{R}^6 .

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Introduction

Theoretical Approach

Step 1

Step 2

Effective Potentials

Numerical Approach

Scattering Model

Results

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

2019-09-02

└ Theoretical Approach

-Step 2

Step 2: Hyperspherical Coordinates

1. The hyperspherical coord. of this point are given by the hyperradius and five hyperangles Ω .
2. The hyperradial coordinate is both rotationally and permutationally invariant and is defined as the square root of the sum of the squared Jacobi vectors.
3. The hyperangles can be defined in many ways and I will not go in to the details here.

Step 2: Hyperspherical Coordinates

- Combine \mathbf{r}_k and \mathbf{R}_k into a 6D position vector in \mathbb{R}^6
 - Hyperspherical coordinates: ρ and Ω
- $$\rho = (\mathbf{r}^2 + \mathbf{R}^2)^{1/2}$$

Step 2: Hyperspherical Coordinates

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Step 1

Step 2

Step 3

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

- Combine \mathbf{r}_k and \mathbf{R}_k into a 6D position vector in \mathbb{R}^6
- Hyperspherical coordinates: ρ and Ω

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

- Separate internal and external coordinates

2019-09-02

└ Theoretical Approach

└ Step 2

└ Step 2: Hyperspherical Coordinates

Step 2: Hyperspherical Coordinates

- Combine \mathbf{r}_k and \mathbf{R}_k into a 6D position vector in \mathbb{R}^6
- Hyperspherical coordinates: ρ and Ω
 $\rho = (\mathbf{r}^2 + \mathbf{R}^2)^{1/2}$
- Separate internal and external coordinates

1. At any instant, three particles form a plane in \mathbb{R}^3 . We can define the internal motion of the particles within this plane in terms of the hyperradial coordinate (size) and two of the angles (shape and particle permutation). The three other angles relate rotations of this plane in a space fixed system.
2. The three other angles relate rotations of this plane in a space fixed system.

Results

- Combine \mathbf{r}_A and \mathbf{R}_B into a 6D position vector in \mathbb{R}^6
- Hyperspherical coordinates: ρ and Ω

$$\rho = (\mathbf{r}^2 + \mathbf{R}^2)^{1/2}$$
- Separate internal and external coordinates
- For $J = 0$ only **internal coordinates** matter \rightarrow 3D Schrödinger equation (SE)

Step 3: The Adiabatic Representation

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Blomdahl

Introduction

Theoretical
Approach

Step 1

Step 2

Step 3

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

Numerical Approach

Exact rep.

2019-09-02

Theoretical Approach

Step 3

Step 3: The Adiabatic Representation

Step 3: The Adiabatic Representation

Navigation icons: back, forward, etc.

1. Now we move on to the final step (in the simplification of the 3BP)

Step 3: The Adiabatic Representation

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Introduction

Theoretical
Approach

Step 1

Step 2

Step 3

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

- The hyperspherical SE:

$$\left(-\frac{1}{2\mu} \frac{\partial^2}{\partial \rho^2} + \frac{\Lambda^2 + \frac{15}{4}}{2\mu \rho^2} + V \right) \psi = E \psi$$

Numerical Approach

Exact rep.

2019-09-02

Theoretical Approach

Step 3

Step 3: The Adiabatic Representation

Step 3: The Adiabatic Representation

• The hyperspherical SE:

$$\left(-\frac{1}{2\mu} \frac{\partial^2}{\partial \rho^2} + \frac{\Lambda^2 + \frac{15}{4}}{2\mu \rho^2} + V \right) \psi = E \psi$$

Navigation icons: back, forward, search, etc.

1. After a clever rescaling of the wfn, the hyperspherical SE can be written like this

Step 3: The Adiabatic Representation

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Step 1

Step 2

Step 3

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

- The hyperspherical SE:

$$\left(-\frac{1}{2\mu} \frac{\partial^2}{\partial \rho^2} + \frac{\lambda^2 + \frac{15}{4}}{2\mu\rho^2} + V \right) \psi = E\psi$$

Numerical Approach

Exact rep.

2019-09-02

Theoretical Approach

Step 3

Step 3: The Adiabatic Representation

Step 3: The Adiabatic Representation

• The hyperspherical SE:

$$\left(-\frac{1}{2\mu} \frac{\partial^2}{\partial \rho^2} + \frac{\lambda^2 + \frac{15}{4}}{2\mu\rho^2} + V \right) \psi = E\psi$$

Navigation icons: back, forward, search, etc.

1. Where lambda is the generalized angular momenta

Step 3: The Adiabatic Representation

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Step 1

Step 2

Step 3

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

- The hyperspherical SE:

$$\left(-\frac{1}{2\mu} \frac{\partial^2}{\partial \rho^2} + \frac{\Lambda^2 + \frac{15}{4}}{2\mu\rho^2} + V \right) \psi = E\psi$$

- Trick: Treat ρ as an adiabatic parameter!

Numerical Approach

Exact rep.

2019-09-02

Theoretical Approach

Step 3

Step 3: The Adiabatic Representation

Step 3: The Adiabatic Representation

- The hyperspherical SE:

$$\left(-\frac{1}{2\mu} \frac{\partial^2}{\partial \rho^2} + \frac{\Lambda^2 + \frac{15}{4}}{2\mu\rho^2} + V \right) \psi = E\psi$$

- Trick: Treat ρ as an adiabatic parameter!

Numerical Approach

Exact rep.

1. Now, the trick is to treat the hyperradius as an adiabatic parameter!
2. That is, we fix ρ in a Born-Oppenheimer like manner

Step 3: The Adiabatic Representation

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Step 1

Step 2

Step 3

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

- The hyperspherical SE:

$$\left(-\frac{1}{2\mu} \frac{\partial^2}{\partial \rho^2} + \frac{\Lambda^2 + \frac{15}{4}}{2\mu\rho^2} + V \right) \psi = E\psi$$

- Trick: Treat ρ as an adiabatic parameter!
- Solve the adiabatic eq.

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

Numerical Approach

Exact rep.

2019-09-02

Theoretical Approach

Step 3

Step 3: The Adiabatic Representation

Step 3: The Adiabatic Representation

- The hyperspherical SE:

$$\left(-\frac{1}{2\mu} \frac{\partial^2}{\partial \rho^2} + \frac{\Lambda^2 + \frac{15}{4}}{2\mu\rho^2} + V \right) \psi = E\psi$$

- Trick: Treat ρ as an adiabatic parameter!
- Solve the adiabatic eq.

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

Numerical Approach

Exact rep.

1. And solve the remaining adiabatic eigenvalue equation

Step 3: The Adiabatic Representation

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Step 1

Step 2

Step 3

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

- The hyperspherical SE:

$$\left(-\frac{1}{2\mu} \frac{\partial^2}{\partial \rho^2} + \frac{\Lambda^2 + \frac{15}{4}}{2\mu\rho^2} + V \right) \psi = E\psi$$

- Trick: Treat ρ as an adiabatic parameter!
- Solve the adiabatic eq.

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

- \rightarrow 3-body BO-like potential

Numerical Approach

Exact rep.

2019-09-02

Theoretical Approach

Step 3

Step 3: The Adiabatic Representation

1. In this way we obtain the three-body equivalent of a BO potential.

Step 3: The Adiabatic Representation

- The hyperspherical SE:

$$\left(-\frac{1}{2\mu} \frac{\partial^2}{\partial \rho^2} + \frac{\Lambda^2 + \frac{15}{4}}{2\mu\rho^2} + V \right) \psi = E\psi$$

- Trick: Treat ρ as an adiabatic parameter!
- Solve the adiabatic eq.

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

- \rightarrow 3-body BO-like potential

Step 3: The Adiabatic Representation cont.

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Step 1

Step 2

Step 3

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

SE

- The total wave function is represented in terms of adiabatic states

$$\psi_n(\rho, \Omega) = \sum_{\nu=0}^{\infty} F_{n\nu}(\rho) \Phi_{\nu}(\rho; \Omega)$$

2019-09-02

└ Theoretical Approach

└ Step 3

└ Step 3: The Adiabatic Representation cont.

Step 3: The Adiabatic Representation cont.

- The total wave function is represented in terms of adiabatic states

$$\psi_n(\rho, \Omega) = \sum_{\nu=0}^{\infty} F_{n\nu}(\rho) \Phi_{\nu}(\rho; \Omega)$$

1. Now, in this way the total wfn can be represented by a sum of adiabatic states

Step 3: The Adiabatic Representation cont.

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Step 1

Step 2

Step 3

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

SE

- The total wave function is represented in terms of **adiabatic states**

$$\psi_n(\rho, \Omega) = \sum_{\nu=0}^{\infty} F_{n\nu}(\rho) \Phi_{\nu}(\rho; \Omega)$$

2019-09-02

└ Theoretical Approach

└ Step 3

└ Step 3: The Adiabatic Representation cont.

1. (shown in red)

Step 3: The Adiabatic Representation cont.

- The total wave function is represented in terms of **adiabatic states**

$$\psi_n(\rho, \Omega) = \sum_{\nu=0}^{\infty} F_{n\nu}(\rho) \Phi_{\nu}(\rho; \Omega)$$

Step 3: The Adiabatic Representation cont.

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Step 1

Step 2

Step 3

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

SE

- The total wave function is represented in terms of adiabatic states

$$\psi_n(\rho, \Omega) = \sum_{\nu=0}^{\infty} F_{n\nu}(\rho) \Phi_{\nu}(\rho; \Omega)$$

2019-09-02

Theoretical Approach

Step 3

Step 3: The Adiabatic Representation cont.

Step 3: The Adiabatic Representation cont.

- The total wave function is represented in terms of adiabatic states

$$\psi_n(\rho, \Omega) = \sum_{\nu=0}^{\infty} F_{n\nu}(\rho) \Phi_{\nu}(\rho; \Omega)$$

- If we substitute this sum into the 3-b SE (click on link)

Step 3: The Adiabatic Representation cont.

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Step 1

Step 2

Step 3

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

- The total wave function is represented in terms of adiabatic states

$$\psi_n(\rho, \Omega) = \sum_{\nu=0}^{\infty} F_{n\nu}(\rho) \Phi_{\nu}(\rho; \Omega)$$

- The hyperradial eigenvalue equation

$$\left(-\frac{1}{2\mu} \frac{\partial^2}{\partial \rho^2} + U_{\mu} - \frac{1}{2\mu} Q_{\mu\mu} \right) F_{n\mu} - \frac{1}{2\mu} \left(\sum_{\nu \neq \mu} 2P_{\mu\nu} \frac{\partial}{\partial \rho} + Q_{\mu\nu} \right) F_{n\nu} = E_n F_{n\mu}$$

SE

2019-09-02

Theoretical Approach

Step 3

Step 3: The Adiabatic Representation cont.

- We will get an exact representation of the 3-body SE if all couplings are included

Step 3: The Adiabatic Representation cont.

- The total wave function is represented in terms of adiabatic states

$$\psi_n(\rho, \Omega) = \sum_{\nu=0}^{\infty} F_{n\nu}(\rho) \Phi_{\nu}(\rho; \Omega)$$

- The hyperradial eigenvalue equation

$$\left(-\frac{1}{2\mu} \frac{\partial^2}{\partial \rho^2} + U_{\mu} - \frac{1}{2\mu} Q_{\mu\mu} \right) F_{n\mu} - \frac{1}{2\mu} \left(\sum_{\nu \neq \mu} 2P_{\mu\nu} \frac{\partial}{\partial \rho} + Q_{\mu\nu} \right) F_{n\nu} = E_n F_{n\mu}$$

Step 3: The Adiabatic Representation cont.

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Step 1

Step 2

Step 3

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

- The total wave function is represented in terms of adiabatic states

$$\psi_n(\rho, \Omega) = \sum_{\nu=0}^{\infty} F_{n\nu}(\rho) \Phi_{\nu}(\rho; \Omega)$$

- The hyperradial eigenvalue equation

$$\left(-\frac{1}{2\mu} \frac{\partial^2}{\partial \rho^2} + U_{\mu} - \frac{1}{2\mu} Q_{\mu\mu} \right) F_{n\mu} - \frac{1}{2\mu} \left(\sum_{\nu \neq \mu} 2P_{\mu\nu} \frac{\partial}{\partial \rho} + Q_{\mu\nu} \right) F_{n\nu} = E_n F_{n\mu}$$

SE

2019-09-02

Theoretical Approach

Step 3

Step 3: The Adiabatic Representation cont.

- The focus of my work has been on this part of this eq.

Step 3: The Adiabatic Representation cont.

- The total wave function is represented in terms of adiabatic states

$$\psi_n(\rho, \Omega) = \sum_{\nu=0}^{\infty} F_{n\nu}(\rho) \Phi_{\nu}(\rho; \Omega)$$

- The hyperradial eigenvalue equation

$$\left(-\frac{1}{2\mu} \frac{\partial^2}{\partial \rho^2} + U_{\mu} - \frac{1}{2\mu} Q_{\mu\mu} \right) F_{n\mu} - \frac{1}{2\mu} \left(\sum_{\nu \neq \mu} 2P_{\mu\nu} \frac{\partial}{\partial \rho} + Q_{\mu\nu} \right) F_{n\nu} = E_n F_{n\mu}$$

Step 3: The Adiabatic Representation cont.

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Step 1

Step 2

Step 3

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

- The total wave function is written in terms of a set of three-body effective potentials

$$W_\nu(\rho) = U_\nu(\rho) - \frac{1}{2\mu} Q_{\nu\nu}(\rho) = U_\nu(\rho) - \frac{1}{2\mu} P_{\nu\nu}^2(\rho)$$

- The hyperradial eigenvalue equation

$$\left(-\frac{1}{2\mu} \frac{\partial^2}{\partial \rho^2} + U_\mu - \frac{1}{2\mu} Q_{\mu\mu} \right) F_{n\mu} - \frac{1}{2\mu} \left(\sum_{\nu \neq \mu} 2P_{\mu\nu} \frac{\partial}{\partial \rho} + Q_{\mu\nu} \right) F_{n\nu} = E_n F_{n\mu}$$

SE

2019-09-02

Theoretical Approach

Step 3

Step 3: The Adiabatic Representation cont.

1. In the adiabatic approximation we define the three-body effective potentials are defined as
2. These potentials are used for determining the single channel solutions of (below)

Step 3: The Adiabatic Representation cont.

- The total wave function is represented in terms of adiabatic states

$$\Psi_\alpha(\rho, \Omega) = \sum_{\nu=0}^{\infty} F_{\nu\alpha}(\rho) \Phi_\nu(\rho, \Omega)$$

- The hyperradial eigenvalue equation

$$\left(-\frac{1}{2\mu} \frac{\partial^2}{\partial \rho^2} + U_\mu - \frac{1}{2\mu} Q_{\mu\mu} \right) F_{n\mu} - \frac{1}{2\mu} \left(\sum_{\nu \neq \mu} 2P_{\mu\nu} \frac{\partial}{\partial \rho} + Q_{\mu\nu} \right) F_{n\nu} = E_n F_{n\mu}$$

Step 3: The Adiabatic Representation cont.

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Step 1

Step 2

Step 3

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

- The total wave function is written in terms of a
a

Three-body effective potentials

$$W_\nu(\rho) = U_\nu(\rho) - \frac{1}{2\mu} Q_{\nu\nu}(\rho) \approx U_\nu(\rho) - \frac{1}{2\mu} \cancel{P_{\nu\nu}^2(\rho)}$$

- The hyperradial eigenvalue equation

$$\left(-\frac{1}{2\mu} \frac{\partial^2}{\partial \rho^2} + U_\mu - \frac{1}{2\mu} Q_{\mu\mu} \right) F_{n\mu} - \frac{1}{2\mu} \left(\sum_{\nu \neq \mu} 2P_{\mu\nu} \frac{\partial}{\partial \rho} + Q_{\mu\nu} \right) F_{n\nu} = E_n F_{n\mu}$$

SE

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Theoretical Approach

Step 3

Step 3: The Adiabatic Representation cont.

Step 3: The Adiabatic Representation cont.

- The total wave function is represented in terms of adiabatic states

$$\psi_s(\rho, \Omega) = \sum_{n=0}^{\infty} F_{sn}(\rho) \Phi_n(\rho, \Omega)$$

- The hyperradial eigenvalue equation

$$\left(-\frac{1}{2\mu} \frac{\partial^2}{\partial \rho^2} + U_\mu - \frac{1}{2\mu} Q_{\mu\mu} \right) F_{n\mu} - \frac{1}{2\mu} \left(\sum_{\nu \neq \mu} 2P_{\mu\nu} \frac{\partial}{\partial \rho} + Q_{\mu\nu} \right) F_{n\nu} = E_n F_{n\mu}$$

1. In this talk I will not explain how the second term is calculated, in the calculations I have performed it is small and we will ignore it from here on

Convergence In the Asymptotic Limit

2019-09-02

- Effective Potentials
 - The Asymptotic Limit
 - Convergence In the Asymptotic Limit

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Introduction

Theoretical
Approach

Effective
Potentials

**The Asymptotic
Limit**

Intermediate
Region
Analytical
Model

Numerical
Approach

Scattering
Model

Results

1. (The following discussion concerns short-ranged two-body interactions, where $|a| \gg r_0$)
2. The behaviour of the 3-b potentials in the asymptotic limit, (i.e., when the hyperradius is much larger than the magnitude a) depend on the sign of a .

Convergence In the Asymptotic Limit

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Introduction

Theoretical
Approach

Effective
Potentials

The Asymptotic
Limit

Intermediate
Region
Analytical
Model

Numerical
Approach

Scattering
Model

Results

For $a < 0$:

$$W_\nu(\rho) \xrightarrow{\rho \rightarrow \infty} \frac{\lambda(\lambda + 4) + \frac{15}{4}}{2\mu\rho^2}$$

2019-09-02

Effective Potentials
└─ The Asymptotic Limit
 └─ Convergence In the Asymptotic Limit

Convergence In the Asymptotic Limit

For $a < 0$:

$$W_\nu(\rho) \xrightarrow{\rho \rightarrow \infty} \frac{\lambda(\lambda + 4) + \frac{15}{4}}{2\mu\rho^2}$$

1. When a has a negative sign there is no weakly bound dimer and the lowest effective potential will converge to the three-body continuum channels, i.e., the kinetic energy for three free particles.

Convergence In the Asymptotic Limit

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Introduction

Theoretical
Approach

Effective
Potentials

The Asymptotic
Limit

Intermediate
Region
Analytical
Model

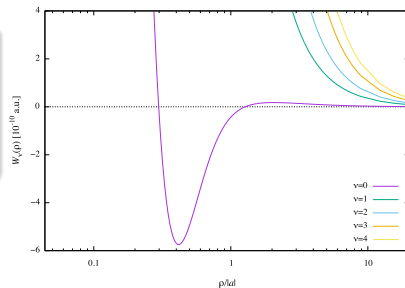
Numerical
Approach

Scattering
Model

Results

For $a < 0$:

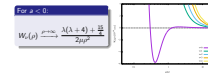
$$W_\nu(\rho) \xrightarrow{\rho \rightarrow \infty} \frac{\lambda(\lambda + 4) + \frac{15}{4}}{2\mu\rho^2}$$



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- └ Effective Potentials
 - └ The Asymptotic Limit
 - └ Convergence In the Asymptotic Limit

Convergence In the Asymptotic Limit



Convergence In the Asymptotic Limit

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Introduction

Theoretical
Approach

Effective
Potentials

The Asymptotic
Limit

Intermediate
Region
Analytical
Model

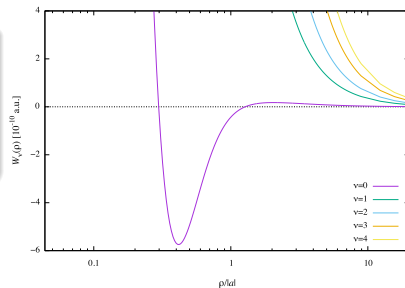
Numerical
Approach

Scattering
Model

Results

For $a < 0$:

$$W_\nu(\rho) \xrightarrow{\rho \rightarrow \infty} \frac{\lambda(\lambda + 4) + \frac{15}{4}}{2\mu\rho^2}$$



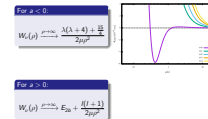
For $a > 0$:

$$W_\nu(\rho) \xrightarrow{\rho \rightarrow \infty} E_{2b} + \frac{l(l + 1)}{2\mu\rho^2}$$

2019-09-02

- Effective Potentials
 - The Asymptotic Limit
 - Convergence In the Asymptotic Limit

Convergence In the Asymptotic Limit

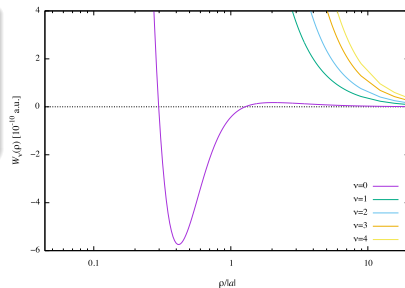


1. However, for systems of 3 identical bosons with a pair-wise attraction that is strong enough to support 2-body bound states, one 3-body effective potential curve will converge asymptotically to each two-body bound state.

Convergence In the Asymptotic Limit

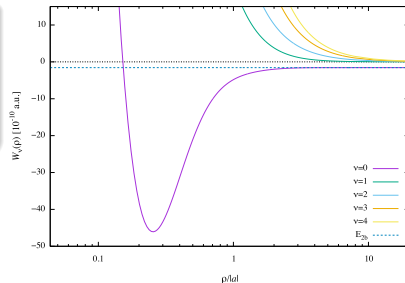
For $a < 0$:

$$W_\nu(\rho) \xrightarrow{\rho \rightarrow \infty} \frac{\lambda(\lambda + 4) + \frac{15}{4}}{2\mu\rho^2}$$



For $a > 0$:

$$W_\nu(\rho) \xrightarrow{\rho \rightarrow \infty} E_{2b} + \frac{l(l + 1)}{2\mu\rho^2}$$

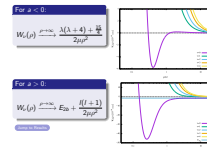


[Jump to Results](#)

2019-09-02

- Effective Potentials
 - The Asymptotic Limit
 - Convergence In the Asymptotic Limit

Convergence In the Asymptotic Limit



Convergence In the Intermediate Region

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Introduction

Theoretical
Approach

Effective
Potentials

The Asymptotic
Limit

**Intermediate
Region**

Analytical
Model

Numerical
Approach

Scattering
Model

Results

Intermediate Interaction Range

$$r_0 \ll \rho \ll |a|$$

[Jump to Results](#)

2019-09-02

Effective Potentials
Intermediate Region
Convergence In the Intermediate Region

Convergence In the Intermediate Region

Intermediate Interaction Range

$$r_0 \ll \rho \ll |a|$$

[Jump to Results](#)

1. Efimov physics comes into play in the intermediate region.
2. In this region the three-body effective potentials are modified by the Efimov physics. It can lead to both attractive and repulsive effective potentials.

Convergence In the Intermediate Region

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Introduction

Theoretical
Approach

Effective
Potentials

The Asymptotic
Limit

Intermediate
Region
Analytical
Model

Numerical
Approach

Scattering
Model

Results

Intermediate Interaction Range

$$r_0 \ll \rho \ll |a|$$

The Lowest Potential's Convergent Form (3 Identical Bosons)

$$W_\nu(\rho) = -\frac{s_0^2 + \frac{1}{4}}{2\mu\rho^2}$$

[Jump to Results](#)

2019-09-02

- Effective Potentials
 - Intermediate Region
 - Convergence In the Intermediate Region

Convergence In the Intermediate Region

Intermediate Interaction Range

$$r_0 \ll \rho \ll |a|$$

The Lowest Potential's Convergent Form (3 Identical Bosons)

$$W_\nu(\rho) = -\frac{s_0^2 + \frac{1}{4}}{2\mu\rho^2}$$

[Jump to Results](#)

1. For 3 identical bosons the effective potential will be attractive and is responsible for the Efimov Effect!

Convergence In the Intermediate Region

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Introduction

Theoretical
Approach

Effective
Potentials

The Asymptotic
Limit

Intermediate
Region
Analytical
Model

Numerical
Approach

Scattering
Model

Results

Intermediate Interaction Range

$$r_0 \ll \rho \ll |a|$$

The Lowest Potential's Convergent Form (3 Identical Bosons)

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[Jump to Results](#)

2019-09-02

- Effective Potentials
 - Intermediate Region
 - Convergence In the Intermediate Region

Convergence In the Intermediate Region

Intermediate Interaction Range

$$r_0 \ll \rho \ll |a|$$

The Lowest Potential's Convergent Form (3 Identical Bosons)

$$W_\nu(\rho) = -\frac{s_0^2 + \frac{1}{4}}{2\mu\rho^2}$$

[Jump to Results](#)

1. And is responsible for the Efimov Effect!

Convergence In the Intermediate Region

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Introduction

Theoretical
Approach

Effective
Potentials

The Asymptotic
Limit

Intermediate
Region
Analytical
Model

Numerical
Approach

Scattering
Model

Results

Intermediate Interaction Range

$$r_0 \ll \rho \ll |a|$$

The Lowest Potential's Convergent Form (3 Identical Bosons)

$$W_\nu(\rho) = -\frac{s_0^2 + \frac{1}{4}}{2\mu\rho^2}$$

Universal Constant (3 Identical Bosons)

$$s_0 \simeq 1.00624$$

[Jump to Results](#)

2019-09-02

- Effective Potentials
 - Intermediate Region
 - Convergence In the Intermediate Region

Convergence In the Intermediate Region

Intermediate Interaction Range

$$r_0 \ll \rho \ll |a|$$

The Lowest Potential's Convergent Form (3 Identical Bosons)

$$W_\nu(\rho) = -\frac{s_0^2 + \frac{1}{4}}{2\mu\rho^2}$$

Universal Constant (3 Identical Bosons)

$$s_0 \simeq 1.00624$$

[Jump to Results](#)

1. The universal constant s_0 sets the size and energy scaling of succeeding Efimov states.

Analytic Model

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Introduction

Theoretical
Approach

Effective
Potentials

The Asymptotic
Limit
Intermediate
Region

**Analytical
Model**

Numerical
Approach

Scattering
Model

Results

Jump to Results

2019-09-02

Effective Potentials
Analytical Model
Analytic Model

Analytic Model

1. We can obtain a similar result analytically by instead of solving the SE we solve the coupled Faddeev equations

Analytic Model

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Introduction

Theoretical
Approach

Effective
Potentials

The Asymptotic
Limit

Intermediate
Region

**Analytical
Model**

Numerical
Approach

Scattering
Model

Results

- The adiabatic potentials ν_n can be determined analytically through the transcendental equation

$$\sqrt{\nu_n} \cos\left(\sqrt{\nu_n} \frac{\pi}{2}\right) - \frac{8}{\sqrt{3}} \sin\left(\sqrt{\nu_n} \frac{\pi}{6}\right) = \sqrt{2} \frac{\rho}{a} \sin\left(\sqrt{\nu_n} \frac{\pi}{2}\right)$$

Jump to Results

2019-09-02

Effective Potentials
Analytical Model
Analytic Model

1. We then obtain the adiabatic potential ν through the transcendental eq.

Analytic Model

• The adiabatic potentials ν_n can be determined analytically through the transcendental equation

$$\sqrt{\nu_n} \cos\left(\sqrt{\nu_n} \frac{\pi}{2}\right) - \frac{8}{\sqrt{3}} \sin\left(\sqrt{\nu_n} \frac{\pi}{6}\right) = \sqrt{2} \frac{\rho}{a} \sin\left(\sqrt{\nu_n} \frac{\pi}{2}\right)$$

Jump to Results

Analytic Model

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Effective
Potentials

The Asymptotic
Limit

Intermediate
Region

**Analytical
Model**

Numerical
Approach

Scattering
Model

Results

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Jump to Results

2019-09-02

Effective Potentials
Analytical Model
Analytic Model

- This adiabatic potential is a function of ρ/a

Analytic Model

♦ The adiabatic potentials ν_n can be determined analytically through the transcendental equation

$$\sqrt{\nu_n} \cos\left(\sqrt{\nu_n} \frac{\pi}{2}\right) - \frac{8}{\sqrt{3}} \sin\left(\sqrt{\nu_n} \frac{\pi}{6}\right) = \sqrt{2} \frac{\rho}{a} \sin\left(\sqrt{\nu_n} \frac{\pi}{2}\right)$$

Jump to Results

Analytic Model

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Effective
Potentials

The Asymptotic
Limit

Intermediate
Region

Analytical
Model

Numerical
Approach

Scattering
Model

Results

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$$\sqrt{\nu_n} \cos\left(\sqrt{\nu_n} \frac{\pi}{2}\right) - \frac{8}{\sqrt{3}} \sin\left(\sqrt{\nu_n} \frac{\pi}{6}\right) = \sqrt{2} \frac{\rho}{a} \sin\left(\sqrt{\nu_n} \frac{\pi}{2}\right)$$

- Three-body effective potential

$$W_\nu(\rho/a) = \frac{(\nu_n(\rho/a) - \frac{1}{4})}{2\mu\rho^2}$$

[Jump to Results](#)

2019-09-02

Effective Potentials
Analytical Model
Analytic Model

- It is related to the 3-body potential
- In the result section I will compare these solutions to my numerically calculated potentials.

Analytic Model

- The adiabatic potentials ν_n can be determined analytically through the transcendental equation

$$\sqrt{\nu_n} \cos\left(\sqrt{\nu_n} \frac{\pi}{2}\right) - \frac{8}{\sqrt{3}} \sin\left(\sqrt{\nu_n} \frac{\pi}{6}\right) = \sqrt{2} \frac{\rho}{a} \sin\left(\sqrt{\nu_n} \frac{\pi}{2}\right)$$

- Three-body effective potential

$$W_\nu(\rho/a) = \frac{(\nu_n(\rho/a) - \frac{1}{4})}{2\mu\rho^2}$$

Numerical Approach; B-spline Collocation

Task = ?

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└ Numerical Approach

└ Numerical Approach; B-spline Collocation

Numerical Approach; B-spline Collocation

Task = ?

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Introduction

Theoretical
Approach

Effective
Potentials

**Numerical
Approach**

Scattering
Model

Results

Numerical Approach; B-spline Collocation

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Introduction

Theoretical
Approach

Effective
Potentials

**Numerical
Approach**

Scattering
Model

Results

Task = Find $W_\nu(\rho)$!

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└ Numerical Approach

└ Numerical Approach; B-spline Collocation

Numerical Approach; B-spline Collocation

Task = Find $W_\nu(\rho)$!

Numerical Approach; B-spline Collocation

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Introduction

Theoretical
Approach

Effective
Potentials

**Numerical
Approach**

Scattering
Model

Results

First: Find a Basis

2019-09-02

└ Numerical Approach

└ Numerical Approach; B-spline Collocation

Numerical Approach; B-spline Collocation

First: Find a Basis

Numerical Approach; B-spline Collocation

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Introduction

Theoretical
Approach

Effective
Potentials

**Numerical
Approach**

Scattering
Model

Results

First: Find a Basis

- $\varphi_{lm} = \varphi_{1l}(\theta)\varphi_{2m}(\phi)$

2019-09-02

└ Numerical Approach

└ Numerical Approach; B-spline Collocation

Numerical Approach; B-spline Collocation

First: Find a Basis

- $\varphi_{lm} = \varphi_{1l}(\theta)\varphi_{2m}(\phi)$

Numerical Approach; B-spline Collocation

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Blomdahl

Introduction

Theoretical
Approach

Effective
Potentials

**Numerical
Approach**

Scattering
Model

Results

First: Find a Basis

- $\varphi_{lm} = \varphi_{1l}(\theta)\varphi_{2m}(\phi)$

Then: Expand

2019-09-02

└ Numerical Approach

└ Numerical Approach; B-spline Collocation

Numerical Approach; B-spline Collocation

First: Find a Basis

• $\varphi_{lm} = \varphi_{1l}(\theta)\varphi_{2m}(\phi)$

Then: Expand

Numerical Approach; B-spline Collocation

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Blomdahl

Introduction

Theoretical
Approach

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

First: Find a Basis

- $\varphi_{lm} = \varphi_{1l}(\theta)\varphi_{2m}(\phi)$

Then: Expand

- $\Phi_\nu(\rho; \theta, \phi) = \sum_{l,m}^{L,M} c_{lm} \varphi_{lm}$

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└ Numerical Approach

└ Numerical Approach; B-spline Collocation

Numerical Approach; B-spline Collocation

First: Find a Basis

- $\varphi_{lm} = \varphi_{1l}(\theta)\varphi_{2m}(\phi)$

Then: Expand

- $\Phi_\nu(\rho; \theta, \phi) = \sum_{l,m}^{L,M} c_{lm} \varphi_{lm}$

Numerical Approach; B-spline Collocation

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Blomdahl

Introduction

Theoretical
Approach

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

First: Find a Basis

- $\varphi_{lm} = \varphi_{1l}(\theta)\varphi_{2m}(\phi)$

Then: Expand

- $\Phi_\nu(\rho; \theta, \phi) = \sum_{l,m}^{L,M} c_{lm} \varphi_{lm}$

Next: Substitute Φ_ν
into Eq. (4)

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└ Numerical Approach

└ Numerical Approach; B-spline Collocation

Numerical Approach; B-spline Collocation

First: Find a Basis

Then: Expand

Next: Substitute Φ_ν
into Eq. (4)

- $\varphi_{lm} = \varphi_{1l}(\theta)\varphi_{2m}(\phi)$
- $\Phi_\nu(\rho; \theta, \phi) = \sum_{l,m}^{L,M} c_{lm} \varphi_{lm}$

Numerical Approach; B-spline Collocation

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Introduction

Theoretical
Approach

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

First: Find a Basis

- $\varphi_{lm} = \varphi_{1l}(\theta)\varphi_{2m}(\phi)$

Then: Expand

- $\Phi_\nu(\rho; \theta, \phi) = \sum_{l,m}^{L,M} c_{lm} \varphi_{lm}$

Next: Substitute Φ_ν
into Eq. (4)

- $\mathbf{H}_{\text{ad}} \mathbf{c} = \mathbf{U} \mathbf{B} \mathbf{c}$

2019-09-02

└ Numerical Approach

└ Numerical Approach; B-spline Collocation

Numerical Approach; B-spline Collocation

First: Find a Basis

Then: Expand

Next: Substitute Φ_ν
into Eq. (4)

• $\varphi_{lm} = \varphi_{1l}(\theta)\varphi_{2m}(\phi)$

• $\Phi_\nu(\rho; \theta, \phi) = \sum_{l,m}^{L,M} c_{lm} \varphi_{lm}$

• $\mathbf{H}_{\text{ad}} \mathbf{c} = \mathbf{U} \mathbf{B} \mathbf{c}$

Finally: Solve the Generalized Eigenvalue Eq.

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First: Find a Basis

- $\varphi_{lm} = \varphi_{1l}(\theta)\varphi_{2m}(\phi)$

Then: Expand

- $\Phi_\nu(\rho; \theta, \phi) = \sum_{l,m}^{L,M} c_{lm} \varphi_{lm}$

Next: Substitute Φ_ν into Eq. (4)

- $\mathbf{H}_{ad}\mathbf{c} = U\mathbf{B}\mathbf{c}$

Finally: Solve the Generalized Eigenvalue Eq.

- $W(\rho) \approx U(\rho)$

Scattering Model

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Blomdahl

Introduction

Theoretical
Approach

Effective
Potentials

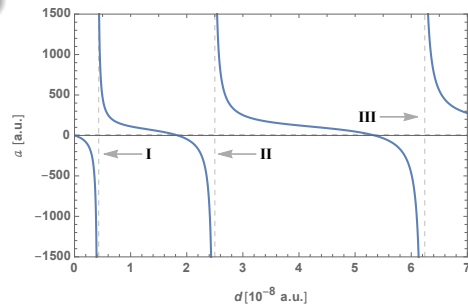
Numerical
Approach

Scattering
Model

Results

Masses

$$m = m(\text{Rubidium} - 87)$$



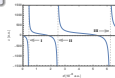
2019-09-02

Scattering Model

Scattering Model

Scattering Model

Masses
 $m = m(\text{Rubidium} - 87)$



Scattering Model

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Effective
Potentials

Numerical
Approach

Scattering
Model

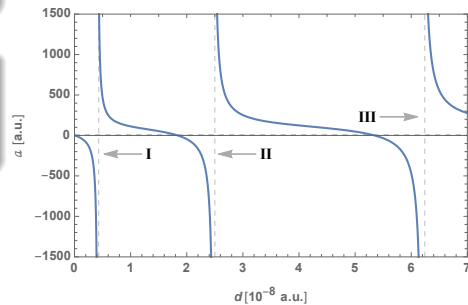
Results

Masses

$$m = m(\text{Rubidium} - 87)$$

Assumption

$$V(\rho, \theta, \psi) = v(r_{12}) + v(r_{23}) + v(r_{31})$$



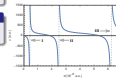
2019-09-02

Scattering Model

Scattering Model

Scattering Model

Masses
 $m = m(\text{Rubidium} - 87)$
Assumption
 $V(\rho, \theta, \psi) = v(r_{12}) + v(r_{23}) + v(r_{31})$



Scattering Model

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

Masses

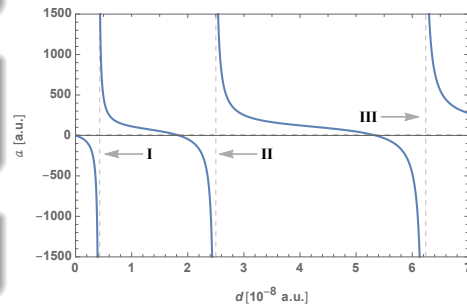
$$m = m(\text{Rubidium} - 87)$$

Assumption

$$V(\rho, \theta, \psi) = v(r_{12}) + v(r_{23}) + v(r_{31})$$

2B Model Potential

$$v(r) = d \cosh^{-2}(r/r_0)$$

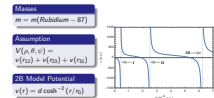


2019-09-02

Scattering Model

Scattering Model

Scattering Model



Scattering Model

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Introduction

Theoretical
Approach

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

Masses

$$m = m(\text{Rubidium} - 87)$$

Assumption

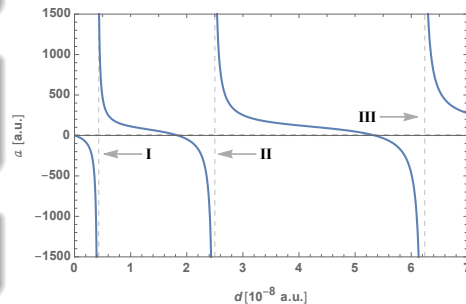
$$V(\rho, \theta, \psi) = v(r_{12}) + v(r_{23}) + v(r_{31})$$

2B Model Potential

$$v(r) = d \cosh^{-2}(r/r_0)$$

Interaction Range

$$r_0 = 55 \text{ a.u.}$$



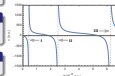
2019-09-02

└ Scattering Model

└ Scattering Model

Scattering Model

Masses
$m = m(\text{Rubidium} - 87)$
Assumption
$V(\rho, \theta, \psi) = v(r_{12}) + v(r_{23}) + v(r_{31})$
2B Model Potential
$v(r) = d \cosh^{-2}(r/r_0)$
Interaction Range
$r_0 = 55 \text{ a.u.}$



Convergence and Accuracy

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Introduction

Theoretical
Approach

Effective
Potentials

Numerical
Approach

Scattering
Model

Results

Convergence
and Accuracy
Comparison to
the Analytical
Model

- For $a \rightarrow \pm\infty$ we expect that the lowest effective potential curve will converge towards the Efimovian form
- This behaviour is easier to recognize if the potentials are multiplied by $2\mu\rho^2$ and plotted as

$$\xi(\rho) = 2\mu\rho^2 W_\nu(\rho) + \frac{1}{4} \quad (1)$$

since these curves should approach the universal value $-s_0^2 (\simeq -1.0125)$ in the intermediate region

To Figures

2019-09-02

Results
Convergence and Accuracy
Convergence and Accuracy

Convergence and Accuracy

- For $a \rightarrow \pm\infty$ we expect that the lowest effective potential curve will converge towards the Efimovian form
 - This behaviour is easier to recognize if the potentials are multiplied by $2\mu\rho^2$ and plotted as
- $$\xi(\rho) = 2\mu\rho^2 W_\nu(\rho) + \frac{1}{4} \quad (1)$$
- since these curves should approach the universal value $-s_0^2 (\simeq -1.0125)$ in the intermediate region

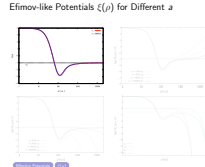
Efimov-like Potentials $\xi(\rho)$ for Different a

2019-09-02

Results

Convergence and Accuracy

Efimov-like Potentials $\xi(\rho)$ for Different a



Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

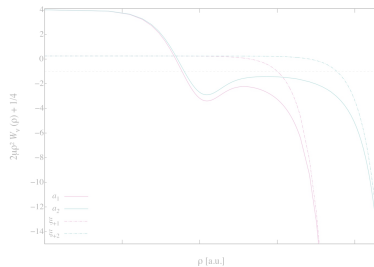
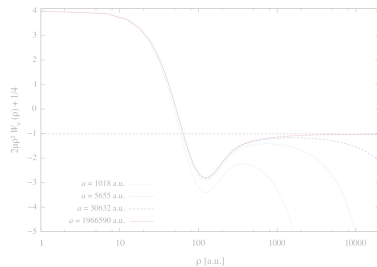
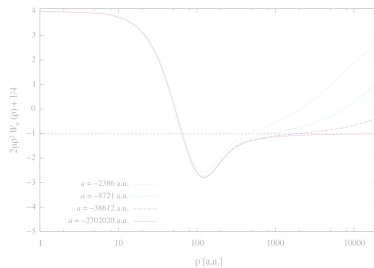
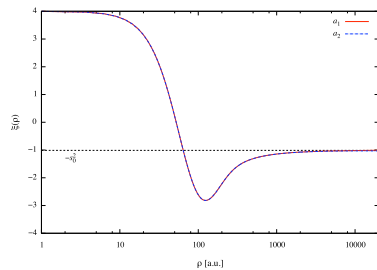
Effective
Potentials

Numerical
Approach

Scattering
Model

Results

Convergence
and Accuracy
Comparison to
the Analytical
Model



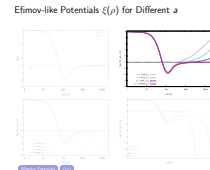
Effective Potentials

$\xi(\rho)$

Efimov-like Potentials $\xi(\rho)$ for Different a

2019-09-02

- Results
 - Convergence and Accuracy
 - Efimov-like Potentials $\xi(\rho)$ for Different a



Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

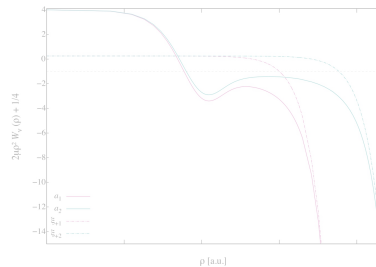
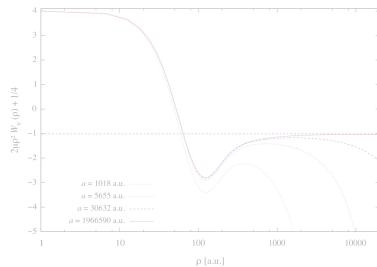
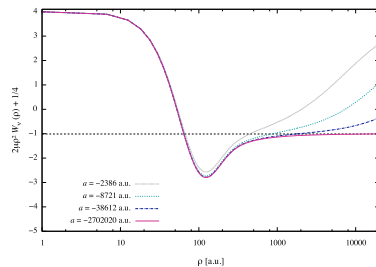
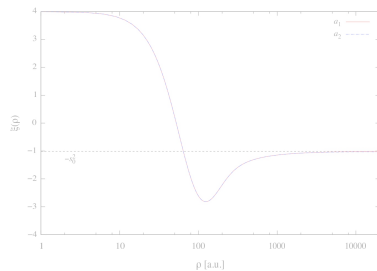
Effective
Potentials

Numerical
Approach

Scattering
Model

Results

Convergence
and Accuracy
Comparison to
the Analytical
Model



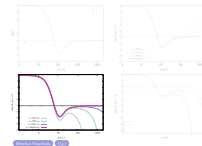
Effective Potentials $\xi(\rho)$

Efimov-like Potentials $\xi(\rho)$ for Different a

2019-09-02

- Results
 - Convergence and Accuracy
 - Efimov-like Potentials $\xi(\rho)$ for Different a

Efimov-like Potentials $\xi(\rho)$ for Different a



Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

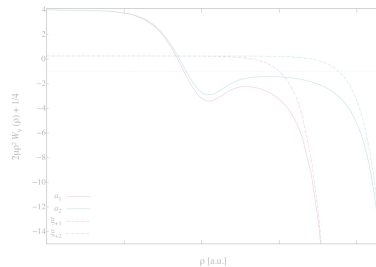
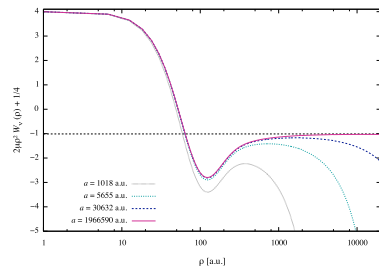
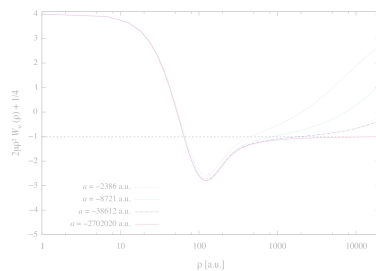
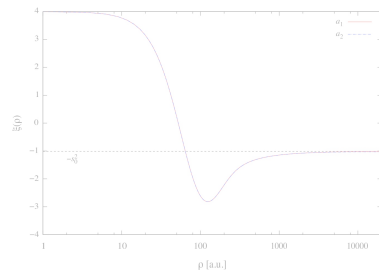
Effective
Potentials

Numerical
Approach

Scattering
Model

Results

Convergence
and Accuracy
Comparison to
the Analytical
Model



Effective Potentials

$\xi(\rho)$

Efimov-like Potentials $\xi(\rho)$ for Different a

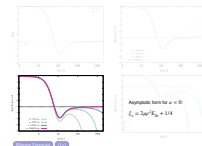
2019-09-02

Results

Convergence and Accuracy

Efimov-like Potentials $\xi(\rho)$ for Different a

Efimov-like Potentials $\xi(\rho)$ for Different a



Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

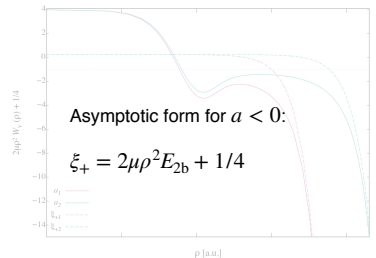
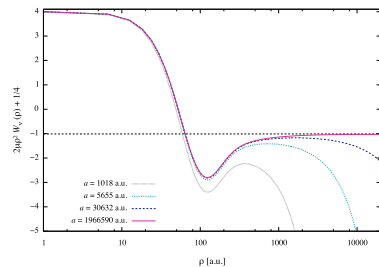
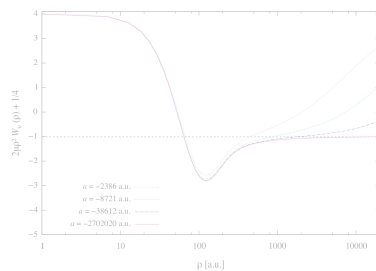
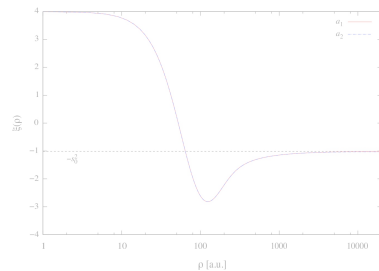
Effective
Potentials

Numerical
Approach

Scattering
Model

Results

Convergence
and Accuracy
Comparison to
the Analytical
Model



Asymptotic form for $a < 0$:

$$\xi_+ = 2\mu\rho^2 E_{2b} + 1/4$$

Effective Potentials

$\xi(\rho)$

Efimov-like Potentials $\xi(\rho)$ for Different a

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

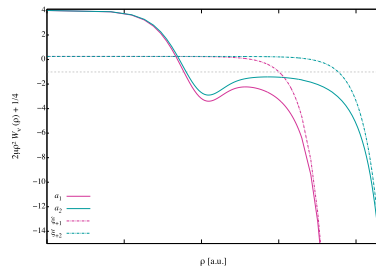
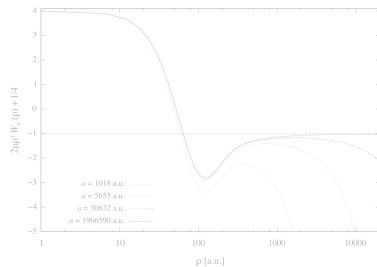
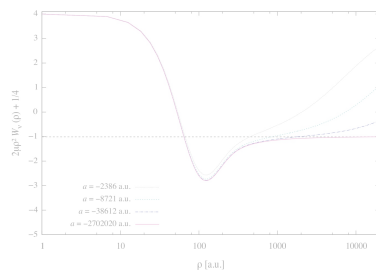
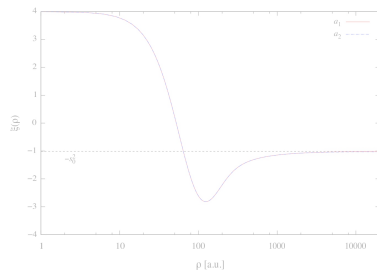
Effective
Potentials

Numerical
Approach

Scattering
Model

Results

Convergence and Accuracy
Comparison to the Analytical
Model



Effective Potentials

$\xi(\rho)$

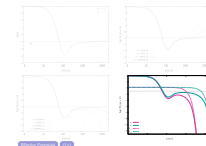
2019-09-02

Results

Convergence and Accuracy

Efimov-like Potentials $\xi(\rho)$ for Different a

Efimov-like Potentials $\xi(\rho)$ for Different a



Comparison to the Analytical Model (1)

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Effective
Potentials

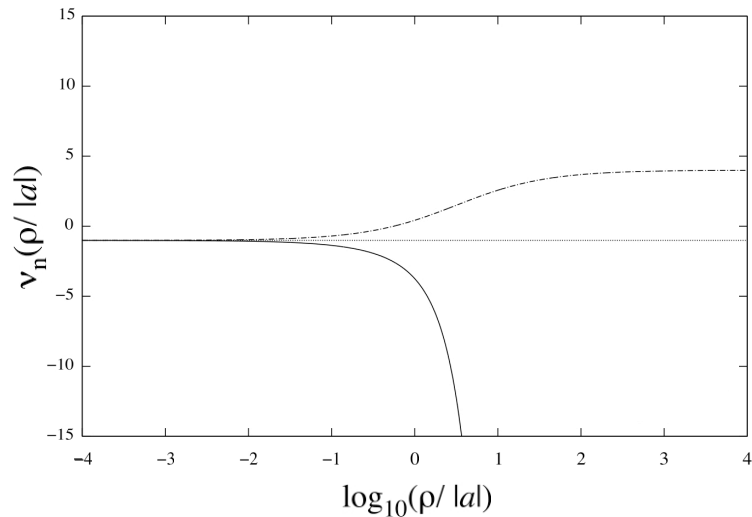
Numerical
Approach

Scattering
Model

Results

Convergence
and Accuracy

Comparison to
the Analytical
Model



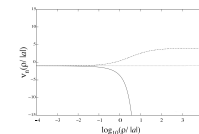
2019-09-02

Results

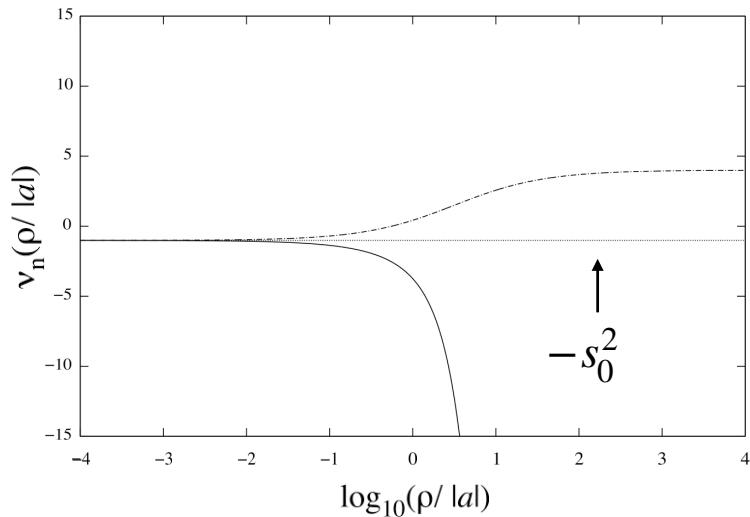
Comparison to the Analytical Model

Comparison to the Analytical Model (1)

Comparison to the Analytical Model (1)



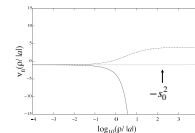
Comparison to the Analytical Model (1)



2019-09-02

- Results
 - Comparison to the Analytical Model
 - Comparison to the Analytical Model (1)

Comparison to the Analytical Model (1)



Comparison to the Analytical Model (1)

Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Effective
Potentials

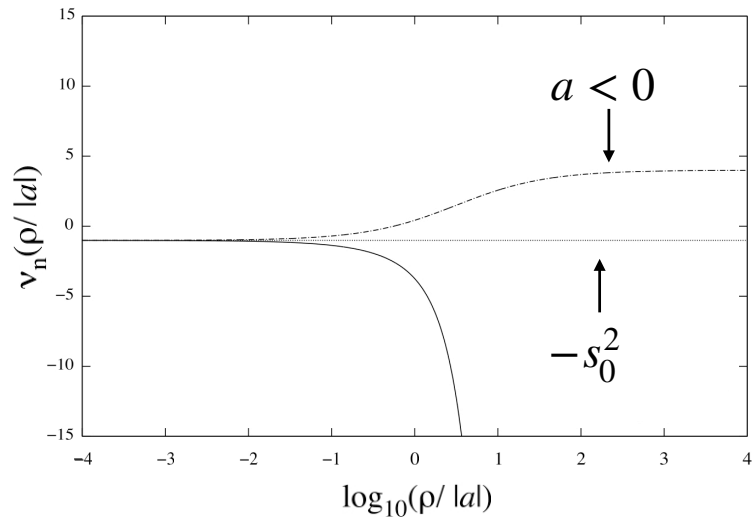
Numerical
Approach

Scattering
Model

Results

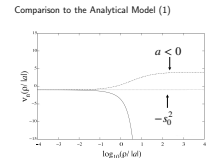
Convergence
and Accuracy

Comparison to
the Analytical
Model

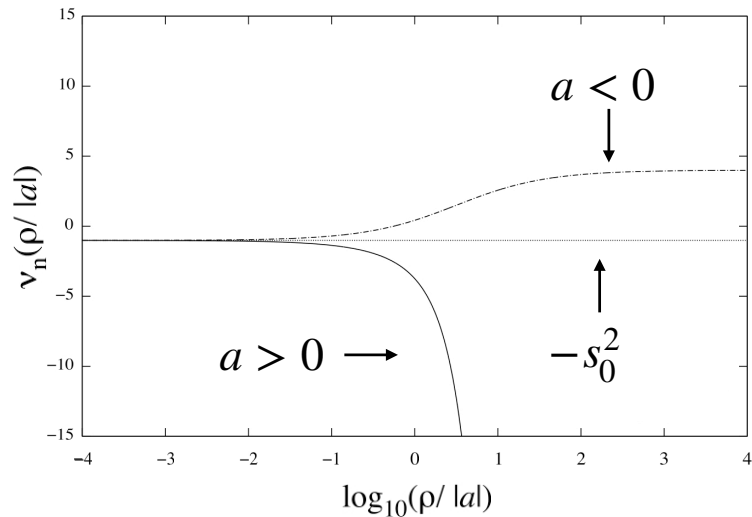


2019-09-02

- Results
 - Comparison to the Analytical Model
 - Comparison to the Analytical Model (1)

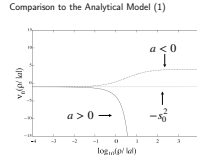


Comparison to the Analytical Model (1)



2019-09-02

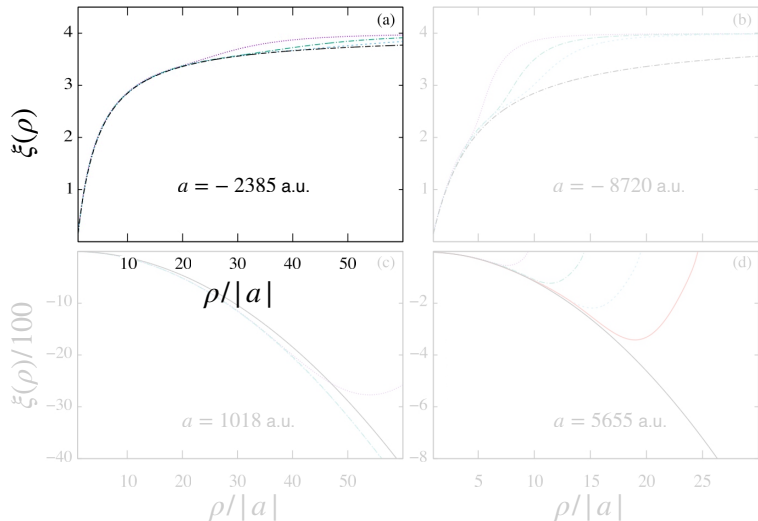
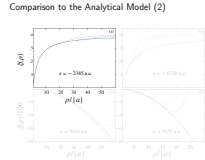
- Results
 - Comparison to the Analytical Model
 - Comparison to the Analytical Model (1)



Comparison to the Analytical Model (2)

2019-09-02

- Results
 - Comparison to the Analytical Model
 - Comparison to the Analytical Model (2)



Kajsa-My Blomdahl

Introduction

Theoretical Approach

Effective Potentials

Numerical Approach

Scattering Model

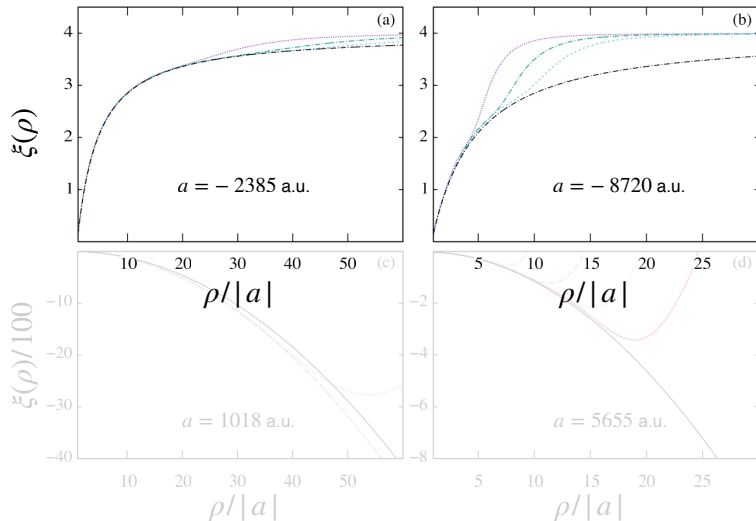
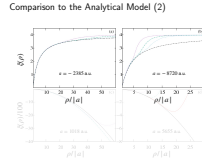
Results

Convergence and Accuracy
Comparison to the Analytical Model

Comparison to the Analytical Model (2)

2019-09-02

- Results
 - Comparison to the Analytical Model
 - Comparison to the Analytical Model (2)



Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Effective
Potentials

Numerical
Approach

Scattering
Model

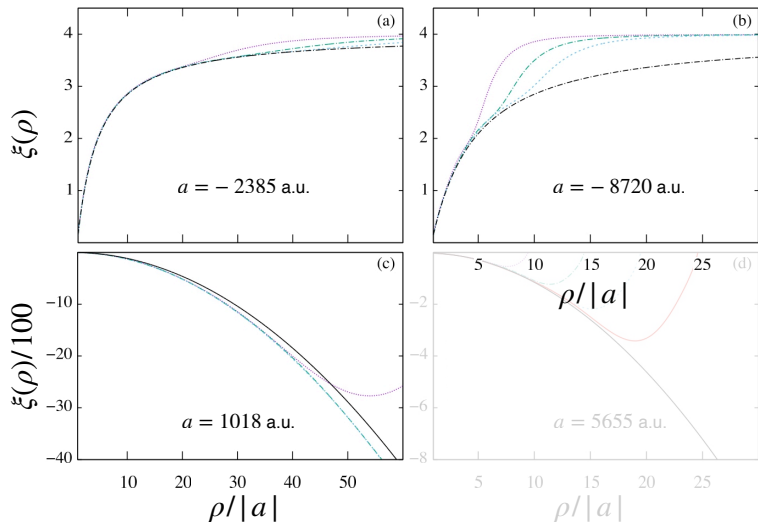
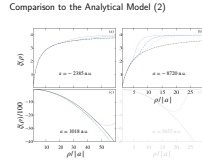
Results

Convergence
and Accuracy
Comparison to
the Analytical
Model

Comparison to the Analytical Model (2)

2019-09-02

- Results
 - Comparison to the Analytical Model
 - Comparison to the Analytical Model (2)



Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Effective
Potentials

Numerical
Approach

Scattering
Model

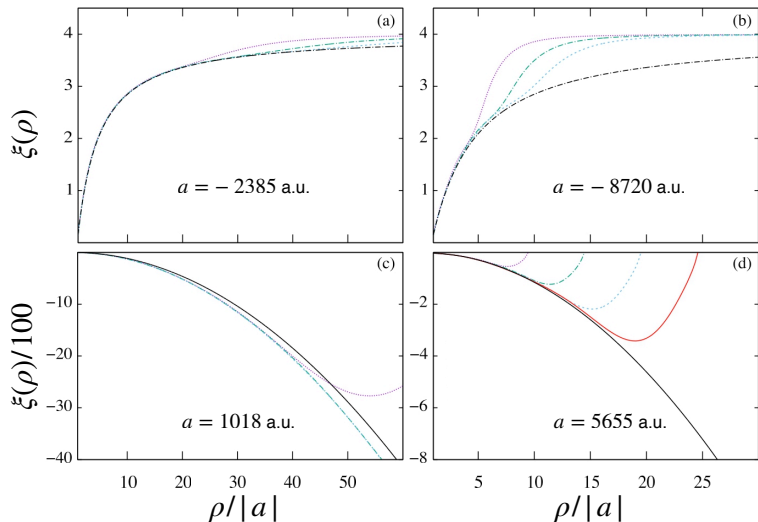
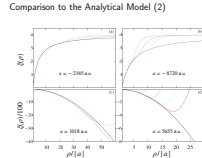
Results

Convergence
and Accuracy
Comparison to
the Analytical
Model

Comparison to the Analytical Model (2)

2019-09-02

- Results
 - Comparison to the Analytical Model
 - Comparison to the Analytical Model (2)

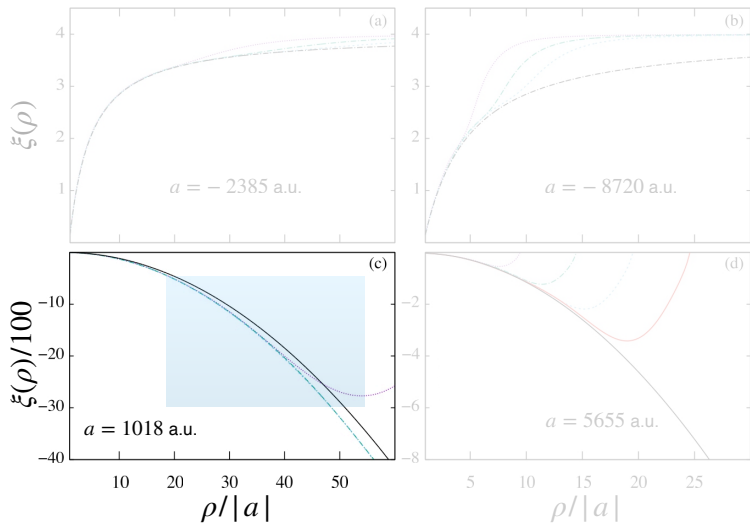
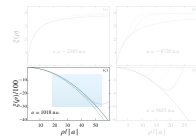


Comparison to the Analytical Model (2)

2019-09-02

- Results
 - Comparison to the Analytical Model
 - Comparison to the Analytical Model (2)

Comparison to the Analytical Model (2)



Kajsa-My
Blomdahl

Introduction

Theoretical
Approach

Effective
Potentials

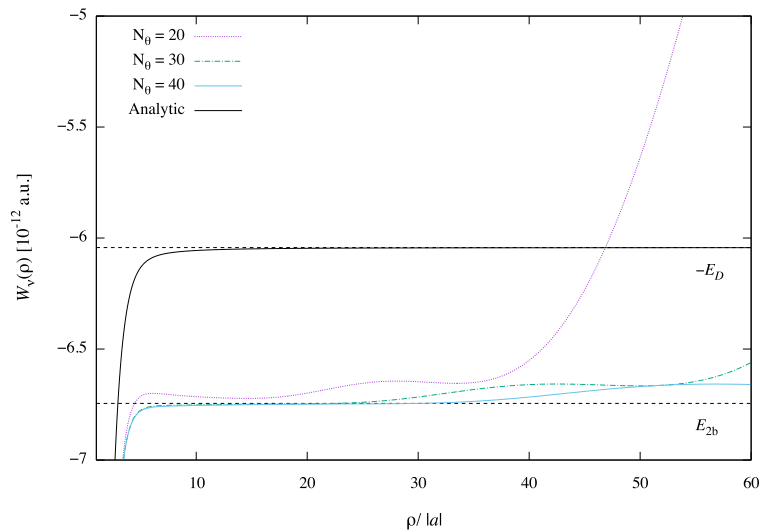
Numerical
Approach

Scattering
Model

Results

Convergence
and Accuracy
Comparison to
the Analytical
Model

Comparison to the Analytical Model (3)



2019-09-02

- Results
 - Comparison to the Analytical Model
 - Comparison to the Analytical Model (3)

