

Few-Body Physics of Cold Atoms: Techniques and Results that May be of Interest to Nuclear Physics/Physicists

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In collaboration with graduate students Debraj Rakshit, Xiangyu (Desmond) Yin and Kevin Daily. Trapped boson work with Phil Johnson and Eite Tiesinga.

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Outline of This Talk

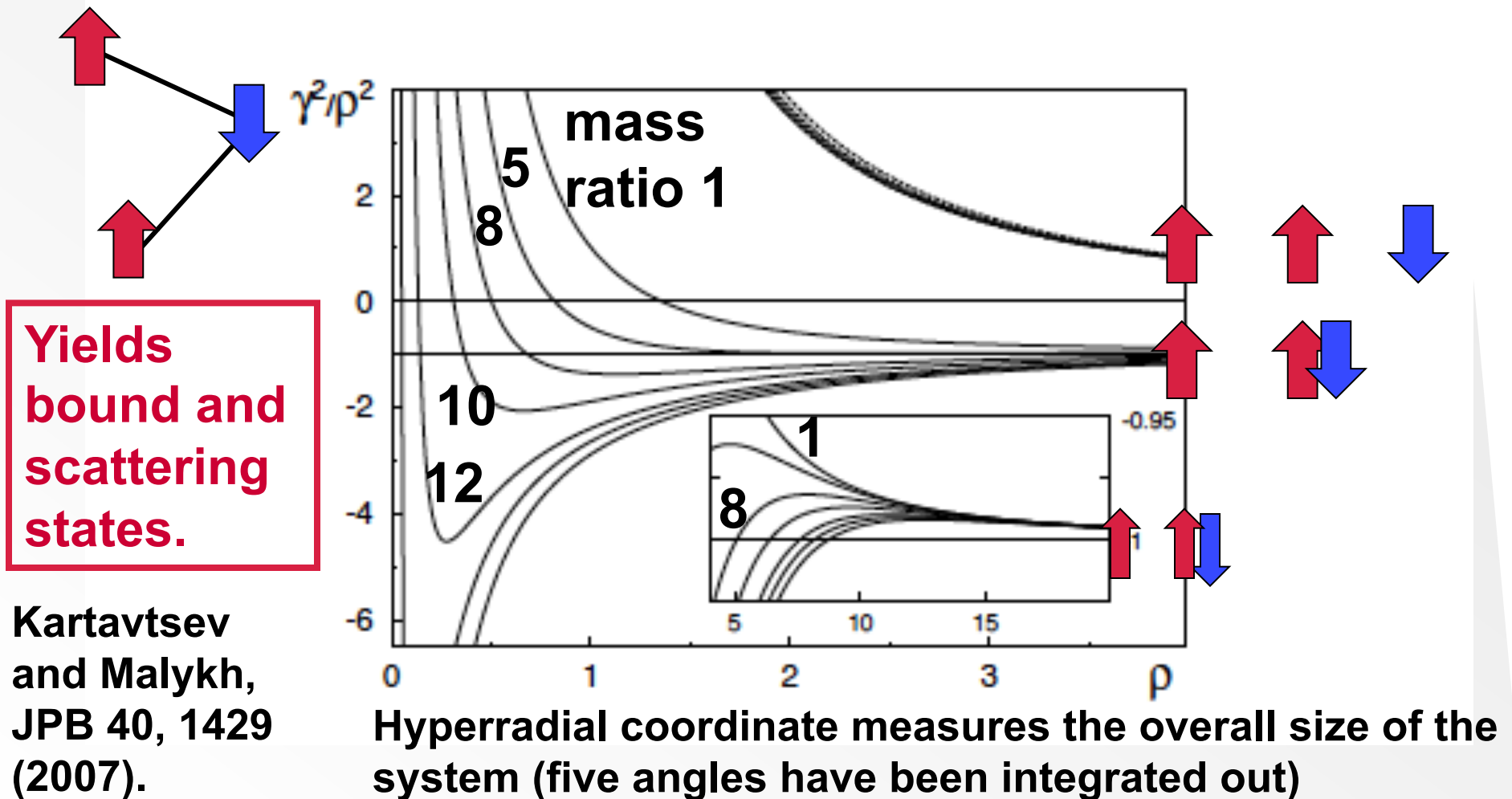
- **Approach to solving four- and five-particle bound and scattering problems:**
 - Combining hyperspherical coordinates, explicitly correlated Gaussian basis functions and stochastic variational technique.
 - Formalism and first results.
- **Bosons in a spherically symmetric harmonic trap:**
 - Confronting effective field theory results with highly accurate numerical results for finite-range interactions.
- **Few-particle system in a box with periodic boundary conditions:**
 - A possible path towards obtaining accurate results.

General Consideration

- **We are interested in low-energy phenomena (justified for ultracold atomic samples):**
 - **Physics is governed by just a few (one) partial waves.**
- **The details of the two-body atom-atom interaction do not matter.** Universal if s-wave scattering length $a_s \gg$ range of two-body potential r_0 .
- **Can replace van der Waals (vdW) potential by model potential.**
 - **vdW potential: hundreds of bound states.**
 - **model potential: zero or one bound states.**
- **In nuclear physics:** Might be able to get away with “simple soft potentials” that reproduce low-energy phase shifts.

Hyperspherical Coordinate Approach and Effective Potential Curves

Two heavy identical fermions and one light impurity with positive s-wave scattering length (zero-range interactions):



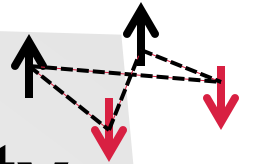
General Formalism: Similar to Born-Oppenheimer Approximation

- Hyperspherical coordinate approach: **hyperradius R** and **hyperangles Ω** .
- Idea: $H = T_{\Omega} + T_R + V_{\text{int}} = H_{\text{adia}}(R) + T_R$
- Step 1: Solve $H_{\text{adia}}(R) \Phi_v(R; \Omega) = U_v(R) \Phi_v(R; \Omega)$ (this is like integrating out the fast electronic degrees of freedom).
- Step 2: Solve $(T_R + U_v(R) + \Sigma_v, \text{coupling}_{v',v}) F_{vq}(R) = E_{vq} F_{vq}(R)$ (this is like solving the nuclear Schroedinger equation).
- For convenience, write $U_v(R) = \hbar^2[(s_v(R))^2 - 1/4] / (2\mu R^2)$

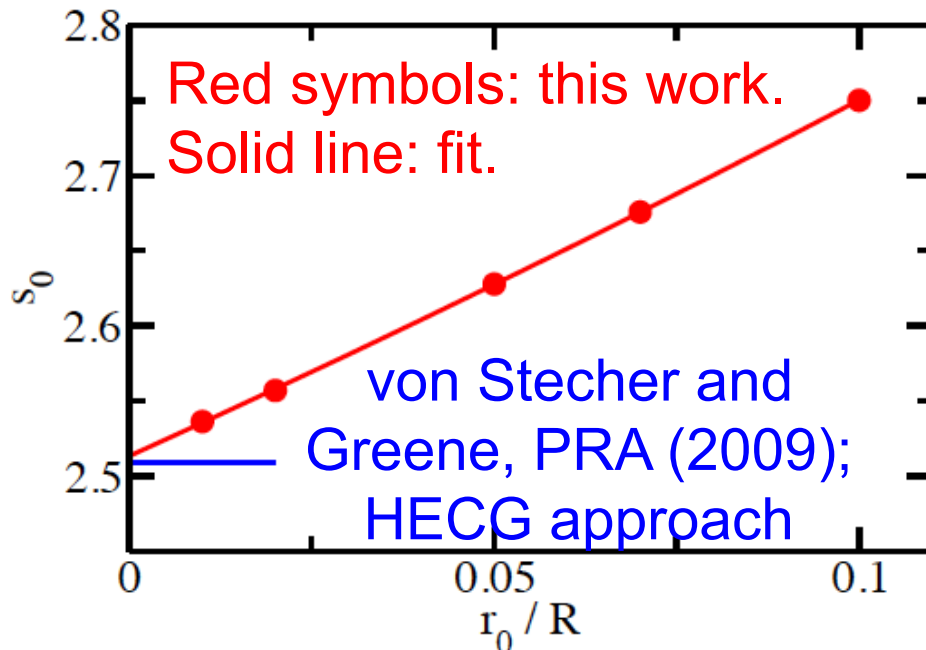
How Do We Solve Hyperangular Schrodinger Equation?

- Use **explicitly correlated Gaussians** to expand hyperangular channel functions [see von Stecher and Greene, PRA (2009) for treatment of 0^+ states].
- $\Phi_v(\mathbf{R};\Omega) = \sum_k c_k [f(\underline{\mathbf{x}}, \underline{\mathbf{u}}_1^{(k)}, \underline{\mathbf{u}}_2^{(k)})] \exp[-\frac{1}{2} \underline{\mathbf{x}}^T \underline{\mathbf{A}}^{(k)} \underline{\mathbf{x}}] |_{\mathbf{R}}$
- Transform basis functions to hyperspherical coordinates and perform $2N-1$ hyperangular integrals analytically.
- For $N=4$ ($N=5$), this leave one (two) numerical integration(s).
- Explicitly correlated Gaussian depend on non-linear variational parameters: Optimize using stochastic variational “trial and error” approach [minimize $U_v(\mathbf{R})$].

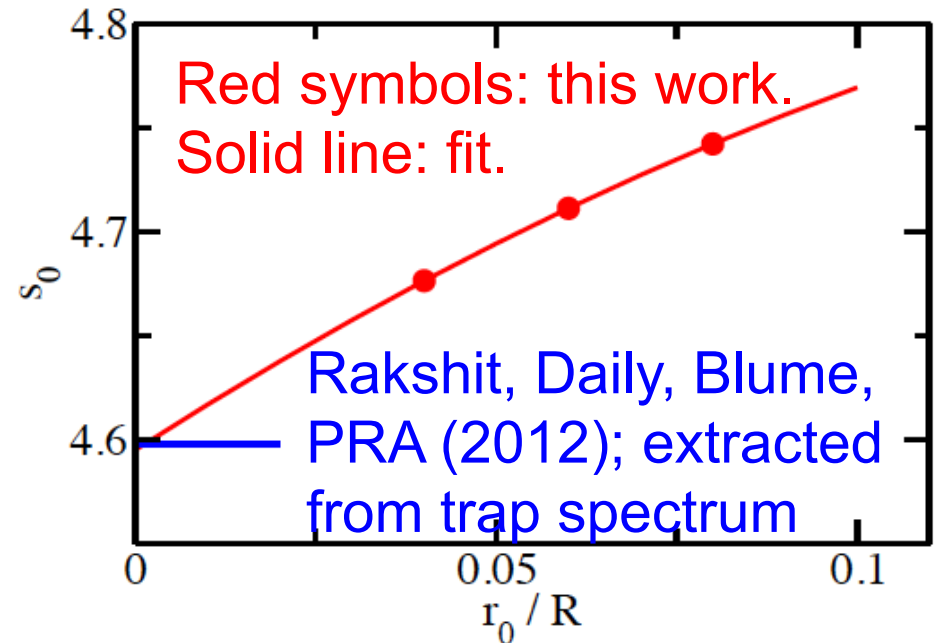
Proof-of-Principle Calculation for Equal-Mass (2,2) System at Unitarity



0^+ symmetry:



1^- symmetry:

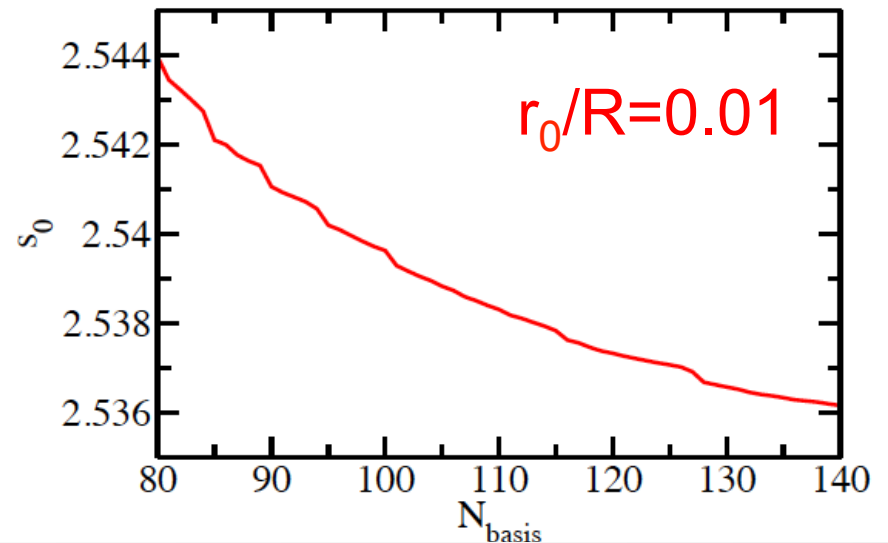
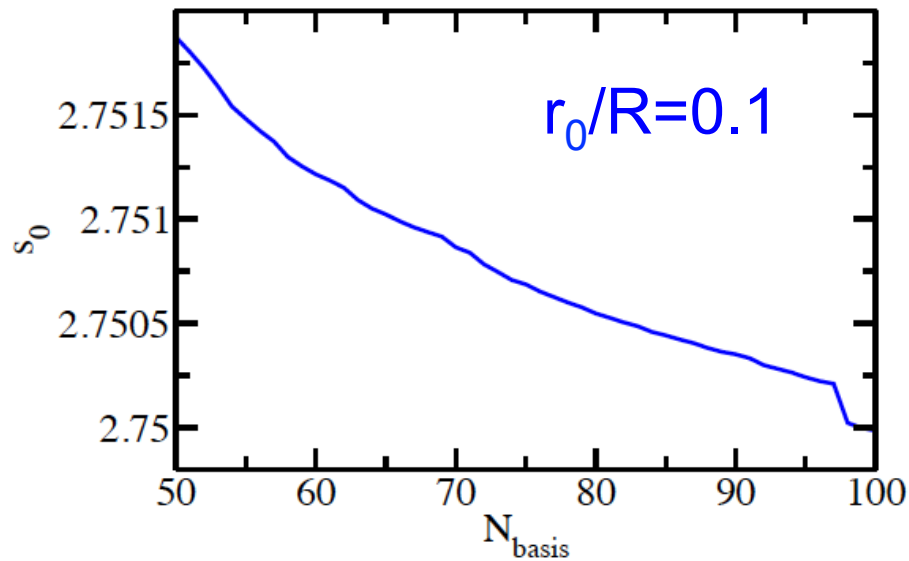
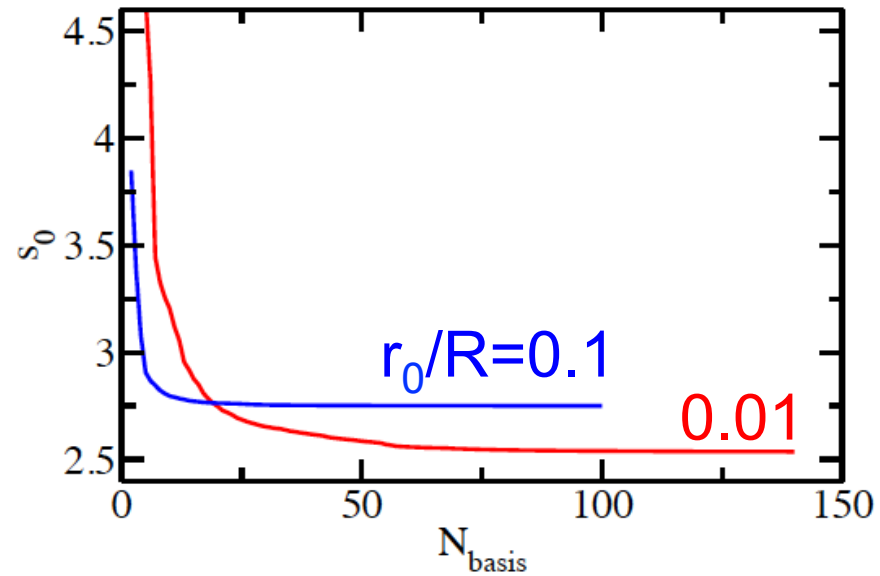


Hyperspherical explicitly correlated Gaussian approach can be applied to states with finite angular momentum.

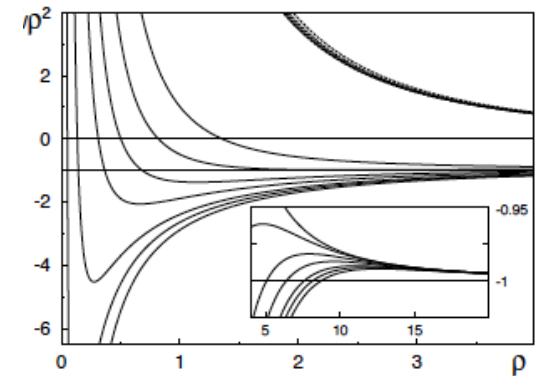
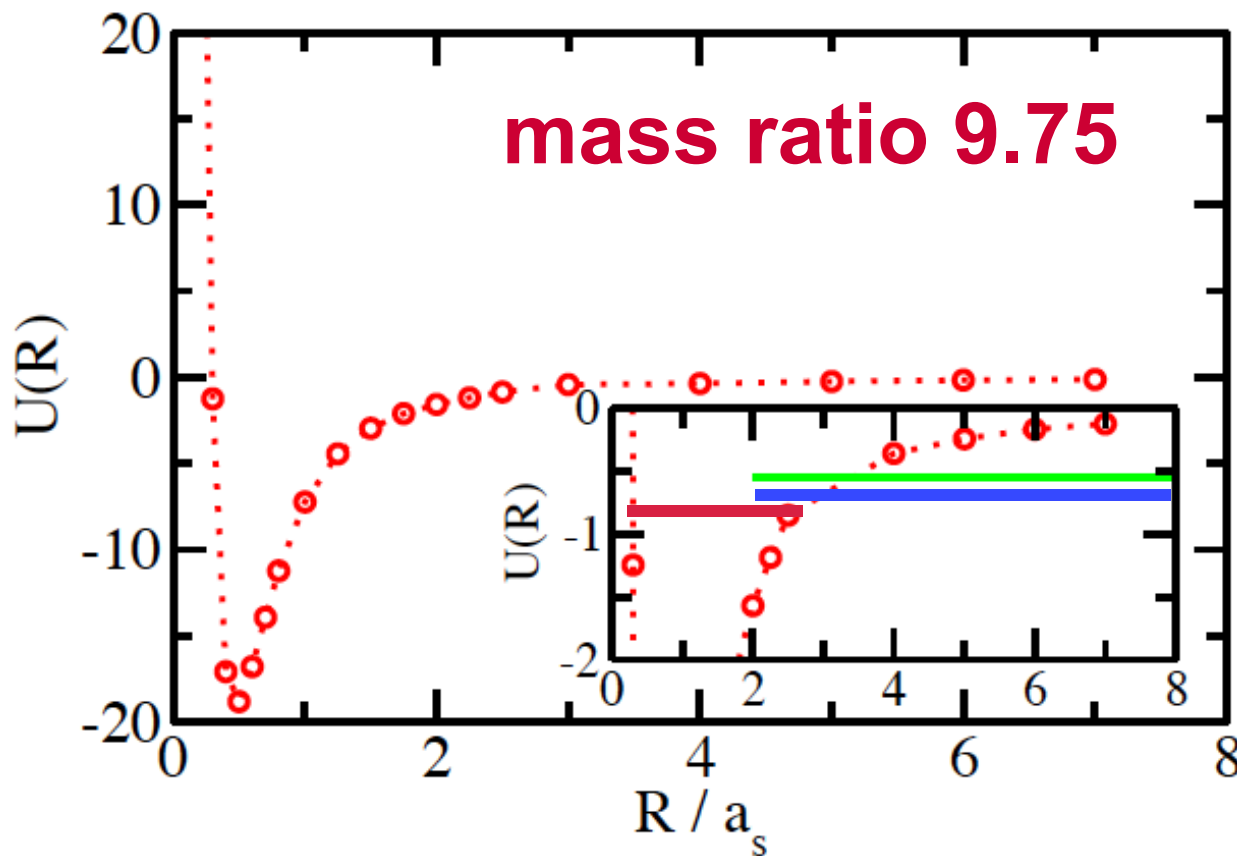
Finite L matrix elements are tedious to derive (applicable to “any N”)... numerics is tractable for N=4, (5)...

Rakshit and Blume, unpublished.

Convergence of Eigenvalue of Hyperangular Schroedinger Equation



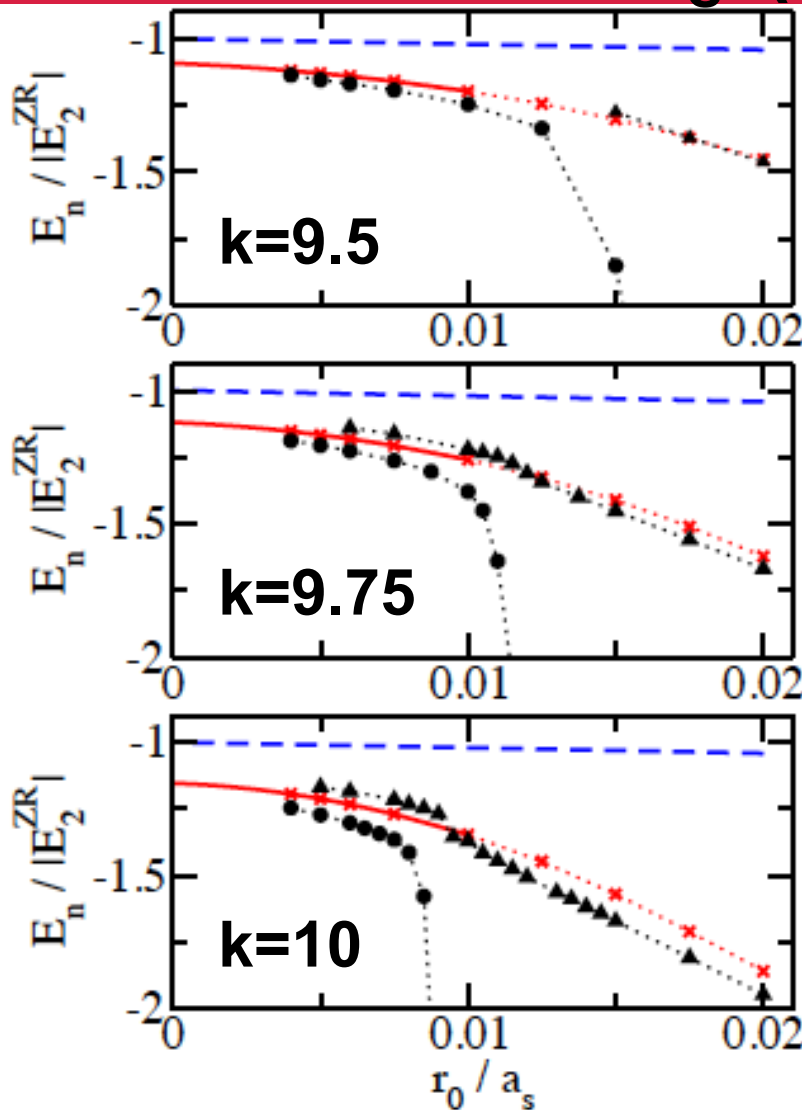
Potential Curve for (3,1) System with 1^+ Symmetry and Positive a_s



Dimer threshold.
Trimer threshold.
Expect: Four-body bound state.

This is work in progress: Go to larger hyperradii; calculate excited curves and coupling elements; and solve coupled channel equations in R .

Heavy-Light (3,1) System with $L^{\Pi}=1^+$ and Positive a_s (no fixed R!)



Dashed blue: Two-body state.

Red: Universal three-body states [see Kartavtsev and Malykh, JPB 40, 1429 (2007)].

Black: Away from resonance-like feature, universal four-body states.

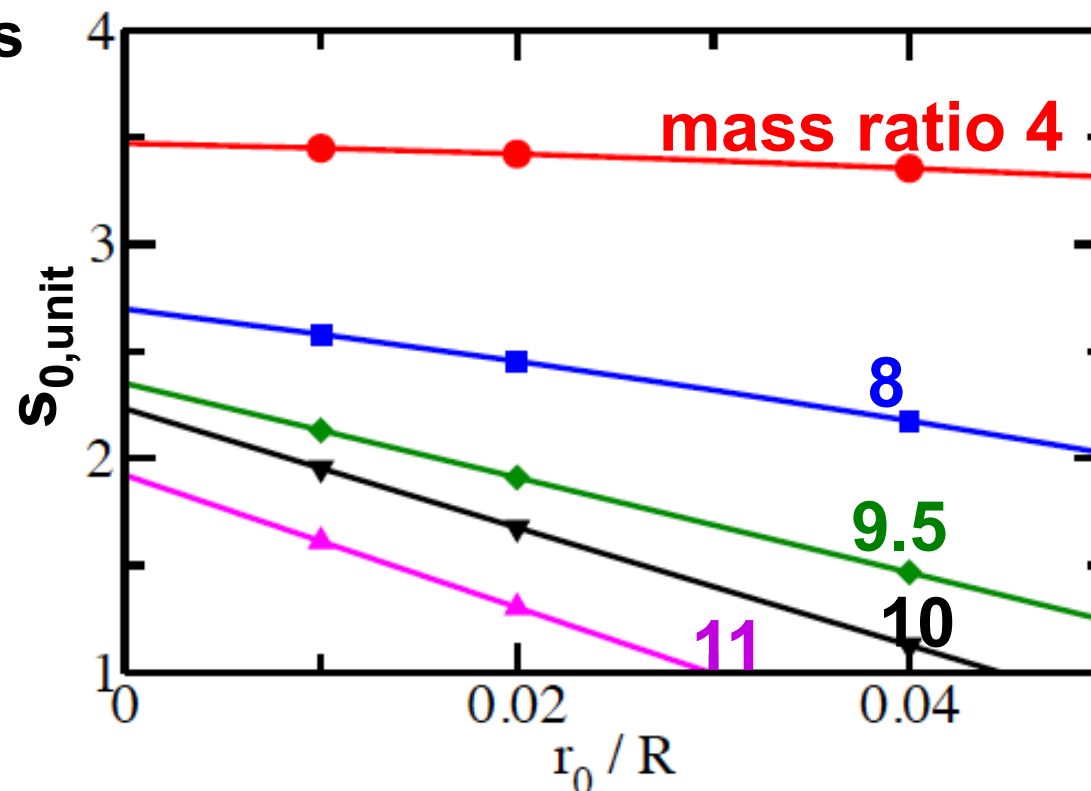
- Universal four-body bound states exist for mass ratio >9.5 .
- Properties are fully determined by a_s .
- Four-body states are tied to three-body states.

Under Which Conditions Do Universal States Exist?

- $(T_R + U_v(R) + \Sigma_v, \text{coupling}_{v,v}) F_{vq}(R) = E_{vq} F_{vq}(R)$
- For finite a_s , small R and $r_0=0$:
- $U_v(R) + \Sigma_v, \text{coupling}_{v,v} \sim \hbar^2[(s_{0,\text{unit}})^2 - 1/4] / (2\mu R^2)$
- $S_{0,\text{unit}} > 1$ [for (2,1), mass ratio $\kappa < 8.6$]: Only “regular” solution contributes (wave fct. vanishes at small R).
- $1 > s_{0,\text{unit}} > 0$ ($8.6 < \kappa < 13.607$): In principle, “regular” and “irregular” solutions can contribute (depends on two-body potential). See work by Petrov, Nishida, Tan, Son, Werner, Castin,...
- Our earlier work on (2,1) systems with Gaussian interactions at unitarity shows that regular solution dominates for mass ratios considered here [see Blume and Daily, PRL and PRA (2010)].

Hyperangular Eigenvalue for Various Mass Ratios: (3,1) System with $L^{\square}=1^+$

Interspecies s-wave scattering length is infinitely large.



Preliminary

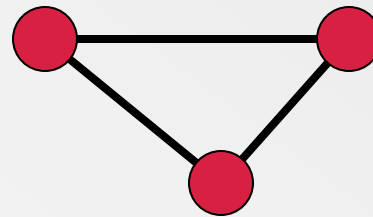
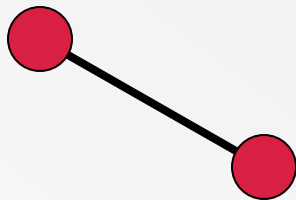
Conclusion: Universal bound states in heavy light mixtures with positive interspecies s-wave sc. length exist for mass ratio > 9.5 .

Conclusion supported by (i) close link between 3- and 4-body free-space energy, (ii) hyperradial densities, (iii) s_0 value at unitarity.

Harmonically Trapped Bose Gas with Small s-wave Scattering Length

Well known:

Interaction energy (IE) of N bosons $\neq N(N-1)/2 \times$ IE of 2 bosons



boson 3 affects how bosons 1 and 2 interact (boson 3 is not a spectator).

Question:

How to “divide” IE of N identical bosons in an isotropic harmonic trap into two-body, three-body, four-body,... contributions?

Our approach:

Apply perturbation theory for small a_s (this is conveniently done by applying formalism of second quantization to Hamiltonian with zero-range interactions); renormalization via effective field theory ideas.

Series in a_s and Effective Range r_{eff} : Effective N-Body Interactions

$$E(N) = E^{\text{NI}} + U_2 N_{\text{pair}} + U_3 N_{\text{trimer}} + U_4 N_{\text{tetramer}} + \dots,$$

1st order PT
2nd order PT
3rd order PT

where U_N are effective N-body interactions:

$$U_2 = c_{2,(1)} a_s/a_{\text{ho}} + c_{2,(2)} (a_s/a_{\text{ho}})^2 + c_{2,(3)} (a_s/a_{\text{ho}})^3 + \dots$$

$$+ d_{2,(1,2)} (r_{\text{eff}} a_s^2)/a_{\text{ho}}^3 + \dots$$

$$U_3 = c_{3,(2)} (a_s/a_{\text{ho}})^2 + c_{3,(3)} (a_s/a_{\text{ho}})^3 + \dots$$

$$U_4 = c_{4,(3)} (a_s/a_{\text{ho}})^3 + \dots$$

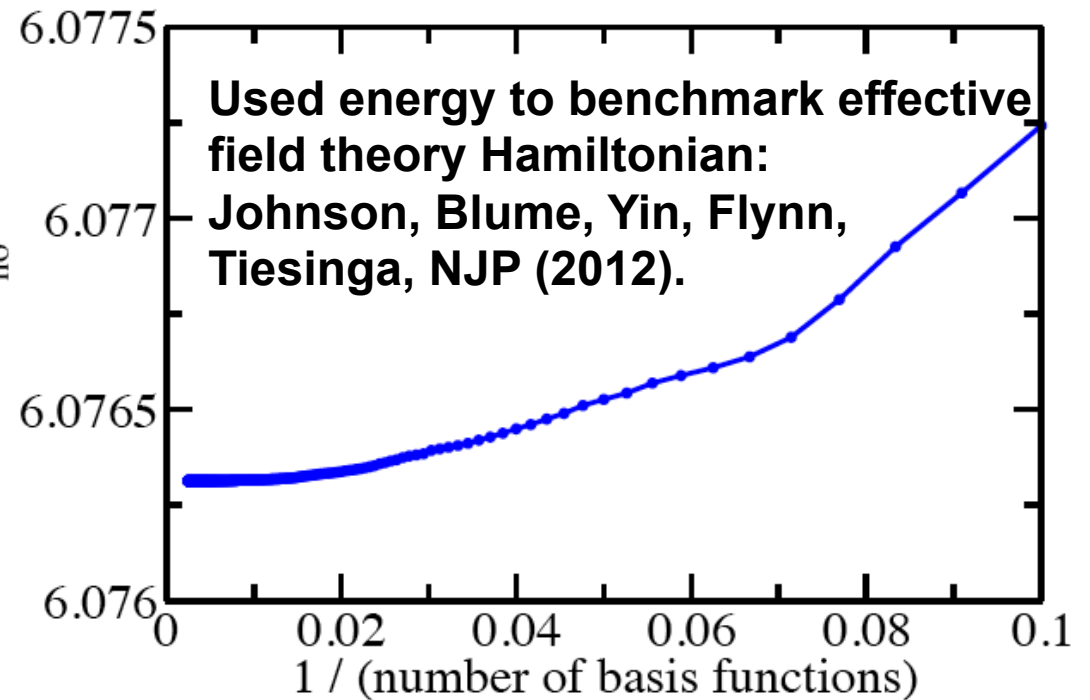
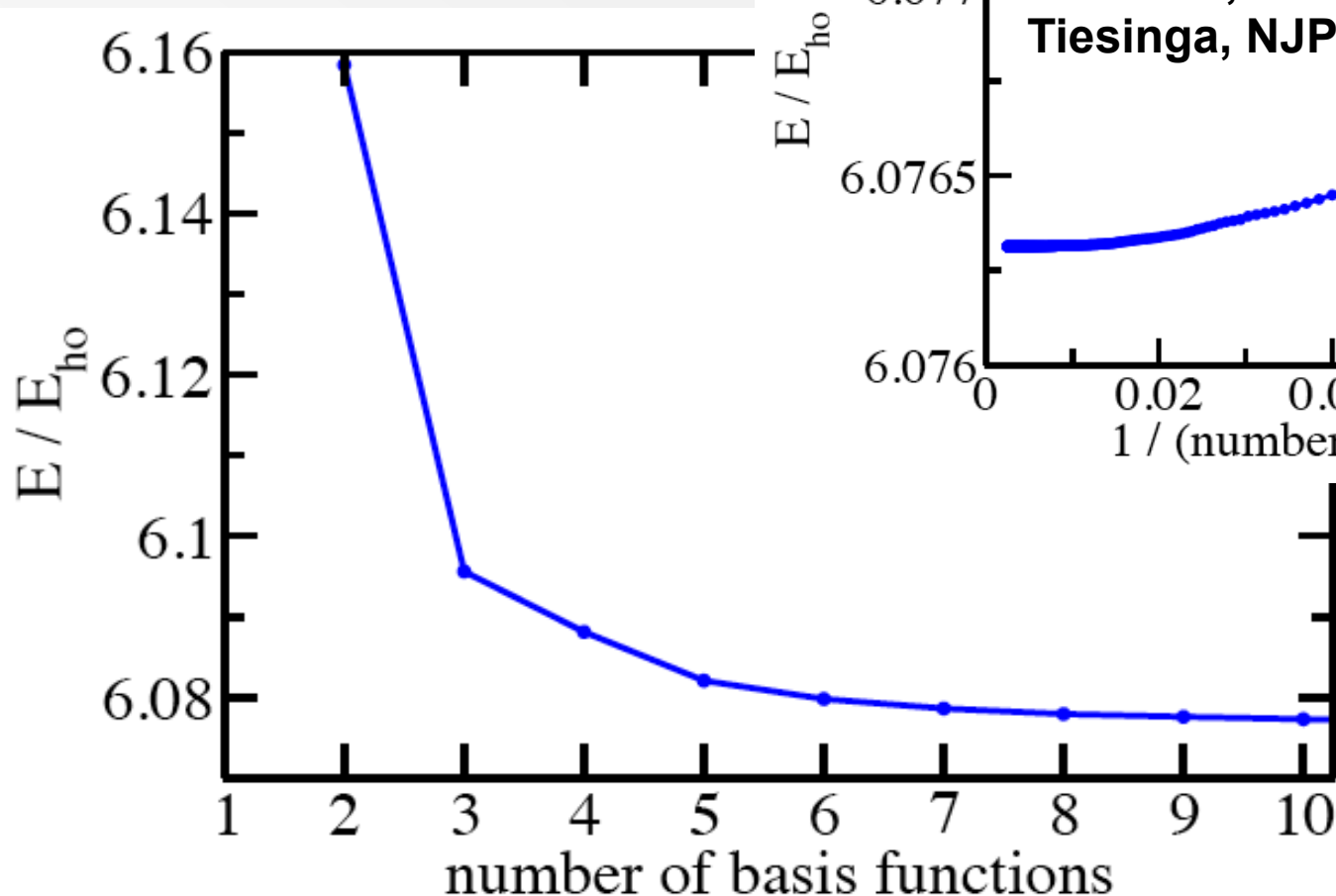
Leading-order effective four-body interaction “competes”
with effective range term: $k \cot(\delta(k)) = -1/a_s + r_{\text{eff}} k^2/2$.

Johnson, Tiesinga, Porto, Williams, New J. Phys. 11, 093022 (2009);

Johnson, Blume, Yin, Flynn, Tiesinga, New J. Phys. 14, 053037 (2012).

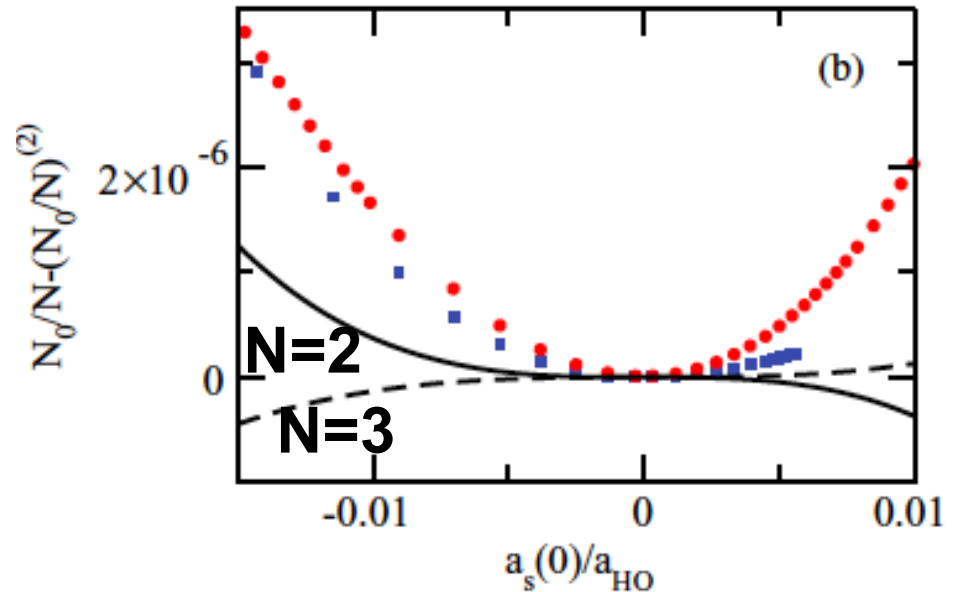
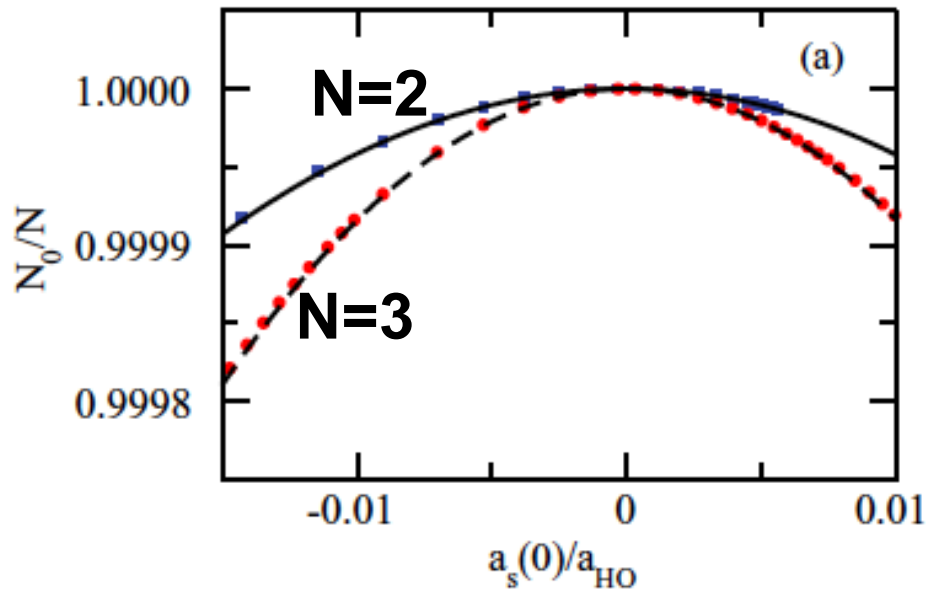
Harmonically Trapped Five-Boson System: Illustration of Convergence

$$r_0 = 0.01 a_{ho}$$
$$a_s = 0.0096 a_{ho}$$



For each N_b , try a few 1000 and keep the best.
 $\Delta E \sim 2 \times 10^{-8} h\nu$.
 $(a_s/a_{ho})^4 \sim 10^{-8}$.

Condensate Fraction N/N_0 of Weakly-Interacting Trapped Bose Gas

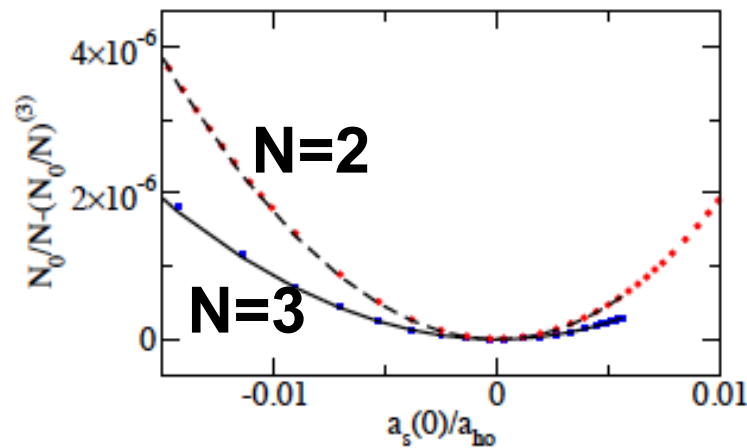


$$\langle \hat{a}_p^\dagger \hat{a}_q \rangle = \frac{\langle \psi_0^{(k)} | \hat{a}_p^\dagger \hat{a}_q | \psi_0^{(k)} \rangle}{\langle \psi_0^{(k)} | \psi_0^{(k)} \rangle}$$

$$N_0/N = 1 - 0.420004(N-1) \left[\frac{a_s(0)}{a_{HO}} \right]^2 + \left[-0.373241(N-1) + 0.439464(N-1)(N-2) \right] \left[\frac{a_s(0)}{a_{HO}} \right]^3 + \dots$$

Condensate Fraction N/N_0 of Weakly-Interacting Trapped Bose Gas

- Expect: N/N_0 is determined by a_s and r_{eff} . But new parameter...



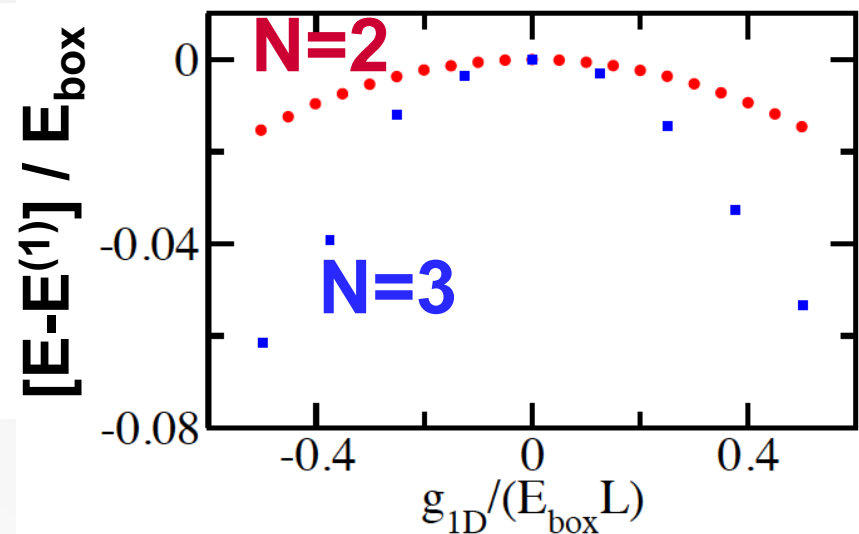
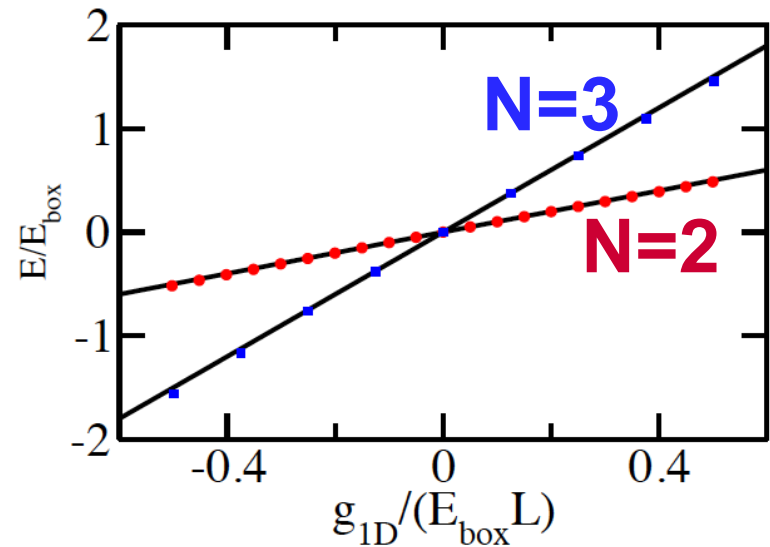
$$\begin{aligned}
 N_0/N = & 1 - 0.420004(N-1) \left[\frac{a_s(0)}{a_{ho}} \right]^2 \\
 & + [-0.373241(N-1) \\
 & + 0.439464(N-1)(N-2)] \left[\frac{a_s(0)}{a_{ho}} \right]^3 \\
 & + [0.406786(N-1) + \gamma_3^{(4)}(N-1)(N-2) \\
 & + \gamma_4^{(4)}(N-1)(N-2)(N-3)] \left[\frac{a_s(0)}{a_{ho}} \right]^4 \\
 & + 2(N-1)\text{Re}(D_0) \\
 & - (3/2) \times 0.420004(N-1) \frac{r_e [a_s(0)]^3}{a_{ho}^4}
 \end{aligned}$$

not needed to describe energy
(two-body parameter) →

- Broader implication:** Two low-energy Hamiltonian that yield the same energy do not necessarily yield the same condensate fraction, momentum distribution,...

Few-Particle System in a Box with Periodic Boundary Conditions

- Application of explicitly correlated Gaussian to periodic systems.
- Few-boson system in a box (so far, 1D).
- Extension to 3D is possible.
- Weakly-interacting 3D Bose gas studied by Savage et al. and Tan, motivated by lattice calculations.



Summary

- **Explicitly correlated Gaussian evaluated at fixed hyperradius R provide promising basis to be used in hyperspherical framework:**
 - Provides access to bound state and scattering continuum ($N=4$ and 5).
- **Construction and testing of effective low-energy Hamiltonian:**
 - Observables besides the energy.
 - Highly accurate benchmark calculations.
- **Few-body systems with periodic boundary conditions:**
 - A potential alternative approach...