The large two-body s-wave scattering length limit: Bose droplets with Efimov character

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(Ideal) Three-Body Efimov Plot: Universally Linked Sequence of States

Spectrum is determined by $a_s$ and one (!) three-body parameter.
What is the Underlying Three-Body Hamiltonian for Identical Bosons?

- Non-relativistic quantum mechanics:
  \[ H = T_1 + T_2 + T_3 + g\delta(r_{12}) + g\delta(r_{23}) + g\delta(r_{31}). \]

- 1D: One three-body bound state for negative \( g \) (McGuire):
  \[ E_3 = -\frac{4\hbar^2}{m(a_{1D})^2}. \]

- 2D: Two three-body bound states for negative \( g \) (Bruch and Tjon, Nielsen et al.):
  \[ E_3 = 16.523E_2 \text{ and } 1.270E_2. \]

- 3D: Infinitely many three-body bound states (geometric sequence), whose absolute position depends on a three-body parameter.
This Talk

1.) Direct observation of a three-body Efimov state: Helium trimer excited state (positive two-body s-wave scattering length).

2.) At unitarity, extension to larger N:
   Provided the BBB ground state is a (nearly) pure Efimov state, are the N-boson ground states universal?
   Ground state of N-body van der Waals systems at unitarity?

Spectrum is determined by $a_s$ and one (!) three-body parameter.
Signatures of Three-Body Efimov Physics

• Experiments to date:
  ▪ **Losses** near three-atom threshold (negative scattering length side): Geometric scaling factor of $\sim 22.7$ has been observed (pioneering work by Grimm et al.).
  ▪ **Losses** near atom-dimer threshold.

• Many other possibilities:
  ▪ Three-body Efimov states are predicted to have impact on transition from polaron branch to molecule branch (Levinsen et al.).
  ▪ Three-body Efimov states are predicted to have impact on virial coefficient, and hence equation of state (Castin et al.).
**$^{4}\text{He}_3$ Rare Gas Trimer (not Ultracold)**

- Liquid helium: $E/N = -7\text{K}$.
- It was suggested in the 1970s that the excited state of $^{4}\text{He}_3$ is an Efimov state.
- $^{4}\text{He}$-$^{4}\text{He}$ binding energy: $E_{\text{dimer}} = -1.3\text{mK}$.
- $^{4}\text{He}$ is special due to the fact that $a_s/r_{\text{eff}} \approx 12.5$ (naturally large!).
- Two-body s-wave scattering length $a_s = 171a_0$.
- Two-body effective range $r_{\text{eff}} = 15.2a_0$.
- Two-body van der Waals length $r_{\text{vdW}} = 5.1a_0$.
- Two $L=0$ bound states with $E_{\text{trimer}} = -131.8\text{mK}$ and $-2.65\text{mK}$.

**How to make and probe helium trimer?**
Placing the Helium Trimers on the Three-Body Efimov Plot

Three-body parameter is chosen such that ZR energy agrees with energy of scaled helium trimer excited state.

\[ \beta V_{\text{He-He}}(r_{12}) + \beta V_{\text{He-He}}(r_{23}) + \beta V_{\text{He-He}}(r_{31}) \]

Symbols:
- Scaled helium
- True helium (ground and excited states)

Line: Universal ZR theory (Braaten, Hammer)

\( V_{\text{He-He}}(r) \) is multiplied by \( \beta \).

Blume, Few-Body Syst. (2015);
Esry, Lin, Greene, PRA 54, 394 (1996);
Naidon, Hiyama, Ueda, PRA 86,012502 (2012).
Experimental Approach for Detecting and Characterizing the Efimov State

Grating serves as mass selector (N times atom mass): He$_3$ signal contains ground state trimer and excited state trimer. Laser beam ionizes trimer: Coulomb explosion of $^4$He$_3$ (3 ions).

The ionization is instantaneous and the He-ions are distributed according to the quantum mechanical eigen states of the ground and excited helium trimer. Large $r_{12}$, $r_{23}$ and $r_{31}$ correspond to small $1/r_{12}+1/r_{23}+1/r_{31}$. 
The ground state is large. The excited state is huge (eight times larger). Assuming an “atom-dimer geometry”, the tail can be fit to extract the binding energy of the excited helium trimer. Fit to experimental data yields 2.6(2)mK. Theory 2.65mK.
Divide all three interparticle distances by largest $r_{ij}$ and plot $k^{th}$ atom (positive y).
Corresponds to placing atoms i and j at ($-1/2,0$) and $(1/2,0)$.

Ground state and excited states have distinct characteristics.
Connection Between Helium Trimers and Ultracold Atoms?

Experiments on various cold atom systems find: $a^{(1)}/r_6 \sim -9.6$ (Grimm group, and then others). Now referred to as van der Waals universality.

<table>
<thead>
<tr>
<th>THEORY</th>
<th>$\kappa^{(1)} r_6$</th>
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Zero-range theory: $\kappa^{(n)} a^{(n)} = -1.50763$

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Helium trimer ground state (1) ~ “ground” alkali trimer (1). Helium trimer excited state (2) ~ zero-range theory.
More than Three Identical Bosons: What Do We Know?

- Non-relativistic quantum mechanics: \[ H = \sum_j T_j + \sum_{j<k} g \delta(r_{jk}). \]

- 1D: N-body bound state for negative g (McGuire): \[ E_N/N = -\hbar^2/(N^2-1)/[6m(a_{1D})^2]. \]

- 2D: Two three- and two four-body bound states for negative g (Platter et al.). Large N limit (Hammer and Son): \[ E_{N+1}/E_N = 8.567. \]

- 3D:
  - N=4 sector has been studied quite extensively (Hammer et al., von Stecher et al., Deltuva): Two four-body states tied to each Efimov trimer (calculations for resonance states with finite-range two-body potentials by Deltuva).
  - Much less is known for N>4.
Four-atom resonances have been observed experimentally in cold atom experiments by Grimm’s group. Theory: von Stecher et al., Platter et al., Deltuva.

At unitarity:

\[ E_{\text{tetramer}}(\text{“gr.”}) = 4.61 E_{\text{trimer}} \]
\[ E_{\text{tetramer}}(\text{“exc.”}) = 1.002 E_{\text{trimer}} \]
Four-atom resonances have been observed experimentally in cold atom experiments by Grimm’s group. Theory: von Stecher et al., Platter et al., Deltuva.

At unitarity:

\[ E_{\text{tetramer}}(\text{“gr”}) = 4.61E_{\text{trimer}} \]
\[ E_{\text{tetramer}}(\text{“exc”}) = 1.002E_{\text{trimer}} \]
Literature Results for “Efimov-Like” States: Energy per Particle at Unitarity

If the predictions were truly universal, the curves would collapse to a single curve.

Gattobigio et al.: \( E_N/N \sim \# N + \text{correction} \); semi-empirical based on gr. st. calcs. (PRA 2014).

Nicholson: \( E_N/N \sim \# N \); from log-normal distribution of noise (PRL 2012).

von Stecher: Two-body and three-body short-range interactions; based on gr. st. calcs. (JPB 2010).
Start Simpler: N Identical Bosons with Large Scattering Length

- Ideally, treat: $H = \sum_j T_j + \sum_{j<k} g\delta(r_{jk})$ plus three-body zero-range BC.
- Simpler: $H = \sum_j T_j + \sum_{j<k} V(r_{jk})$; $V=$He-He van der Waals potential.

Well known literature results:

Small $N$ ($N<10$):
$E/N \sim \# N$.

Large $N$: $E/N \sim -7K$

(E/N changes by four orders of magnitude).

Quantum liquid: No shell structure!
What About Infinite S-Wave Scattering Length for van der Waals Interactions?

Two-body van der Waals potential $V(r) = \frac{c_p}{r^p} - \frac{c_6}{r^6}$ with infinite $a_s$ and one zero-energy two-body bound state (fixed $c_6$ and mass $m$):

- $p=12$ (Lenard-Jones)
- $p=10$
- $p=8$

N-body energies scaled by three-body energy:

- $p=12$: $E_3 / E_{vdW} = (0.230)^2$
- $p=10$: $E_3 / E_{vdW} = (0.233)^2$
- $p=8$: $E_3 / E_{vdW} = (0.245)^2$

The power $p$ matters!

Nearly perfect collapse of scaled ground state energy.
N Identical Bosons with Infinitely Large s-Wave Scattering Length

• Non-relativistic quantum mechanics in the spirit of Efimov (two-body zero-range interactions): \( H = \sum_j T_j + \sum_{j<k} g\delta(r_{jk}). \)

• Build zero-range interactions into two-body propagator. We use path integral Monte Carlo approach extrapolated to zero temperature (Yan and Blume, PRA (2015)).

• To avoid Thomas collapse, use repulsive three-body regulator (we don’t know how to treat three-body zero-range boundary condition…):
  ▪ Use three-body regular so that \( N=3 \) system is as close as possible to ideal Efimov trimer; see work by von Stecher (hardcore regular or repulsive powerlaw potential).
Approximate Scale Invariance for N=3: Three-Body Finite-Range Regulator

• We use two-body zero-range interactions.
• Repulsive three-body potential pushes the trimer out.

Three-body energy ratio of ground state (n=1) and first excited state (n=2) deviates by ~0.11% from universal energy spacing (<1 out of 515).

Scale invariance is broken weakly by regulator.
We consider ground states (not resonance states).

Three-body hardcore potential is hard to treat numerically by PIMC approach.

Use $1/(R_{ijk})^p$ regulator in three-body sector:

$$(R_{ijk})^2 = (r_{ij})^2 + (r_{jk})^2 + (r_{ki})^2.$$

The three-body regulator leads to very weak breaking of the scale invariance in three-body sector. The effect is enhanced for $N>3$. 

Yan and Blume, PRA 2015 and in preparation.
Smooth Distribution Functions: No Shell Structure

No evidence of shell structure or layering. Three-body regulator changes "size" but leaves $P_{\text{angle}}$ nearly unchanged.

$P_{\text{pair}} \quad N=13$

$P_{\text{triple}} \quad N=13$

$P_{\text{angle}} \quad p=6$

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N-Body Lengths in Terms of Characteristic/Intrinsic Lengths

• Three-body regulator (p=6): \( L_6 = (mC_6/\hbar^2)^{1/4}/2 \).

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<th>N=15</th>
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<td>( r_{ij} / L_6 )</td>
<td>16</td>
<td>10</td>
</tr>
<tr>
<td>( R_{ijk} / L_6 )</td>
<td>18</td>
<td>11</td>
</tr>
<tr>
<td>( (\rho_{\text{max}})^{-1/3} / L_6 )</td>
<td>7</td>
<td>4.5</td>
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• N-body state is large and largely located in classically forbidden region.

Despite separation of scales, a surprisingly (?) large dependence of \( (E_N/N)/(E_3/3) \) on the three-body regulator is seen. Common feature: Structureless broad “blobs” (shrink/stretch).
Nearly Perfect Collapse of $P_{\text{pair}}$ if Scaled by N-Body Binding Momentum

Amplitude is largely located in classically forbidden region.

$p=4$

$p=8$

2-body ZR + 3-body repulsive regulator
Nearly Perfect Collapse of $P_{\text{pair}}$ if Scaled by N-Body Binding Momentum

Amplitude is largely located in classically forbidden region.

Different classes in N-body sector.
Different “classes”:

2-body ZR + 3-body repulsive regulator:
N=2: Fully universal.
N=3: Ground state trimer is nearly identical to ideal Efimov trimer.
N>3: “Sensitivity” of $E_N/E_3$ increases with increasing N.

2-body van der Waals:
N=2: Nearly fully universal.
N=3: Structure of ground state trimer differs from ideal Efimov trimer; van der Waals universality for sufficiently repulsive short-range potential.
N>3: $E_N/E_3$ nearly collapse.

2-body Gaussian: $E_N \sim N^2$ for $N>6$. 
Summary

• Boson droplets (N>3) at unitarity:
  ▪ Throughout this talk: Investigated ground state manifold.
  ▪ Next step: Look at N-body states tied to excited Efimov trimers.

• Observation of helium trimer excited state (positive $a_s$):
  ▪ Structural properties deduced from experiment and theory agree.
  ▪ More focus on structural properties in the future?
\[ \kappa_{\text{predict}} = \kappa_3 + \kappa_3 (N - 3) (\kappa_4 / \kappa_3 - 1); \] see Gattobigio et al. (2015).

Three- and four-body binding momentum serve as input.
N-Body Sector with Infinitely Large Two-Body s-Wave Scattering Length

• We developed Monte Carlo approach that can deal with two-body zero-range interactions (use exact two-body zero-range propagator).

• Consider N-body ground states:
  - We calculated N-body energies and structural properties for $C_6/(R_{ijl})^k$ three-body regulators, $k=4-8$.
  - Trimer size is about 26 times larger than $L_k$ (good separation of scales).

Yangqian Yan, D. Blume: PRA 90, 013620 (2014); PRA 91, 043607 (2015); and in preparation.
Energy per Particle from our Monte Carlo Calculations

If the N-body energy was fully determined by the three-body parameter, then the curves would collapse to a single curve.

Doesn’t happen with the literature data.

Doesn’t happen with our data.

Surprisingly (?) large sensitivity on details of three-body regulator.
Length Scales?

Factor of 10... Apparently not enough.
Summary

From (quantum/physical chemistry to) quantum liquids to quantum gases

N-body energy is scaled by three-body energy. E/N curves deviate in functional form and coefficients. WHY?


How Do the Three-Body Correlations of an Ideal Efimov Trimer Look Like?

infinitely many lobes

all angles occur

Next: What about finite $a_s$?
How Do the Three-Body Correlations of an Ideal Efimov Trimer Look Like?

\[ E_3 = \left( \frac{\hbar \kappa_3}{2} \right)^2 / m \]

- infinitely many lobes
- all angles occur

Next: What about finite \( a_s \)?
This is the perfect Efimov scenario.

Discrete scale invariance (the zero-range interactions do not define a length scale for the trimer): The hyperradial Hamiltonian becomes \( s_0 = 1.006 \ldots \)

Infinite number of three-body bound states with spacing \( 22.7^2 \).

Each hyperradial wave function has infinitely many nodes.

\[
\int |\Psi|^2 d^3r = 1
\]

\[
\delta (r - 2) \frac{2}{r}
\]

\[
\delta (r - a) \delta (r - b) \delta (r - c)
\]

\[
\phi_1 (r) \phi_2 (r)
\]

\[
\phi_1 (r) \phi_2 (r)
\]

Here, \( \lambda = \exp(\pi/s_0) \approx 22.7 \)
Pretend: $a_s$ is Infinitely Large and $r_{\text{eff}}$ Vanishes

• …this is the perfect Efimov scenario.

• Discrete scale invariance (the zero-range interactions do not define a length scale for the trimer): The hyperradial Hamiltonian becomes ($s_0=1.006…$)

$$H_R(R) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial R^2} - \frac{\hbar^2}{2mR^2} \left( s_0^2 + \frac{1}{4} \right)$$

$$H_R(\lambda R) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial (\lambda R)^2} - \frac{\hbar^2}{2m(\lambda R)^2} \left( s_0^2 + \frac{1}{4} \right) = \lambda^{-2} H(R)$$

If $F(R)$ is a solution with energy $E_3^{(n)}$, $F(\lambda R)$ is a solution with energy $E_3^{(n+1)} = \lambda^{-2} E_3^{(n)}$. Here, $\lambda = \exp(\pi/s_0) \approx 22.7$

Infinite number of three-body bound states with spacing $22.7^2$.

Each hyperradial wave function has infinitely many nodes.
Smooth Pair and Triple Distribution Functions for N=13

Quantitative differences. Qualitatively similar. In particular: No evidence of shell structure or layering.

Peak density displays saturation:

\[ \left( \frac{4\pi^2 P_{12}(R)}{\kappa_3^r} \right)^2 \]

\[ \left( \frac{\rho_\text{max}}{\kappa_3^3} \right)^2 \]

Gaussian
Dependence of N=13 Angular Distribution on Three-Body Regulator

Fairly small dependence on three-body regulator – angular correlations appear less sensitive than overall size...
Angular Correlations of Three-Body System at Unitarity

The ground and excited states look notably different. The excited state essentially coincides with zero-range theory distribution.
N-Dependence of Angular Distribution for $k=6$ Three-Body Regulator

For comparison:
Motivating Questions

• Unique three-body states: Do they lead to predictable N-body behavior?

• Based on the knowledge of just a few parameters, can we predict N-body properties?

• How many particles are “many”?

• Weakly-bound systems with long-range interactions?

• What role does dimensionality play?

• What role does the particle statistics play?
Thanks to Collaborators

• He trimer Efimov state:

• Extensions to more bodies:
  ▪ Yangqian Yan, D. Blume: PRA 90, 013620 (2014); PRA 91, 043607 (2015); and in preparation.

• Early work on van der Waals systems:
Size of van der Waals Trimer as a Function of Inverse Scattering Length

He-He potential [JCP 136, 224303 (2012)] + overall scaling factor.

\[(R_{\text{hyper}})^2 = \frac{\left[ \sum_{i<j} (r_{ij})^2 \right]}{3^{1/2}}\]

Universal theory:
\[\kappa_*= -1.56(5)/a_*\]

This yields:
\[0.0323/a_0\]
\[0.0424/a_0\]

Calculation:
\[0.0439/a_0\]
\[0.0426/a_0\]

\[a_*= -48.31a_0\]
\[a_/r_{vdw} = -9.796\]
\[a_/r_{vdw} = -166\]
\[(a_/r_{vdw})/22.694 = -7.30\]

“true” helium trimers

1. excited state

ground state
The ground and excited states look notably different. The excited state essentially coincides with zero-range theory distribution.
Objectives of This Talk: Extended/Generalized Efimov Scenario

“Standard” Efimov scenario:
Three identical bosons with zero-range contact interactions:

\[ T_1 \quad T_2 \quad D \]

- Efimov scenario for \( B_N \) system:
  - How do the N-body energies depend on the regularization in the three-body sector?

- Efimov scenario for \( B_N X \) system (specifically, Cs\(_N\)Li):
  - Do four-body states exist that are universally tied to CsCsLi Efimov states?
  - If so, where do the four-atom resonances lie relative to the three-atom resonances?
Want to Go Beyond N=3: Possible Approaches...

“Standard” Efimov scenario:
Three identical bosons with zero-range contact interactions:

Ideally: Solve the N-body problem with two-body ZR interactions analytically...

Treat N-body resonance states [for N=4, Deltuva, Few-Body Syst. 54, 569 (2013); for N=5 and 6, von Stecher, PRL 107, 200402 (2011)].

Treat the ground state using FR two-body potentials and “correct” for non-universal effects (Gattobigio/Kievsky).

Analyze noise (Nicholson).

Make $T_1$ close to universal using repulsive three-body force [von Stecher, JPB 43, 101002 (2010)].
\( E_N \) for \( N \) Bosons (\( a_s = \infty \)): “Universal” Energy Predictions from the Literature

**Pairwise Gaussian:**
\[ E_N \sim N^2 \text{ (non-universal).} \]
PRA 90, 013620 (2014).

**Gattobigio & Kievsky:**
finite-range corrections included (\( E_4 \) made to match Deltuva result).
PRA 90, 010101(R) (2014).

**Nicholson:**
\[ E_N = E_4 N/2(N/2-1)/2. \]
PRL 109, 073002 (2012)

**von Stecher:**
DMC results for 3b HC. JPB 43, 101002 (2010).

This talk:
Monte Carlo calculations for two-body ZR interactions and different regularizations in three-body sector.
BBB ($a_s=\infty$): Two-Body ZR Interactions and Three-Body Hardcore Potential

- Hyperangular equation can be solved analytically (yields $s_0$ value).
- Hyperradial equation can be solved analytically.

Energy ratio of ground state ($n=1$) and first excited state ($n=2$) deviates by $\sim 0.11\%$ from universal energy spacing ($<1$ out of 515)
BBB \( (a_s = \infty) \): Two-Body ZR Interactions and Three-Body Powerlaw Potential

\[ V(R) = C_k / R^k \]

\( C_k \) sets the energy scale

For large \( k \), the three-body powerlaw potential behaves like the hardcore potential.

For \( k = 2 \), the powerlaw potential "modifies" \( s_0 \) (does not regularize...).

For \( k \sim 3-4 \), we see some deviations from universal energy ratio for \( n = 2 \) and 1.
BBB \((a_s = \infty)\): Two-Body FR Interactions and Three-Body Gaussian Potential

Range \(R_0\) of repulsive three-body Gaussian is fixed. Range \(r_0\) of attractive two-body Gaussian is varied.

This is where Gattobigio et al. work. Trimer size \(<R> = 2.66r_0.\)

\[ R^2 = \frac{1}{3} \sum_{i<j} (r_{ij})^2 \]

A small repulsive three-body potential affects the ground and excited states differently.
Two-Body ZR Interactions and Three-Body Powerlaw Potential

- What happens in the N-body sector for different three-body powerlaw potentials?
- Restrict ourselves to N-body ground states.
- Calculate $E_{N}^{(1)}/E_{3}^{(1)}$.

We use the Path Integral Monte Carlo (PIMC) approach, extrapolated to zero temperature, to treat N-body system: Pair approximation with analytical two-body zero-range propagator.
Benchmarking the Two-Body Zero-Range Propagator

- Two-body propagator calculated analytically for 1d and 3d systems (harmonically trapped or free space).
- Can be used in real or imaginary time evolution.
- We have primarily used it in applications where imaginary time is identified with inverse T.

- Example: Pair distribution function for harmonically trapped three-boson system.

  Infinitely large $a_s$ and three-body $C_6/R^6$ powerlaw potential.
Energy Predictions from the Literature

Pairwise Gaussian: $E_N \sim N^2$.

Gattobigio & Kievsky (next talk): finite-range corrections included ($E_4$ made to match Deltuva result).

Nicholson (noise): $E_N = E_4N/2(N/2-1)/2$.

Our work:
Monte Carlo calculations for two-body ZR interactions and different regularizations in three-body sector.
Purely repulsive three-body powerlaw potential: $V(R) = C_k / R^k$.

As $N$ increases, the dependence of the $N$-body energy on the power of the repulsive three-body potential increases.

For large $N$, the larger $k$ energies deviate notably from hardcore DMC energies (dash-dotted line).
Connection Between Helium Trimers and Ultracold Atoms?

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<td>-169</td>
<td>-1.57</td>
<td>23.5</td>
<td>1/17.1</td>
</tr>
<tr>
<td>LJ (0 b. st.)</td>
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<td>-9.49</td>
<td>-2.18</td>
<td>0.00981</td>
<td>-160</td>
<td>-1.57</td>
<td>23.4</td>
<td>1/16.8</td>
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\[
\frac{\text{m}^2 \text{V}^2 \text{C}}{\text{A}^2 \text{R}} = \frac{\text{m}^2 \text{V}^2 \text{C}}{\text{A}^2 \text{R}}
\]

\[
L = \frac{g}{E^{\frac{3}{4}} (\text{energy}^{\frac{1}{4}})}
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\]

\[
L = \frac{g}{E^{\frac{3}{4}} (\text{energy}^{\frac{1}{4}})}
\]
Hyperradial Density for N Bosons \((a_s=\infty)\)

Three-body powerlaw potential with \(k=6\). N-body hyperradius 
\[ R^2 = \frac{[\sum_{i<j} (r_{ij})^2]}{N}. \]
\(\kappa\) is the three-body binding momentum.

\[ \frac{1}{\kappa} = 16.4L^6, \] where \(L^6\) is length scale of three-body powerlaw potential, \(L^6 = (mC^6/\hbar^2)^{1/4}\).

N=3 distribution is broadest. 
N-body hyperradial density becomes more compact and moves to larger \(R\).
Radial Density ($a_s=\infty$): k=6 Three-Body Powerlaw Potential

Radial density normalized to number of particles.

Radial peak density saturates around $N=10-15$.

The peak density for $N=15$ is 3 times larger than peak density for $N=3$.

Note: The errorbars are non-negligible.
Midway Summary ($a_s=\infty$): N Identical Bosons with Two-Body ZR Interactions

• N-body energies show notable dependence on how the three-body system is regularized (we looked at different repulsive powerlaw potentials in hyperradius of three-body subsystems).

• Radial peak density, normalized to number of particles, saturates around $N=10-15$ for $k=6$.

• Also monitored hyperradial density, two- and three-body correlations,…

• Conclusion: To see “truly” universal behavior, need to go to N-body states tied to excited Efimov trimer?
Unequal Masses: B
\textsubscript{N}X System with Large Mass Ratio

- Recent experiments by the Chicago (arXiv:1402.5943) and Heidelberg [PRL 112, 250404 (2014)] groups on CsLi mixture measure three-atom resonances.

- Ideal Efimov scenario:
  - Two large s-wave scattering lengths.
  - Scaling factor of 23.669 for mass ratio 133/6 as opposed to 515.035 for BBB system.

- Provided three-body parameter is fixed, what happens in the B
\textsubscript{N}X sector?
  - Number of four-body bound states, if any, that are tied to B\textsubscript{2}X trimer?
  - Four-atom resonances?
  - When does four-body state hit trimer state?
BBB versus BBX ($a_s=\infty$): ZR Two-Body and HC Three-Body Potential

The amplitude of the hyperradial density in the “inner lobe” is larger for BBX than for BBB. More favorable (i.e., smaller) energy level spacing introduces new computational challenge...

BBB: $\sim0.11\%$
BBX: $\sim1.9\%$

BBX calculations are for CsLi mass ratio.
BBX \( (a_s=\infty) \): Gaussian Two-Body and Gaussian Three-Body Potential

Three-body repulsive Gaussian: Range \( R_0 \) is fixed and height \( V_0 \) is varied (below \( R^2 \sim \Sigma_{i<j}(r_{ij})^2 \); not hyperradius…). Range and depth of attractive two-body Gaussian are fixed.

- **Explicitly correlated Gaussian basis set**

Calculations are for \( 133/6 \) (CsLi) mass ratio.
Expand Wave Function in Basis: Explicitly Correlated Gaussians

- Basis functions:

  \[ \Phi_k(x) = \exp(-x^T A^{(k)} x / 2) \]

  \( x \) collectively denotes \( N-1 \) Jacobi coordinates.

  \( A \) denotes \((N-1) \times (N-1)\) dimensional parameter matrix.

  Use physical insight to choose \( d_{ij} \) efficiently.

- For each basis function \( \varphi_k \) (\( L^{\Pi}=0^+ \)), we have \( N(N-1)/2 \) parameters.

  For \( N=4, N_{\text{basis}}=1000 \), \( L^{\Pi}=0^+ \): 6000 non-linear variational parameters.

Sum over interparticle distances: \( \sum_{i<j} -(r_{ij}/d_{ij})^2 / 2 \)

Total wave fct.:

\[ \Psi = \sum_{k=1}^{N_{\text{basis}}} c_k S \Phi_k(x) \]
Explicitly Correlated Gaussian and Semi-Stochastic Variational Approach

Hamiltonian matrix can be evaluated semi-analytically.

Rigorous upper bound for energy (“controlled accuracy”).

Matrix elements for structural properties can be calculated analytically.

Computational effort increases with number of atoms N:

- Evaluation of Hamiltonian matrix elements involves diagonalizing \((N-1)x(N-1)\) matrix.
- Number of permutations \(N_p\) scales non-linearly (\(N_p = 0, 4, 36, 576, \ldots\) for \(FF', 2F2F', 3F3F', 4F4F', \ldots\) systems).

Approach is powerful for certain few-body problems:
Harmonically trapped 8 particle system (4 spin-up and 4 spin-down fermions) at unitarity as a function of range of two-body Gaussian.

Yin and Blume (preliminary)

Mulkerin et al., PRA 90, 023626 (2014)
BBX ($a_s=\infty$) with Mass Ratio 133/6: Hyperradial Density

Convincing agreement...
Cs$_3$Li ($a_s = \infty$): Gaussian Two-Body and Gaussian Three-Body Potential

Three-body repulsive Gaussian: Range $R_0$ is fixed and height $V_0$ is varied.
Range and depth of attractive two-body Gaussian are fixed.

**Four-body ground state:**

**Four-body excited state:**
CsₙLi \ (a_s=\infty) \n
Pair distribution: Likelihood of finding two particles at distance \( r \) from each other.

Distributions for Cs₃Li ground state resemble those of Cs₂Li ground state.

Distributions for Cs₃Li* excited state are broader.
Generalized Efimov Scenario for CsLi Mixture

Two tetramer states:

\[ a_{4,-}^{(1,1)} \sim 0.55a_{3,-}^{(1)} \]
\[ a_{4,-}^{(1,2)} \sim 0.91a_{3,-}^{(1)} \]

More weakly-bound tetramer becomes unbound on positive scattering length side.

Energy ratios 2.28 and 1.02

Fairly similar to equal boson case...
BBB ($a_s=\infty$): Two-Body FR Interactions and Three-Body Gaussian Potential

For sufficiently large Gaussian three-body barrier, the 2b ZR + 3b hardcore value is approached.

If three-body barrier is high, 2b FR and 2b ZR results behave the same.
Benchmarking the Two-Body Zero-Range Propagator

- Two-body propagator calculated analytically for 1d and 3d systems (harmonically trapped or free space).
- Can be used in real or imaginary time evolution.
- We have primarily used it in applications where imaginary time is identified with inverse $T$.

- Example: Energy of harmonically trapped N-particle system with infinite coupling constant in 1d at $k_B T = E_{ho}$.  

![Graph 1](image1.png)  
![Graph 2](image2.png)
Three-Body Correlation ($a_s = \infty$): k=6 Three-Body Powerlaw Potential

\[ (R_3)^2 = \frac{[(r_{ij})^2 + (r_{jk})^2 + (r_{ki})^2]}{3}. \]

All ijk combinations.
Pair Distribution Function ($a_s = \infty$): $k=3$ Three-Body Powerlaw Potential

![Graph showing the relationship between $4\pi P(r_{12})r_{12}^2/\kappa$ and $\kappa r_{12}$ for different $N$ values. The curves are labeled with $N=3$, $N=10$, and $N=15$.](image)