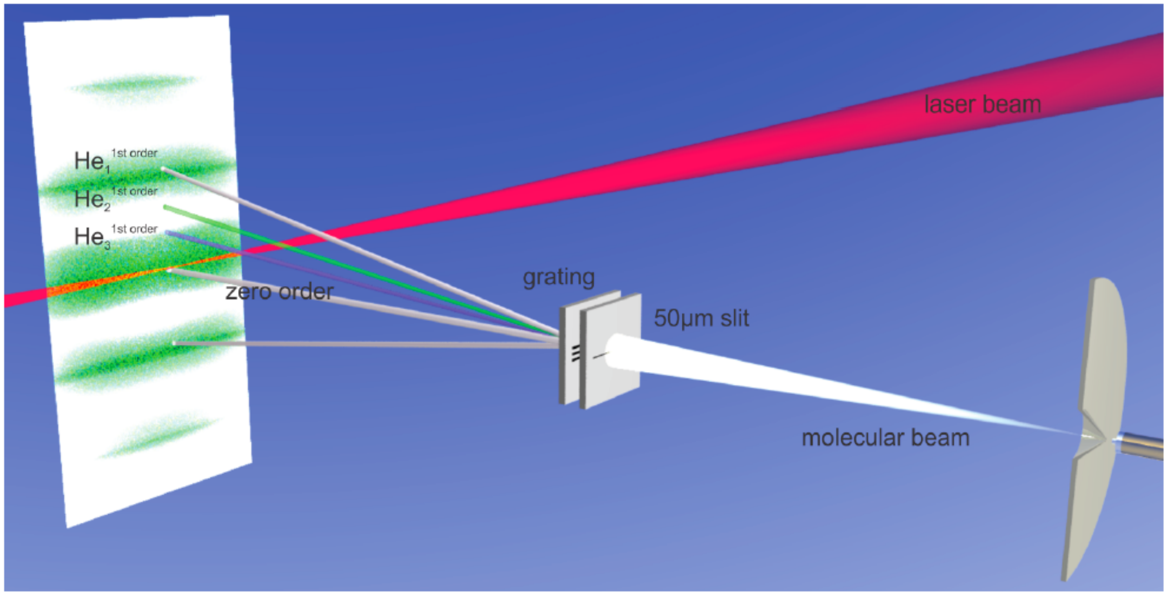

The large two-body s-wave scattering length limit: Bose droplets with Efimov character

Doerte Blume and Yangqian Yan

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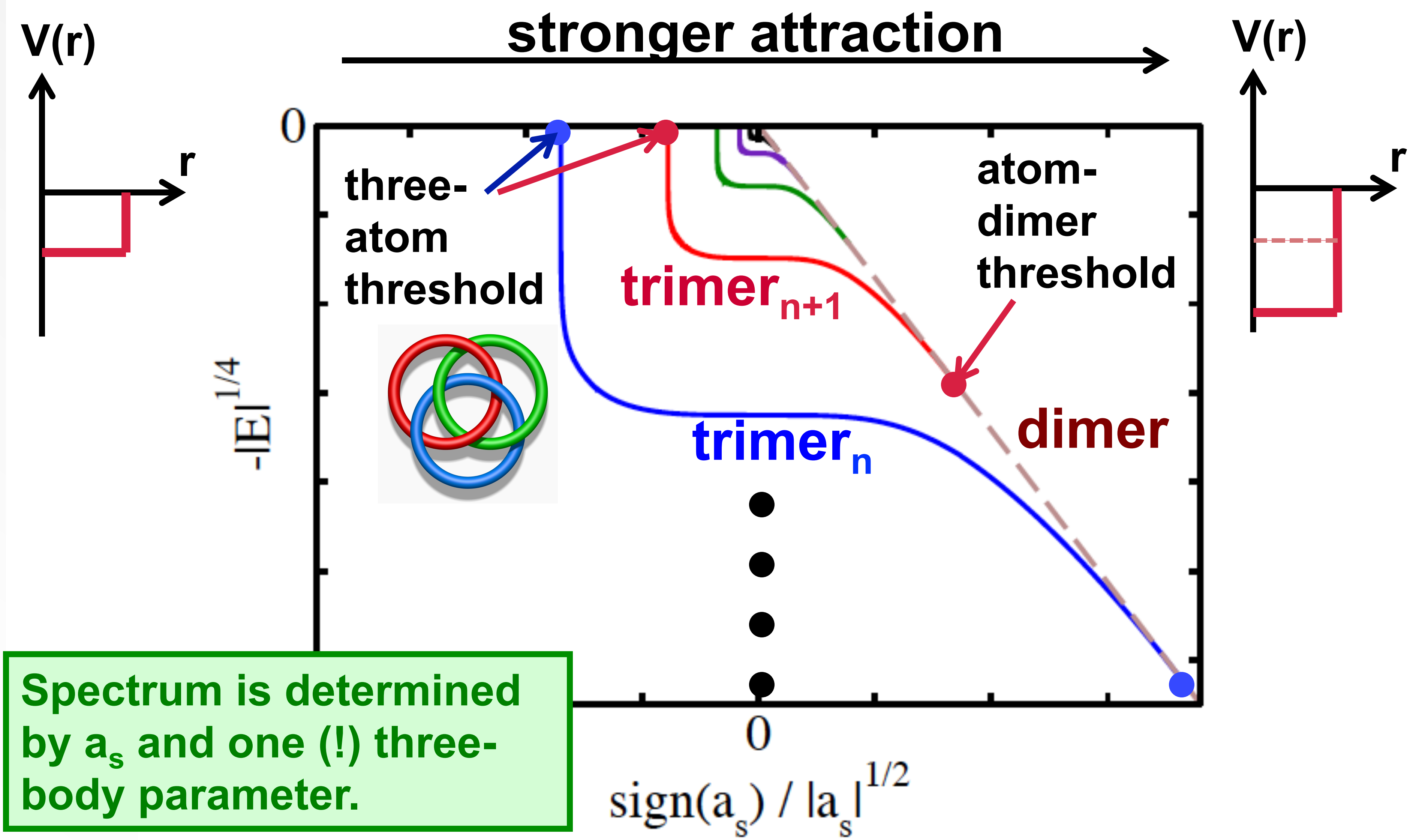
Maksim Kunitski, Reinhard Dörner, S. Zeller, J. Voigtsberger, A. Kalinin, L. Schmidt, M. Schöffler, A. Czasch, W. Schöllkopf, R. Grisenti, T. Jahnke Frankfurt University

Supported by the NSF.

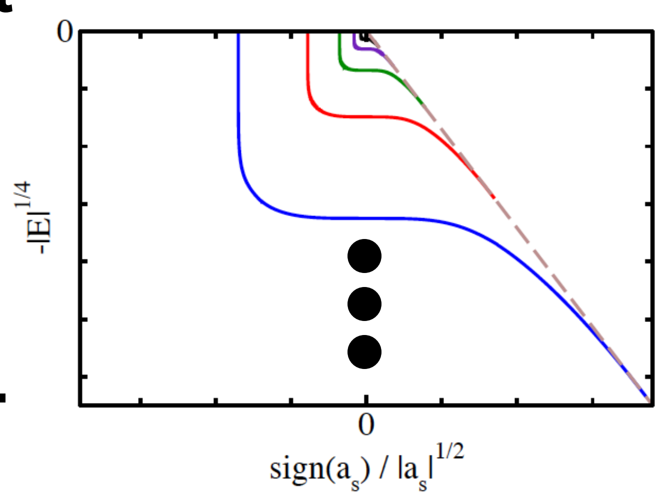
(Ideal) Three-Body Efimov Plot: Universally Linked Sequence of States



Spectrum is determined by a_s and one (!) three-body parameter.

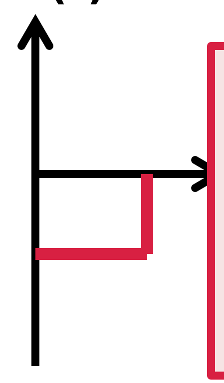
What is the Underlying Three-Body Hamiltonian for Identical Bosons?

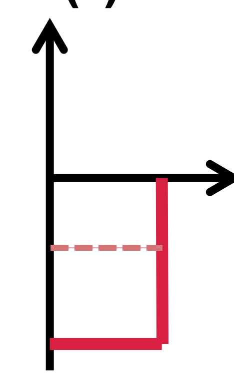
- Non-relativistic quantum mechanics: $H = T_1 + T_2 + T_3 + g\delta(r_{12}) + g\delta(r_{23}) + g\delta(r_{31})$.
- 1D: One three-body bound state for negative g (McGuire): $E_3 = -4\hbar^2/[m(a_{1D})^2]$.
- 2D: Two three-body bound states for negative g (Bruch and Tjon, Nielsen et al.): $E_3 = 16.523 E_2$ and $1.270 E_2$.
- 3D: Infinitely many three-body bound states (geometric sequence), whose absolute position depends on a three-body parameter.

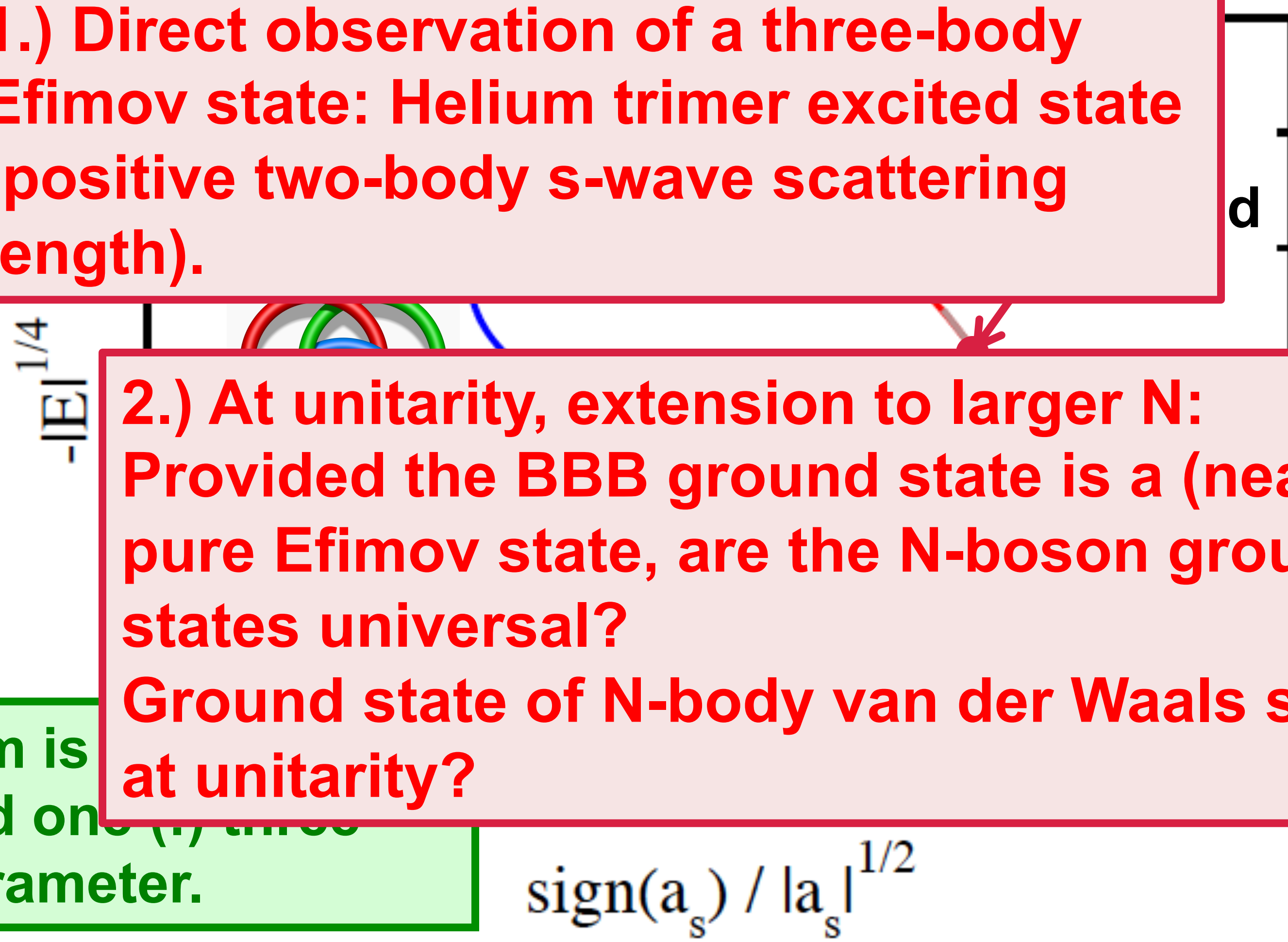


This Talk

stronger attraction →







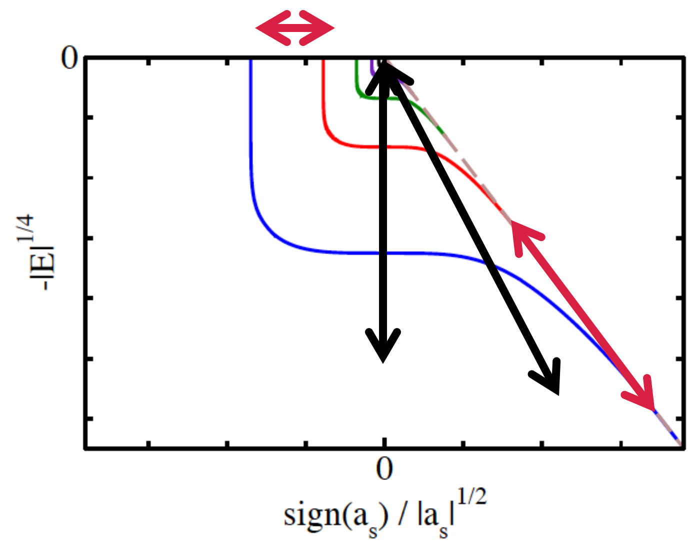
1.) Direct observation of a three-body Efimov state: Helium trimer excited state (positive two-body s-wave scattering length).

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 ... by a_s and one ... three-body parameter.

Signatures of Three-Body Efimov Physics

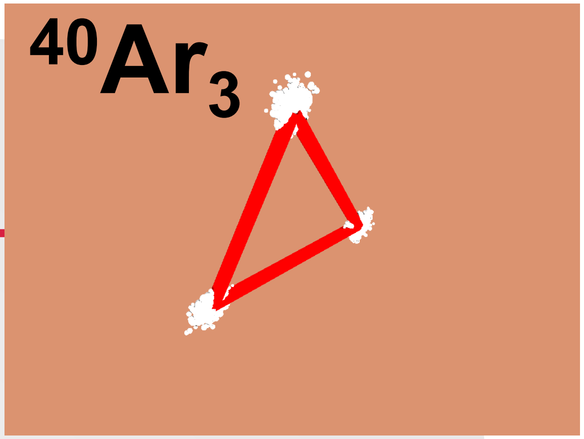
- Experiments to date:
  - **Losses** near three-atom threshold (negative scattering length side): Geometric scaling factor of ~22.7 has been observed (pioneering work by Grimm et al.).
  - **Losses** near atom-dimer threshold.

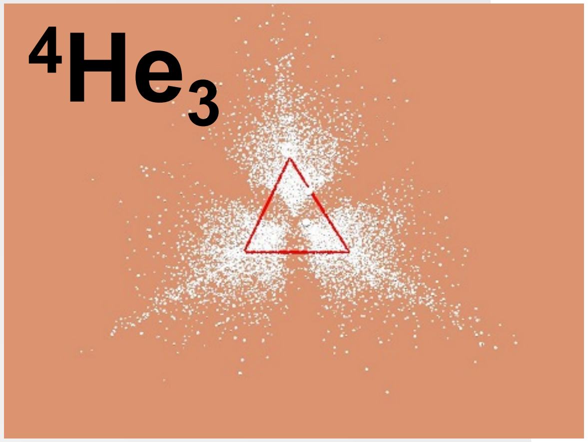


- Many other possibilities:
  - Three-body Efimov states are predicted to have impact on transition from polaron branch to molecule branch (Levinsen et al.).
  - Three-body Efimov states are predicted to have impact on virial coefficient, and hence equation of state (Castin et al.).

$^4He_3$ Rare Gas Trimer (not Ultracold)

- Liquid helium: E/N = −7K.
- It was suggested in the 1970s that the excited state of $^4He_3$ is an Efimov state.
- ^{4}He-^{4}He binding energy: E_{dimer} = −1.3mK.
- ^{4}He is special due to the fact that a_s/r_{eff}~12.5 (naturally large!).
- Two-body s-wave scattering length $a_s=171a_0$.
- Two-body effective range $r_{eff}=15.2a_0$.
- Two-body van der Waals length $r_{vdW}=5.1a_0$.
- Two L=0 bound states with E_{trimer}= −131.8mK and −2.65mK.





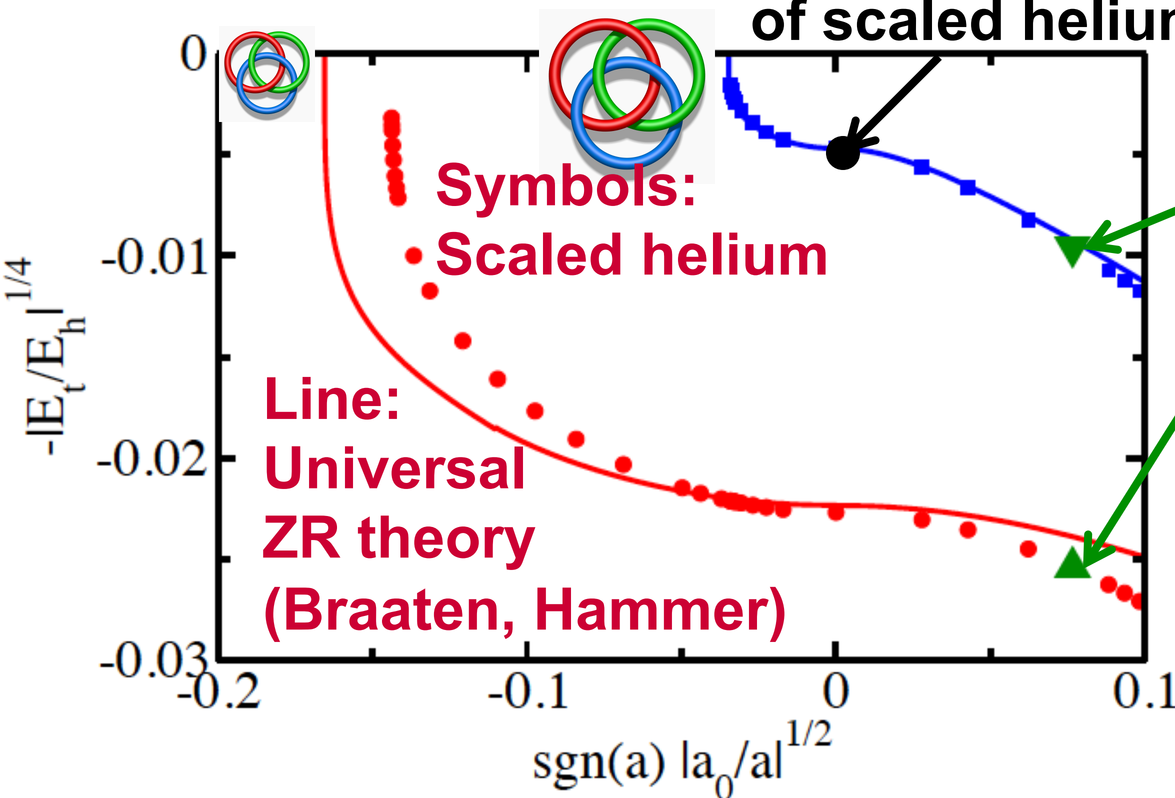
How to make and probe helium trimer?

1 K = 8.6 x 10^{-5} eV

Placing the Helium Trimers on the Three-Body Efimov Plot

$\beta V_{He\text{-}He}(r_{12}) + \beta V_{He\text{-}He}(r_{23}) + \beta V_{He\text{-}He}(r_{31})$.

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



True helium (ground and excited states)

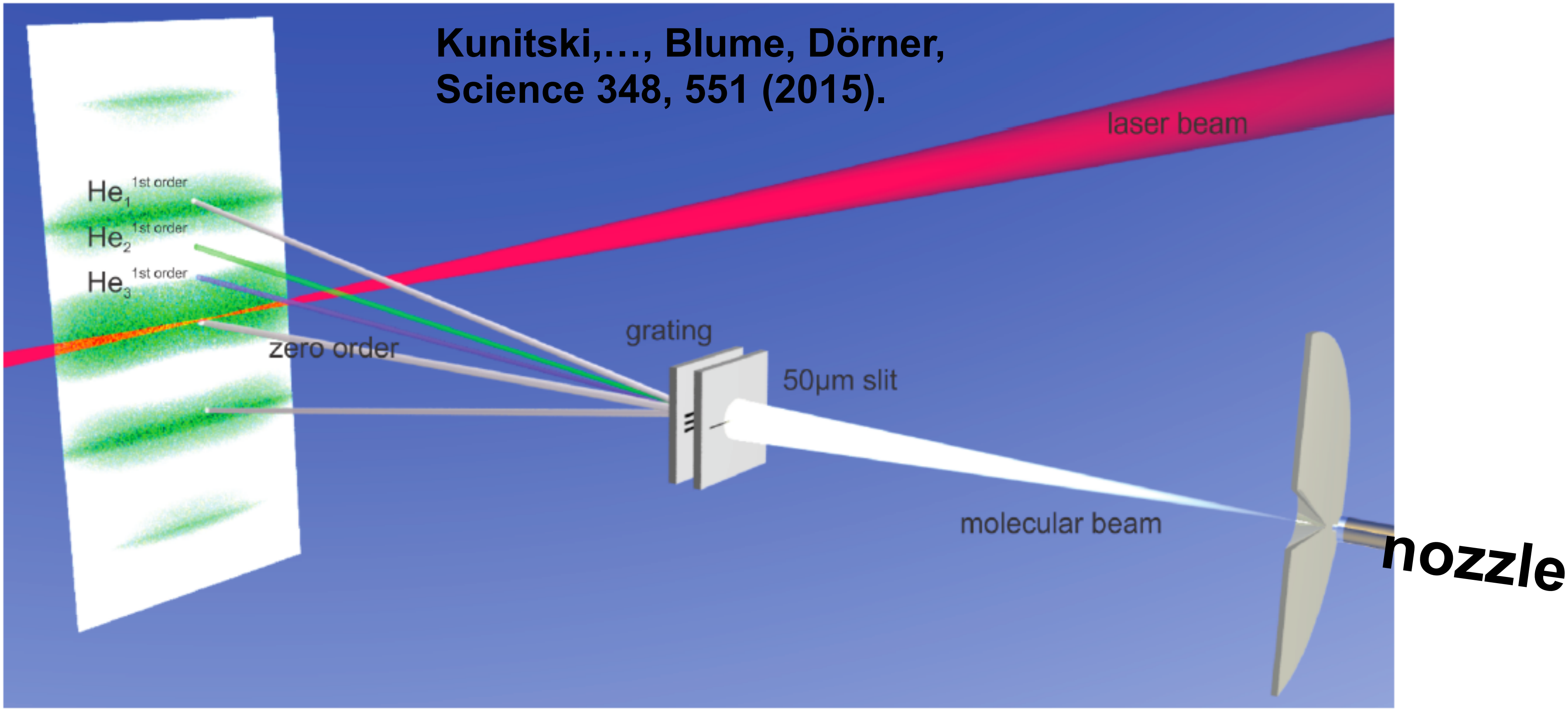
For the excited state, symbols agree with line! Molecular system follows predicted Efimov behavior.

Blume, Few-Body Syst. (2015); Esry, Lin, Greene, PRA 54, 394 (1996); Naidon, Hiyama, Ueda, PRA 86,012502 (2012).

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

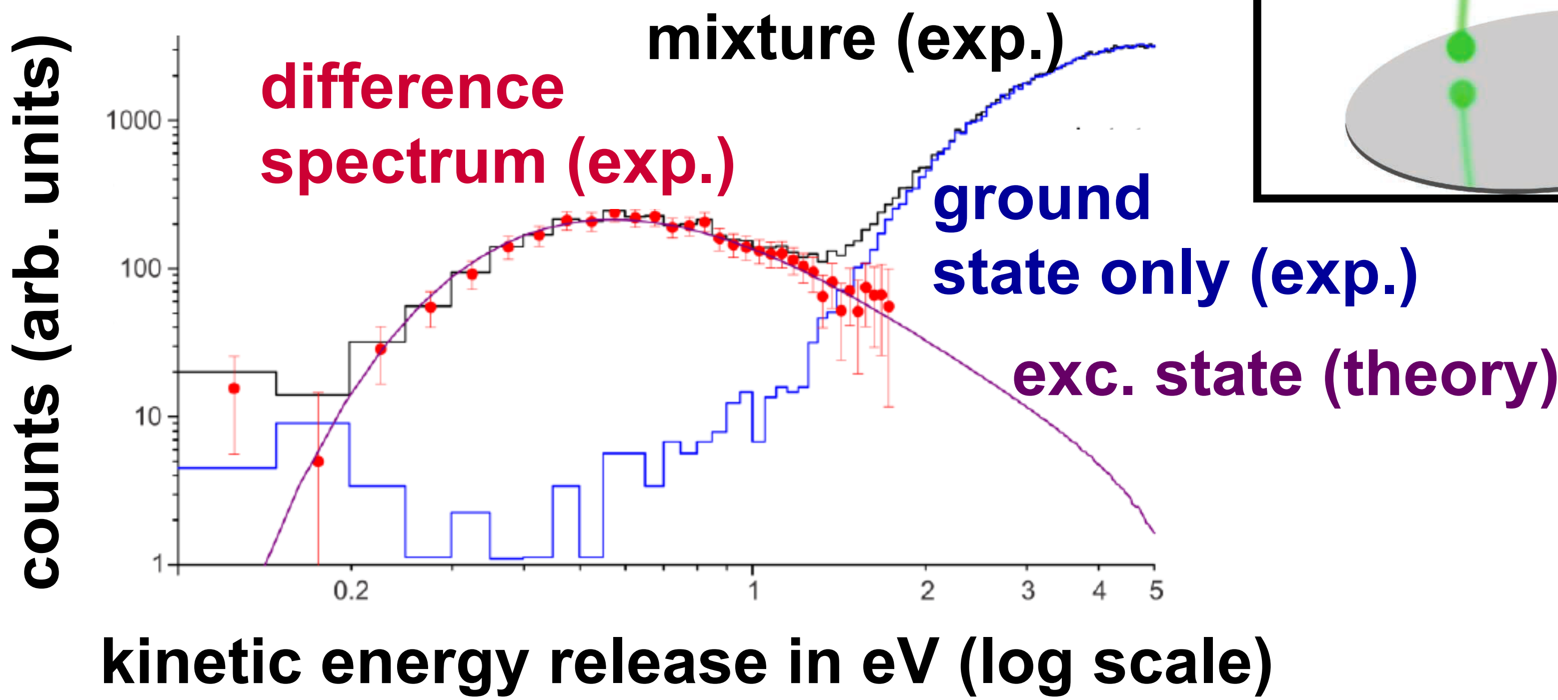
$\beta < 1$ ← → $\beta > 1$

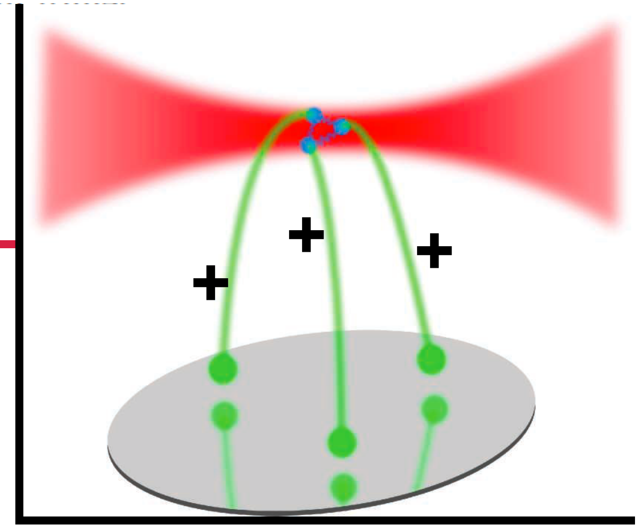
Experimental Approach for Detecting and Characterizing the Efimov State



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 $^4He_3$ (3 ions).

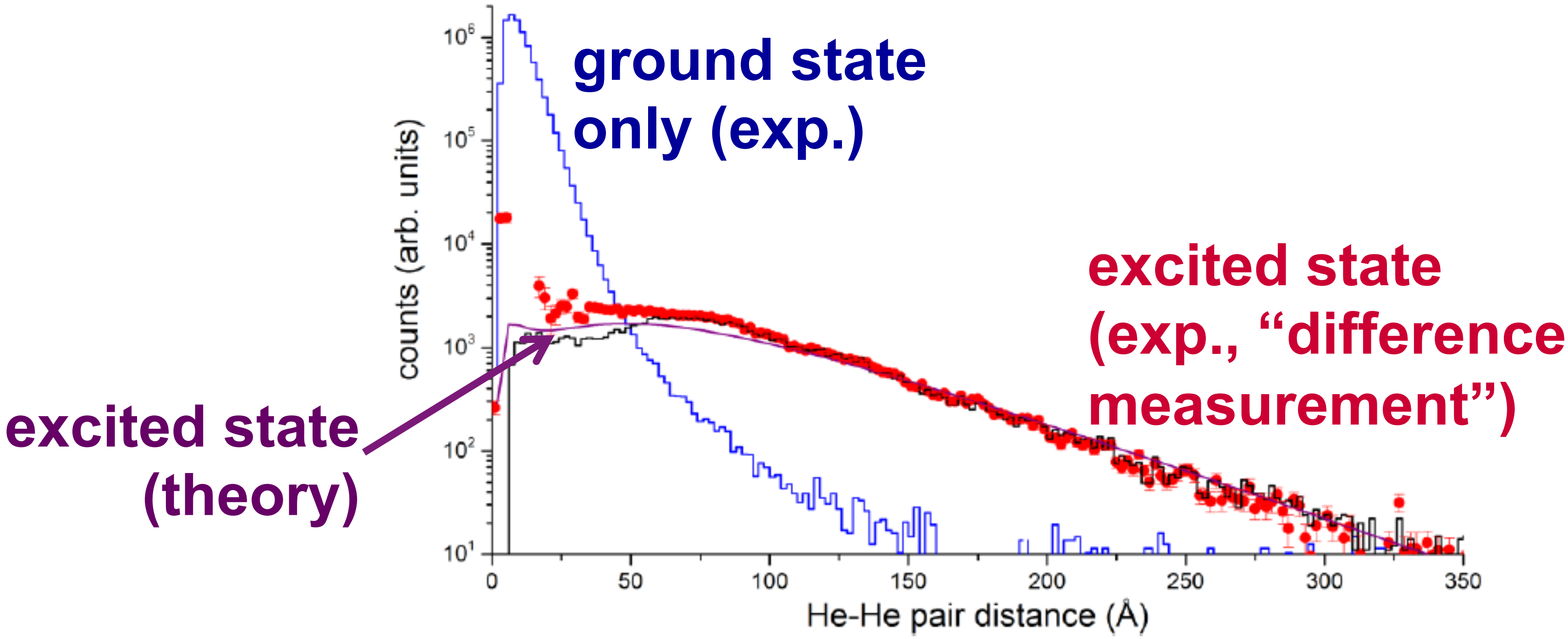
Kinetic Energy Release Measurement





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 $1/r_{12}+1/r_{23}+1/r_{31}$.

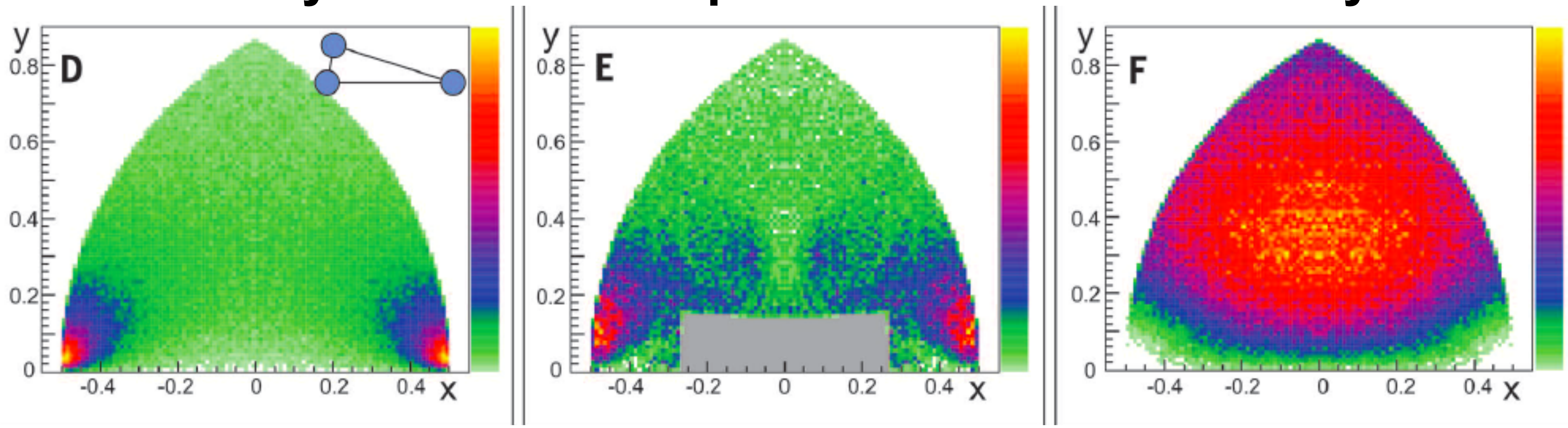
Reconstructing Real Space Properties: Pair Distribution Function of $^4He_3$



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.

Other Structural Properties of $^4He_3$

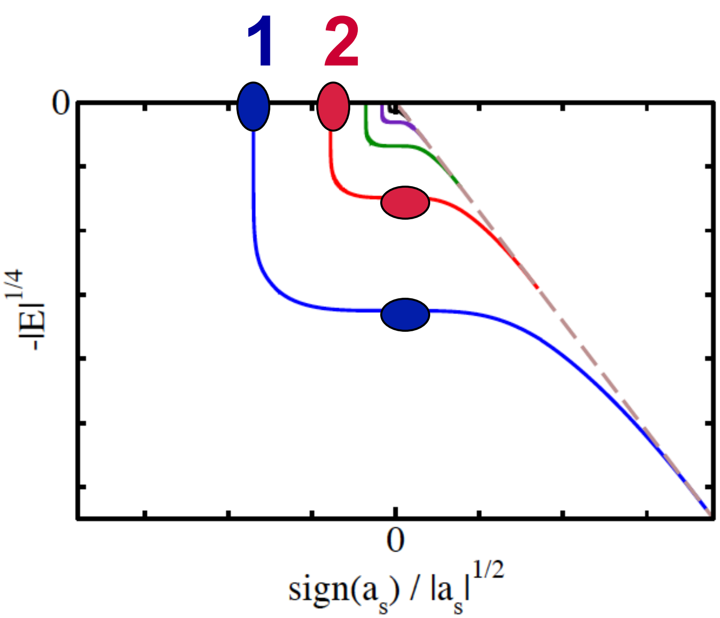
excited state: theory | excited state: experiment | ground state: theory



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.

THEORY	$\kappa^{(1)}r_6$	$a^{(1)}/r_6$	$\kappa^{(1)}a^{(1)}$
Jia Wang et al.	0.226(2)	-9.73(3)	-2.20(2)
Naidon et al.	0.187(1)	-10.85(1)	-2.03(1)

Zero-range theory: $\kappa^{(n)}a^{(n)} = -1.50763$

	$\kappa^{(1)}r_6$	$a^{(1)}/r_6$	$\kappa^{(1)}a^{(1)}$	$\kappa^{(2)}r_6$	$a^{(2)}/r_6$	$\kappa^{(2)}a^{(2)}$	$\kappa^{(1)}/\kappa^{(2)}$	$a^{(1)}/a^{(2)}$
He-He (scale)	0.222	-9.80	-2.12	0.00947	-166	-1.57	23.4	1/17.3

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: $H = \Sigma_j T_j + \Sigma_{j<k} g\delta(r_{jk})$.**
- **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 each Efimov trimer (calculations for resonance states with finite-range two-body potentials by Deltuva).**
  - **Much less is known for N>4.**

Schematic of Four-Boson Energy Spectrum

Four-atom resonances have been observed experimentally in cold atom experiments by Grimm's group.
Theory: von Stecher et al., Platter et al., Deltuva.

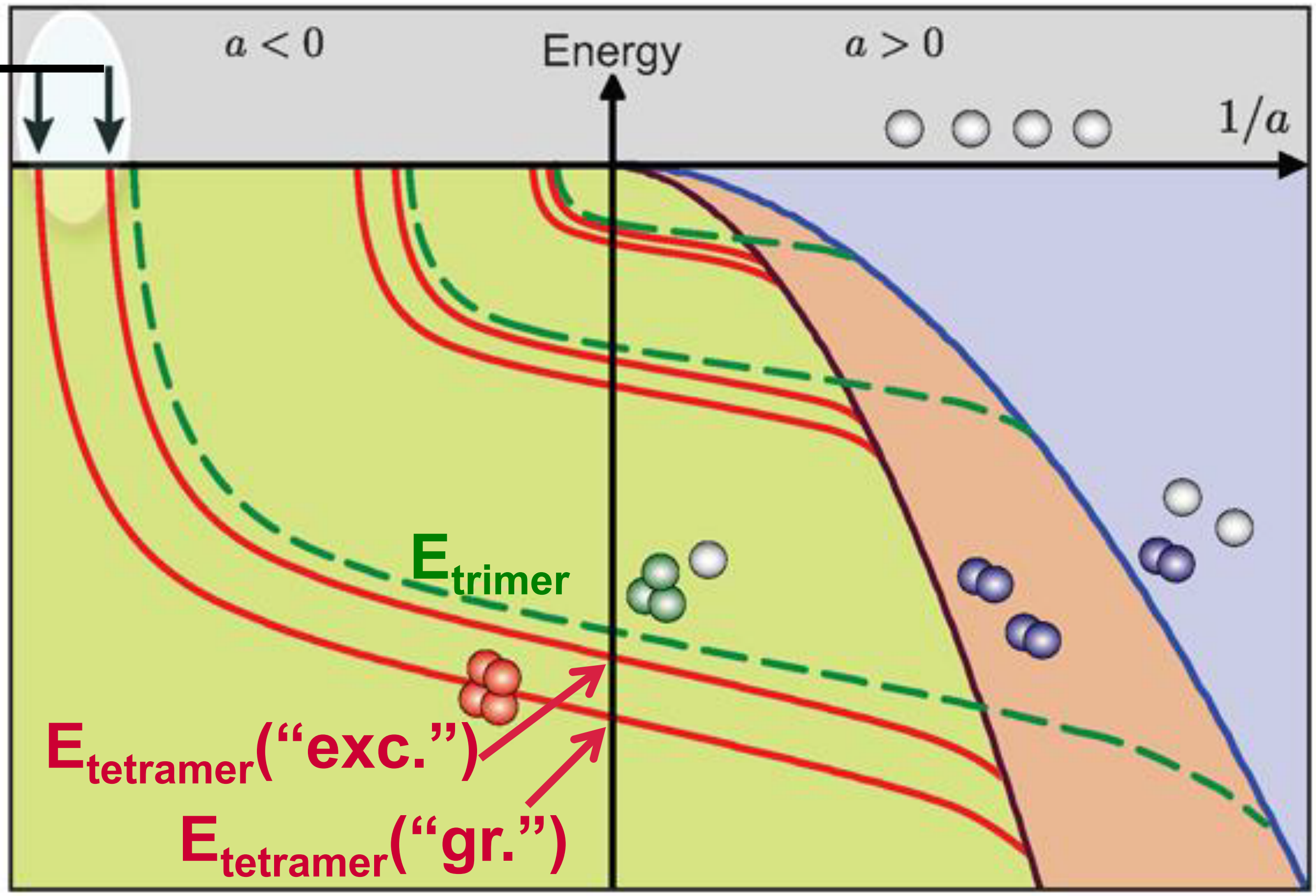


Figure taken from Grimm group.

At unitarity:

$E_{tetramer}$("gr")=4.61E_{trimer}

$E_{tetramer}$("exc")=1.002E_{trimer}

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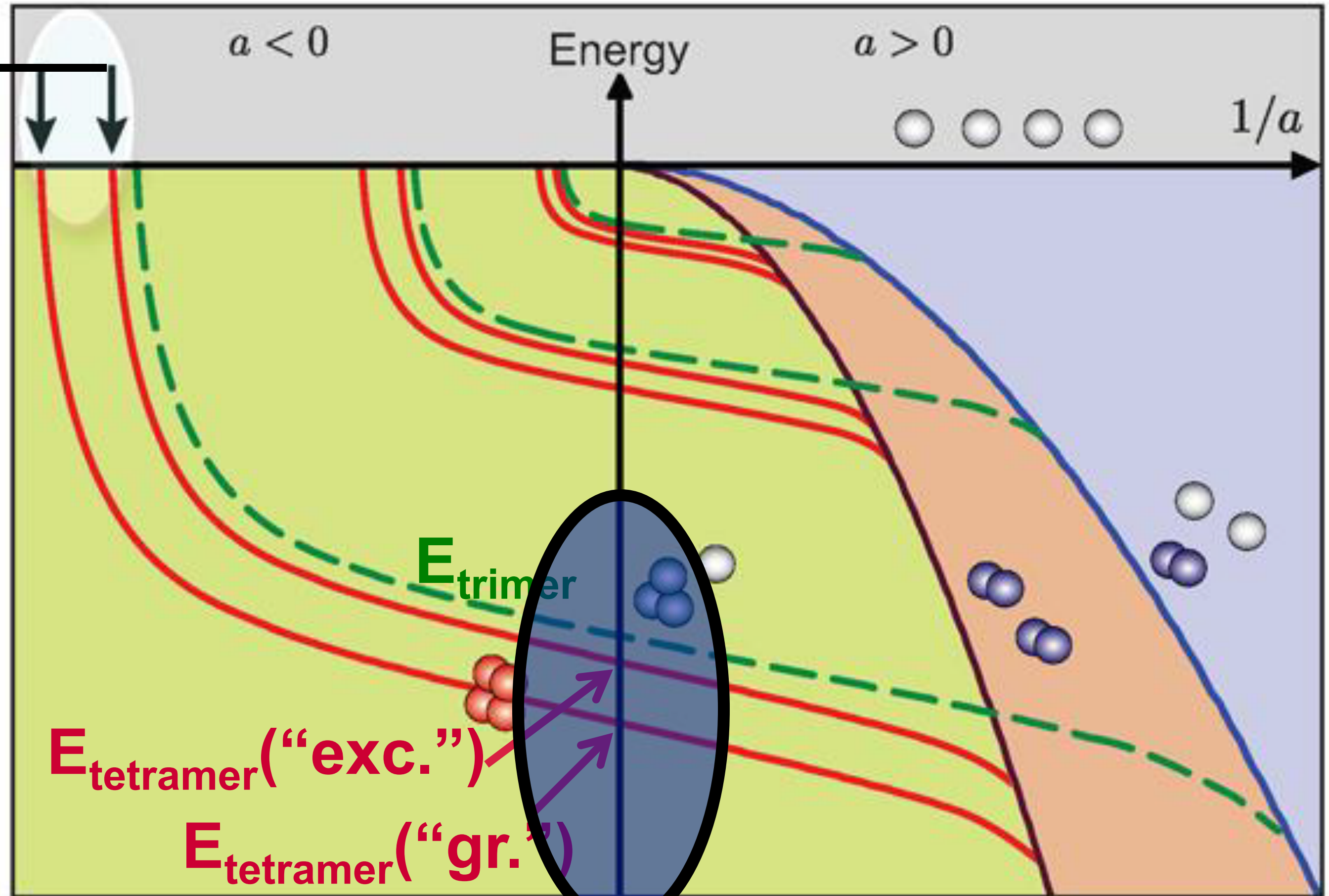
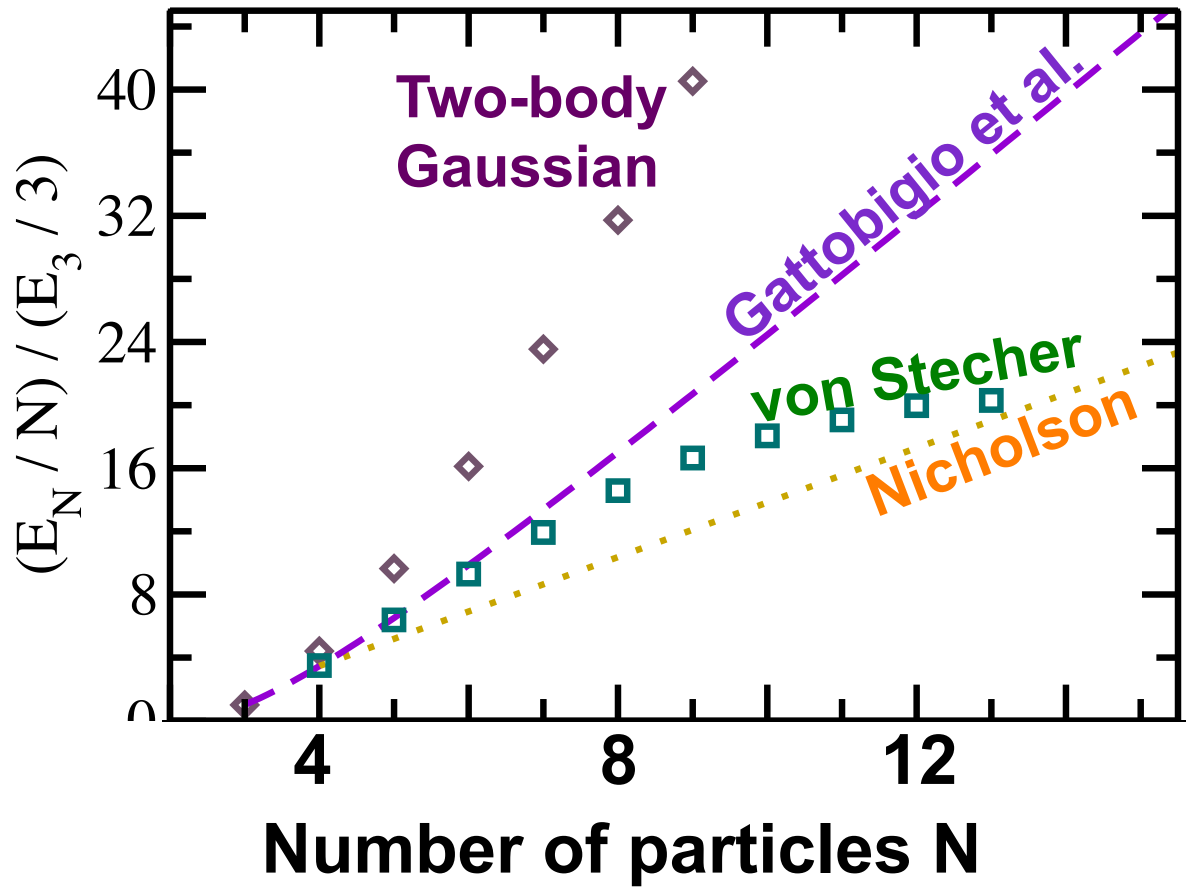


Figure taken from Grimm group.

At unitarity:
$E_{tetramer}$("gr")=4.61E_{trimer}
$E_{tetramer}$("exc")=1.002E_{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.

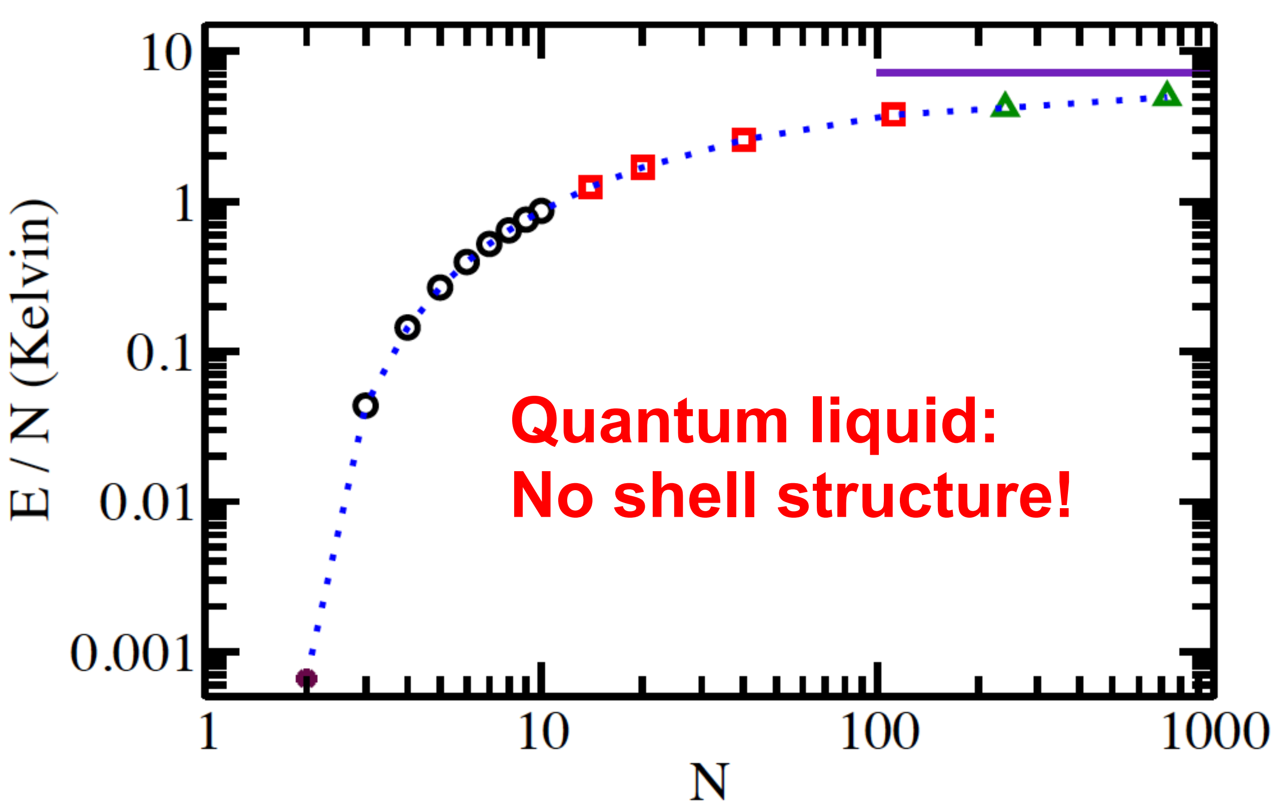
Gattobigio et al.: $E_N/N \sim \# N$ + correction; semi-empirical based on gr. st. calcs. (PRA 2014).

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



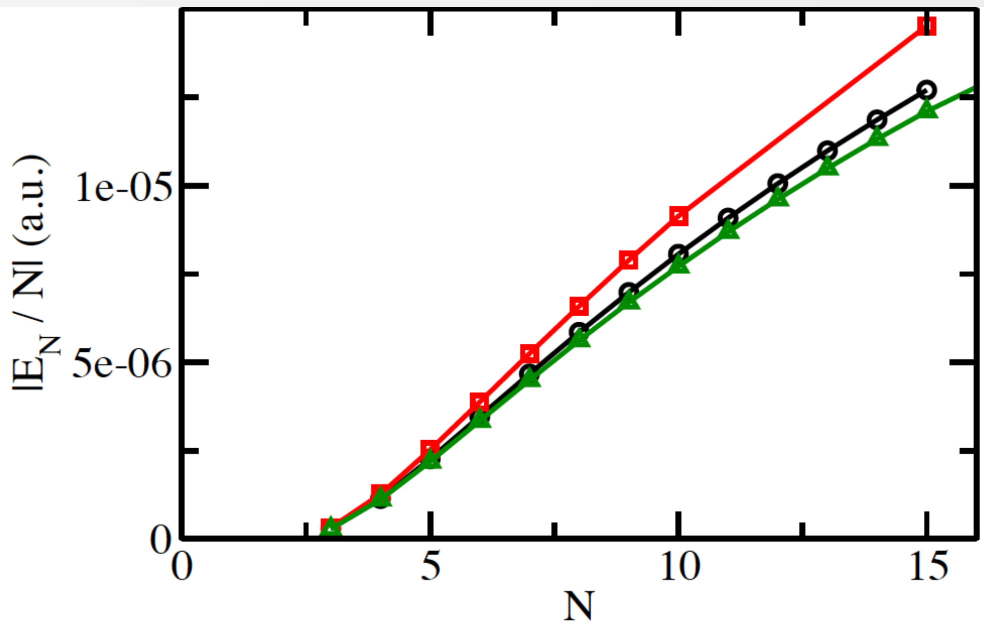
Well known literature results:

Small N (N<10): E/N ~ # N.

Large N: E/N ~ −7K

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

What About Infinite S-Wave Scattering Length for van der Waals Interactions?



Two-body van der Waals potential $V(r)=c_p/r^p-c_6/r^6$ 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.

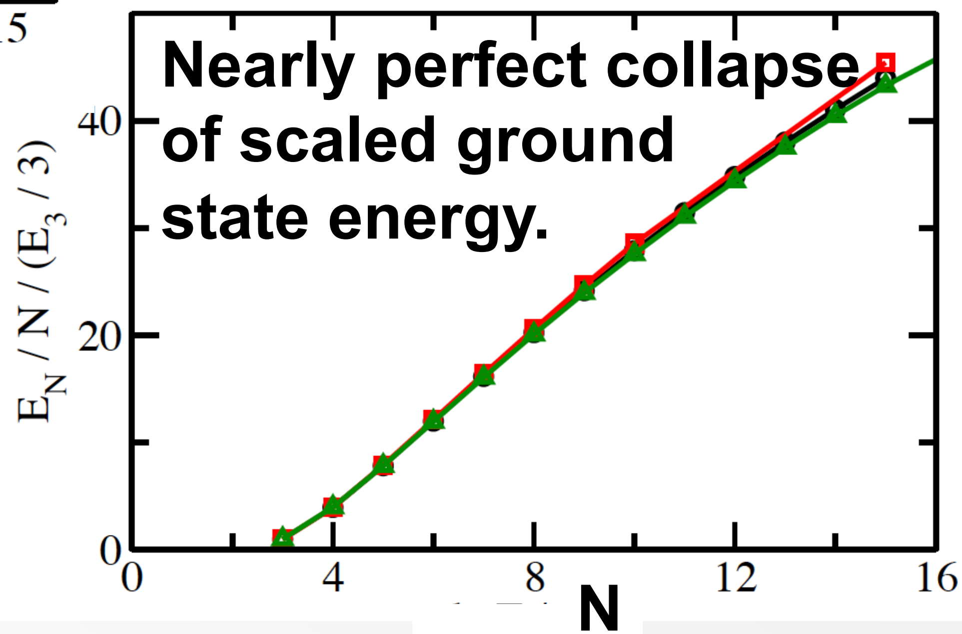
N-body energies scaled by three-body energy:

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!



N Identical Bosons with Infinitely Large s-Wave Scattering Length

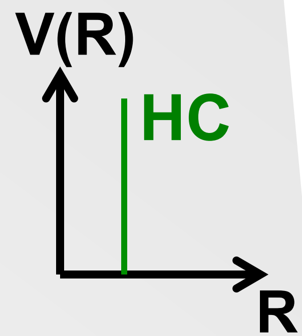
- **Non-relativistic quantum mechanics in the spirit of Efimov (two-body zero-range interactions): $H = \Sigma_j T_j + \Sigma_{j<k} g\delta(r_{jk})$.**

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

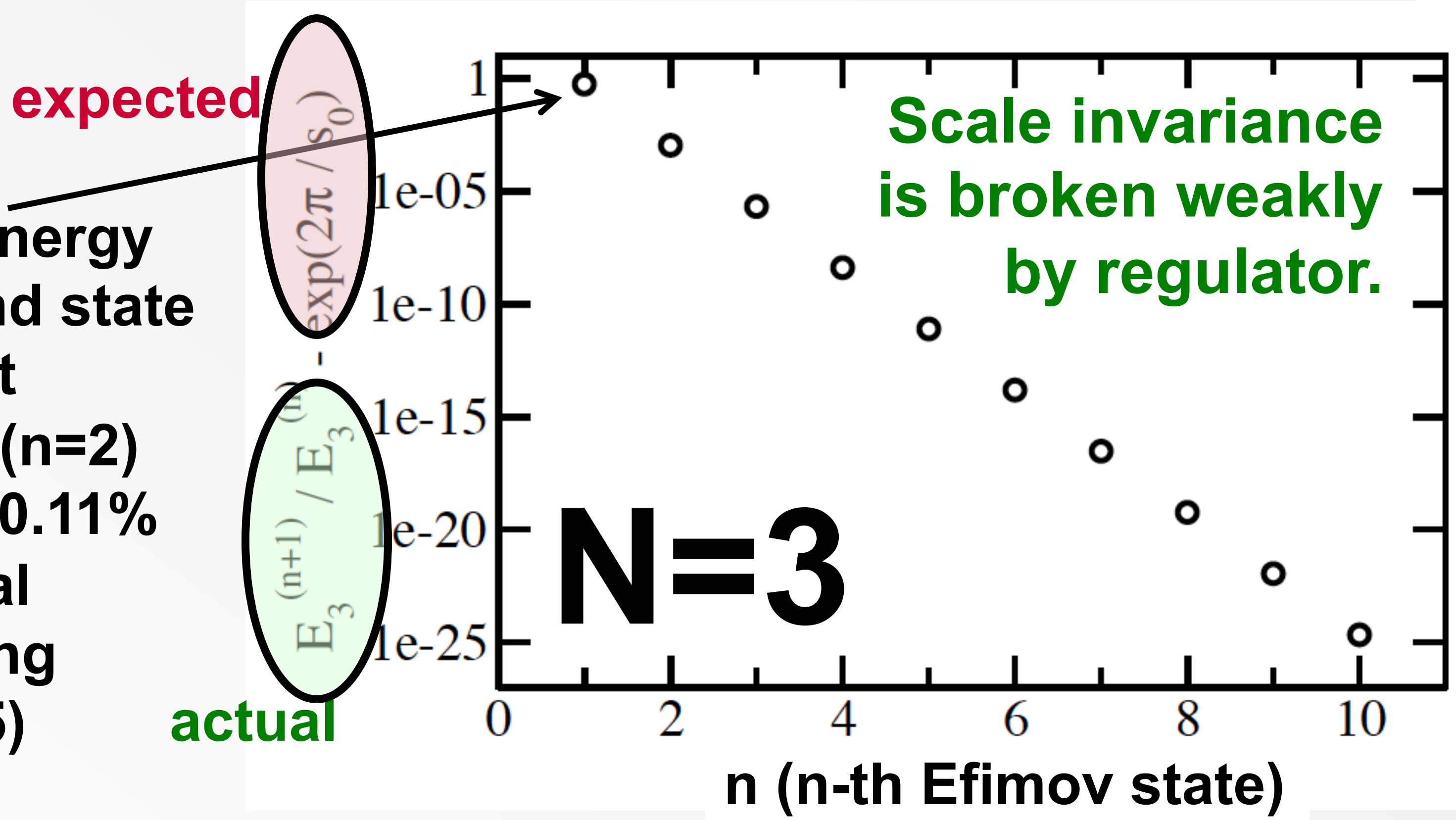
- **To avoid Thomas collapse, use repulsive three-body regulator (we don't know how to treat three-body zero-range boundary condition…):**
  - **Use three-body regular so that N=3 system is as close as possible to ideal Efimov trimer; see work by von Stecher (hardcore regular or repulsive powerlaw potential).**

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.

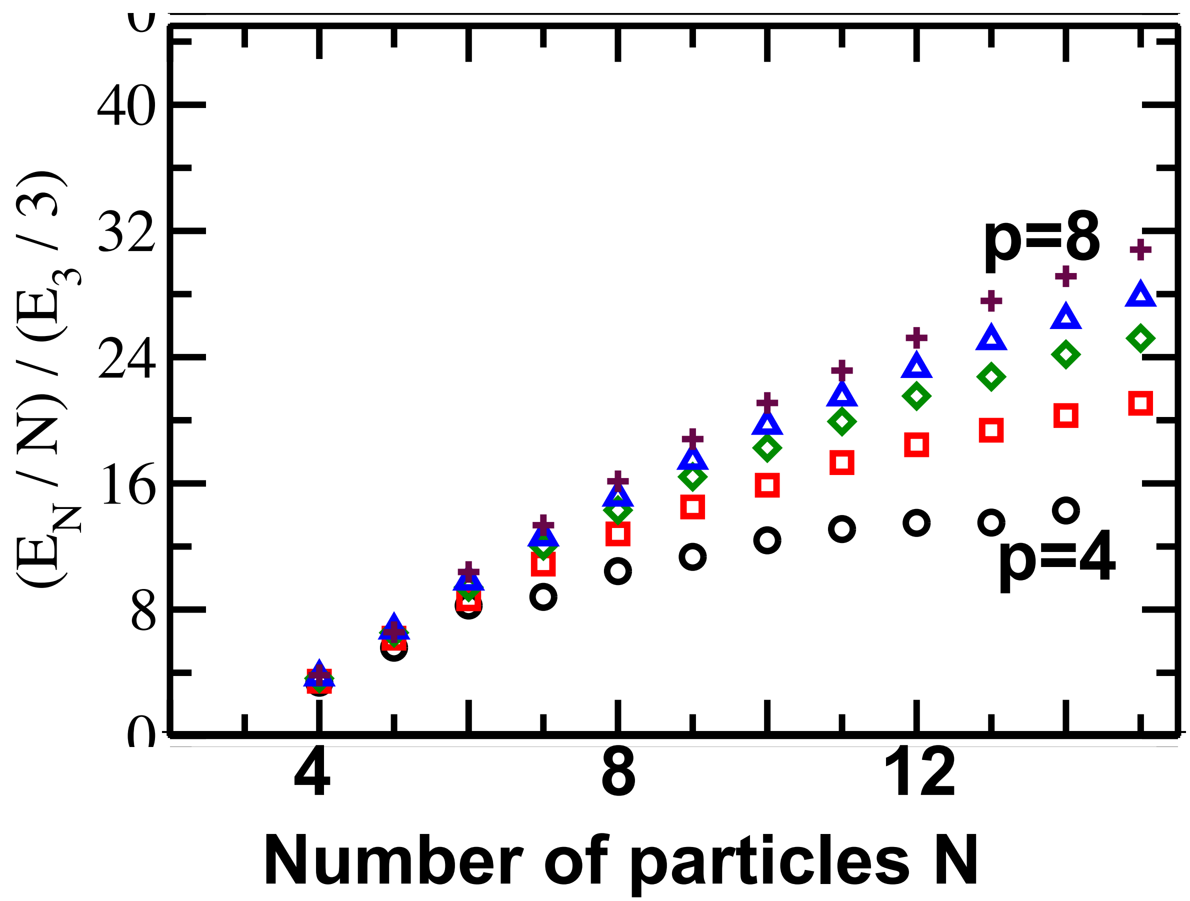


Three-body energy ratio of ground state (n=1) and first excited state (n=2) deviates by ~0.11% from universal energy spacing (<1 out of 515)



Use Two-Body Zero-Range Interactions and Three-Body Finite Regulator

Yan and Blume, PRA 2015 and in preparation.



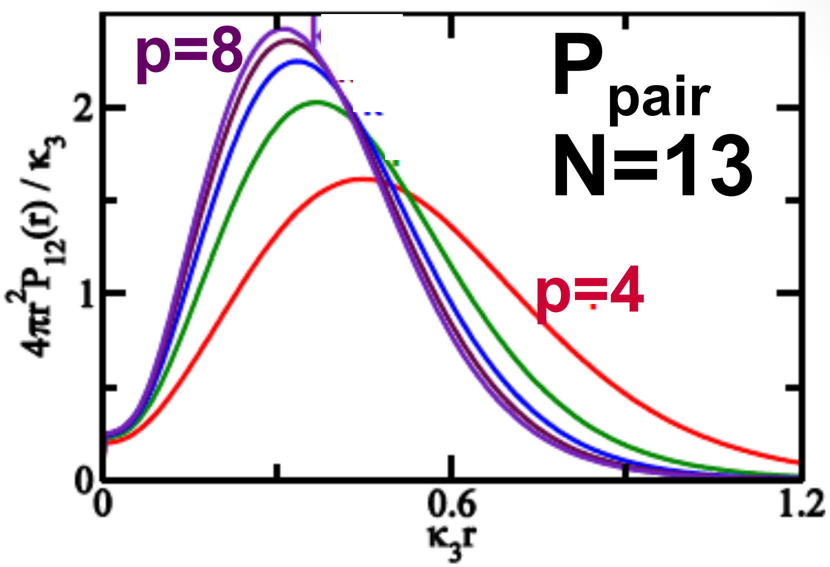
We consider ground states (not resonance states).

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

Use $1/(R_{ijk})^p$ regulator in three-body sector: $(R_{ijk})^2=(r_{ij})^2+(r_{jk})^2+(r_{ki})^2$.

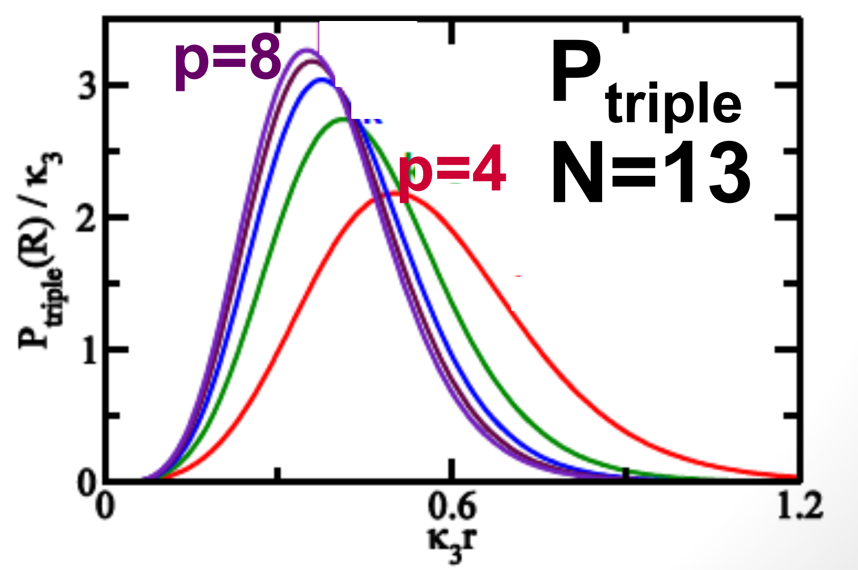
The three-body regulator leads to very weak breaking of the scale invariance in three-body sector. The effect is enhanced for N>3.

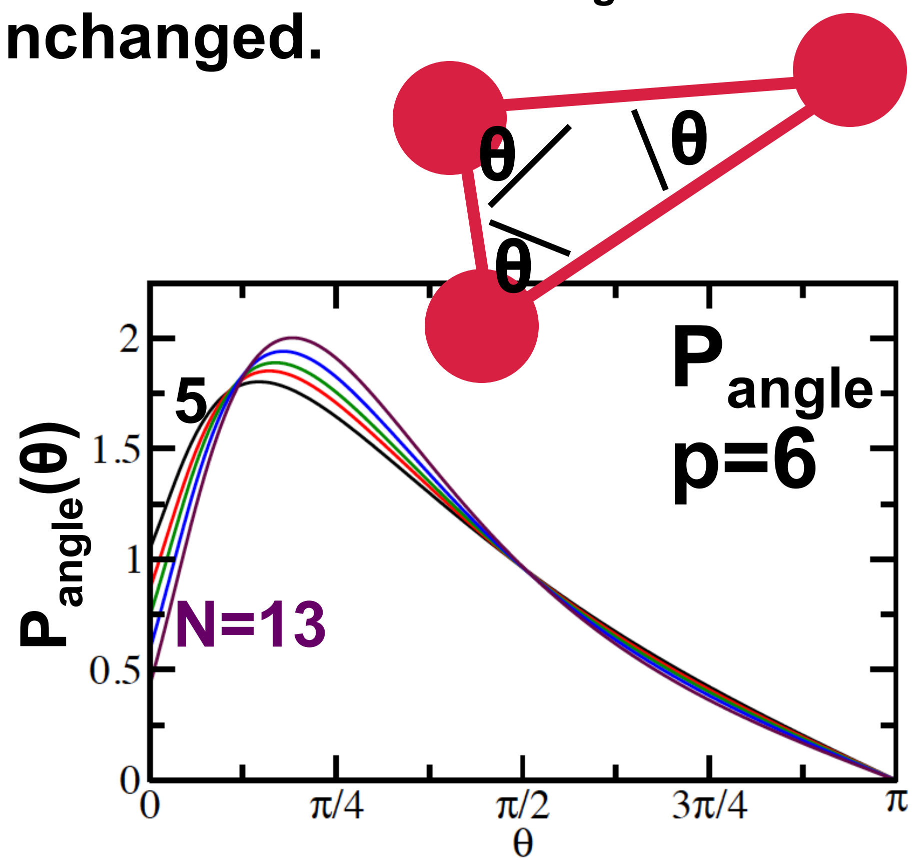
Smooth Distribution Functions: No Shell Structure



No evidence of shell structure or layering.

Three-body regulator changes "size" but leaves P_{angle} nearly unchanged.

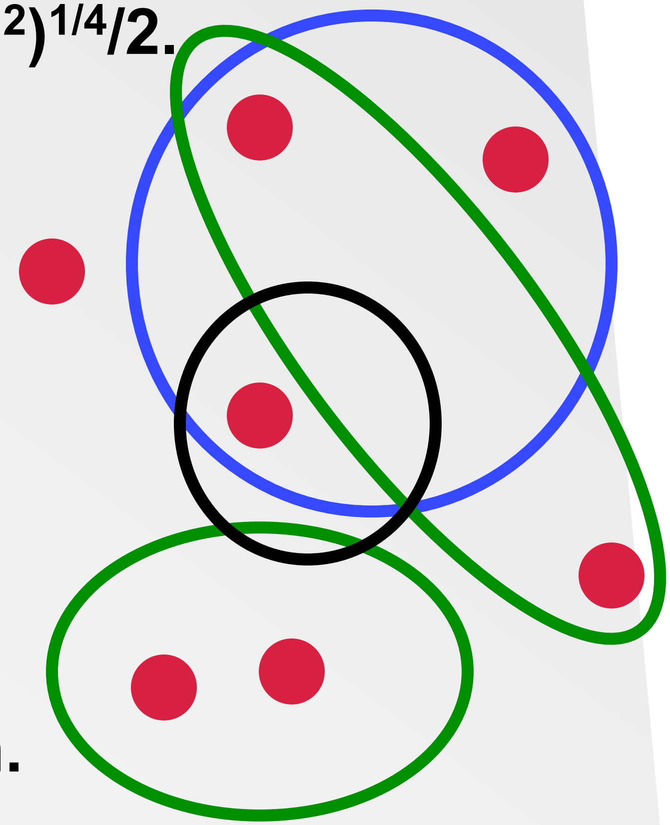




N-Body Lengths in Terms of Characteristic/Intrinsic Lengths

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

	N=3	N=15
r_{ij} / L_6	16	10
R_{ijk} / L_6	18	11
$(\rho_{max})^{-1/3} / L_6$	7	4.5

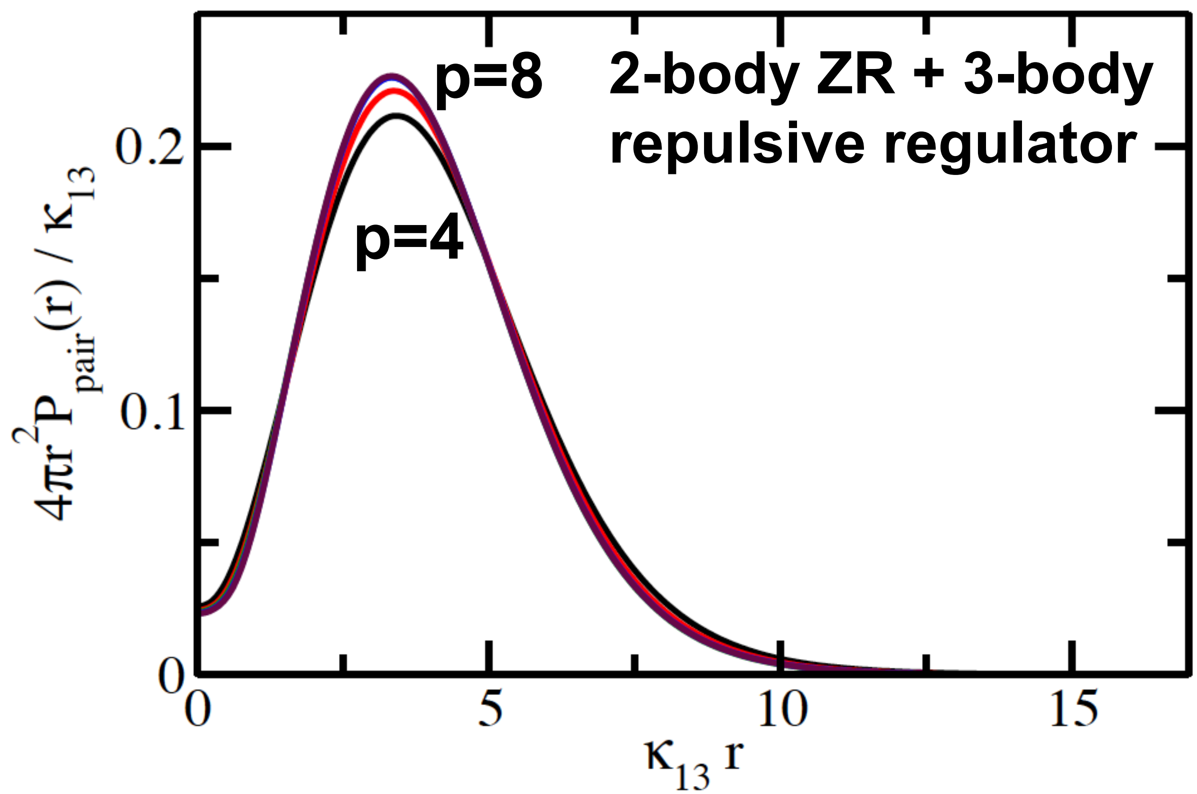


- N-body state is large and largely located in classically forbidden region.

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_{pair} if Scaled by N-Body Binding Momentum

Amplitude is largely located in classically forbidden region.



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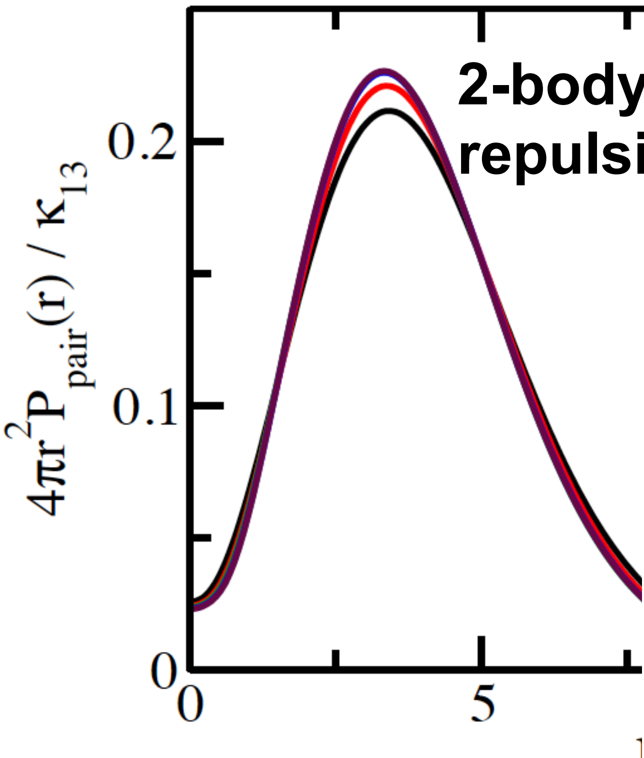
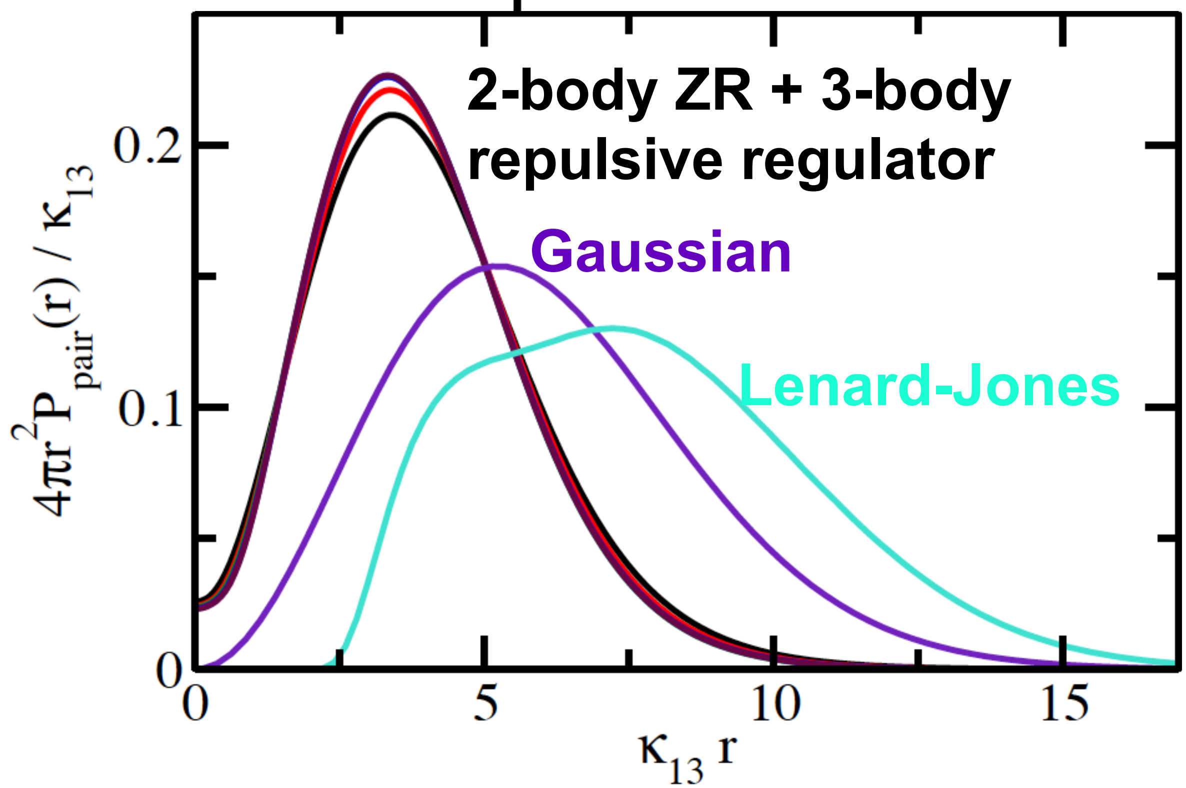
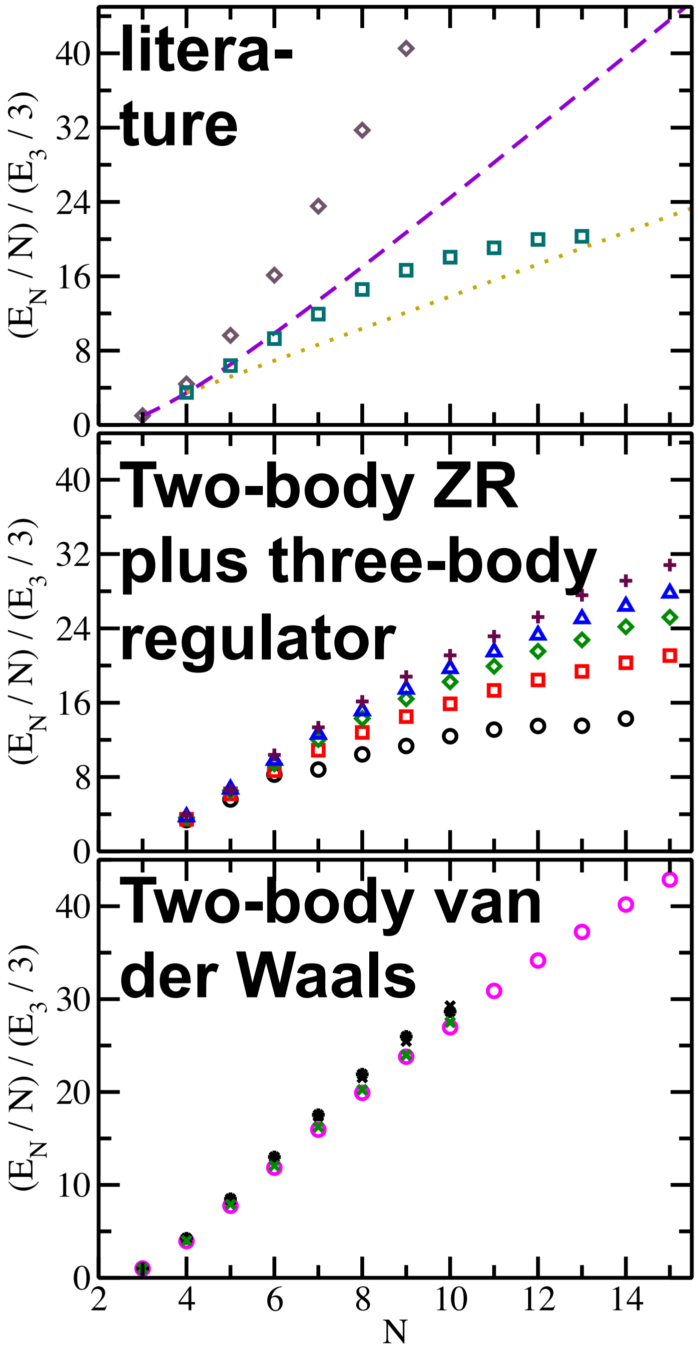




Different classes in N-body sector.



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:

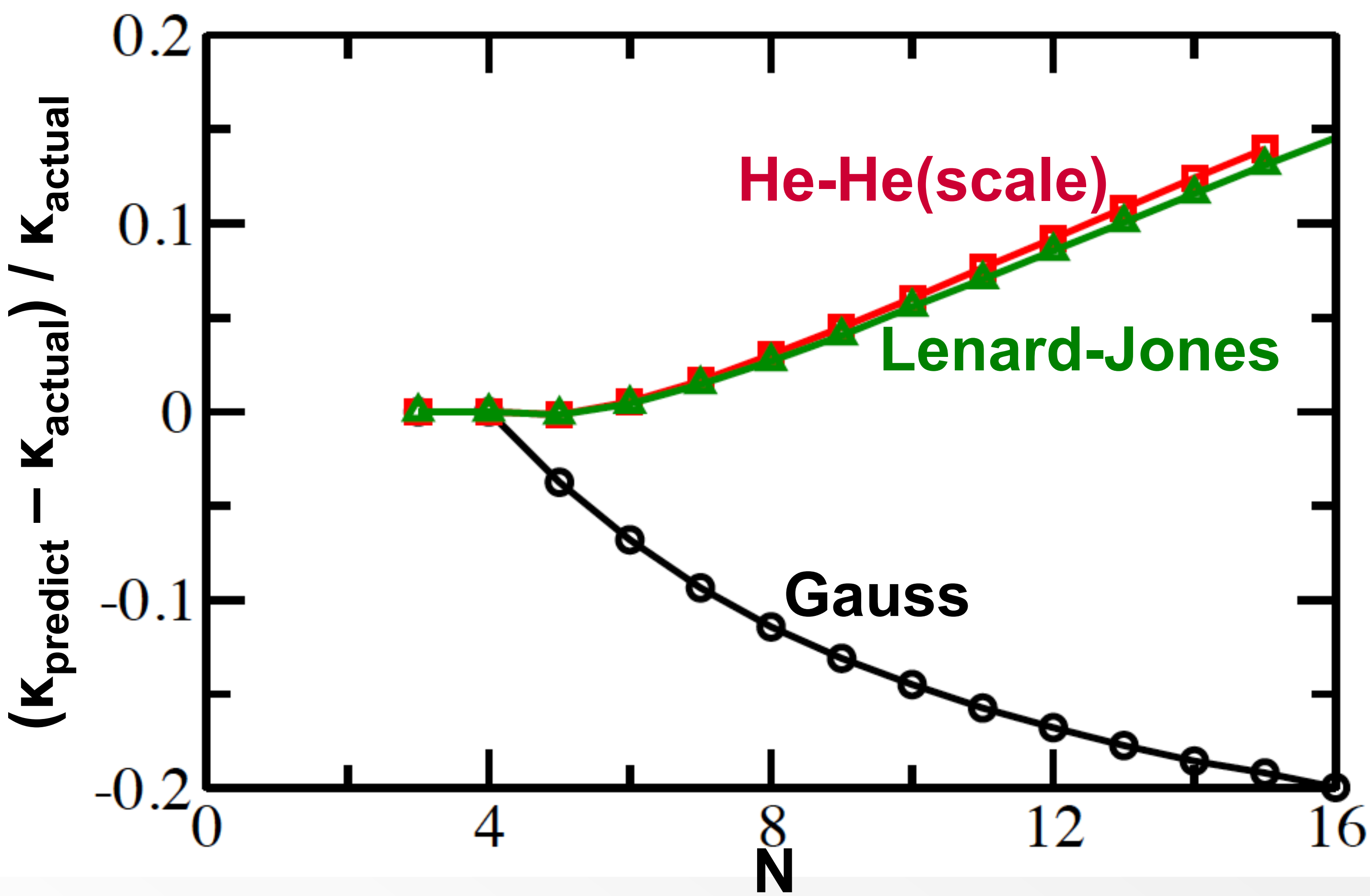
N=2: Nearly fully universal.
N=3: Structure of ground state trimer differs from ideal Efimov trimer; van der Waals universality for sufficiently repulsive short-range potential.
N>3: E_N/E_3 nearly collapse.

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?



$\kappa_{predict} = \kappa_3 + \kappa_3 (N - 3) (\kappa_4 / \kappa_3 - 1)$; see Gattobigio et al. (2015).
Three- and four-body binding momentum serve as input.

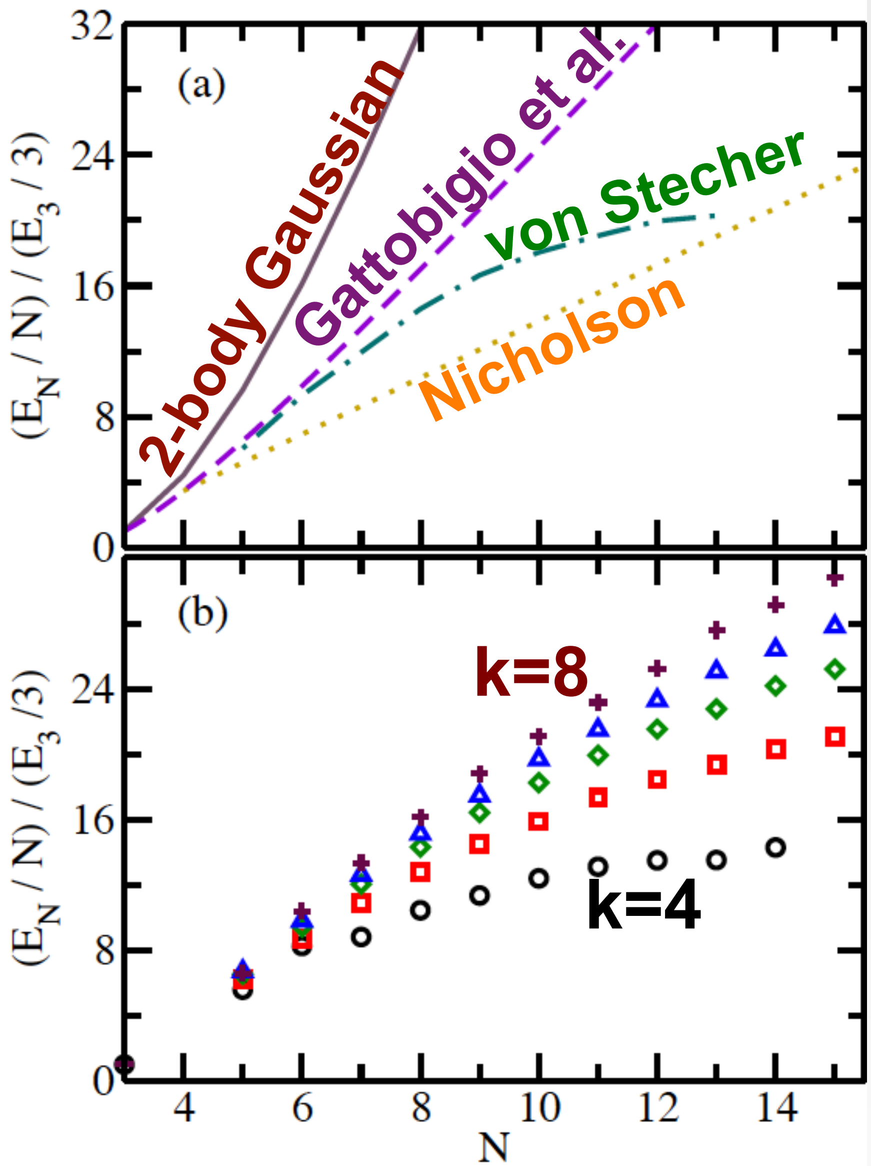
N-Body Sector with Infinitely Large Two-Body s-Wave Scattering Length

- **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



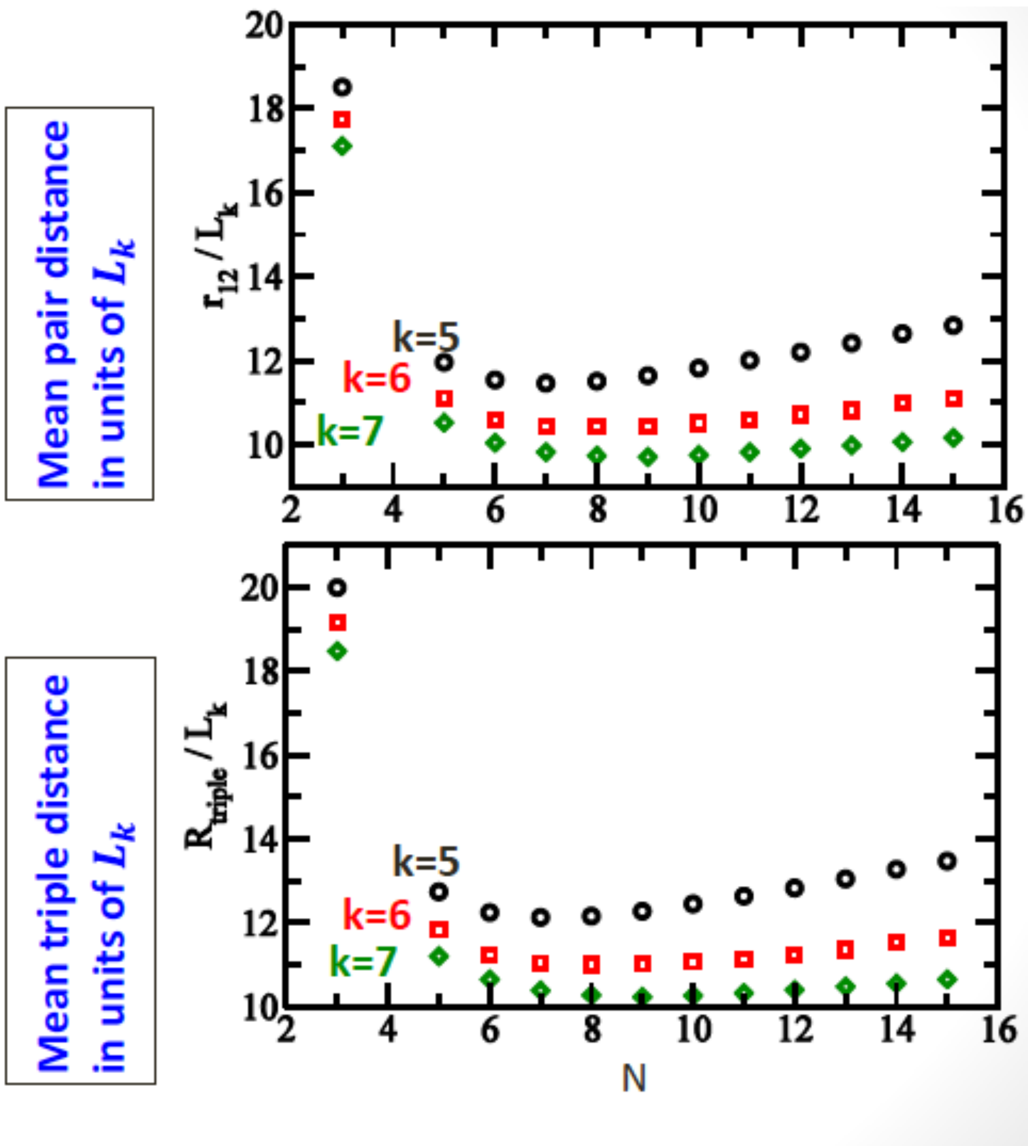
If the N-body energy was fully determined by the three-body parameter, then the curves would collapse to a single curve.

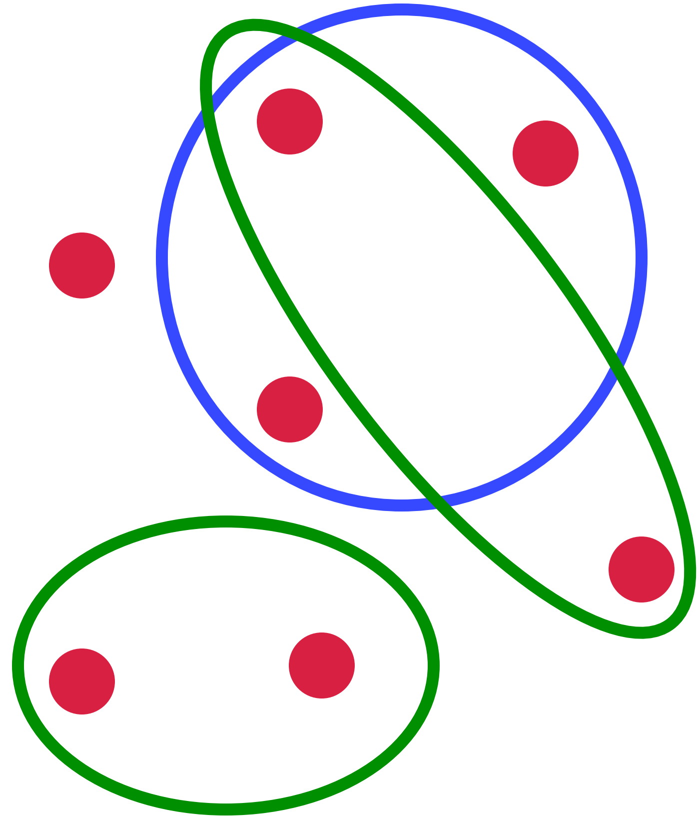
Doesn't happen with the literature data.

Doesn't happen with our data.

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

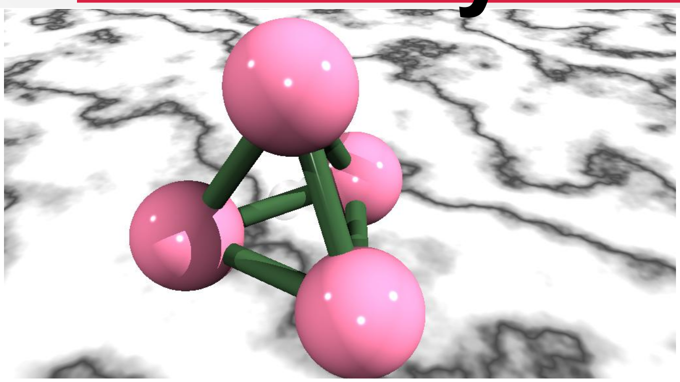
Length Scales?



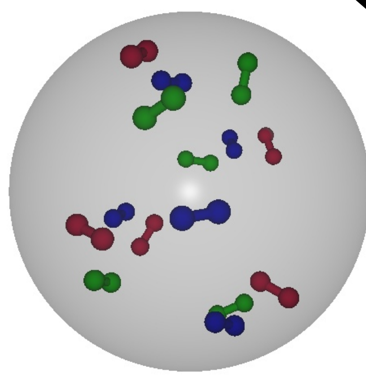


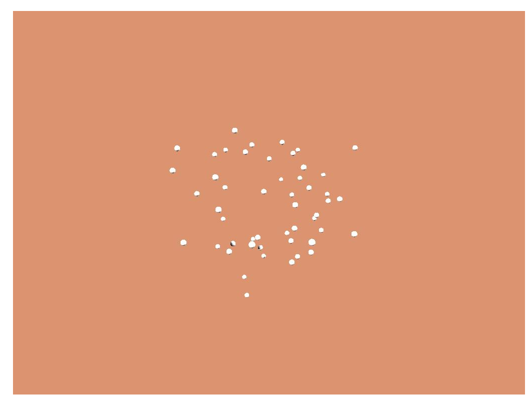
Factor of 10… Apparently not enough.

Summary



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

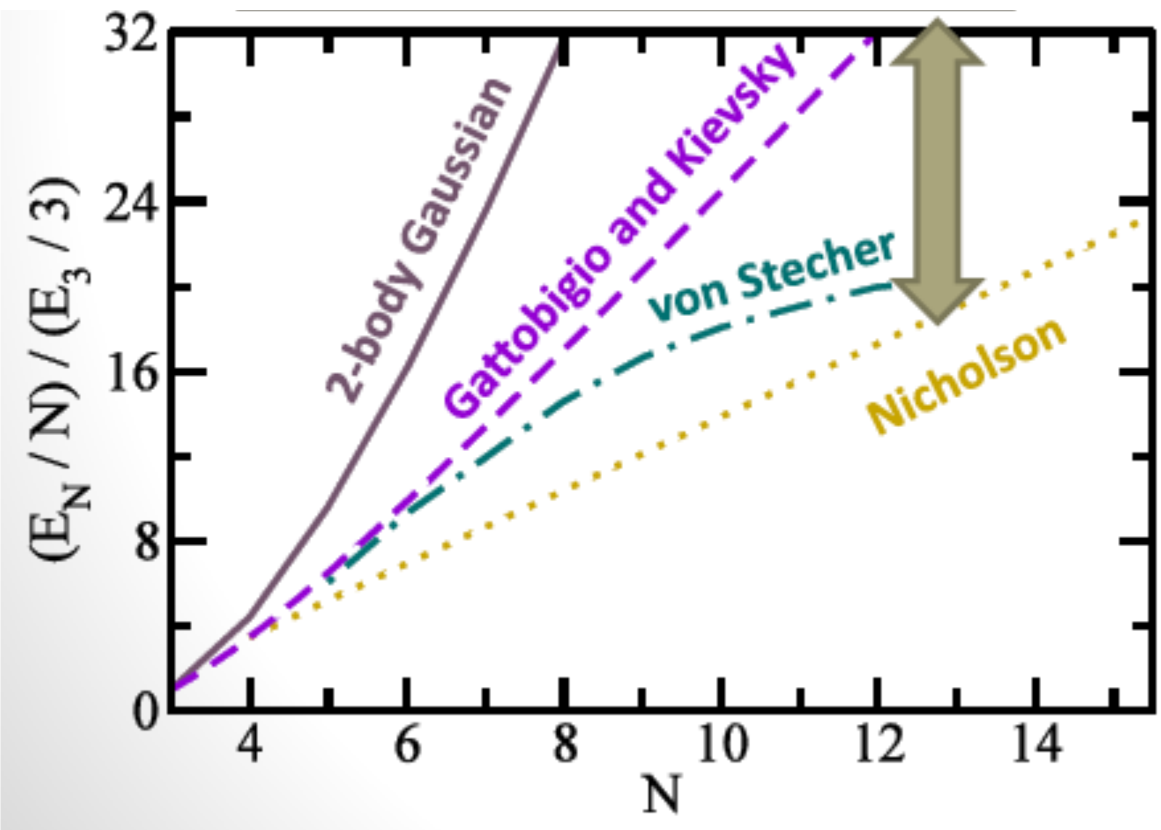




Thanks to collaborators:
Chris Greene, Brett Esry, Maksim Kunitski, Reinhard Doerner, Yangqian Yan, S. Zeller, J. Voigtsberger, A. Kalinin, L. Schmidt, M. Schoeffler, A. Czasch, W. Schoellkopf, R. Grisenti, T. Jahnke.

"Universal" Predictions for Energy of N-Body Droplets with Infinitely Large a_s

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

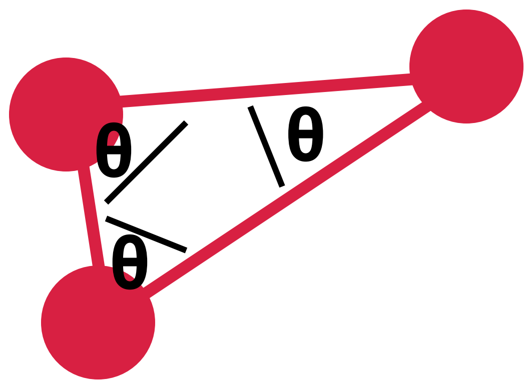


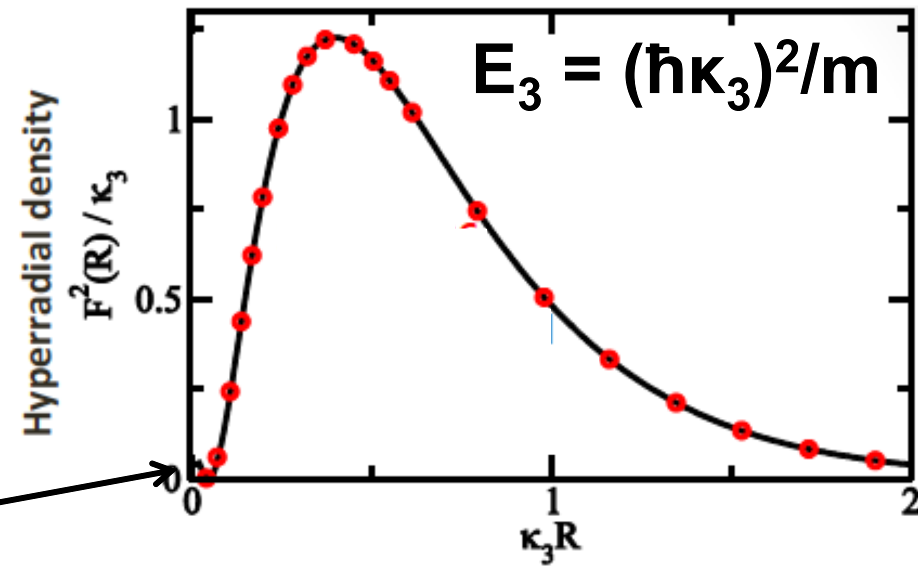
M. Gattobigio and A. Kievsky: $E_N \sim N^2$ based on 2bG (finite-range effects "taken out"), Phys. Rev. A 90, 012502 (2014).

A. Nicholson: $E_N \sim N^2$ based on N-body noise, Phys. Rev. Lett. 109, 073003 (2012).

J. von Stecher: 2-body finite-range interaction with 3-body hardcore, J. Phys. B 43, 101002 (2010).

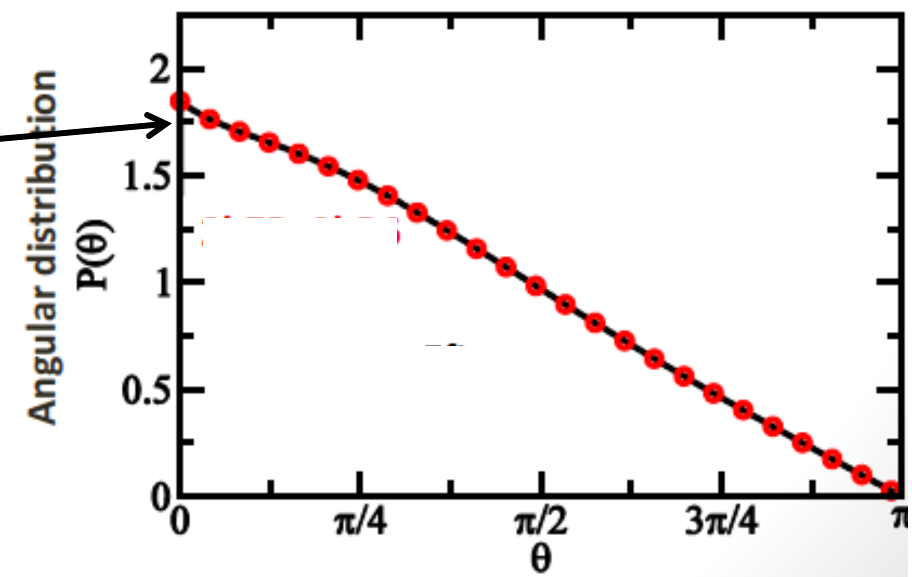
How Do the Three-Body Correlations of an Ideal Efimov Trimer Look Like?





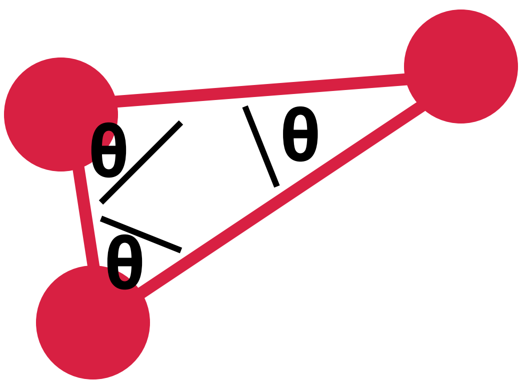
infinitely many lobes

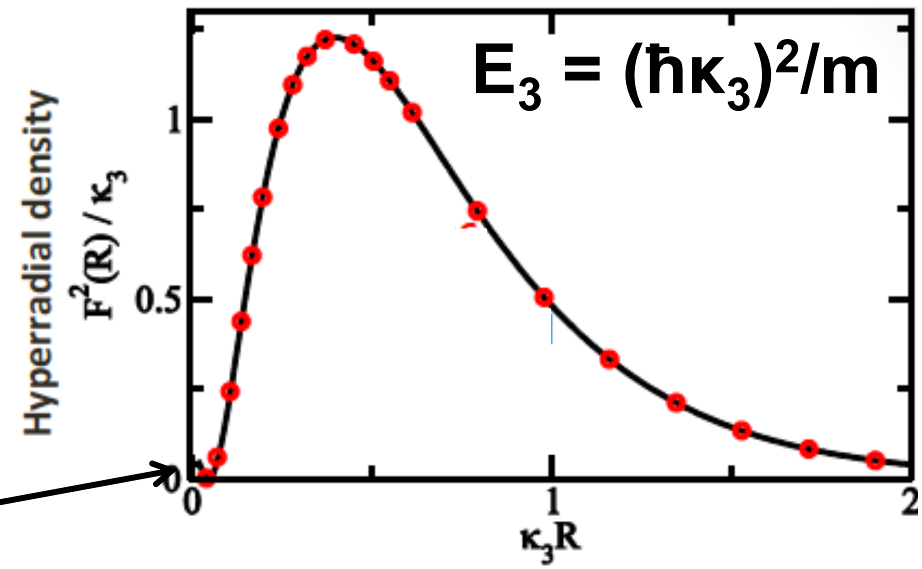
all angles occur



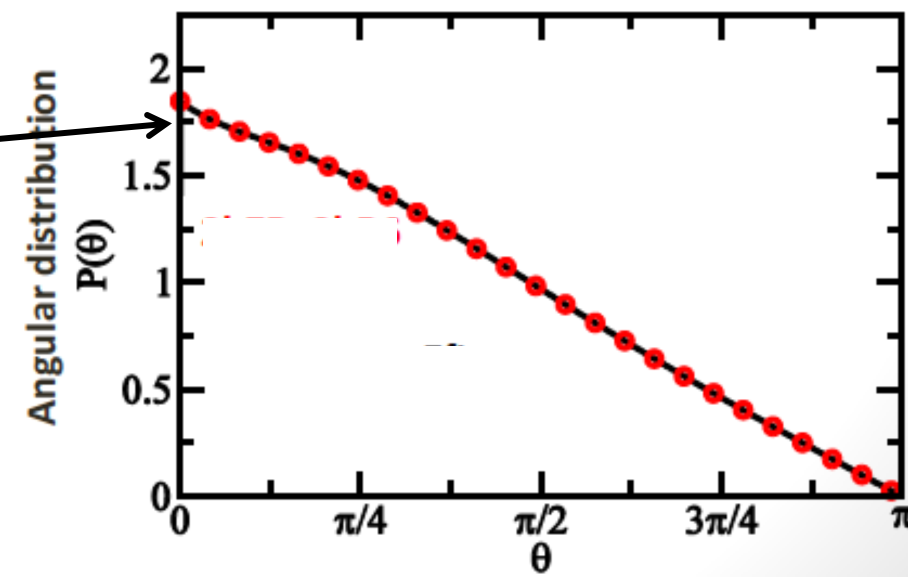
Next: What about finite a_s?

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





infinitely many lobes

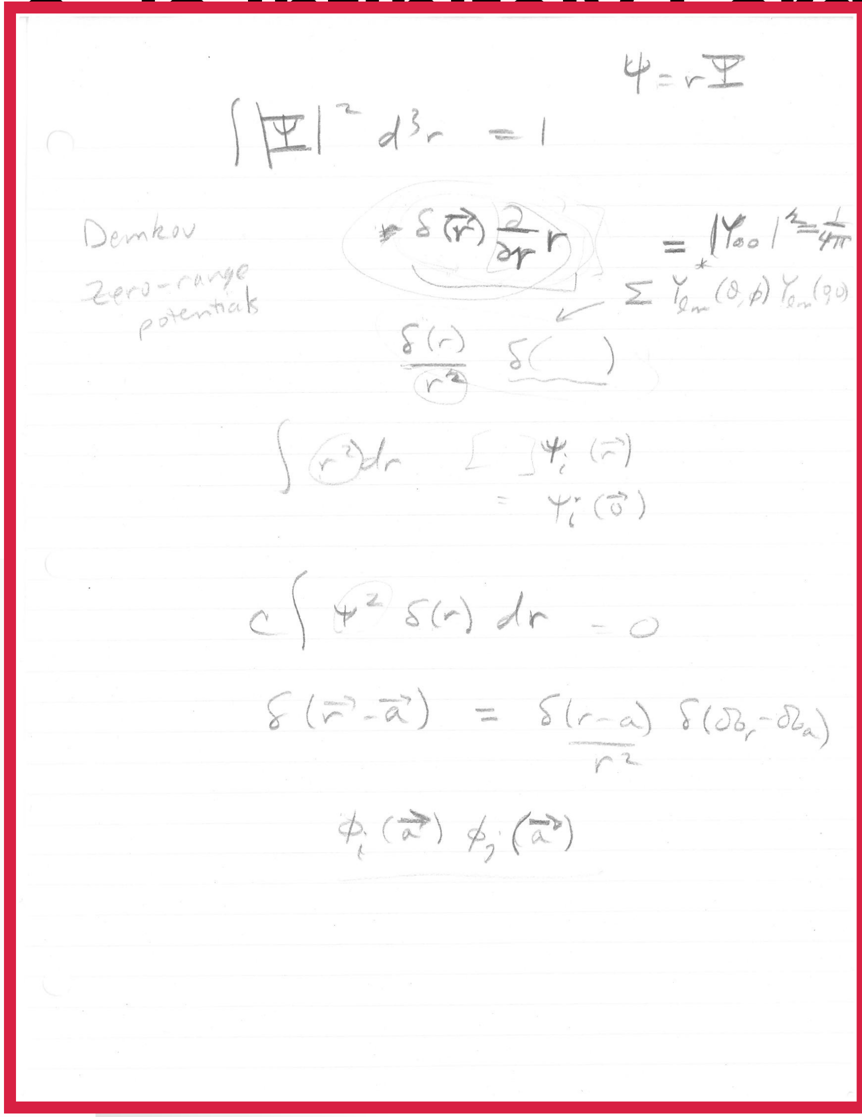


all angles occur

Next: What about finite a_s?

Pretend:

a_s is Infinitely Large and r_{eff} Vanishes



…ov scenario.

… (the **zero-range interactions** …ale for the trimer): The …becomes (s_0=1.006…)

$$\ldots \frac{1}{4}\Big) \ldots = \lambda^{-2} H(\mathrm{R})$$

$$\ldots,$$

$$\ldots = \lambda^{-2}\, E_3^{(n)}.$$

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.

Pretend:
a_s is Infinitely Large and r_{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…)

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

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

If $\mathrm{F}(R)$ is a solution with energy $E_3^{(n)}$,

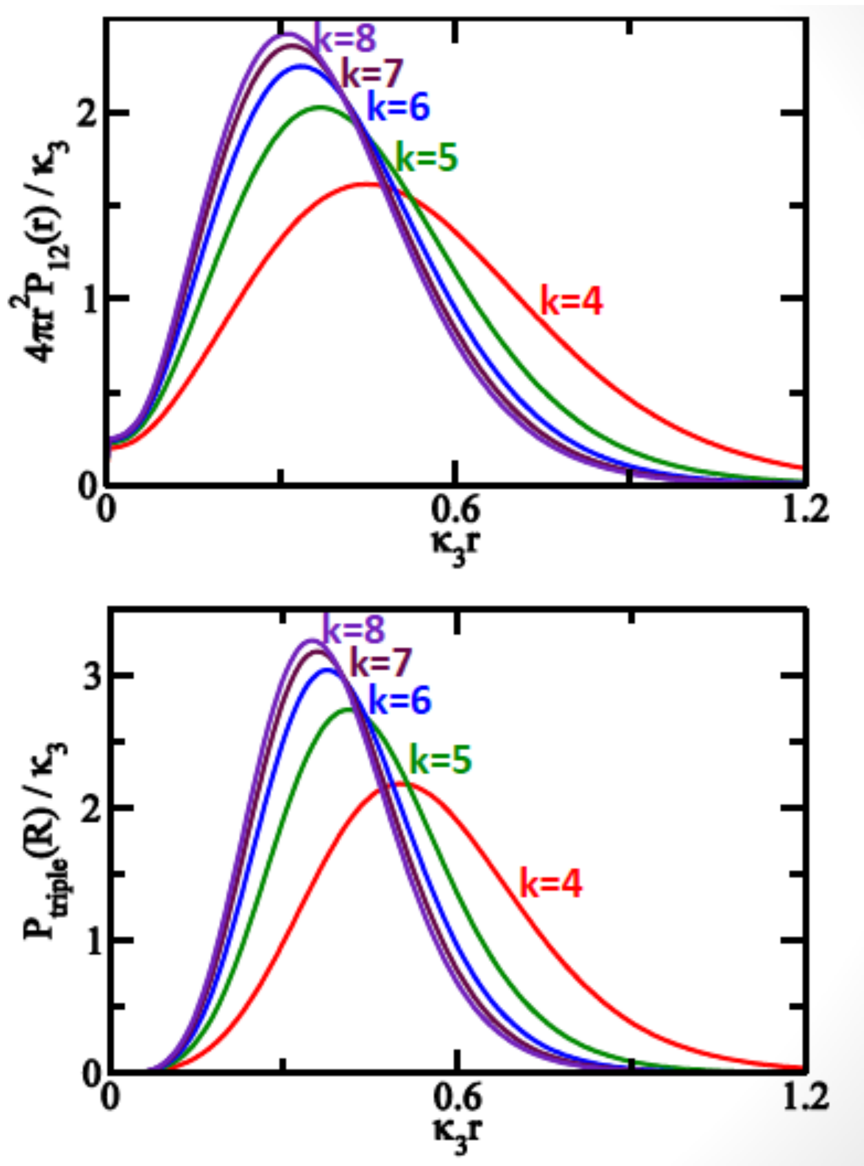
$F(\lambda R)$ is a solution with energy $E_3^{(n+1)} = \lambda^{-2}\, E_3^{(n)}$.

Here, $\lambda = \exp(\pi/s_0) \approx 22.7$

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

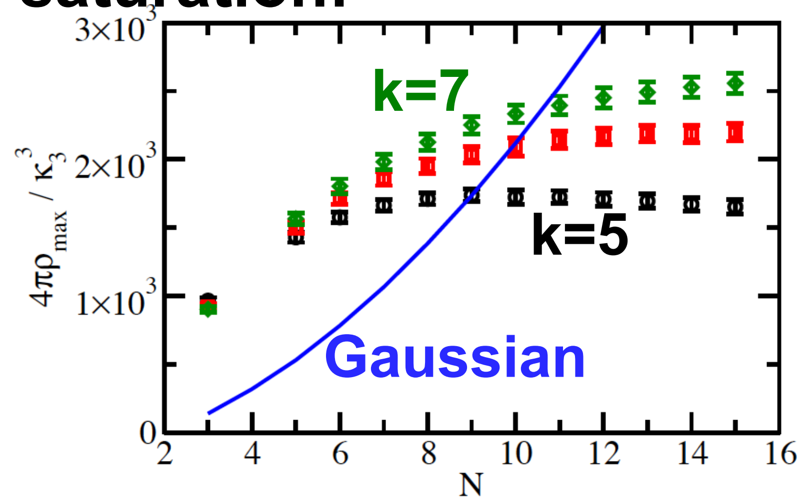
Each hyperradial wave function has infinitely many nodes.

Smooth Pair and Triple Distribution Functions for N=13

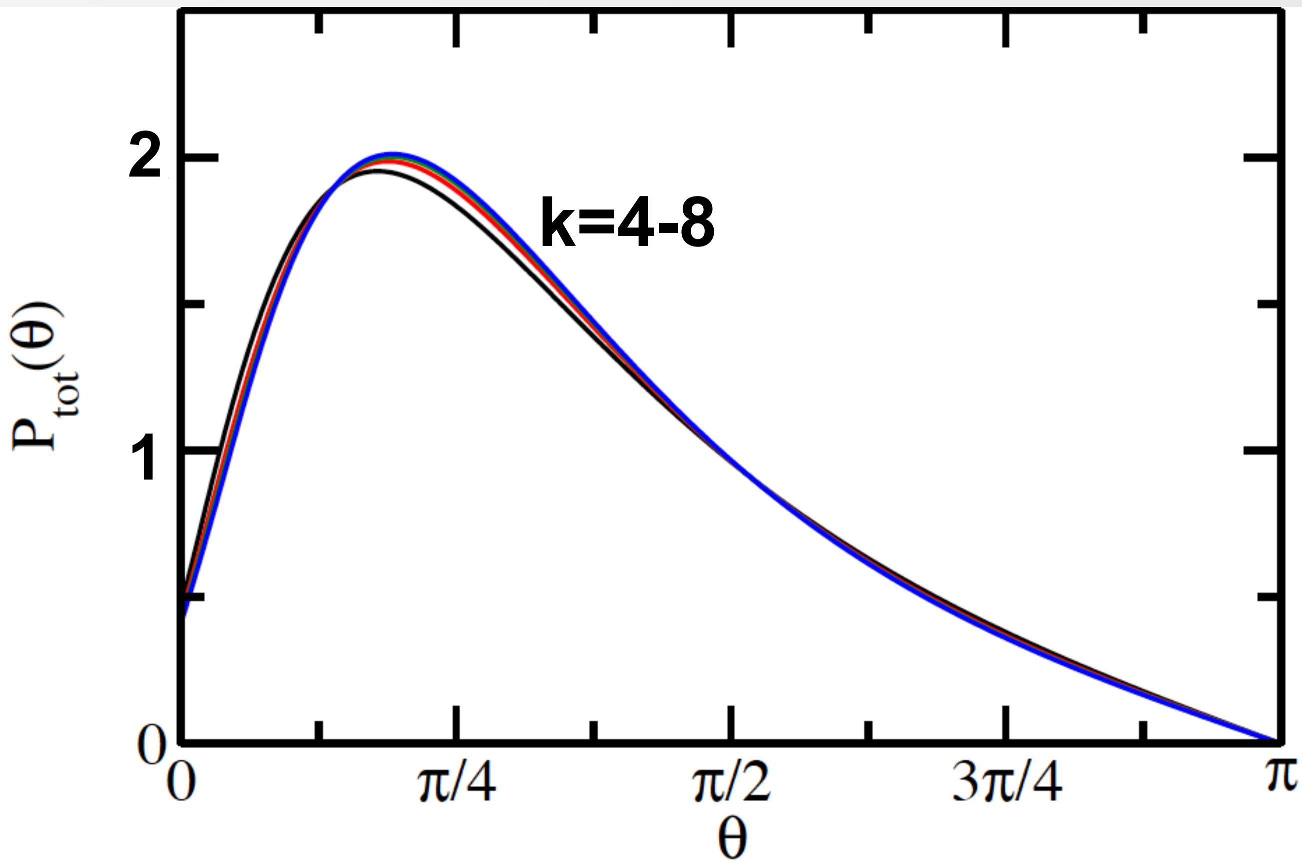


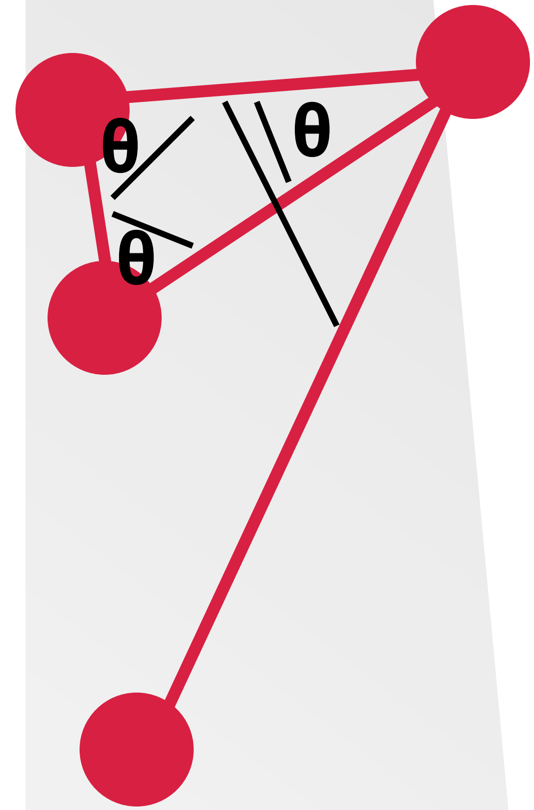
Quantitative differences.
Qualitatively similar.
In particular: No evidence of shell structure or layering.

Peak density displays saturation:



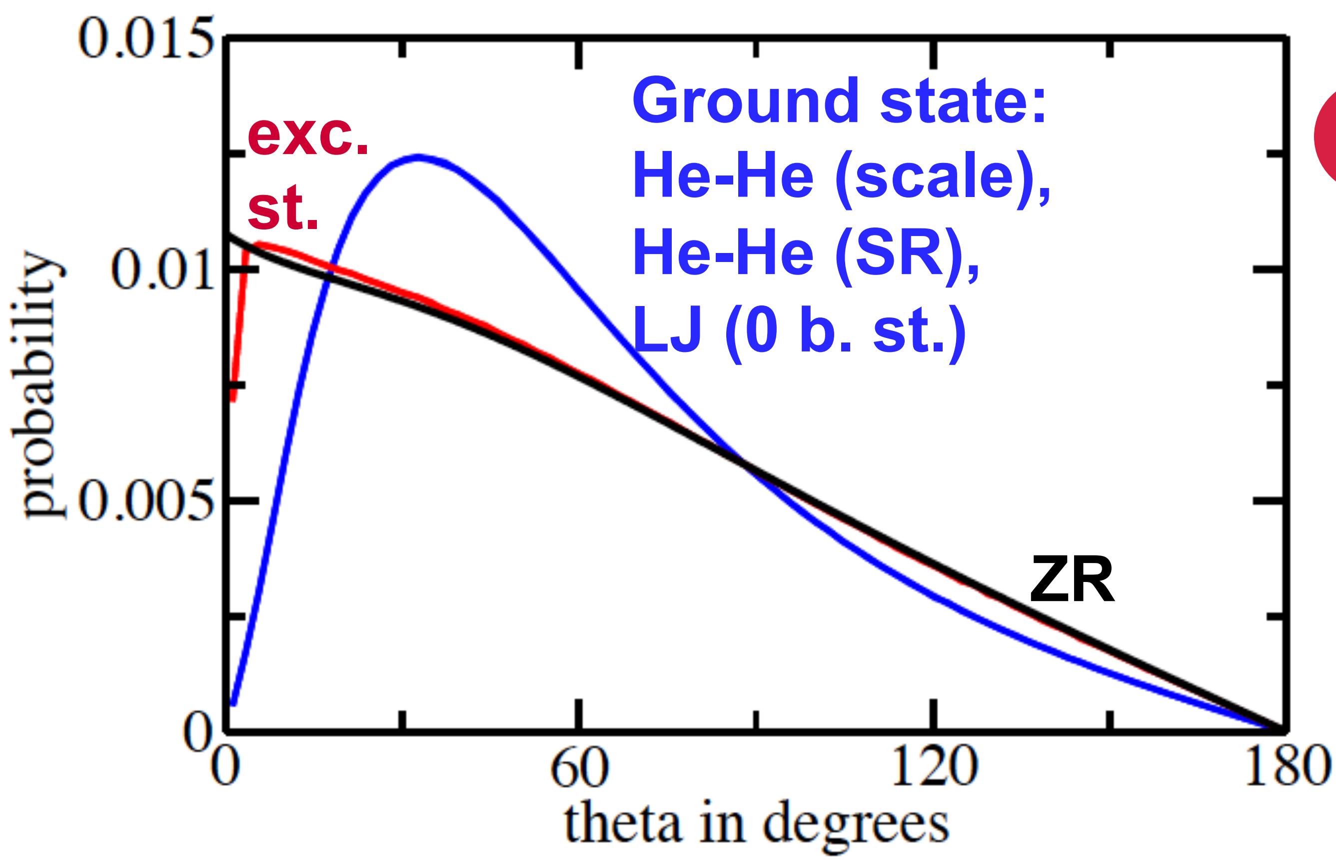
Dependence of N=13 Angular Distribution on Three-Body Regulator

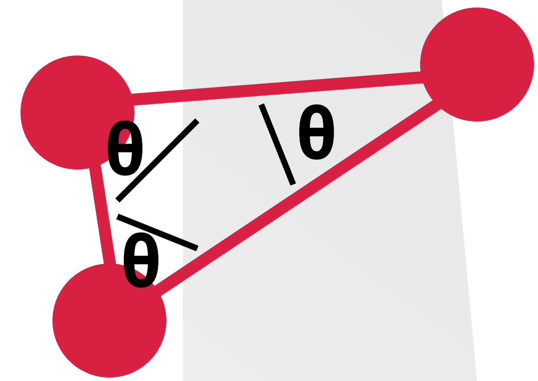




Fairly small dependence on three-body regulator – angular correlations appear less sensitive than overall size…

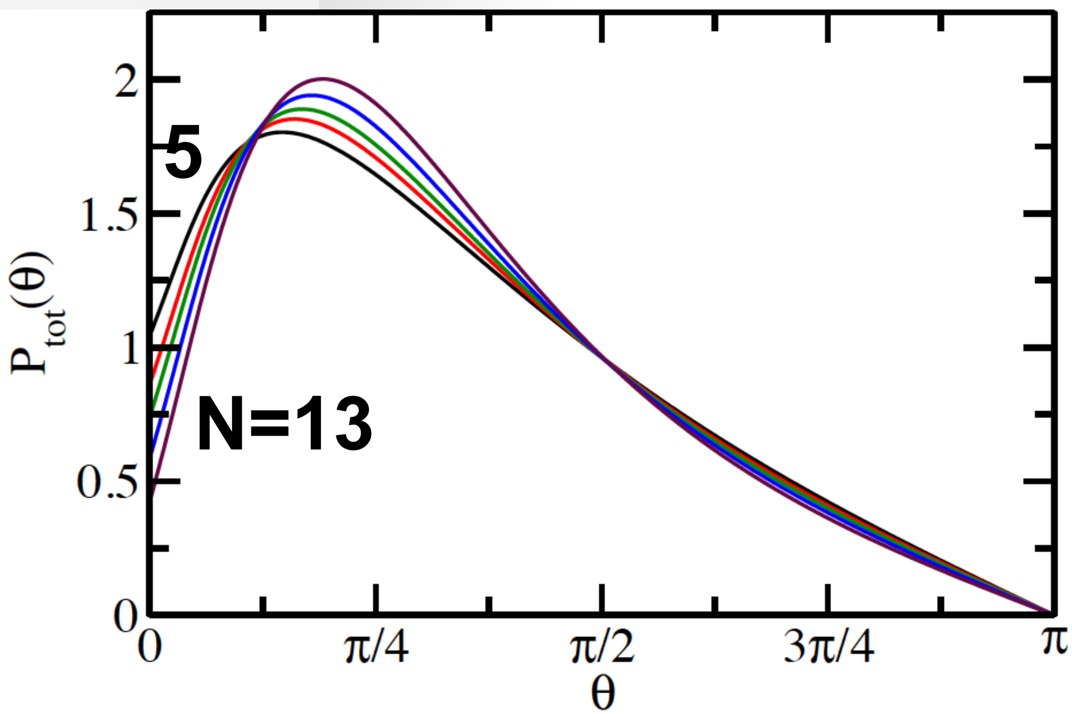
Angular Correlations of Three-Body System at Unitarity

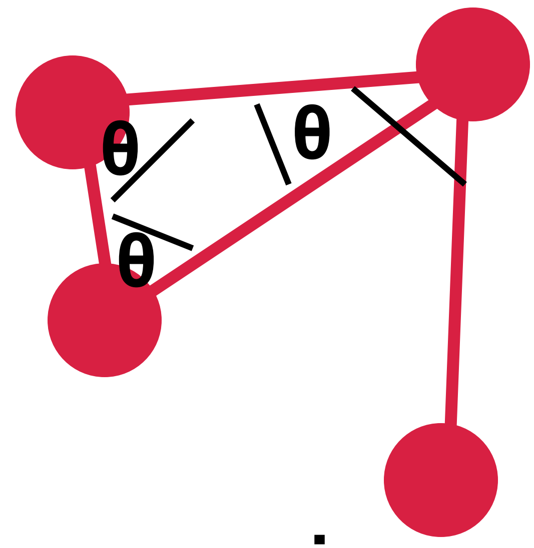




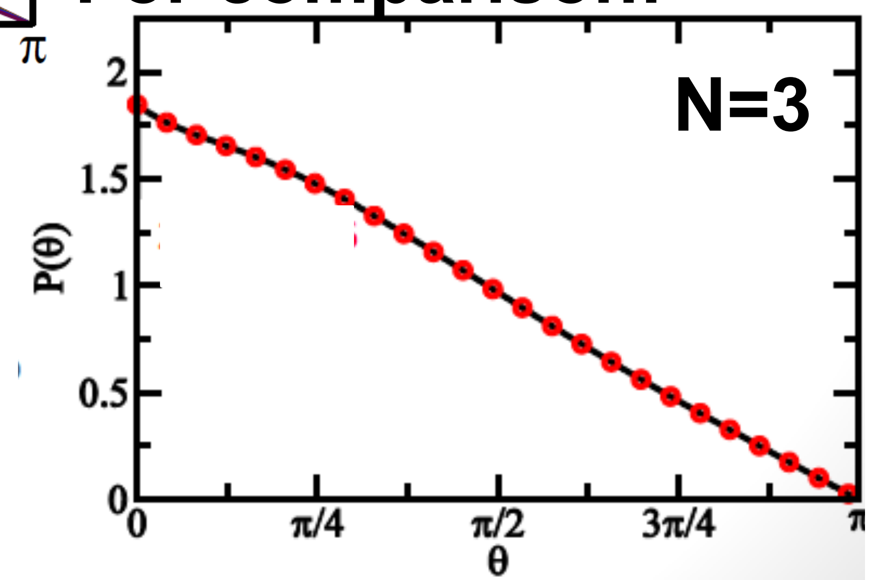
The ground and excited states look notably different. The excited state essentially coincides with zero-range theory distribution.

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:
  - M. Kunitski, S. Zeller, J. Voigtsberger, A. Kalinin, L. Schmidt, M. Schoeffler, A. Czasch, W. Schoellkopf, R. Grisenti, T. Jahnke, D. Blume, R. Doerner: Science 348, 551 (2015)

- 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:
  - D. Blume, C. Greene, B. Esry: JCP 113, 2145 (2000).
  - D. Blume, B. Esry, C. Greene, N. Klaussen, G. Hanna, PRL 89, 163402 (2002).
  - D. Blume, C. Greene, JCP 112, 8053 (2000).

Size of van der Waals Trimer as a Function of Inverse Scattering Length

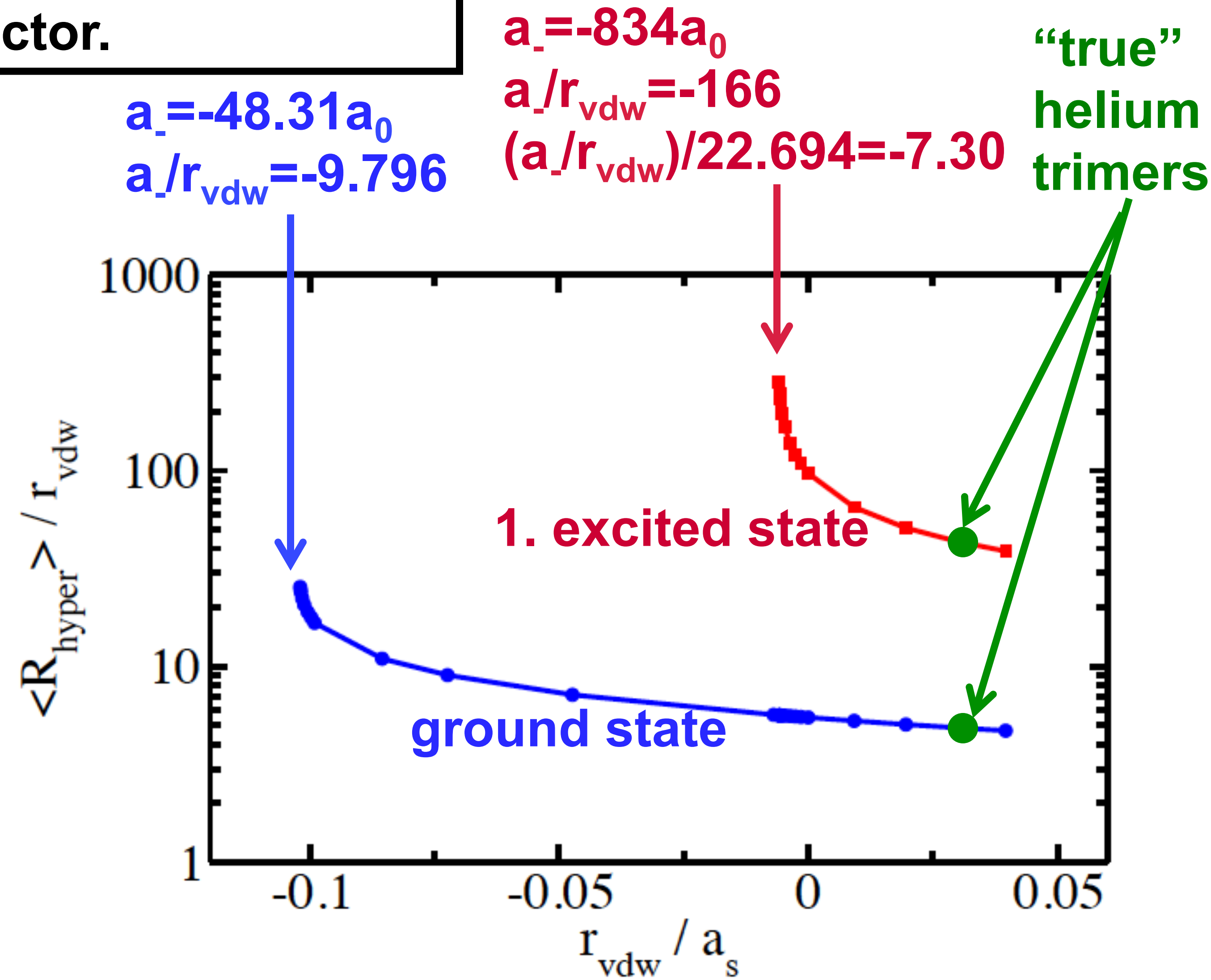
He-He potential [JCP 136, 224303 (2012)] + overall scaling factor.

$(R_{hyper})^2 = [\Sigma_{i<j}(r_{ij})^2] / 3^{1/2}$

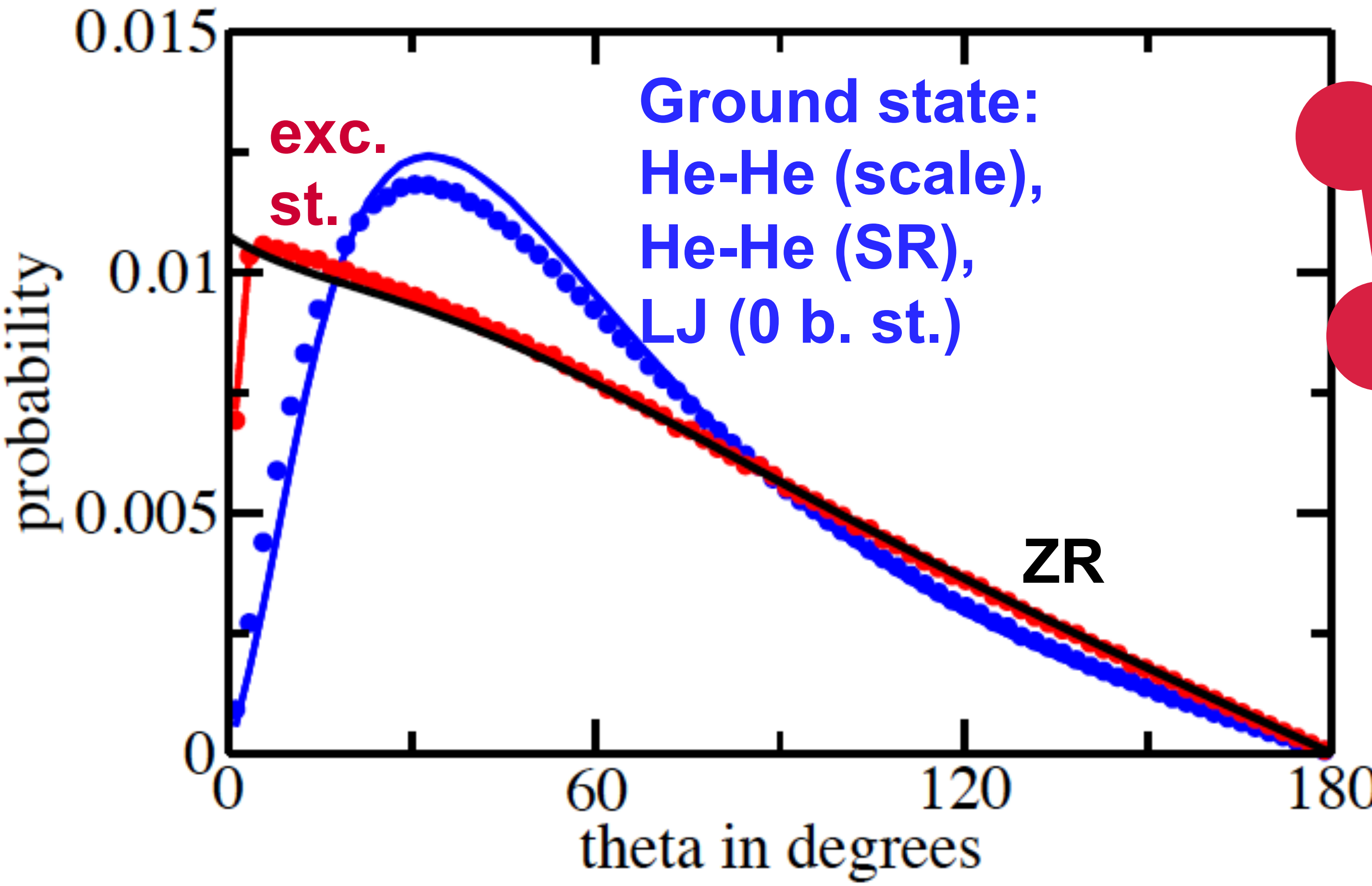
Universal theory:
$\kappa_* = -1.56(5)/a_-$

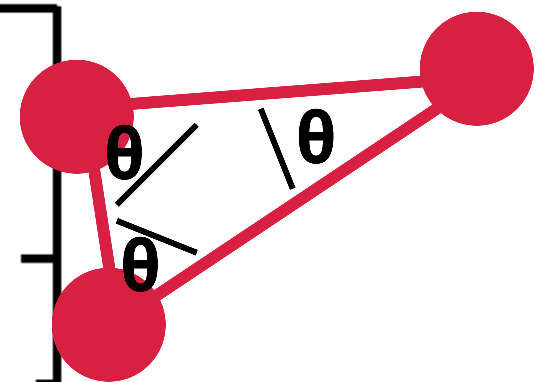
This yields:
$0.0323/a_0$
$0.0424/a_0$

Calculation:
$0.0439/a_0$
$0.0426/a_0$



Angular Correlations of Three-Body System at Unitarity



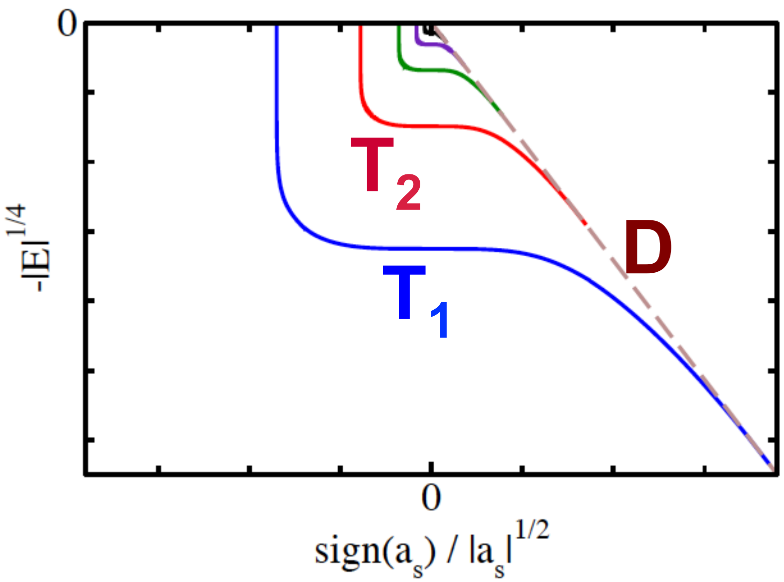


Symbols: Gaussian potential. Not so different…

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

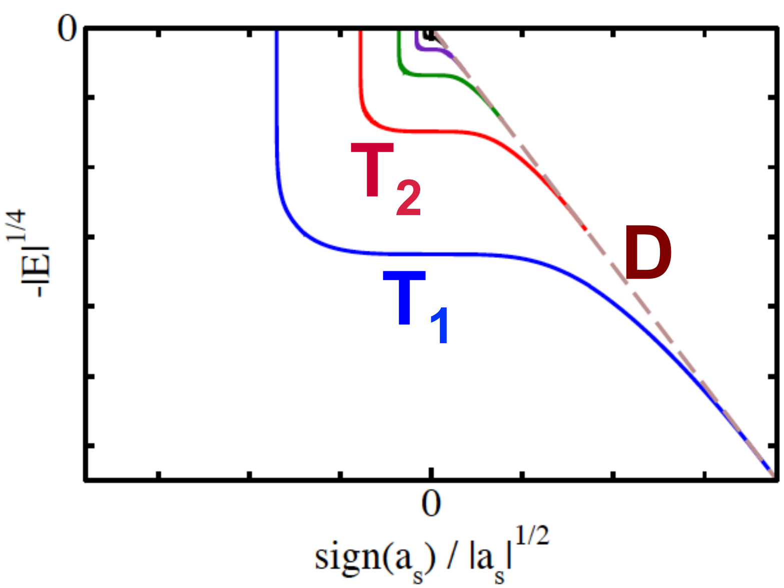
"Standard" Efimov scenario:
Three identical bosons with zero-range contact interactions:



- 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_NX system (specifically, Cs_NLi):
  - 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…

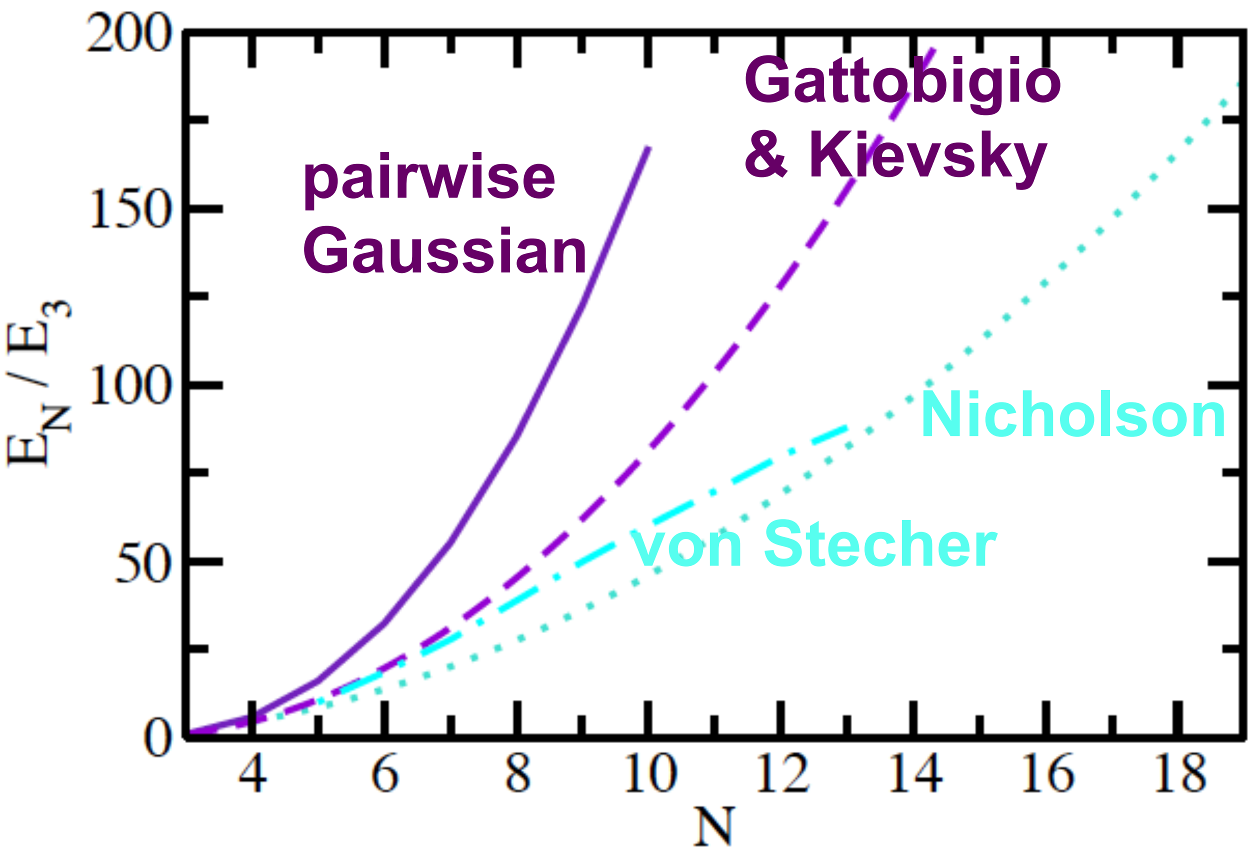
Treat N-body resonance states [for N=4, Deltuva, Few-Body Syst. 54, 569 (2013); for N=5 and 6, von Stecher, PRL 107, 200402 (2011)].

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: $E_N \sim N^2$ (non-universal). PRA 90, 013620 (2014).

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

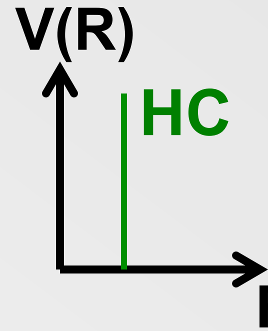
Nicholson (noise): $E_N = E_4 N/2(N/2-1)/2$. PRL 109, 073002 (2012)

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

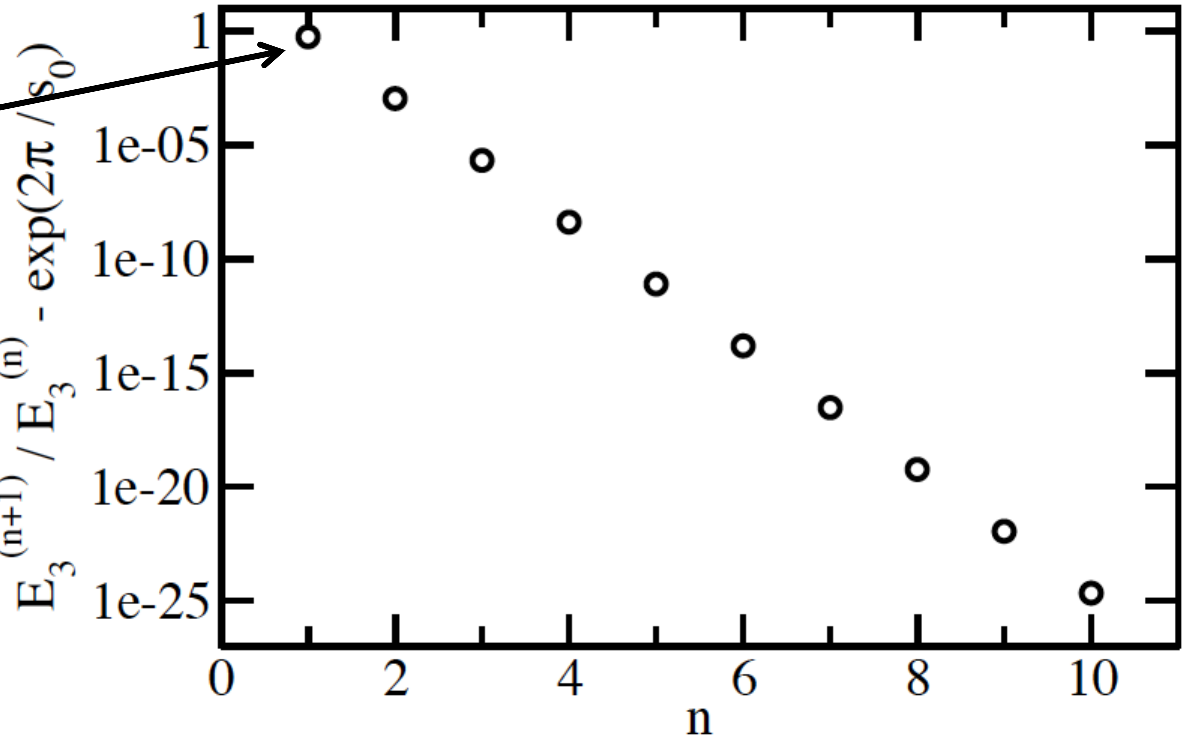
This talk:
Monte Carlo calculations for two-body ZR interactions and different regularizations in three-body sector.

BBB ($a_s=\infty$): Two-Body ZR Interactions and Three-Body Hardcore Potential

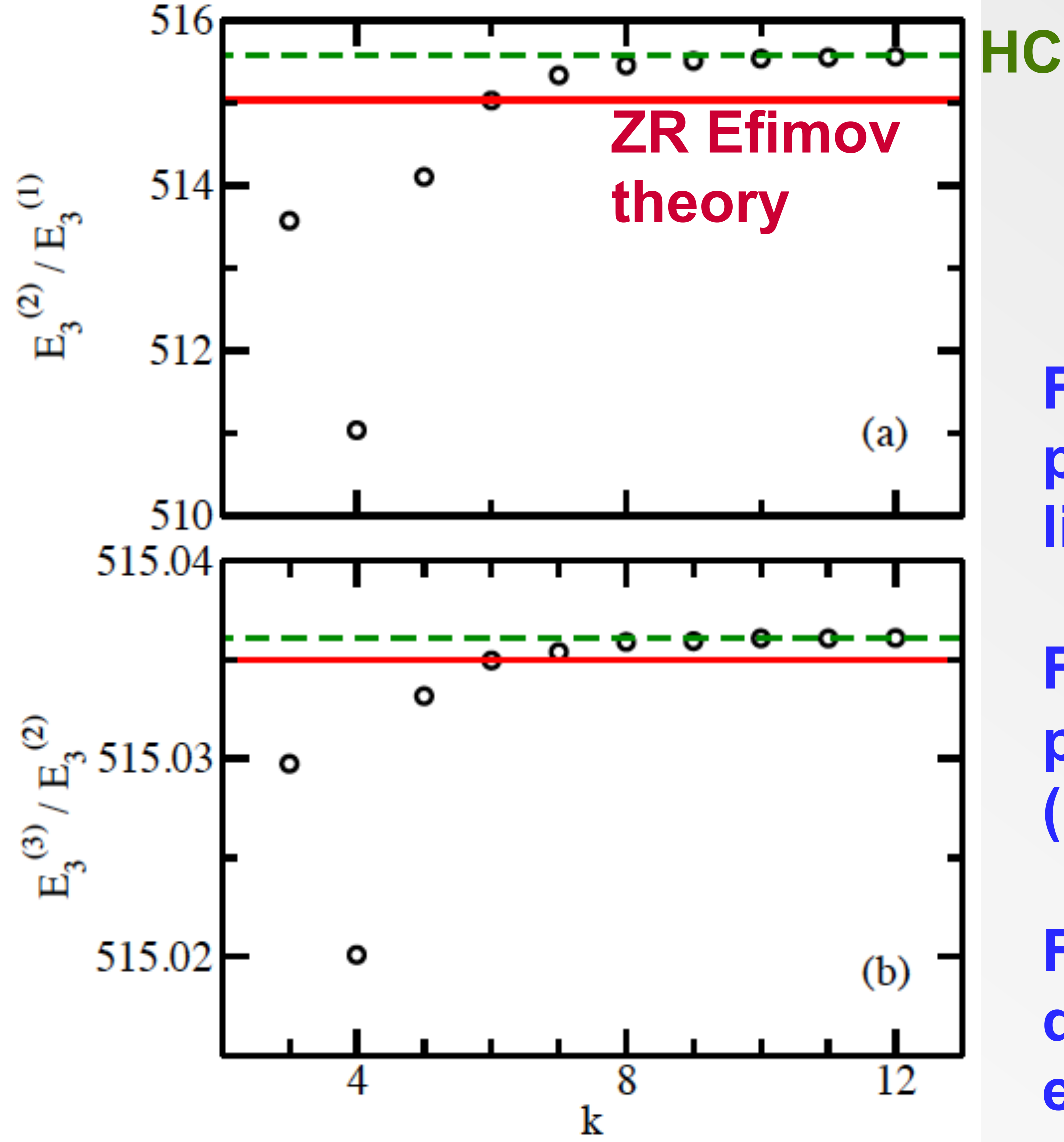
- Hyperangular equation can be solved analytically (yields s_0 value).
- Hyperradial equation can be solved analytically.



Energy ratio of ground state (n=1) and first excited state (n=2) deviates by ~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.

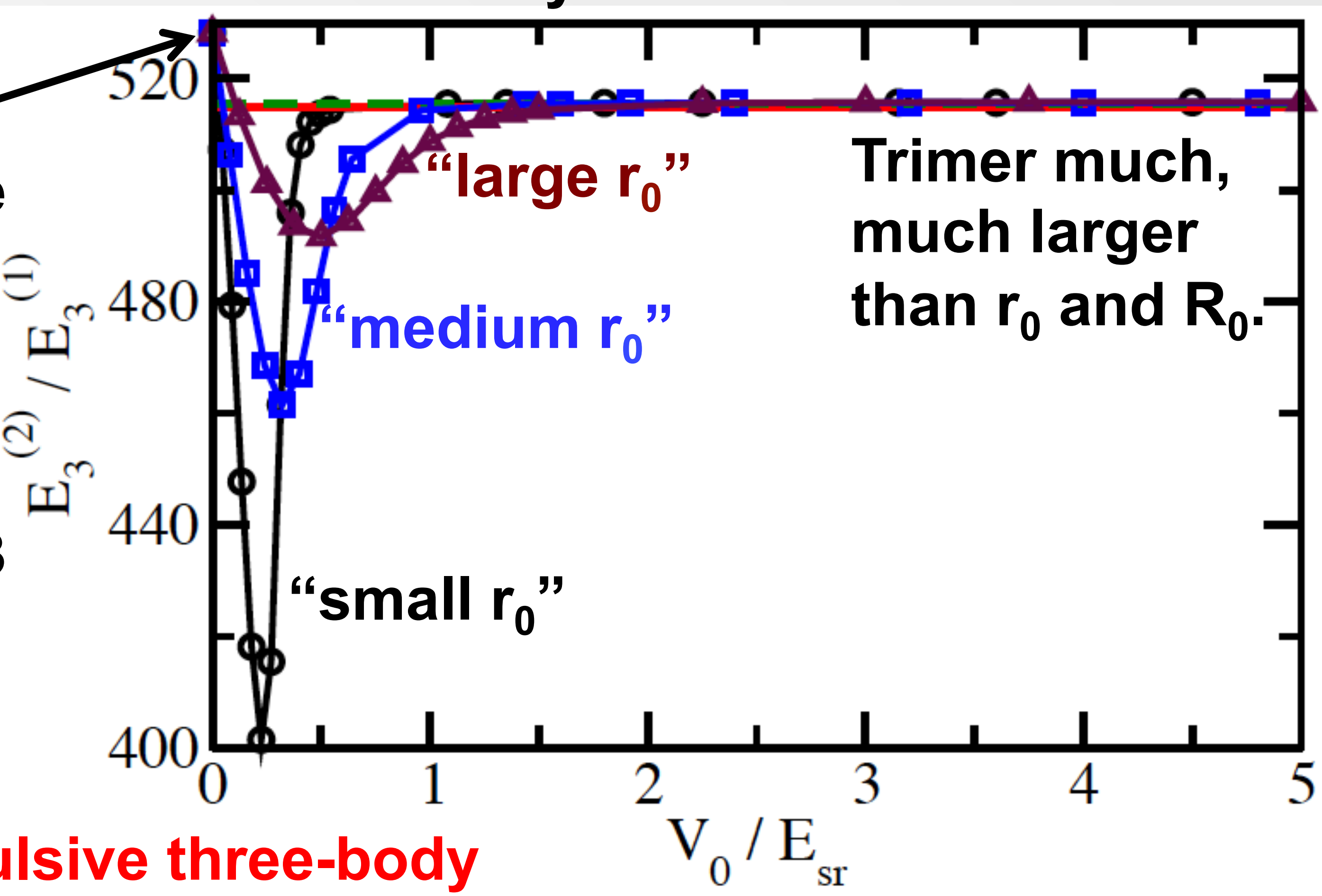
For k=2, the powerlaw potential "modifies" s_0 (does not regularize…).

For k~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.

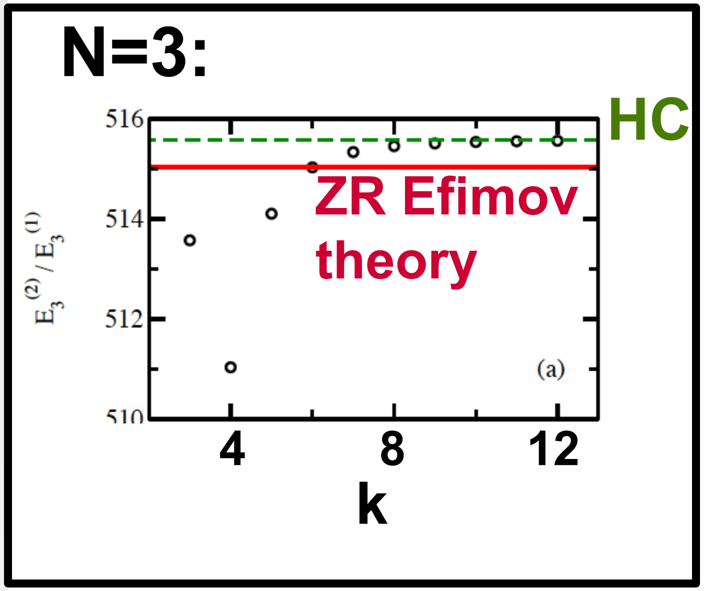
This is where Gattobigio et al. work. Trimer size $\langle R \rangle = 2.66 r_0$. $R^2=[\Sigma_{i<j}(r_{ij})^2]/3$



A small repulsive three-body potential affects the ground and excited states differently.

$a_s=\infty$: 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 $E_N^{(1)}/E_3^{(1)}$.



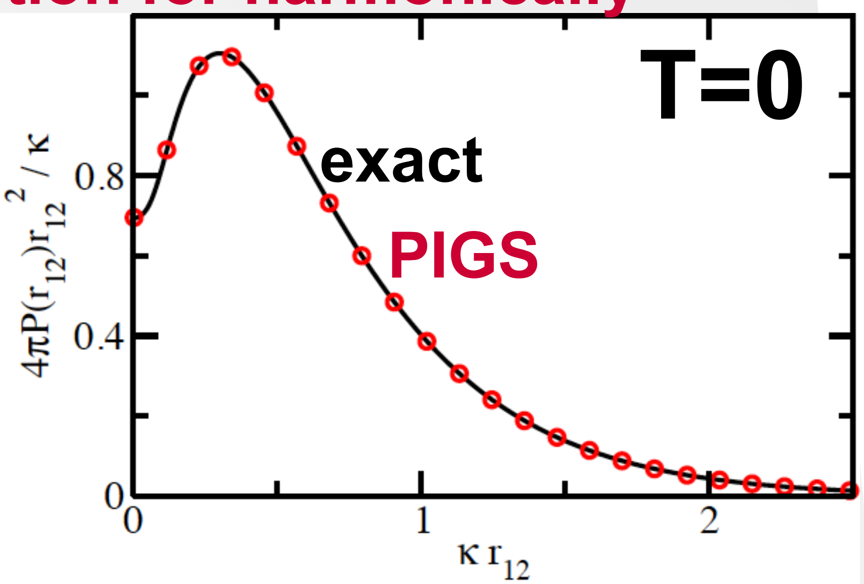
We use the Path Integral Monte Carlo (PIMC) approach, extrapolated to zero temperature, to treat N-body system: Pair approximation with analytical two-body zero-range propagator.

Benchmarking the Two-Body Zero-Range Propagator

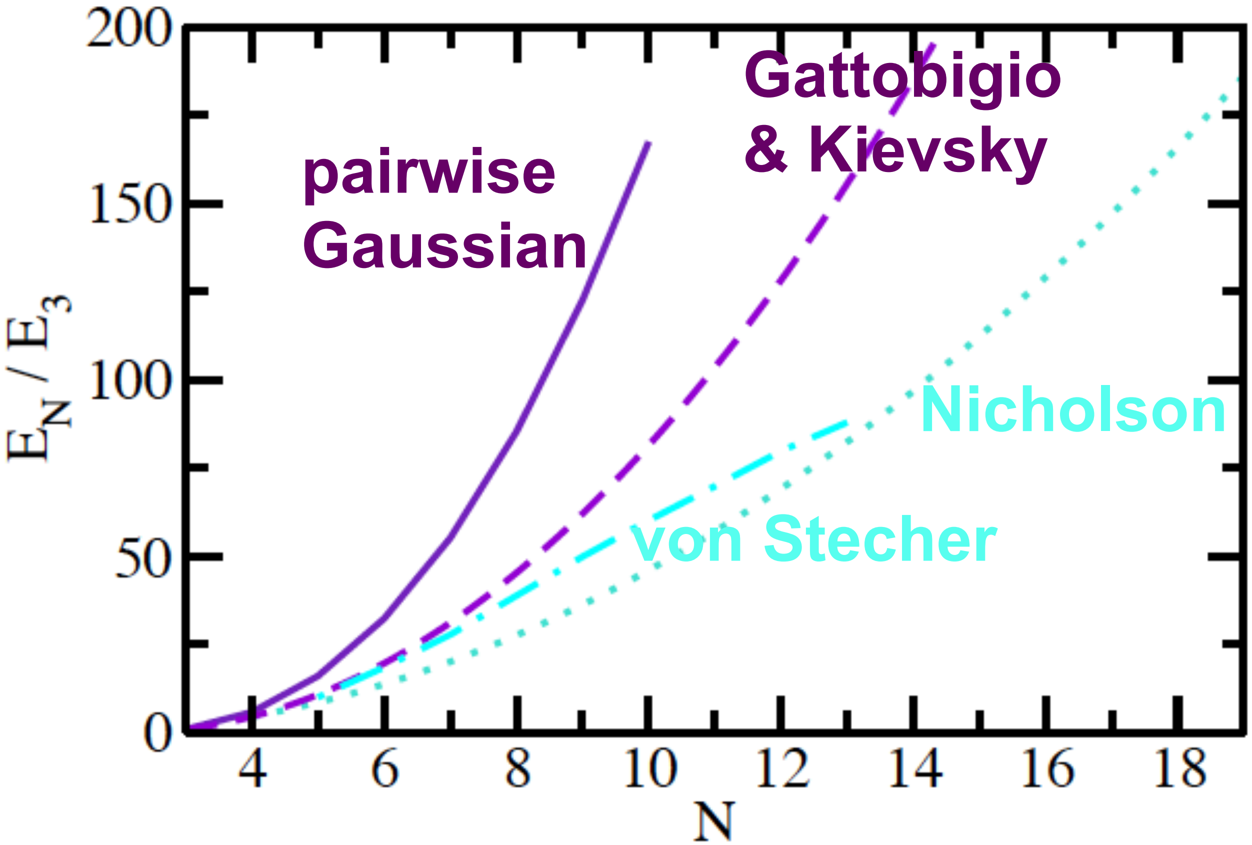
- **Two-body propagator calculated analytically for 1d and 3d systems (harmonically trapped or free space).**
- **Can be used in real or imaginary time evolution.**
- **We have primarily used it in applications where imaginary time is identified with inverse T.**

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

Infinitely large a_s and three-body C_6/R^6 powerlaw potential.



E_N for N Bosons ($a_s=\infty$): "Universal" Energy Predictions from the Literature



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

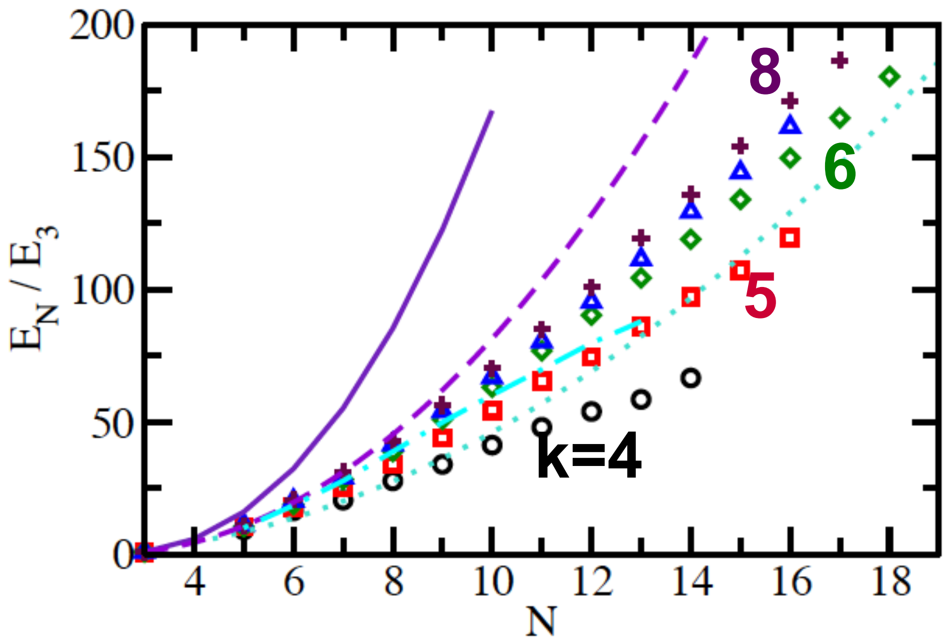
Gattobigio & Kievsky (next talk): finite-range corrections included (E_4 made to match Deltuva result).

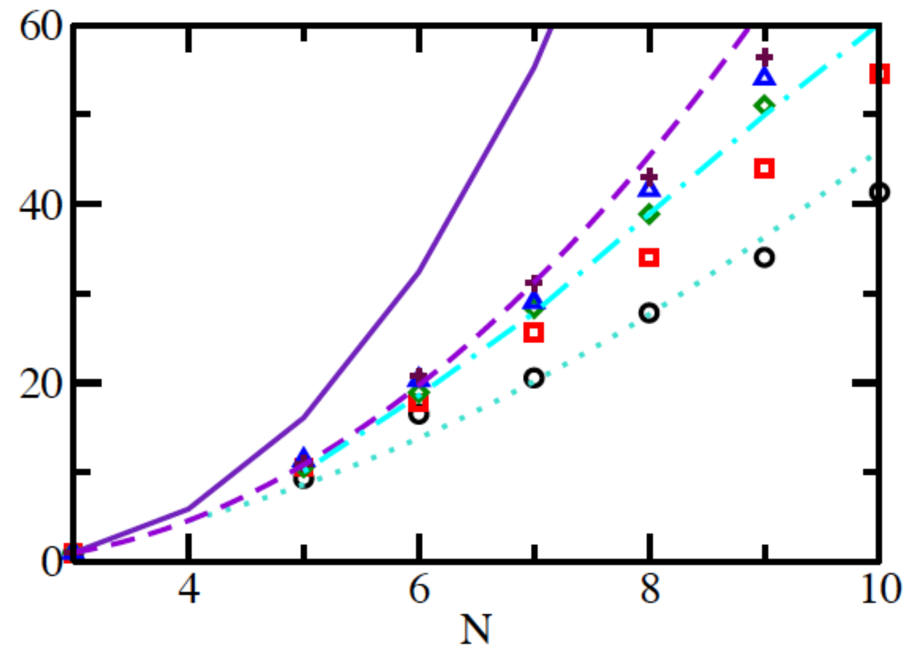
Nicholson (noise): $E_N = E_4 N/2(N/2-1)/2$.

von Stecher: DMC results for three-body HC.

Our work:
Monte Carlo calculations for two-body ZR interactions and different regularizations in three-body sector.

E_N (a_s=∞): Two-Body ZR Interactions and Three-Body Powerlaw Potential



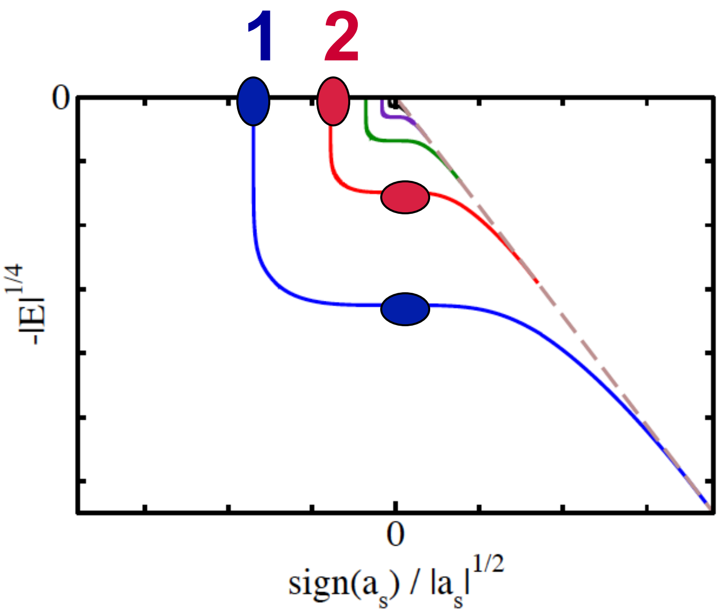


Purely repulsive three-body powerlaw potential: $V(R)=C_k/R^k$.

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).

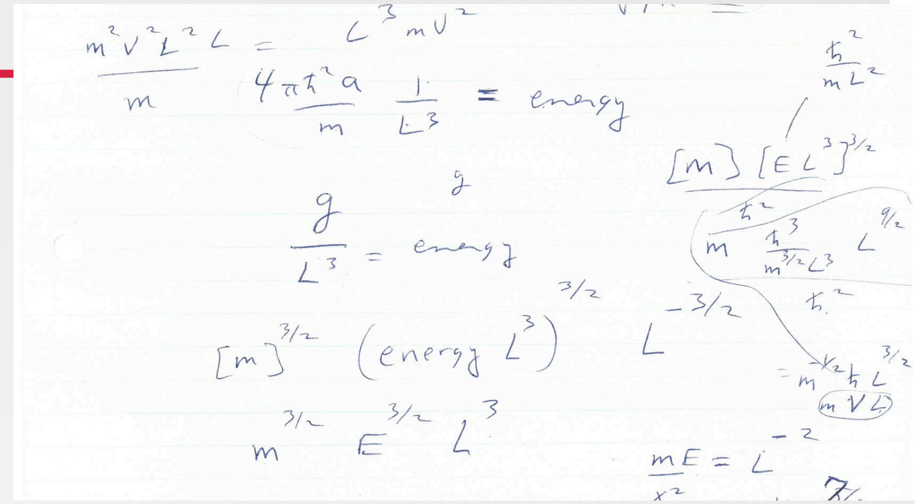
Connection Between Helium Trimers and Ultracold Atoms?



EXPERIMENT	$a^{(1)}/r_6$	$a^{(2)}/r_6$	$a^{(1)}/a^{(2)}$
cesium	-9.53(11)	-200(12)	1/[21.0(1.3)]
lithium	-7.50(5)	-161(1)	1/[21.5(2)]

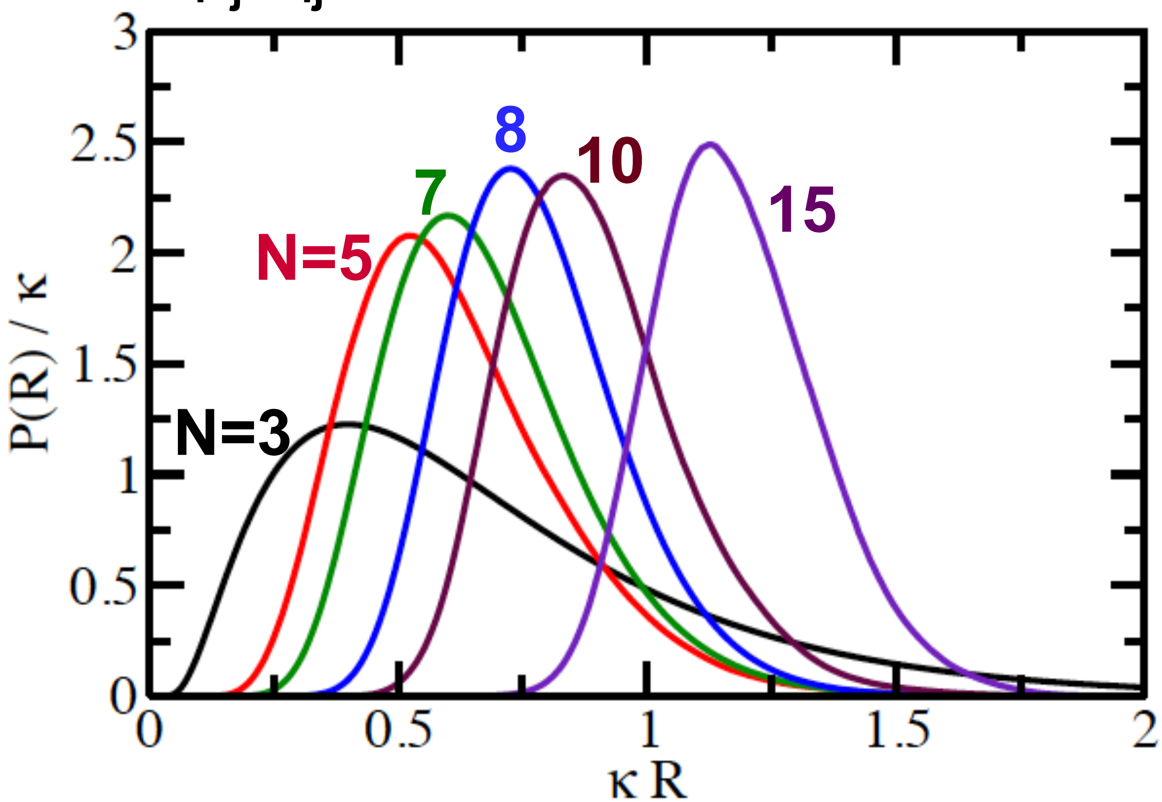
THEORY	$\kappa^{(1)}r_6$	$a^{(1)}/r_6$	$\kappa^{(1)}a^{(1)}$
Wang et al.	0.226(2)	-9.73(3)	-2.20(2)
Naidon et al.	0.187(1)	-10.85(1)	-2.03(1)
ZR theory			-1.50763

	$\kappa^{(1)}r_6$	$a^{(1)}/r_6$	$\kappa^{(1)}a^{(1)}$	$\kappa^{(2)}r_6$	$a^{(2)}/r_6$	$\kappa^{(2)}a^{(2)}$	$\kappa^{(1)}/\kappa^{(2)}$	$a^{(1)}/a^{(2)}$
He-He (scale)	0.222	-9.80	-2.12	0.00947	-166	-1.57	23.4	1/17.3
He-He (SR)	0.218	-9.88	-2.15	0.00928	-169	-1.57	23.5	1/17.1
LJ (0 b. st.)	0.230	-9.49	-2.18	0.00981	-160	-1.57	23.4	1/16.8


= energy
= energy
(energy L^3)

Hyperradial Density for N Bosons ($a_s=\infty$)

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

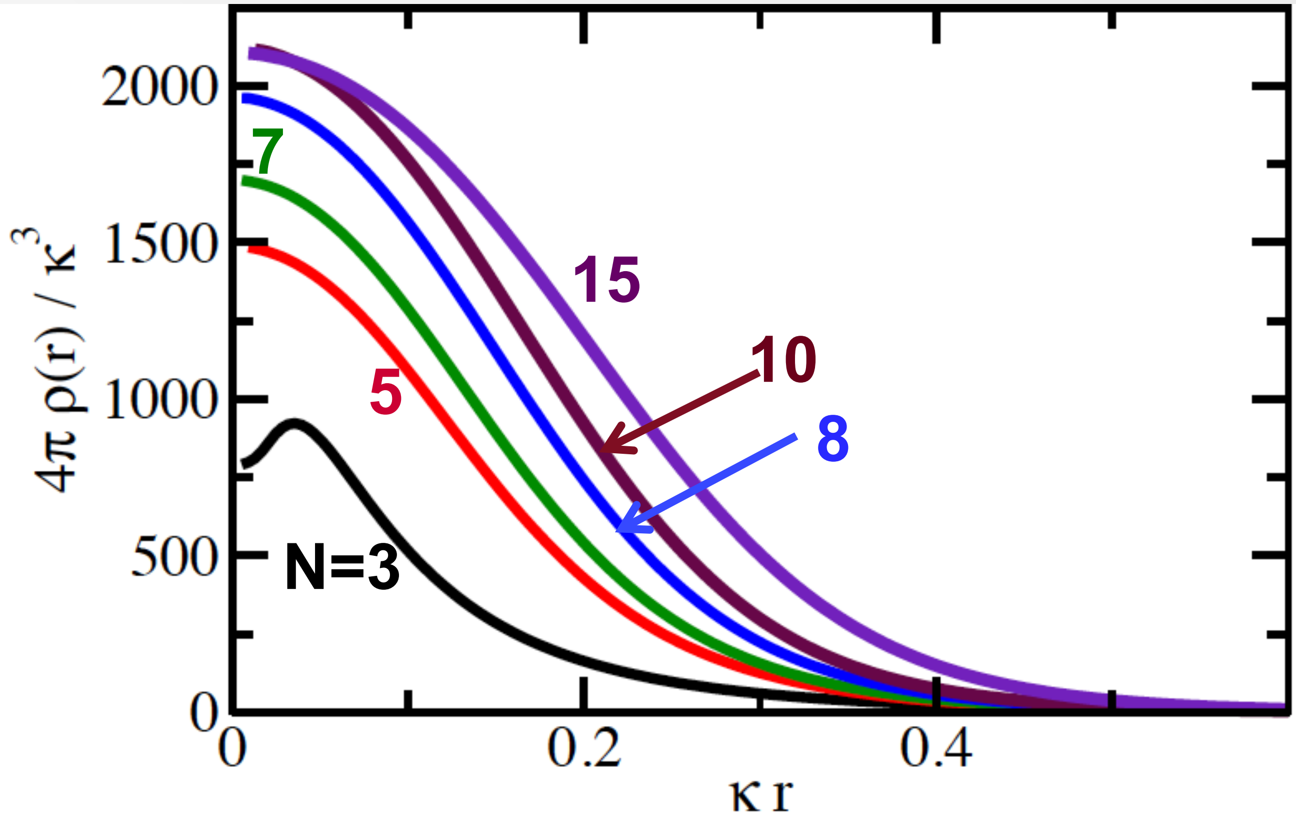


N=3 distribution is broadest.

N-body hyperradial density becomes more compact and moves to larger R.

$1/\kappa = 16.4L_6$, where L_6 is length scale of three-body powerlaw potential, $L_6 = (mC_6/\hbar^2)^{1/4}$.

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.

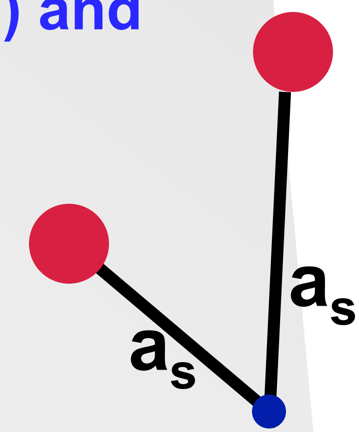
Note: The errorbars are non-negligible.

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?

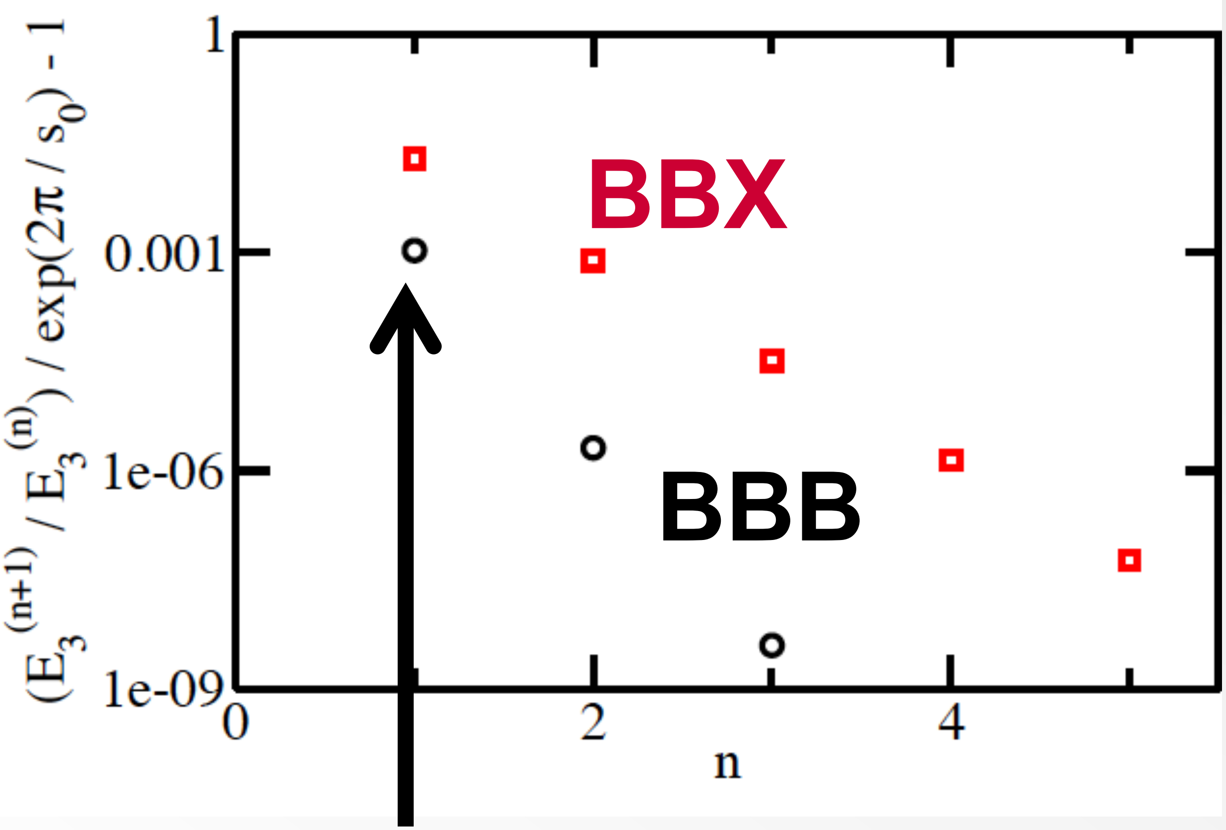
Unequal Masses: $B_N X$ System with Large Mass Ratio

- 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 $B_N X$ sector?
  - Number of four-body bound states, if any, that are tied to $B_2 X$ 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



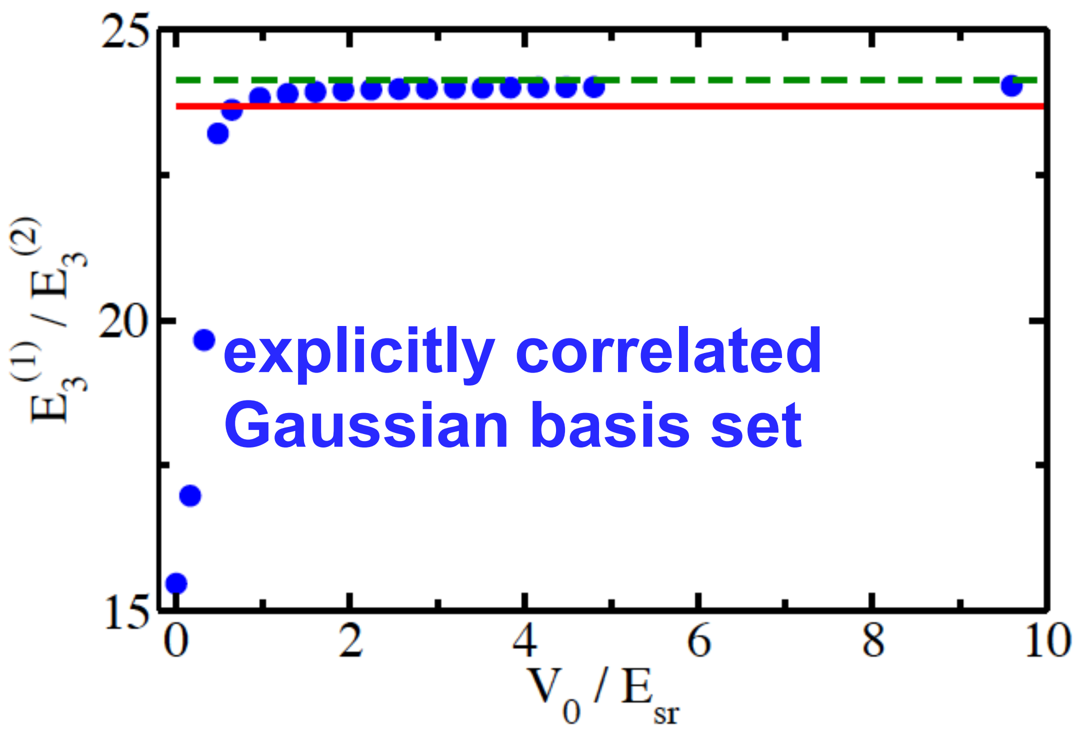
BBB: ~0.11%
BBX: ~1.9%

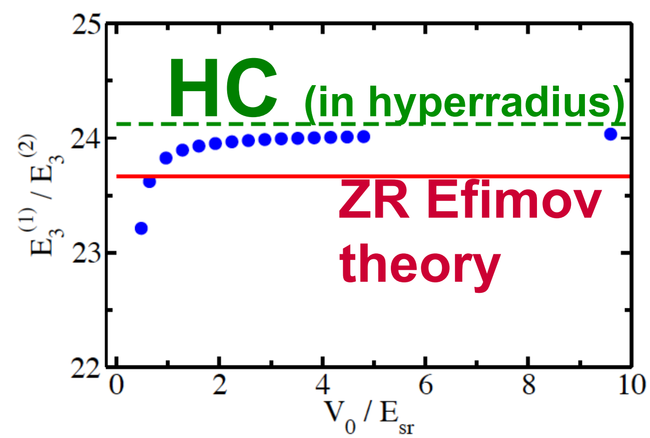
The amplitude of the hyperradial density in the “inner lobe” is larger for BBX than for BBB. More favorable (i.e., smaller) energy level spacing introduces new computational challenge…

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.





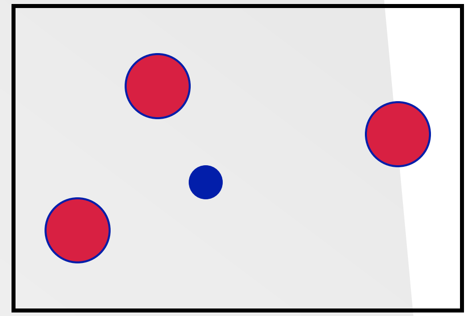
Calculations are for 133/6 (CsLi) mass ratio.

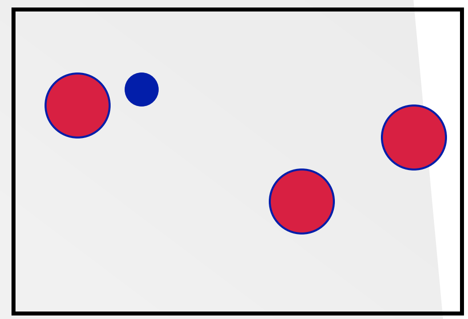
Expand Wave Function in Basis: Explicitly Correlated Gaussians

- Basis functions:
  Simple Gaussian $\Phi_k(\underline{x}) = \exp(-\underline{x}^T A^{(k)} \underline{x}/2)$

See Suzuki and Varga

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





Total wave fct.:

$$\Psi = \sum_{k=1}^{N_{\text{basis}}} c_k \, S \, \Phi_k(\underline{x})$$

- $\underline{x}$ collectively denotes N-1 Jacobi coordinates.
- A denotes (N-1)x(N-1) dimensional parameter matrix.

- Use physical insight to choose d_{ij} efficiently.
- For each basis function φ_k ($L^\Pi=0^+$), we have N(N-1)/2 parameters.
- For N=4, N_{basis}=1000, $L^\Pi=0^+$: 6000 non-linear variational parameters.

Explicitly Correlated Gaussian and Semi-Stochastic Variational Approach

Hamiltonian matrix can be evaluated semi-analytically.

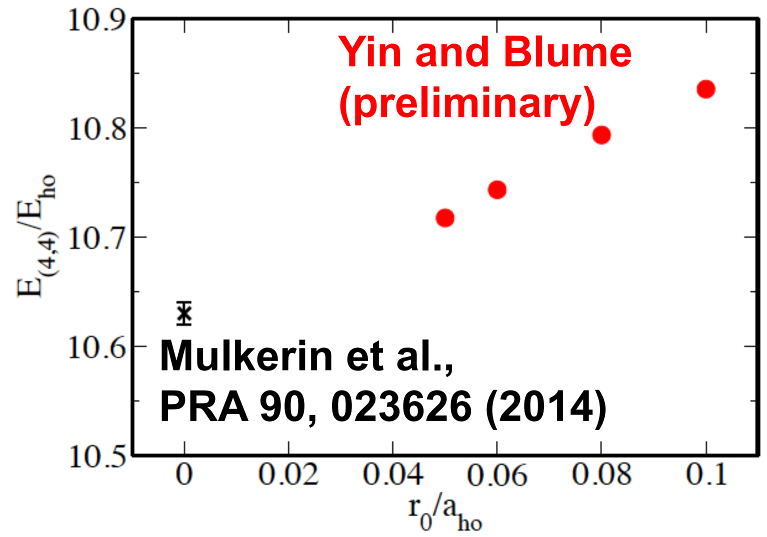
Rigorous upper bound for energy ("controlled accuracy").

Matrix elements for structural properties can be calculated analytically.

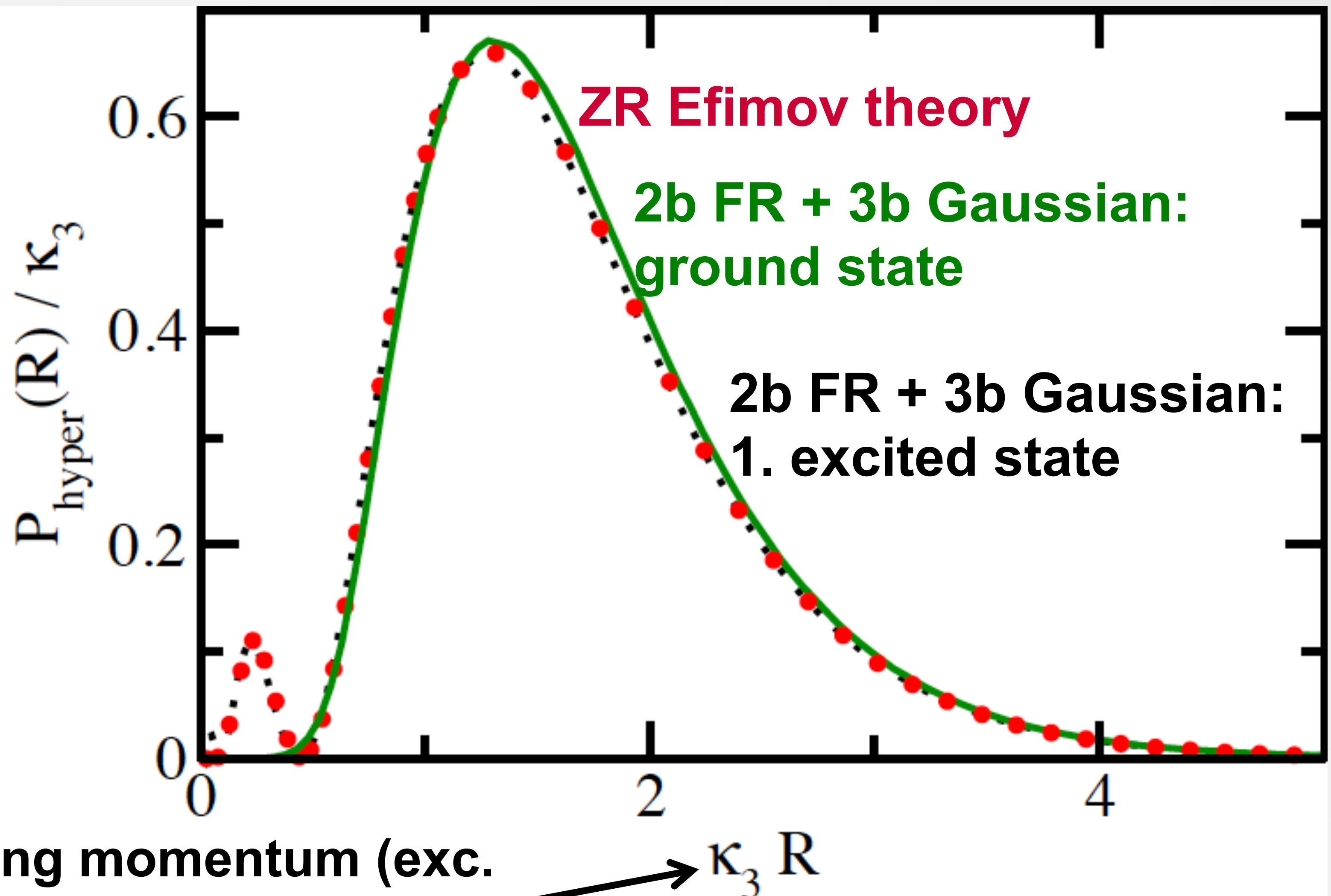
Computational effort increases with number of atoms N:

- 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,… for FF', 2F2F', 3F3F', 4F4F',… 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.



BBX ($a_s=\infty$) with Mass Ratio 133/6: Hyperradial Density



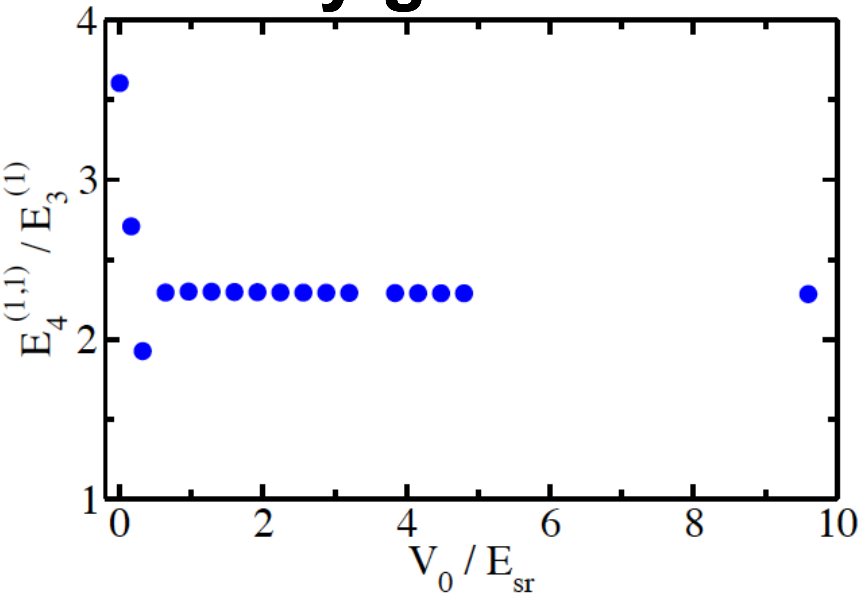
Binding momentum (exc. state energies are made to agree).

Convincing agreement…

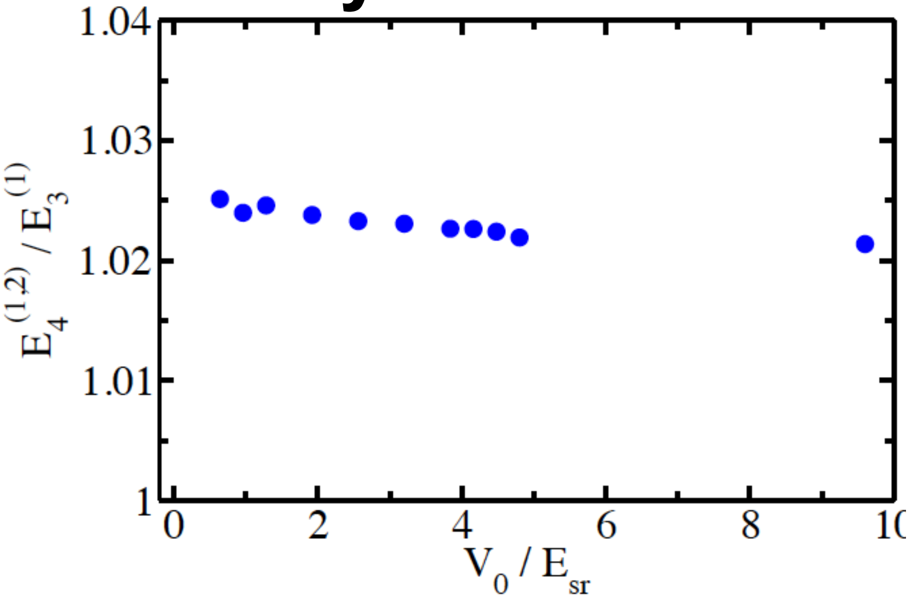
Cs_3Li ($a_s=\infty$): Gaussian Two-Body and Gaussian Three-Body Potential

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:

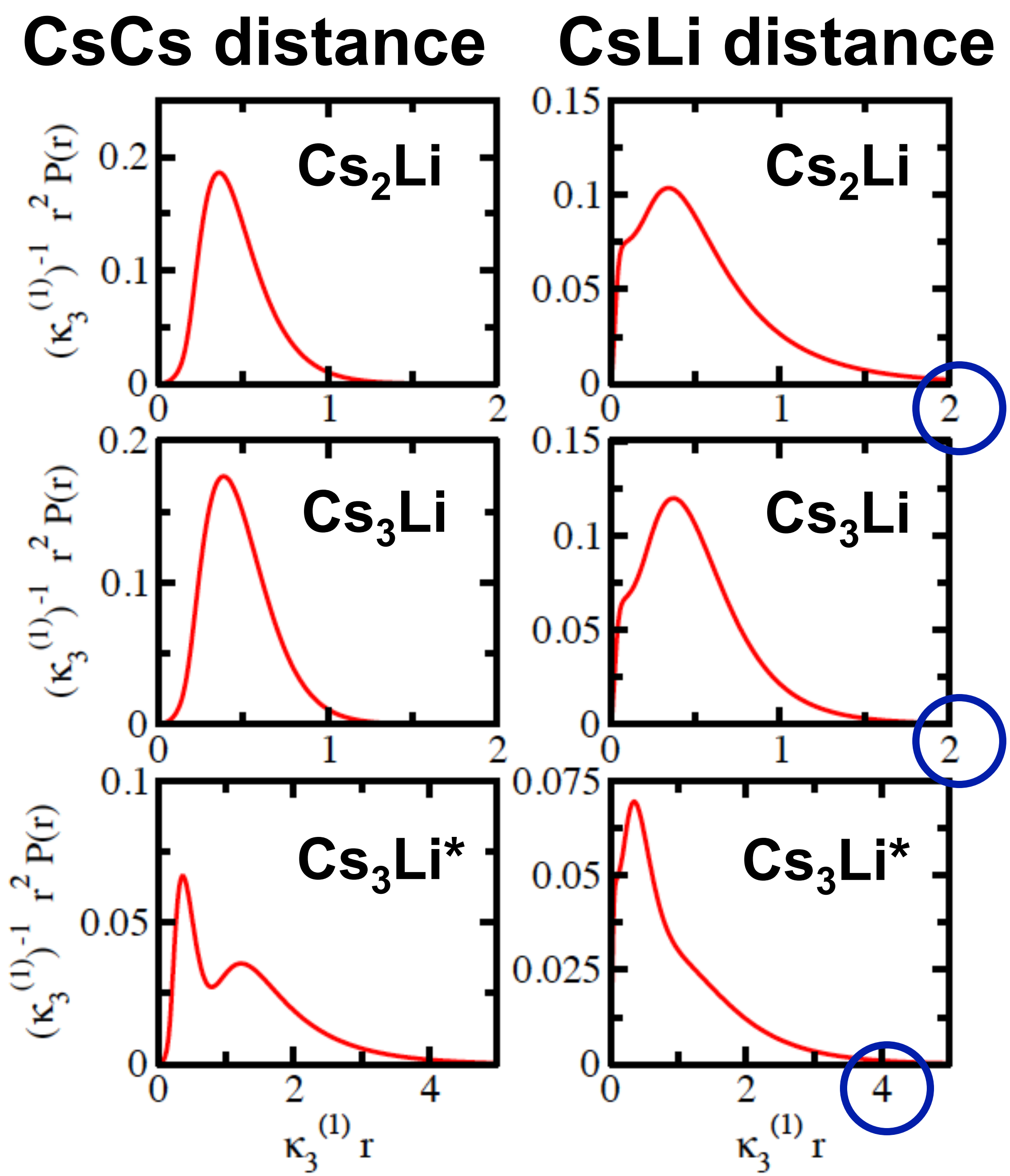


Cs_NLi (a_s=∞)

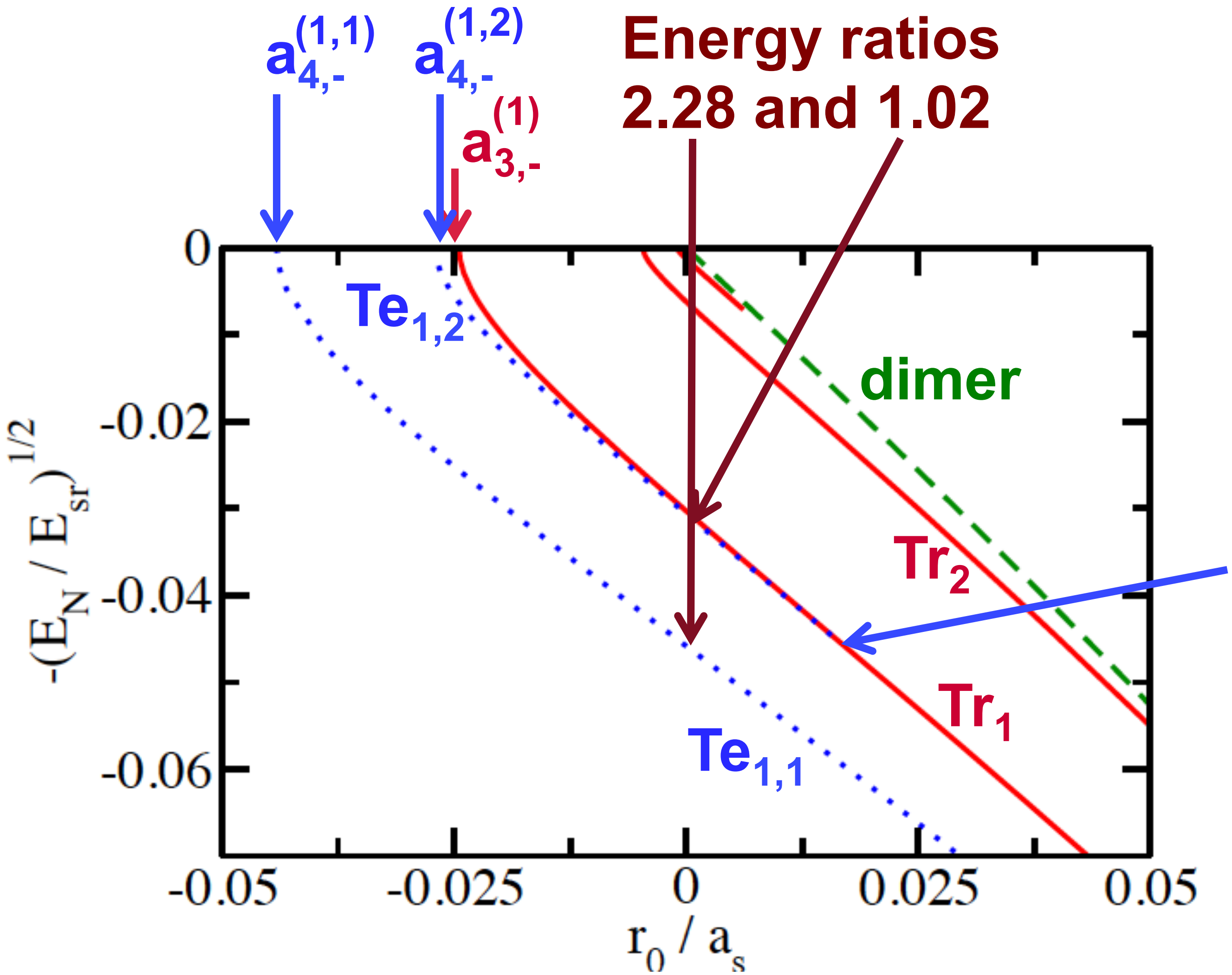
Pair distribution: Likelihood of finding two particles at distance r from each other.

Distributions for Cs_3Li ground state resemble those of Cs_2Li ground state.

Distributions for Cs_3Li^* excited state are broader.



Generalized Efimov Scenario for CsLi Mixture



Two tetramer states:

$a_{4,-}^{(1,1)} \sim 0.55 a_{3,-}^{(1)}$

$a_{4,-}^{(1,2)} \sim 0.91 a_{3,-}^{(1)}$

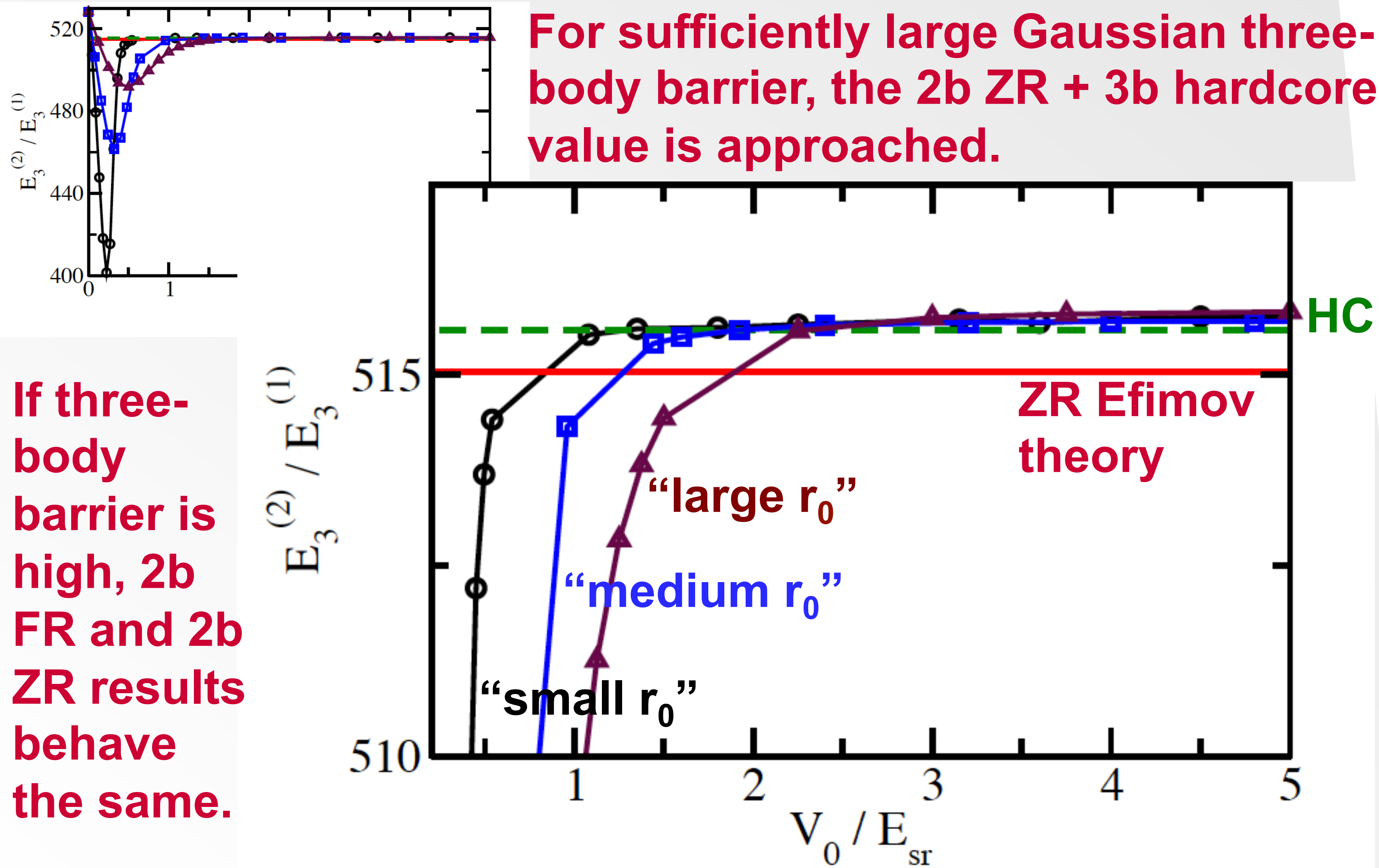
More weakly-bound tetramer becomes unbound on positive scattering length side.

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.

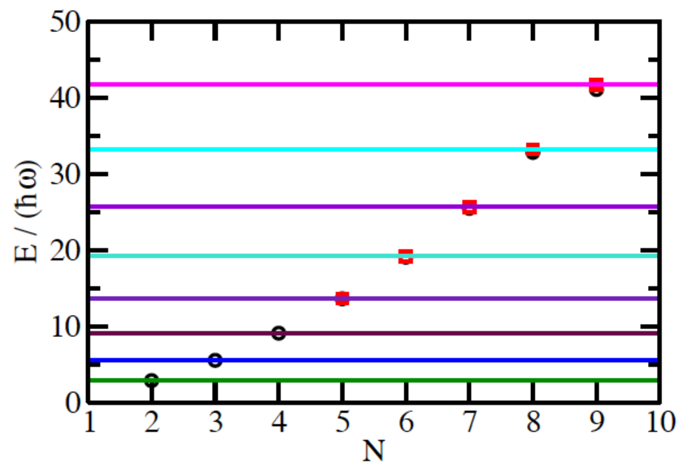
If three-body barrier is high, 2b FR and 2b ZR results behave the same.

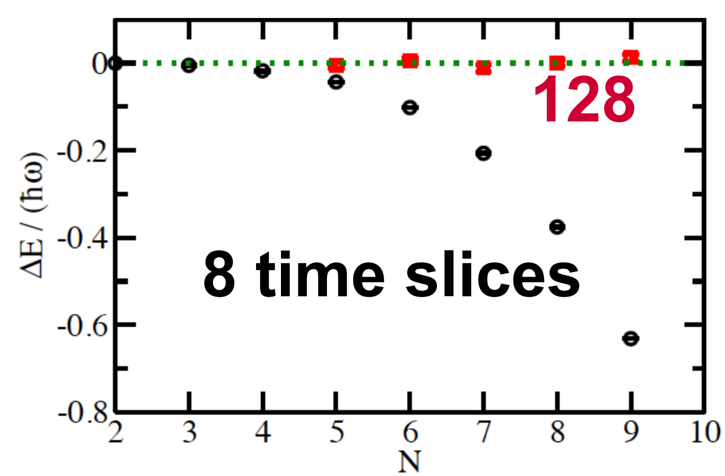


Benchmarking the Two-Body Zero-Range Propagator

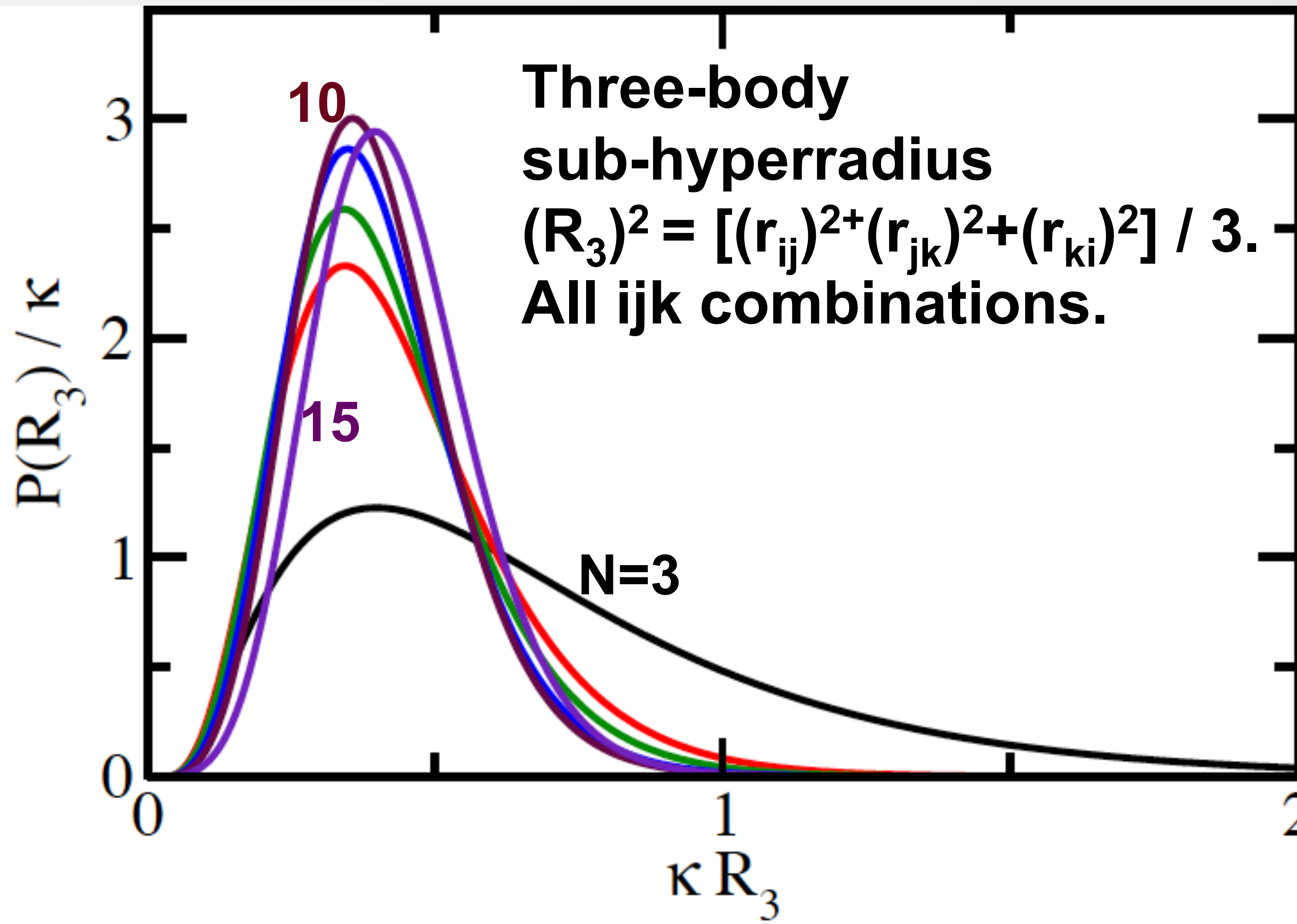
- Two-body propagator calculated analytically for 1d and 3d systems (harmonically trapped or free space).
- Can be used in real or imaginary time evolution.
- We have primarily used it in applications where imaginary time is identified with inverse T.

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





Three-Body Correlation ($a_s=\infty$): k=6 Three-Body Powerlaw Potential



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