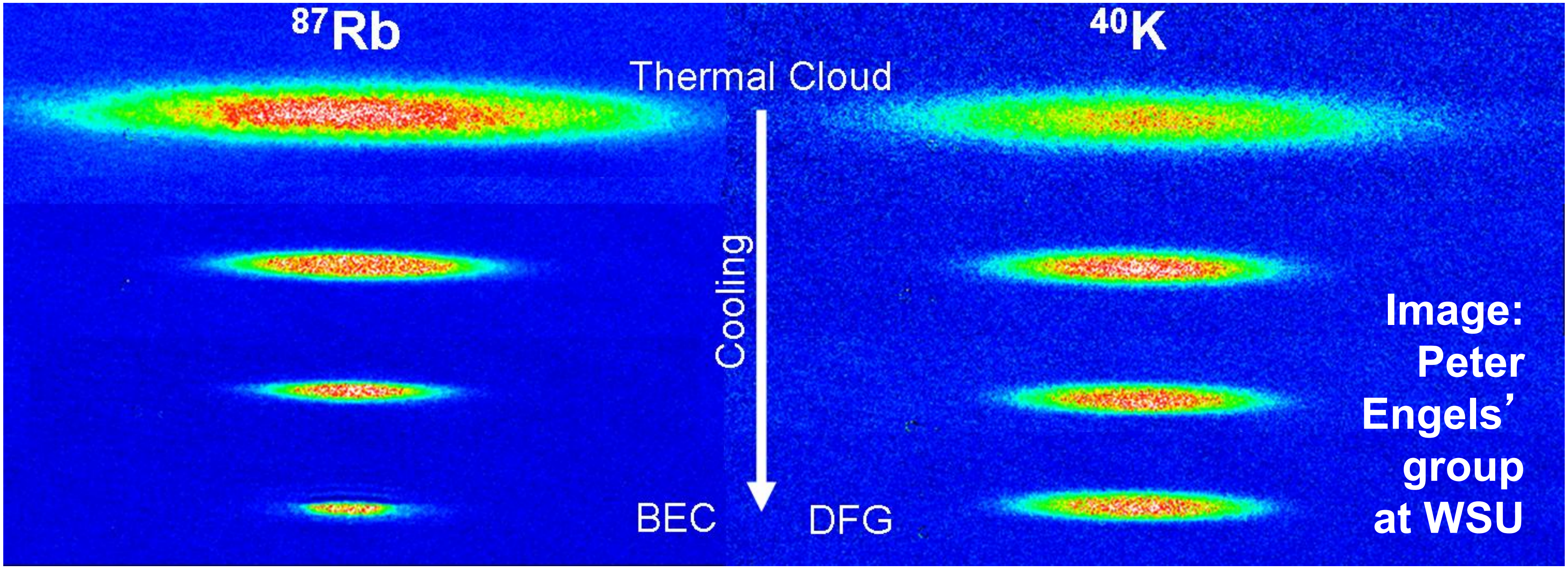

Extended Efimov scenario: Boson droplets without and with an impurity

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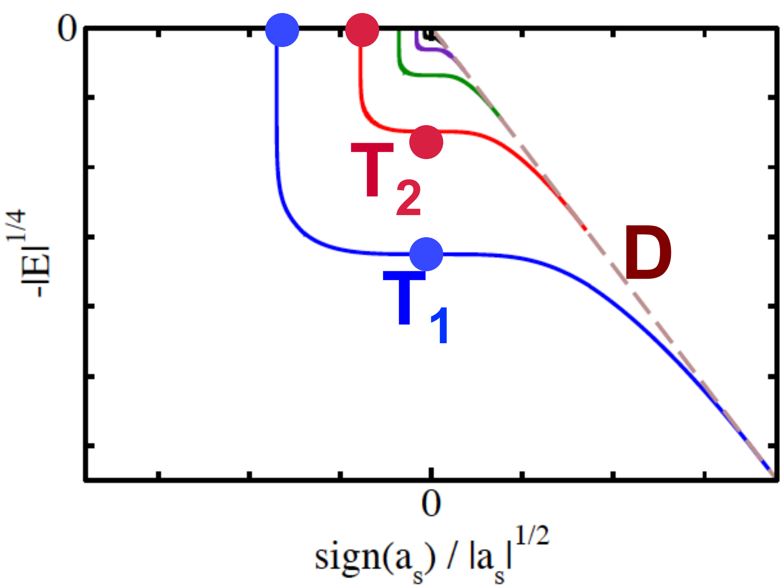
Supported by the NSF.

Beyond the "Zero-Range Efimov Theory"

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



- Most generally: Where do we see discrete scale invariance?
- Realistic interactions (understanding the three-body parameter; structural properties).
- BBB system under (partial) confinement/mixed dimensions.
- Unequal masses/different statistics (BBX, FFX).
- More particles.

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

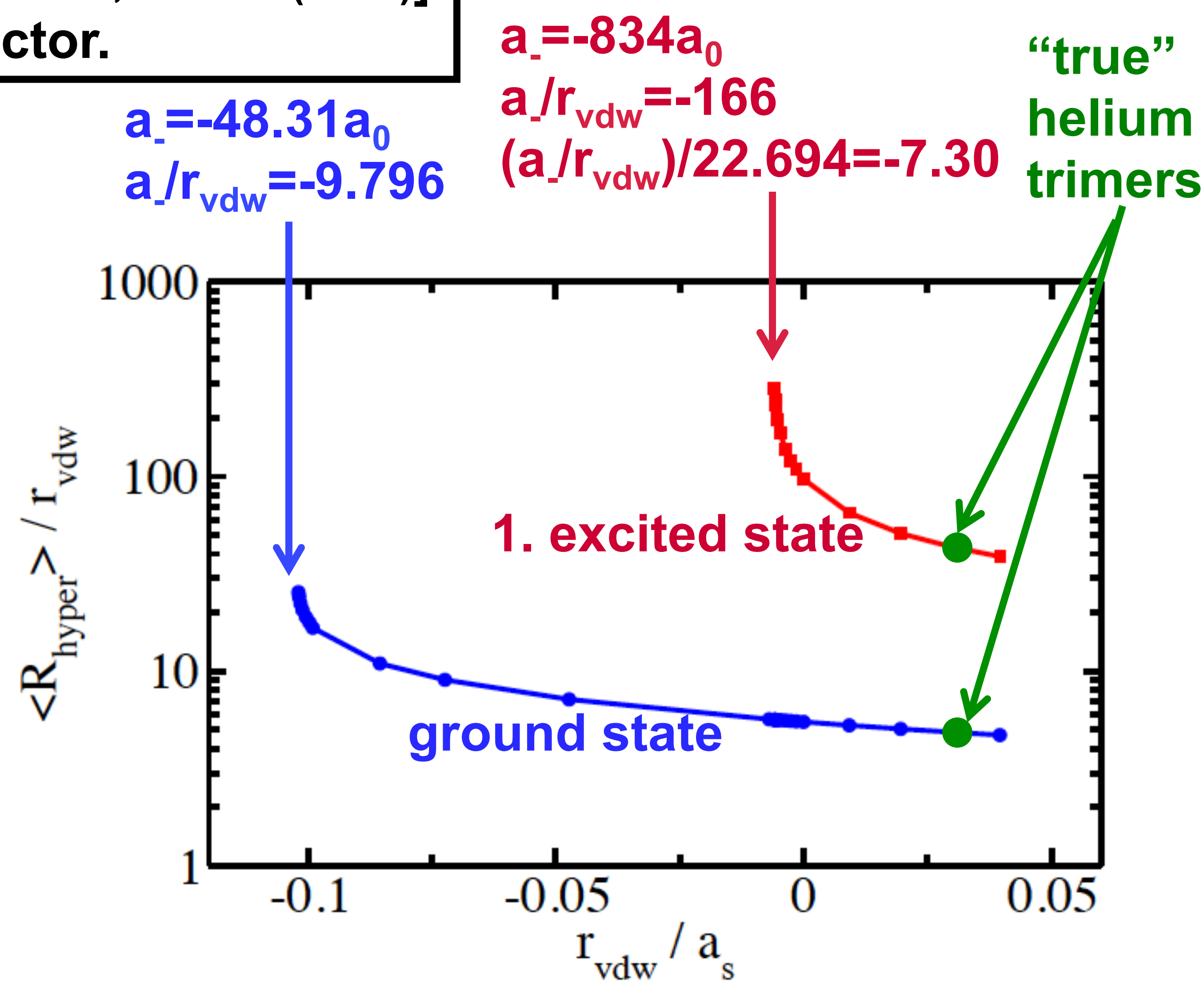
He-He potential [JCP 136, 224303 (2012)] + overall scaling factor.

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

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

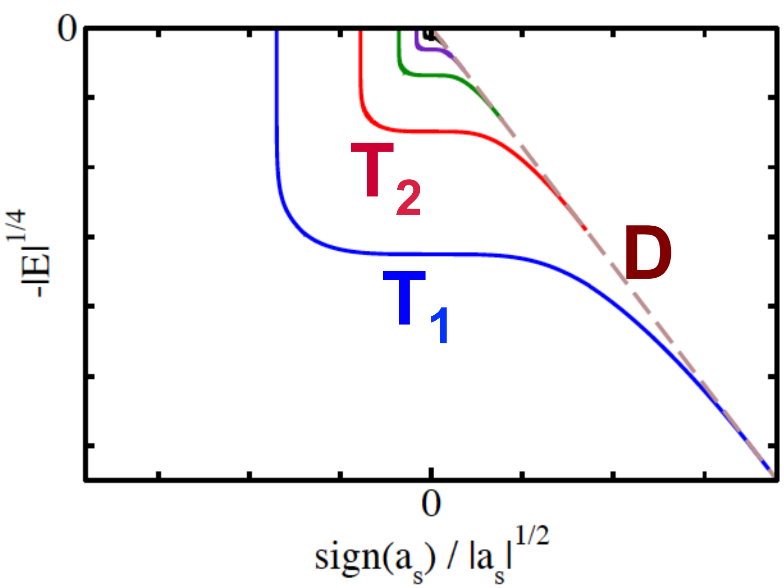
This yields:
$0.0323/a_0$
$0.0424/a_0$

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



Objectives of This Talk: Extended/Generalized Efimov Scenario

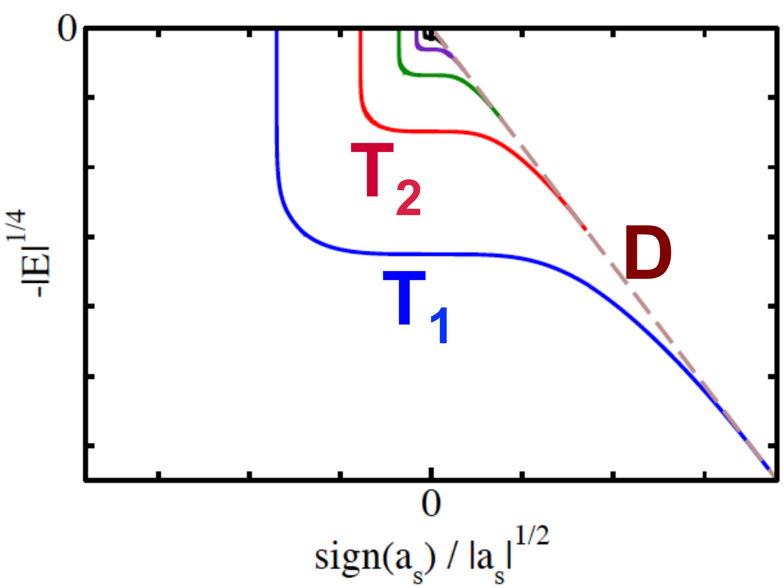
"Standard" Efimov scenario:
Three identical bosons with zero-range contact interactions:



- 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…

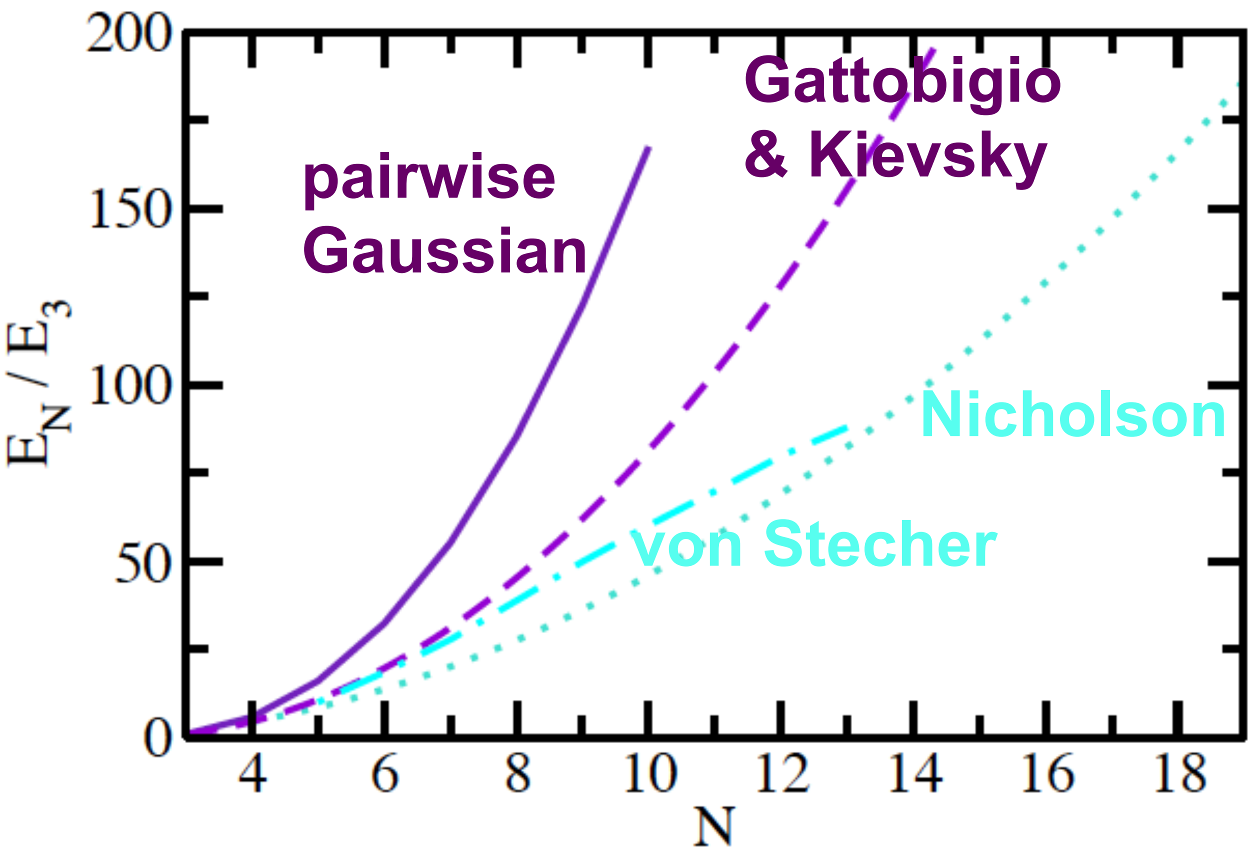
Treat N-body resonance states [for N=4, Deltuva, Few-Body Syst. 54, 569 (2013); for N=5 and 6, von Stecher, PRL 107, 200402 (2011)].

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).

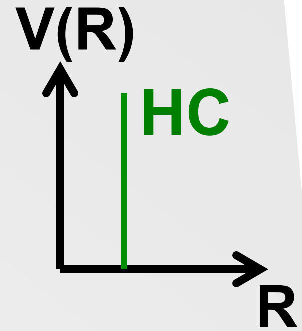
Nicholson (noise):
$E_N = E_4N/2(N/2-1)/2$.
PRL 109, 073002 (2012)

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

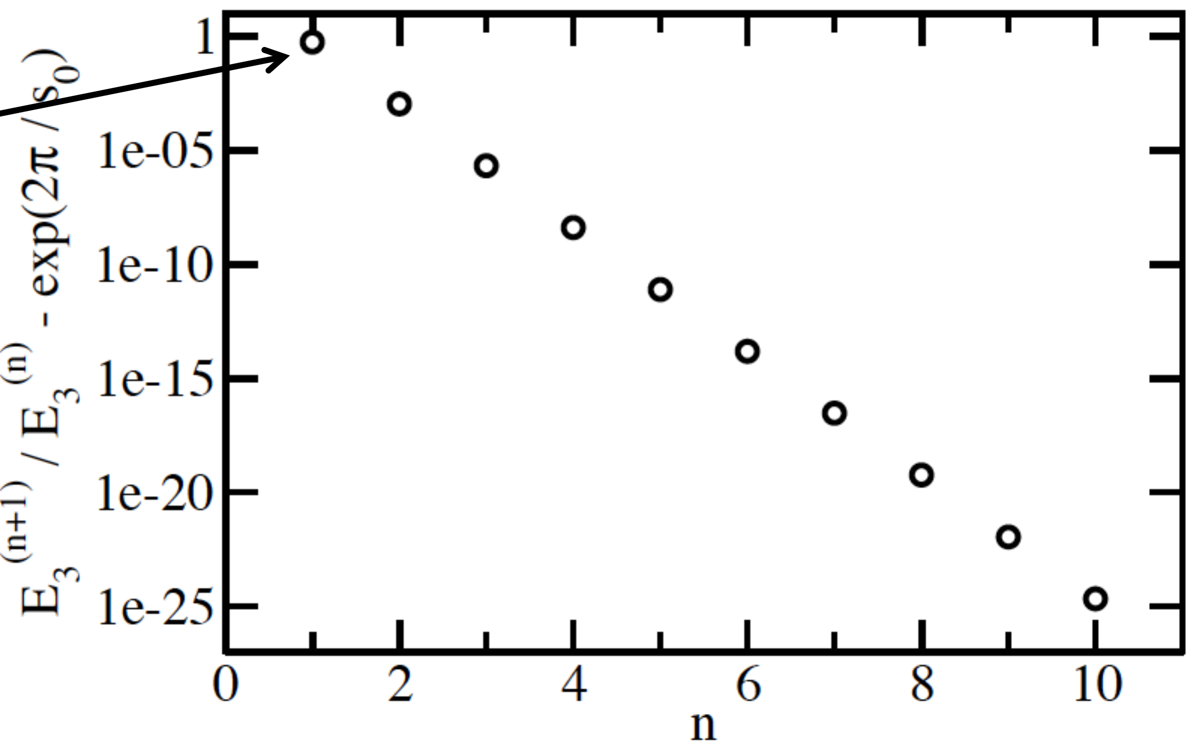
This talk:
Monte Carlo calculations for two-body ZR interactions and different regularizations in three-body sector.

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

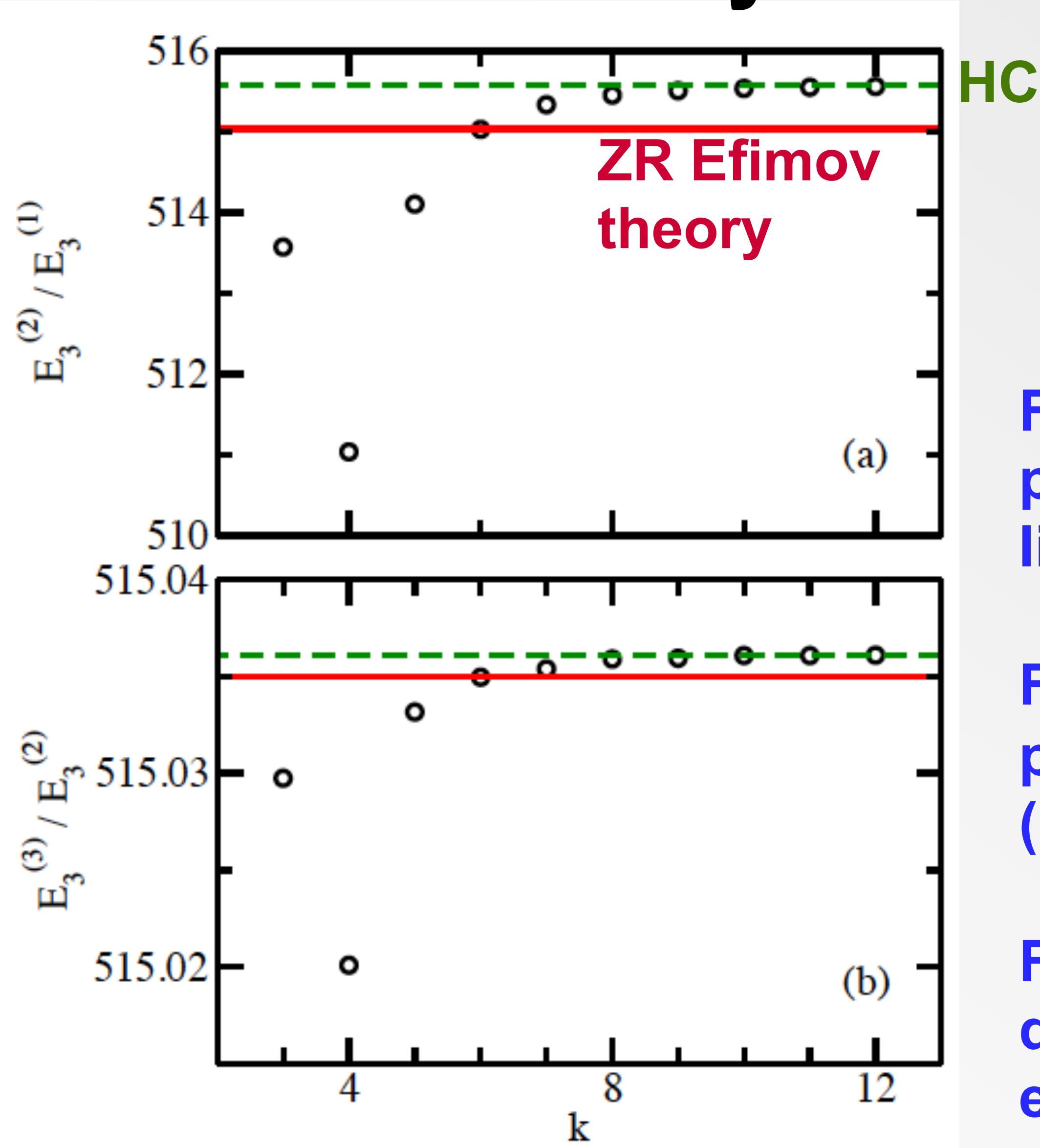
- Hyperangular equation can be solved analytically (yields s_0 value).
- Hyperradial equation can be solved analytically.



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.

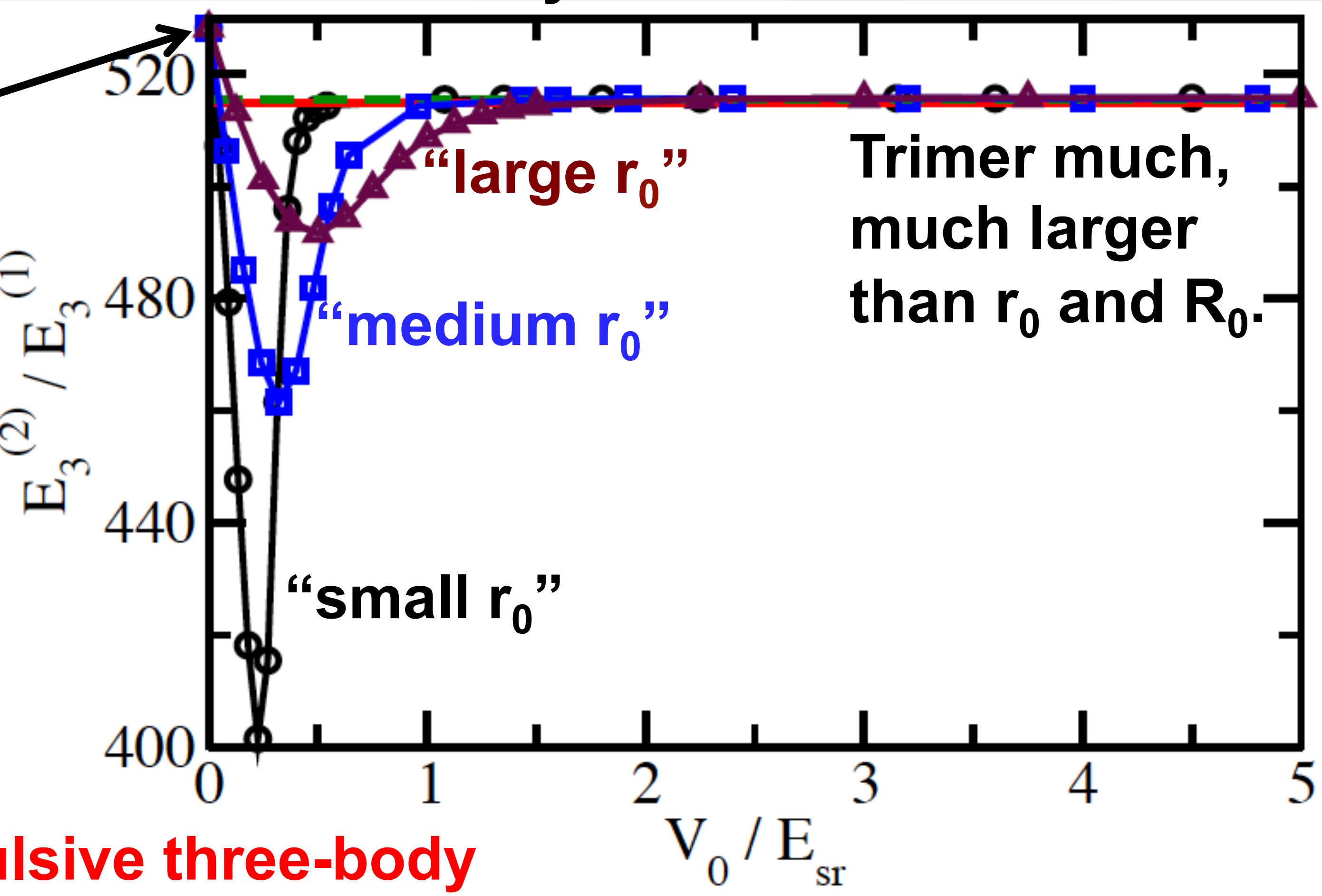
For k=2, the powerlaw potential "modifies" s_0 (does not regularize…).

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.

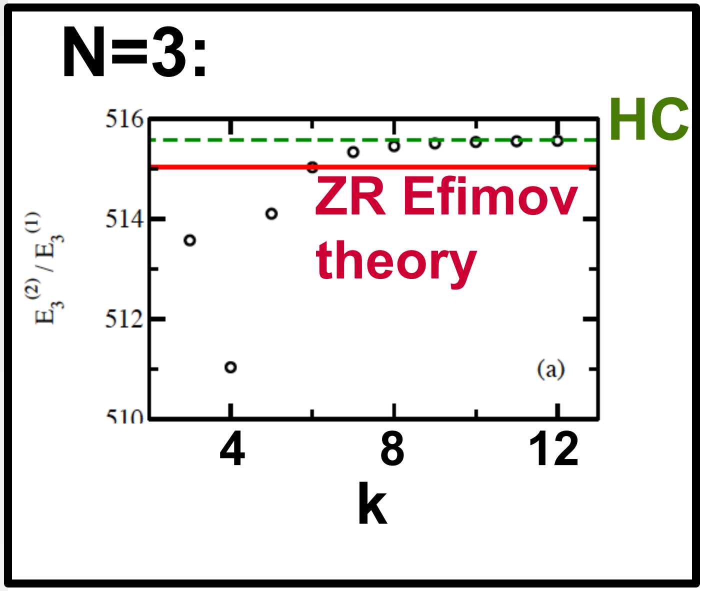
This is where Gattobigio et al. work. Trimer size $\langle R \rangle = 2.66 r_0$. $R^2=[\Sigma_{i<j}(r_{ij})^2]/3$



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 $E_N^{(1)}/E_3^{(1)}$.



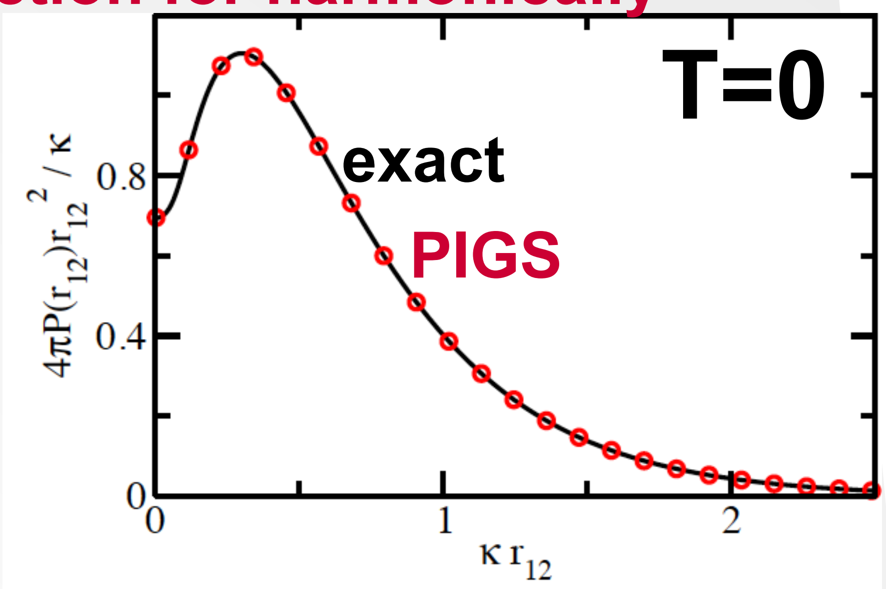
We use the Path Integral Monte Carlo (PIMC) approach, extrapolated to zero temperature, to treat N-body system: Pair approximation with analytical two-body zero-range propagator.

Benchmarking the Two-Body Zero-Range Propagator

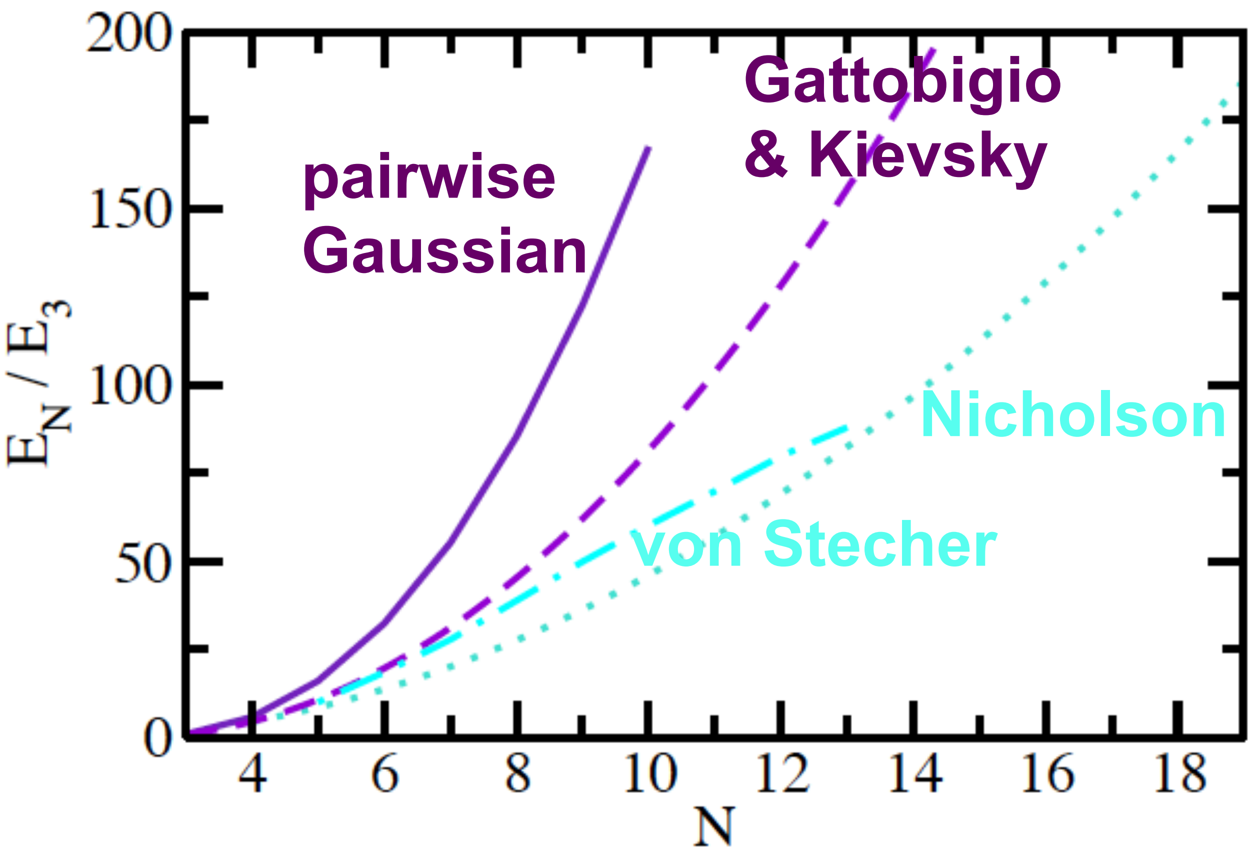
- **Two-body propagator calculated analytically for 1d and 3d systems (harmonically trapped or free space).**
- **Can be used in real or imaginary time evolution.**
- **We have primarily used it in applications where imaginary time is identified with inverse T.**

- **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=∞): "Universal" Energy Predictions from the Literature



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

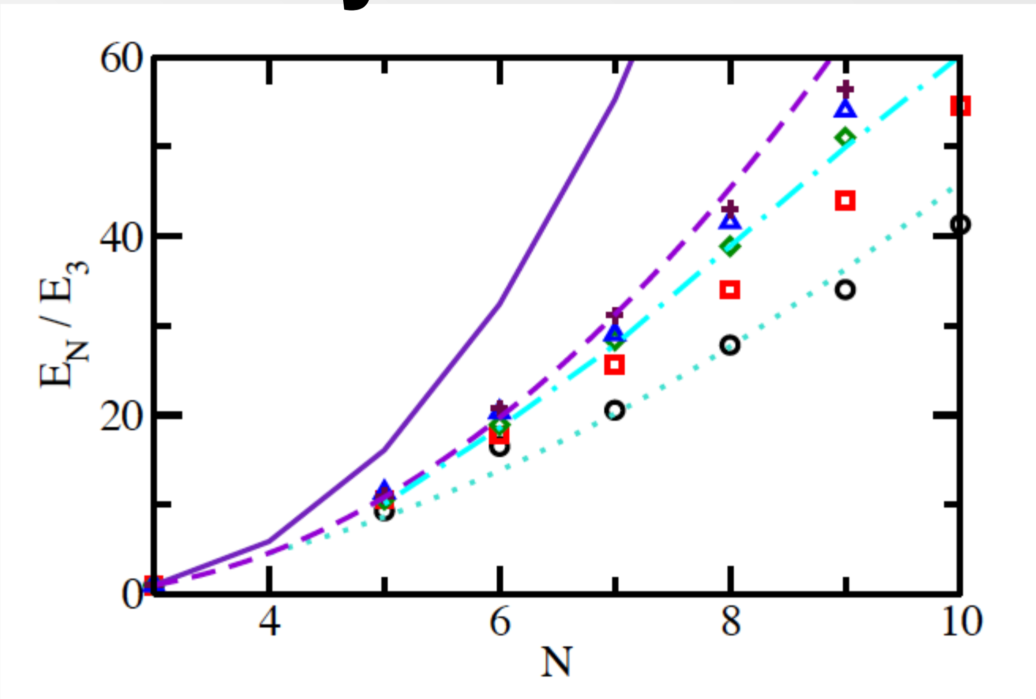
Gattobigio & Kievsky (next talk): finite-range corrections included (E_4 made to match Deltuva result).

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



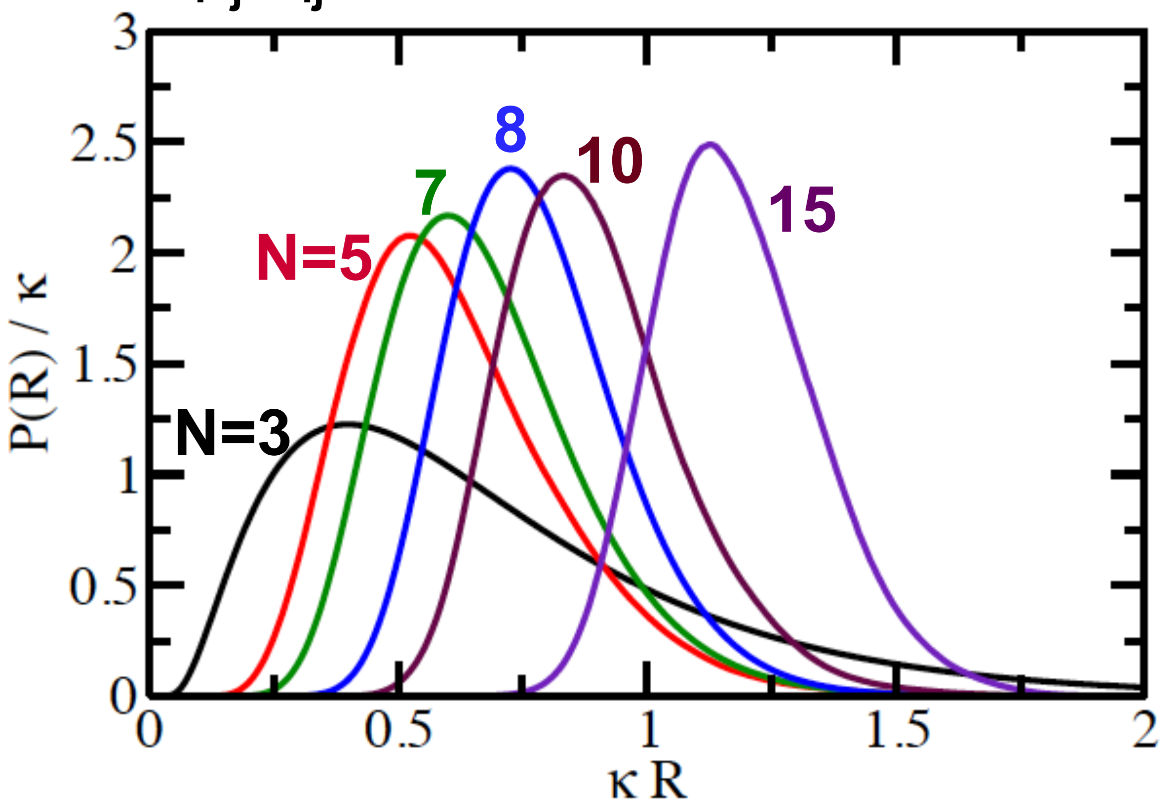
Purely repulsive three-body powerlaw potential: $V(R)=C_k/R^k$.

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).

Hyperradial Density for N Bosons (a_s=∞)

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.

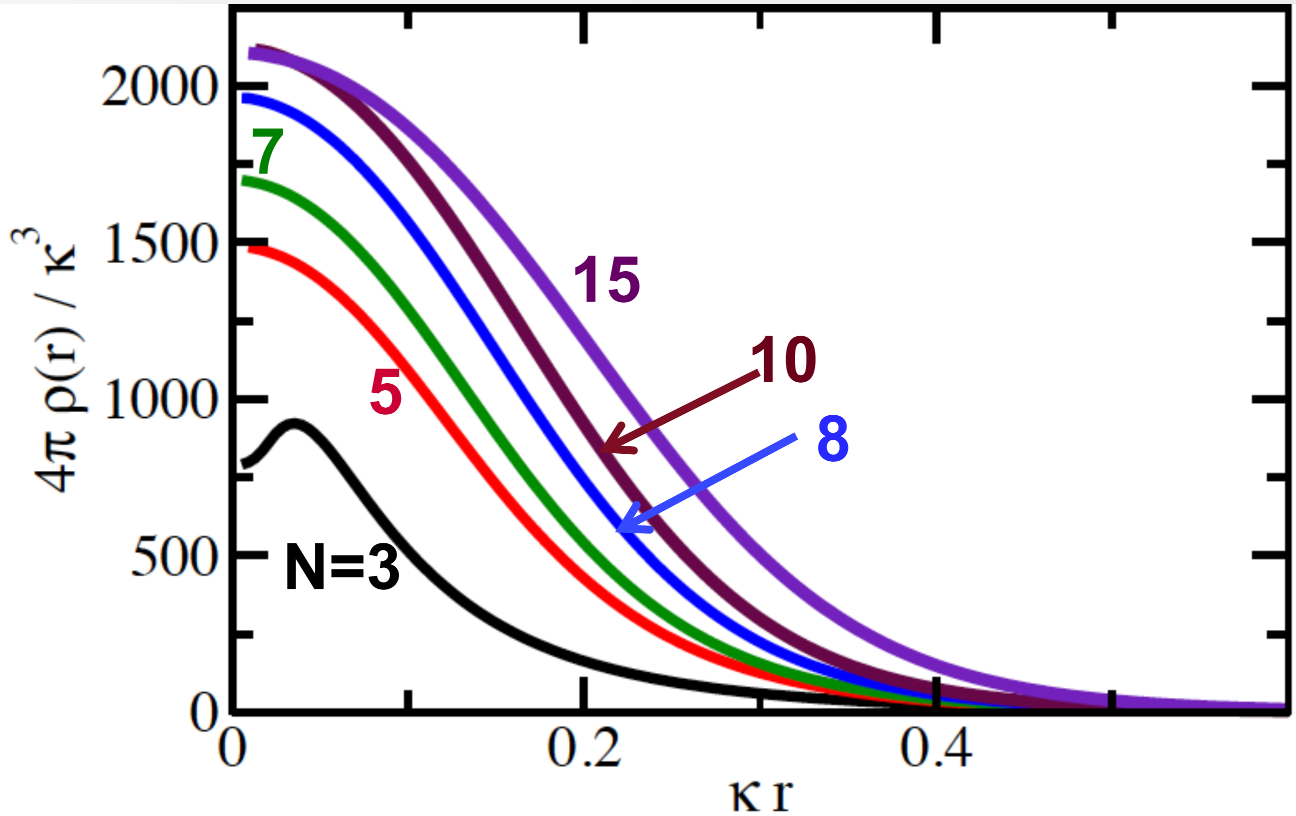


N=3 distribution is broadest.

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).

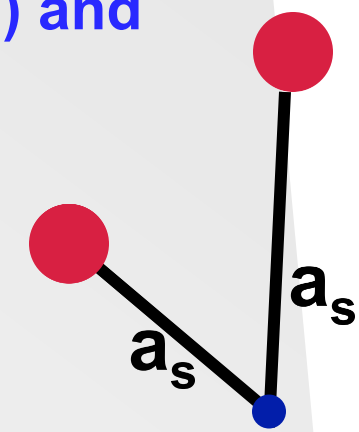
- Radial peak density, normalized to number of particles, saturates around N=10-15 for k=6.

- 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_NX System with Large Mass Ratio

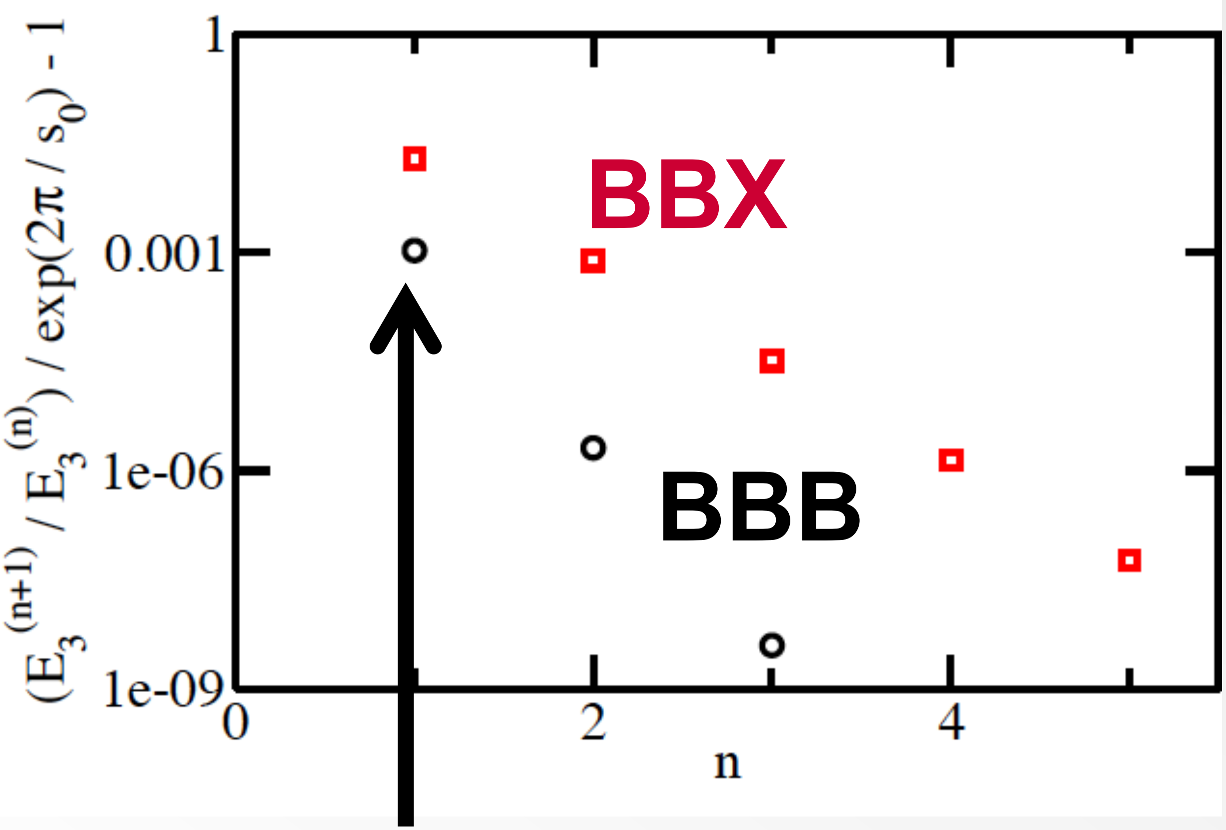
- Recent experiments by the Chicago (arXiv:1402.5943) and Heidelberg [PRL 112, 250404 (2014)] groups on CsLi mixture measure three-atom resonances.



- 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_NX sector?
  - Number of four-body bound states, if any, that are tied to B_2X 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



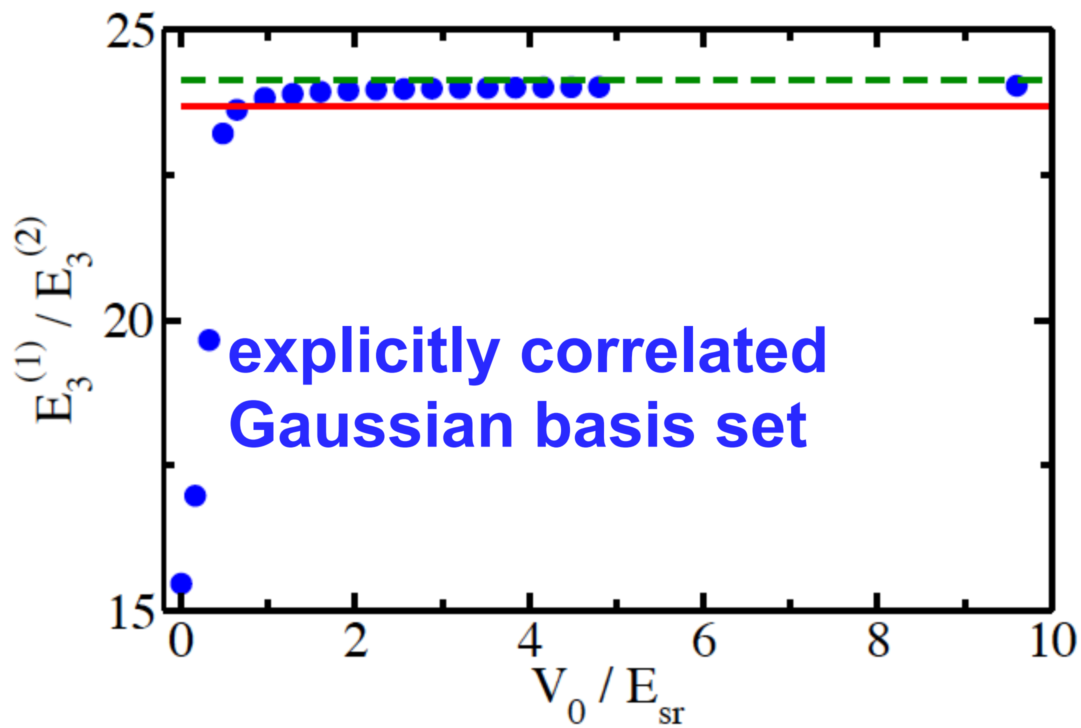
BBB: ~0.11%
BBX: ~1.9%

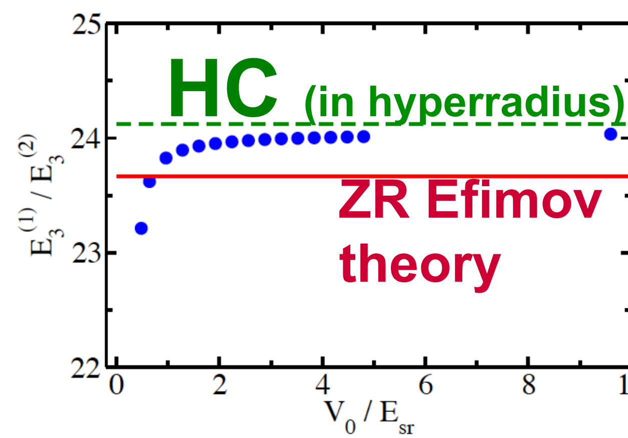
The amplitude of the hyperradial density in the "inner lobe" is larger for BBX than for BBB. More favorable (i.e., smaller) energy level spacing introduces new computational challenge…

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

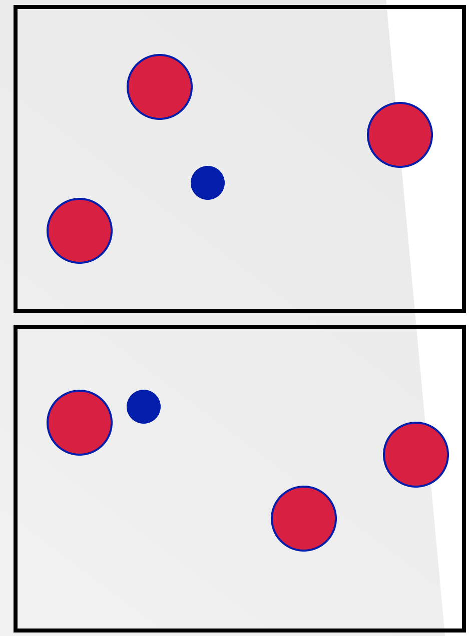
- **Basis functions:**
  Simple Gaussian $\Phi_k(\underline{x}) = \exp(-\underline{x}^T A^{(k)} \underline{x}/2)$

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.

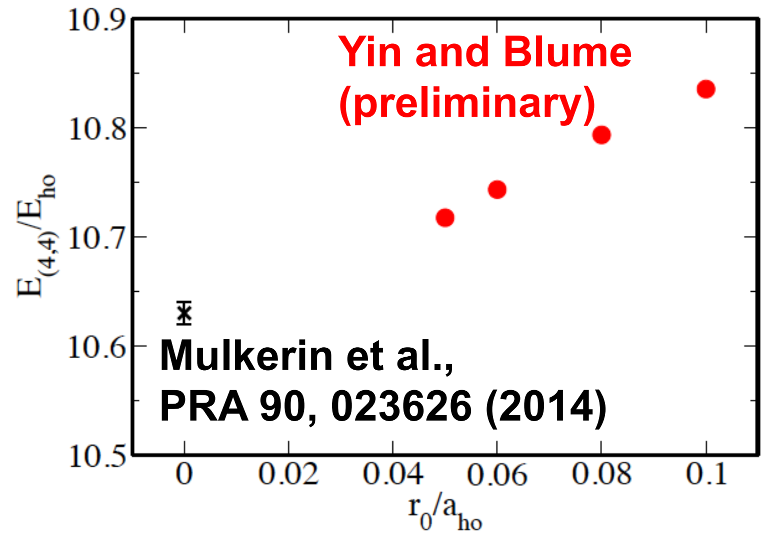
Rigorous upper bound for energy ("controlled accuracy").

Matrix elements for structural properties can be calculated analytically.

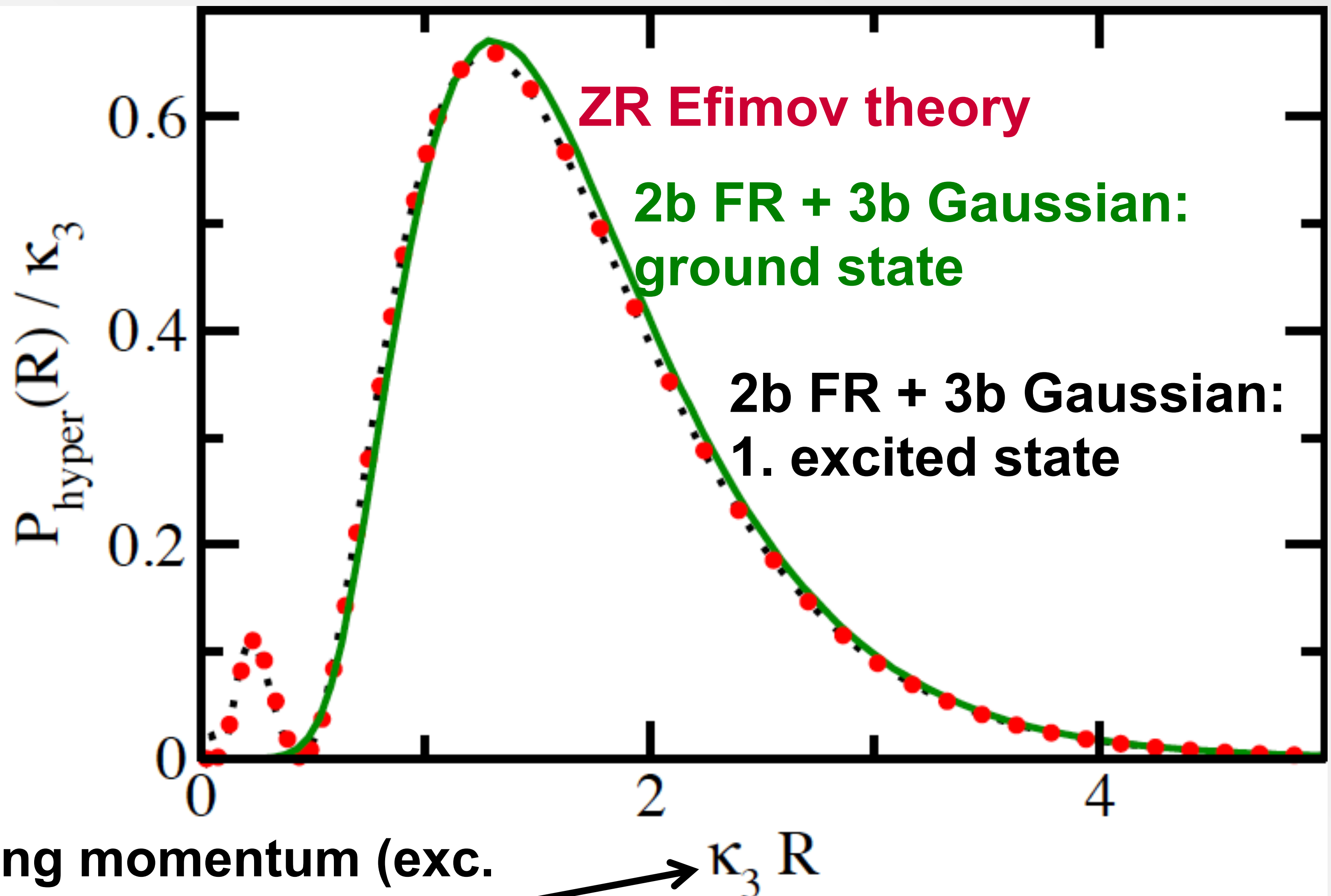
Computational effort increases with number of atoms N:

- 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



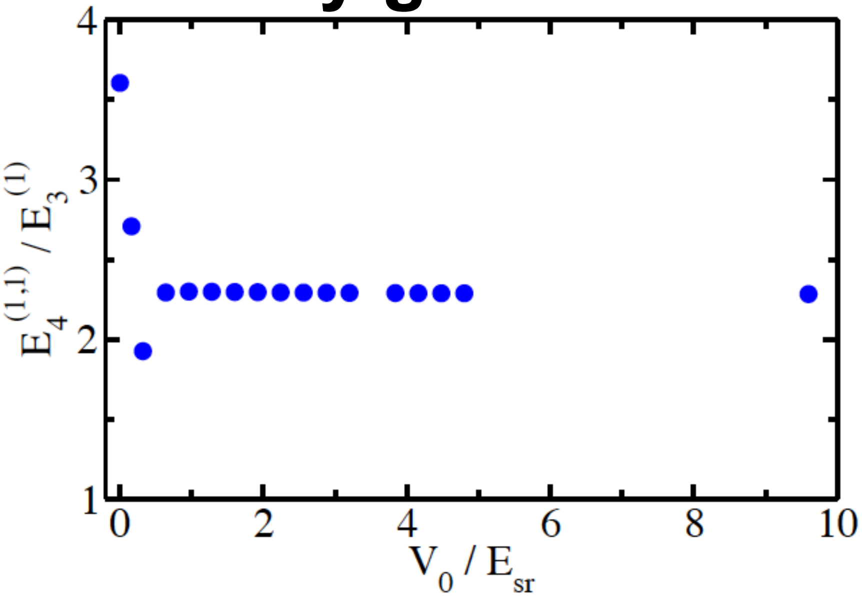
Binding momentum (exc. state energies are made to agree).

Convincing agreement…

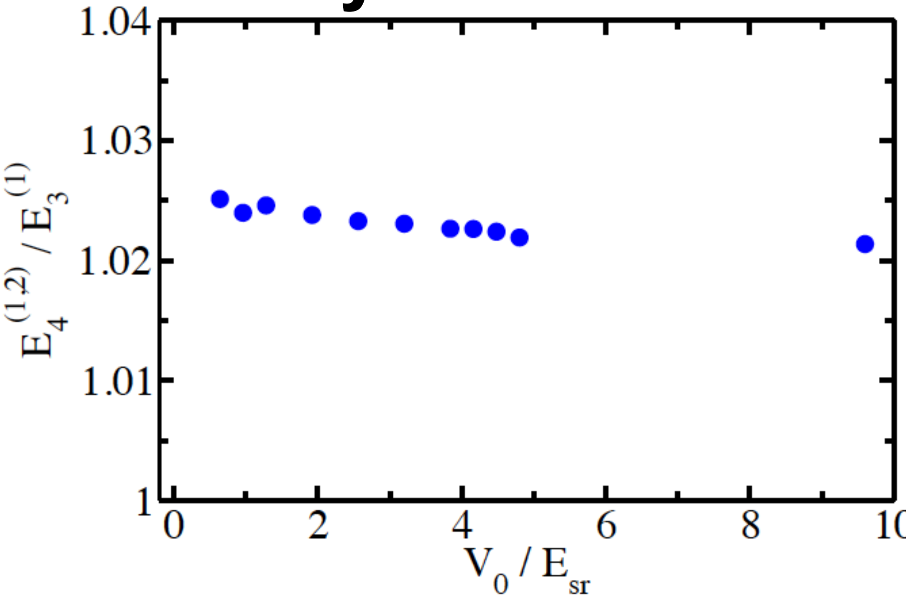
Cs_3Li ($a_s=\infty$): Gaussian Two-Body and Gaussian Three-Body Potential

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:

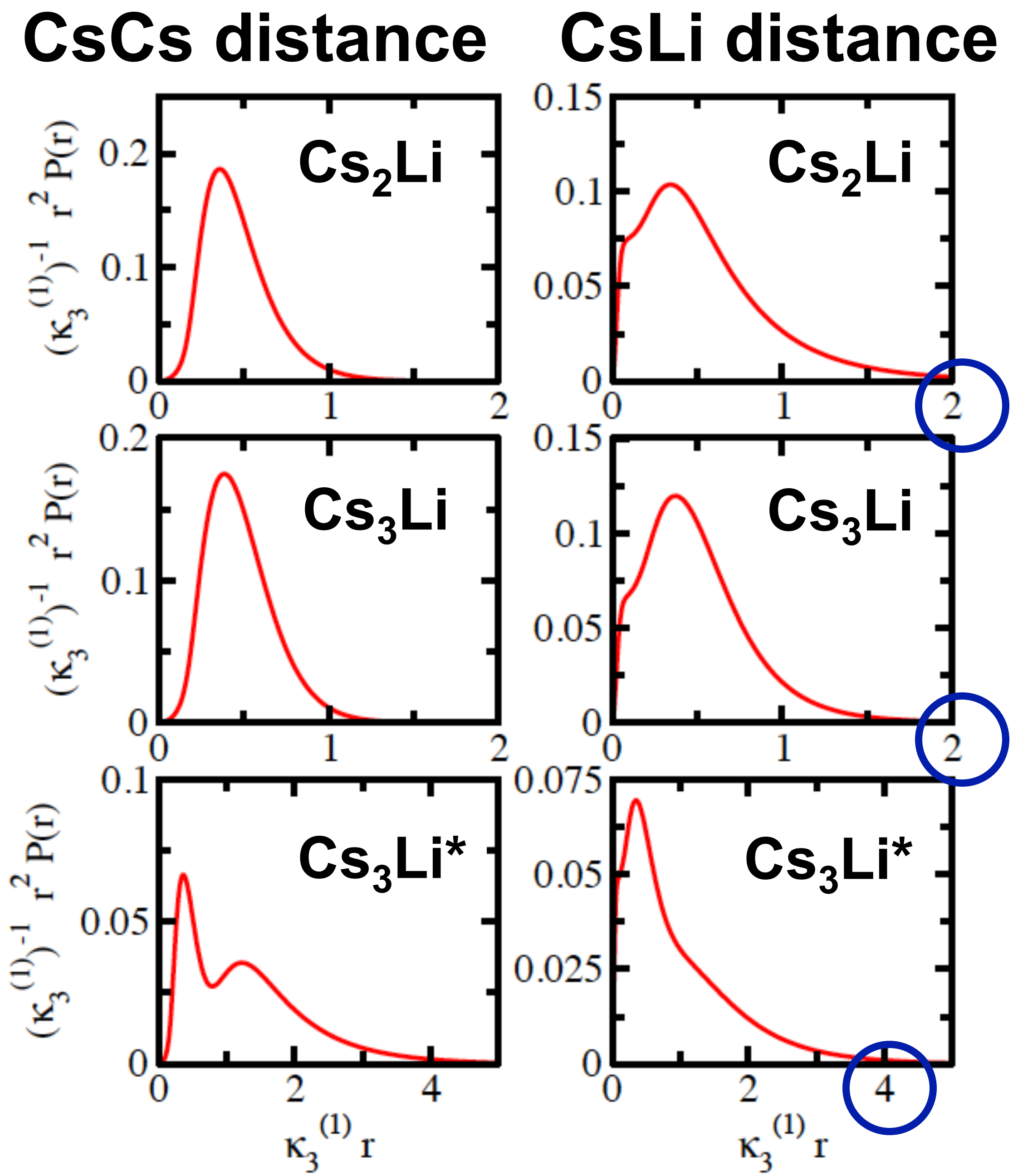


Cs_NLi ($a_s=\infty$)

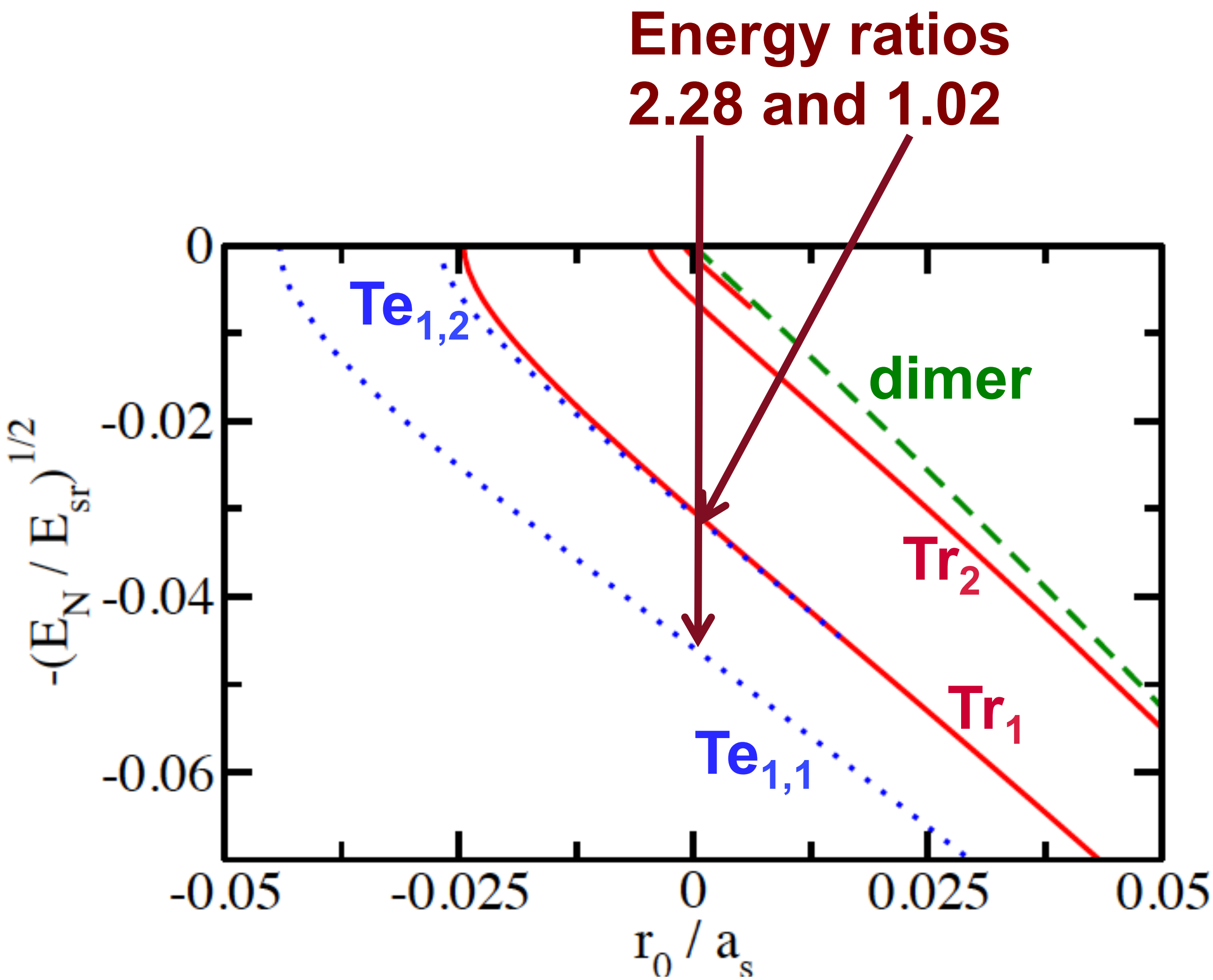
Pair distribution: Likelihood of finding two particles at distance r from each other.

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

Distributions for Cs_3Li^* excited state are broader.

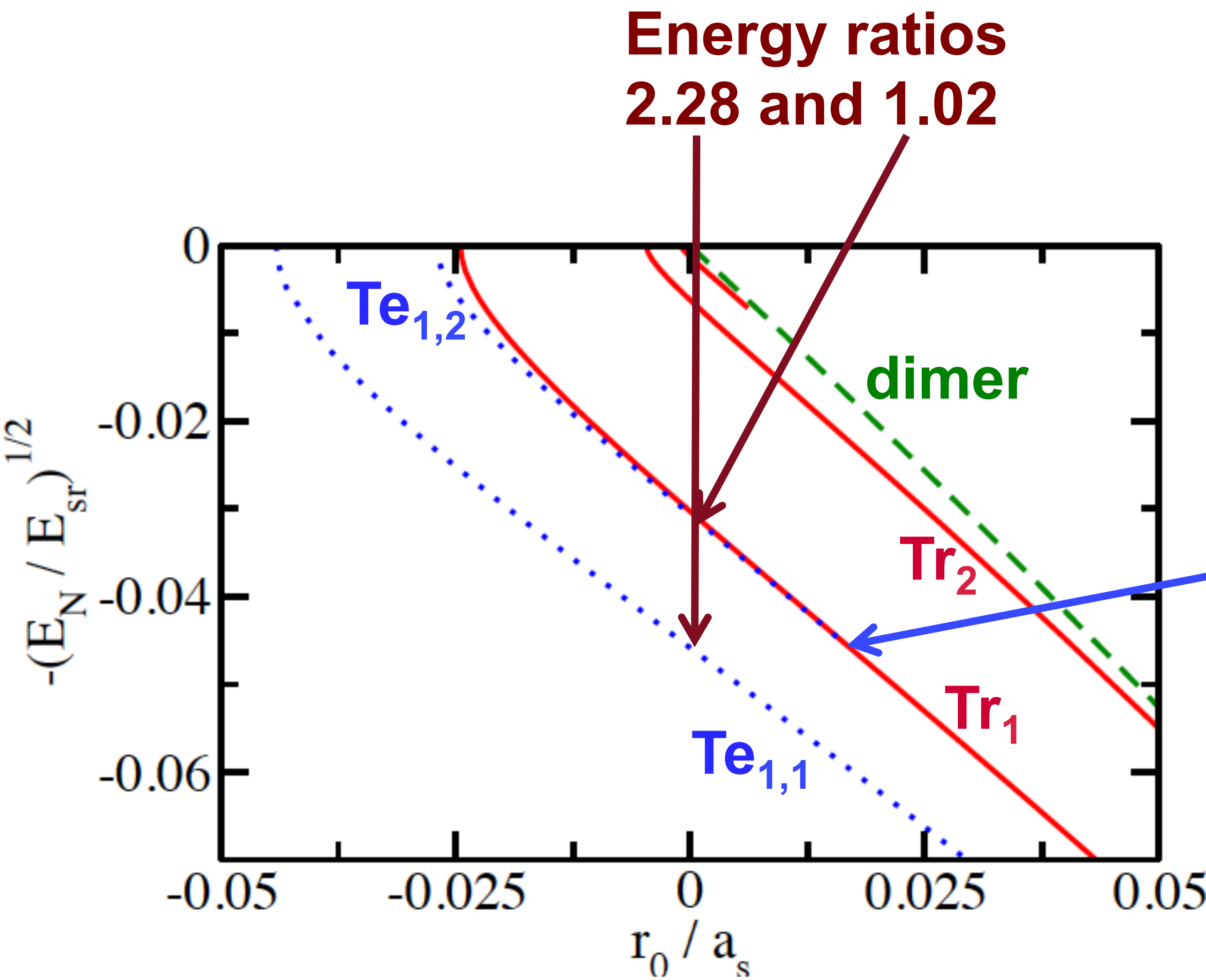


Generalized Efimov Scenario for CsLi Mixture



Two tetramer states.

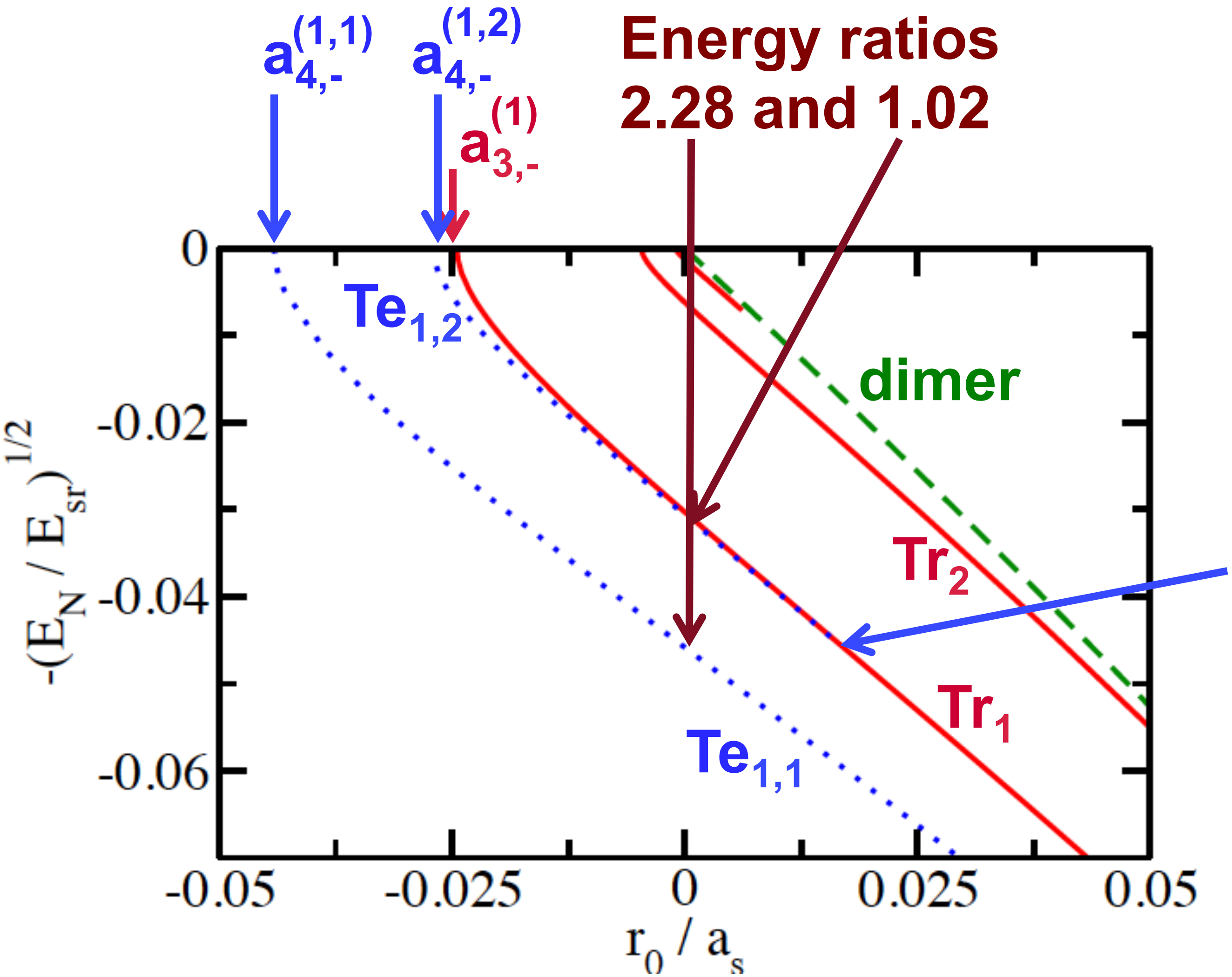
Generalized Efimov Scenario for CsLi Mixture



Two tetramer states.

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

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…

Summary

- Unequal-mass Cs_3Li system (see arXiv:1410.2314):
  - Two four-body states tied to Cs_2Li trimer.
  - Four-atom resonance position of weakly-bound state is close to three-atom resonance position.

- B_N system at unitarity:
  - Dependence of system properties on three-body regulator.
  - Structural properties of Bose droplet.
  - Next step: Look at N-body states tied to excited Efimov trimers.

- Developed two-body zero-range propagator suitable for use in continuum Monte Carlo simulations.