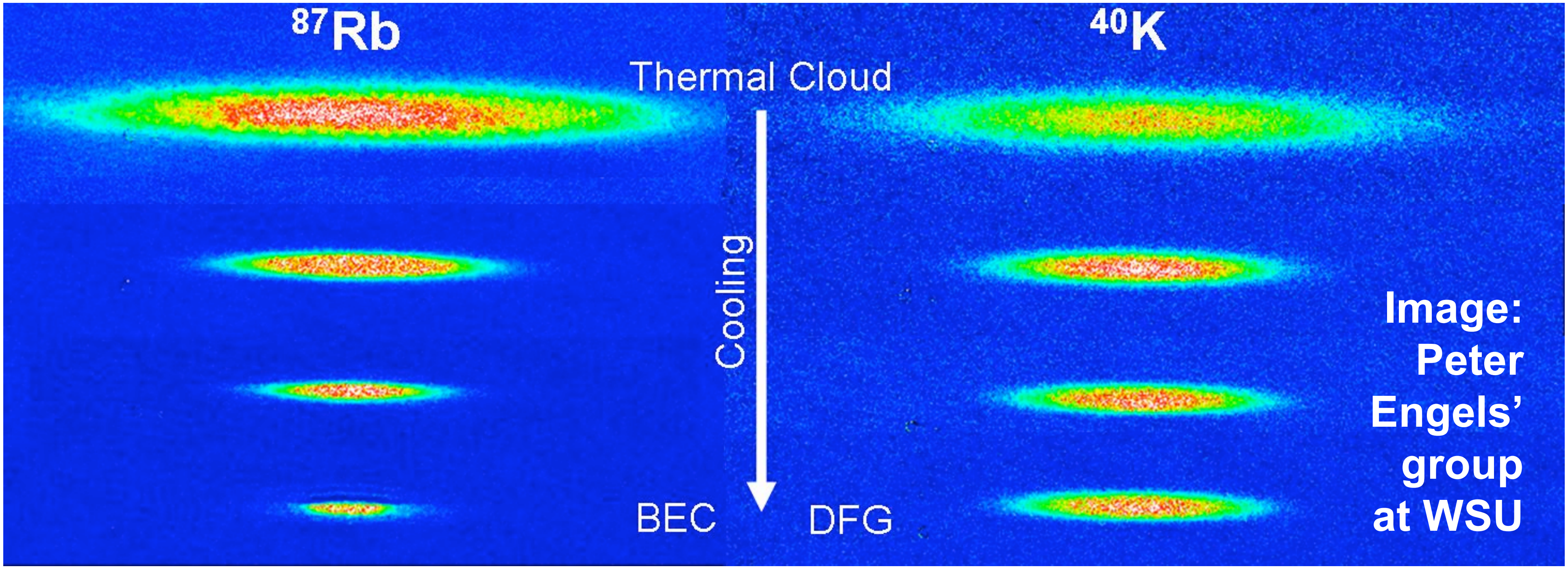

The Trapped Few-Body System

Doerte Blume

Dept. of Physics and Astronomy, Washington State University, Pullman

In collaboration with Kevin Daily and Debraj Rakshit.

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Outline of This Talk

- What is the state of the art of few-body calculations?
- Why do we care about the few-body problem?
- Stochastic variational approach:
  - Basic idea and implementation.
- Examples:
  - Weakly-interacting harmonically trapped few-boson systems.
  - Few-fermion systems with equal masses.
  - Strongly-interacting few-fermion systems with unequal masses.
- Where are we headed?

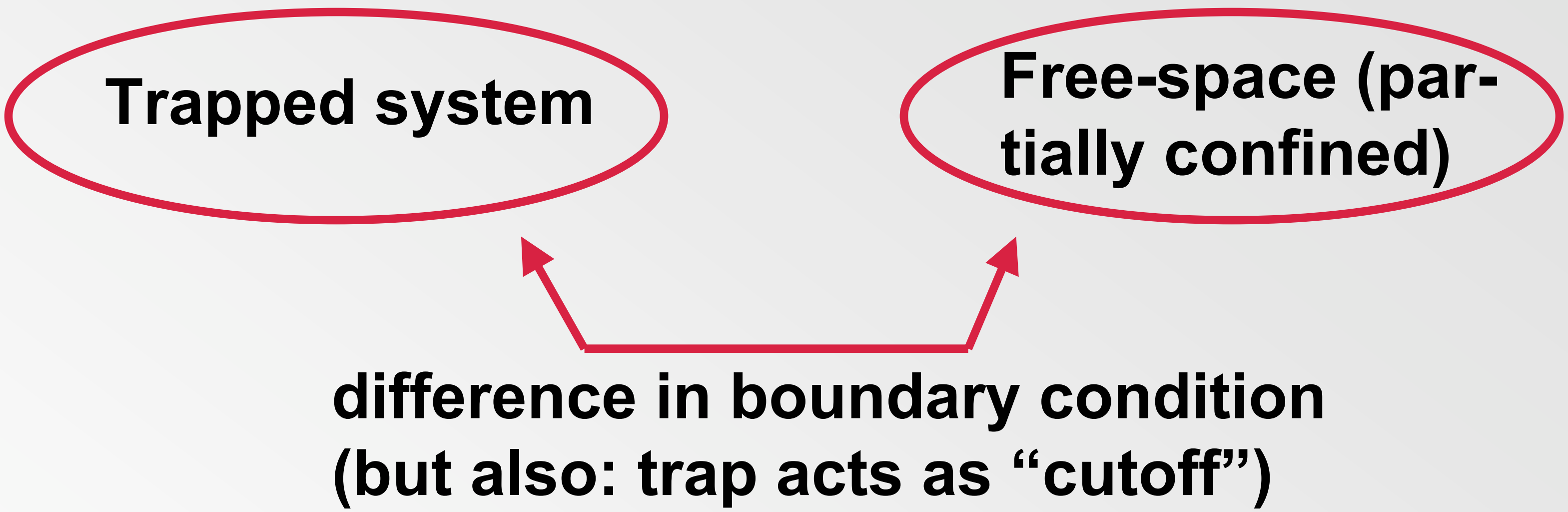
Our Goal:
Characterize Few-Body Systems

- **Motivation:**
  - Bottom-up approach: One step at a time…
  - Often/sometimes: Few determine the properties of many.

- **Experimental realization of few-body systems:**
  - Optical lattices (now “standard” in cold atom labs).
  - Microtraps (beautiful work by Jochim’s group, 1101.2124).

- **Success stories:**
  - Efimov effect (predicted in 1971, first solid evidence in 2006 by Grimm’s group).
  - Metal clusters: How many particles are needed for superconductivity?
  - Helium and para-hydrogen droplets: Microscopic superfluidity.

What is the Status of Few-Body Calculations?



What can be done depends on problem and accuracy wanted…

Scattering calculations are, in general, harder than bound state calculations since scattering calculations require many channels to be treated out to large R.

Scattering calculations: N=3 are standard, N=4 are becoming available.

Techniques for Determining Quantum Mechanics at Zero-Temperature

- Configuration interaction (CI) with effective interactions.
- Effective field theory.
- Grid based techniques (real space and momentum space).
- Various variants of Monte Carlo methods:
  - VMC/DMC/FN-DMC.
  - Lattice based.
- Basis set expansion approach with semi-analytical integrals (stochastic variational approach).

- Parameters:
  - Statistics, mass ratio, trapping geometry, interaction strength, temperature (equivalent to “which part of spectrum is probed”).

Contributions to Many-Body Problem: Few-Body Physics…

- …tells us how many/which parameters are needed in many-body problem: a_s, three-body parameter.
- …explains phenomena that occur in many-body environment: 3- and 4-body recombination.
- …provides input for thermodynamics: High-T virial expansion.
- …provides effective parameters for Bose-Hubbard Hamiltonian.
- …provides input for equation of state of two-component gas on BEC side: atom-dimer and dimer-dimer sc. lengths.
- …provides benchmark results for methods that can treat small and large particle samples: (FN-)DMC, lattice MC, DFT,…

Semi-Stochastic Variational Approach

Non-relativistic low-energy few-body Hamiltonian:

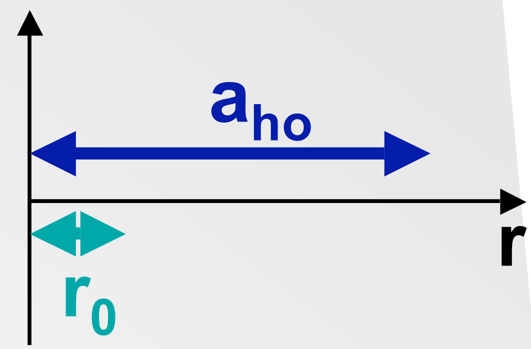
$$H = \Sigma_i (T_i + V_{trap,i}) + \Sigma_{l<j} V_{twobody,ij} \; ; \quad V_{twobody} = V_0 \exp[-(0.5r/r_0)^2]$$

Spherically symmetric.

Sum over unlike spin pairs/all particles.

Short-range and single channel (applicable to broad resonance). ZR for $r_0 \rightarrow 0$.

Idea:



Use basis set expansion approach that involves Gaussian of different widths in interparticle distances.

Large number of non-linear parameters.
Non-orthogonal basis set.

Method first introduced to cold atom community for bosons by Sorensen, Fedorov and Jensen, AIP Conf. Proc. No. 777, p. 12 (2005). See also work on fermions by von Stecher and Greene, PRL 99, 090402 (2007). For details see: Suzuki and Varga (Springer, 1998); von Stecher, Greene, Blume, PRA 77, 043619 (2008).

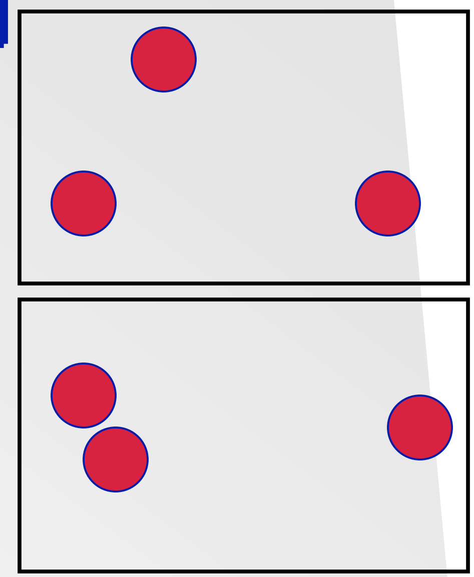
Semi-Stochastic Variational Approach

- Symmetrized basis function with $L^{\Pi}=0^{+}$ symmetry (Gaussian with many non-linear parameters) $\varphi_k = \Sigma_{Np} \exp(-\underline{x}^T A^{(k)} \underline{x}/2)$

Total wave fct.:

$$\Psi = \sum_{k=1}^{N_{\text{basis}}} c_k \mathcal{A}\left[\varphi_k(\vec{x})\right]$$

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



- $\underline{x}$ 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, we have N(N-1)/2 parameters.
- For N=4 and N_{basis}=1000: 6000 variational, non-linear parameters.

Semi-Stochastic Variational Approach

Hamiltonian matrix can be evaluated semi-analytically.

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

Matrix elements for structural properties and momentum distribution can be calculated analytically.

Computational effort increases with N:

- Evaluation of Hamiltonian matrix elements involves diagonalizing (N-1)x(N-1) matrix.
- More degrees of freedom require more basis functions.
- Number of permutations N_p scale non-linearly (N_p=2, 6, 24, 120,… for BB, BBB, BBBB, BBBBB,…).

Outline of Algorithm

- Pick basis function φ_1 and calculate E_1.

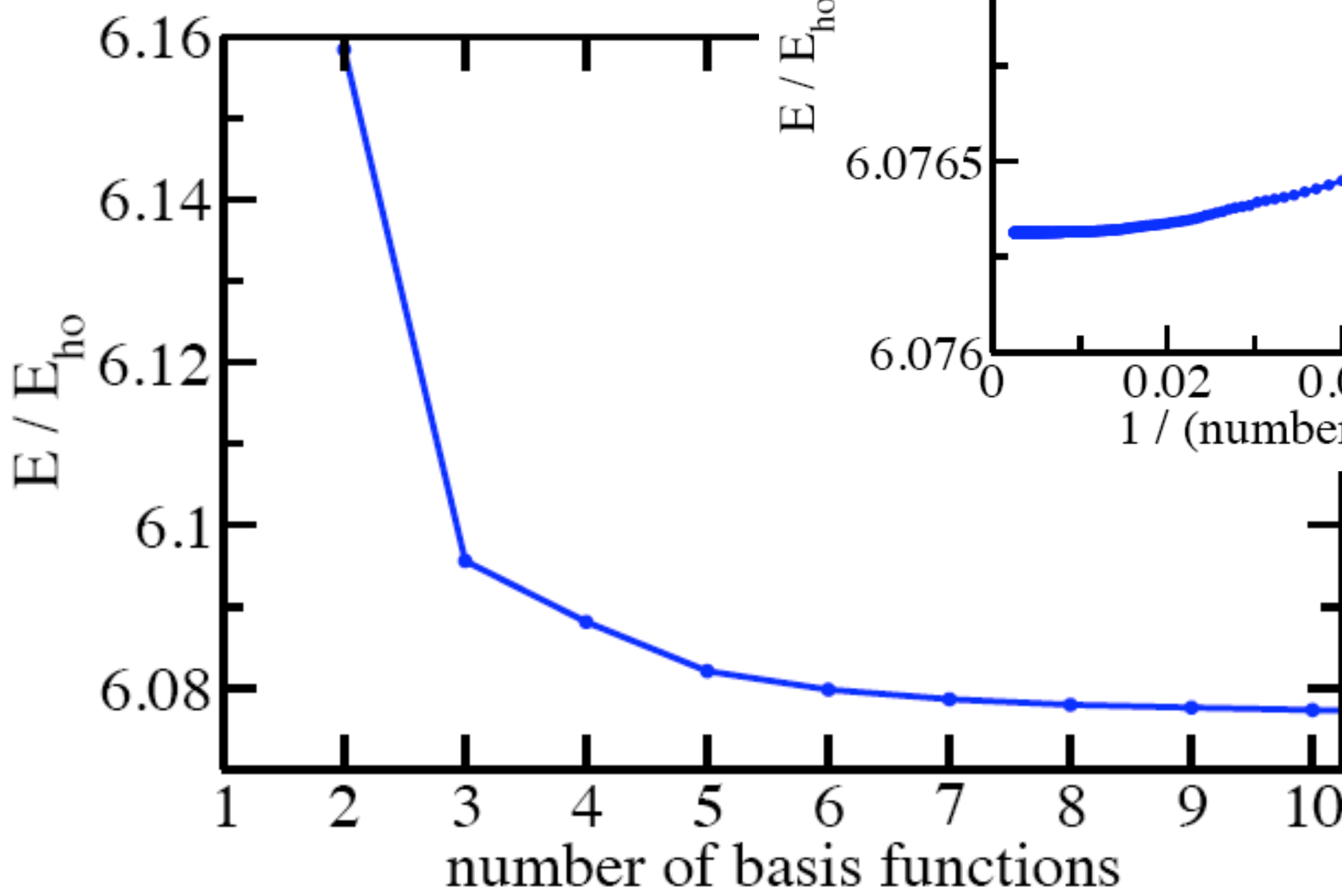
- Goal: Add φ_2.
- Procedure:
  - Pick $\varphi_{2,1},\ldots, \varphi_{2,n}$ (n~1-10000).
  - Calculate $E_{2,1},\ldots,E_{2,n}$ by solving determinantal equation.
  - Determine $\varphi_2=\varphi_{2,j}$ such that $E_2=E_{2,j}\leq E_{2,1},\ldots,E_{2,n}$.
  - Diagonalize Hamiltonian matrix: eigenvalues $\underline{E}_2$ and eigenvectors $\underline{C}_2$.

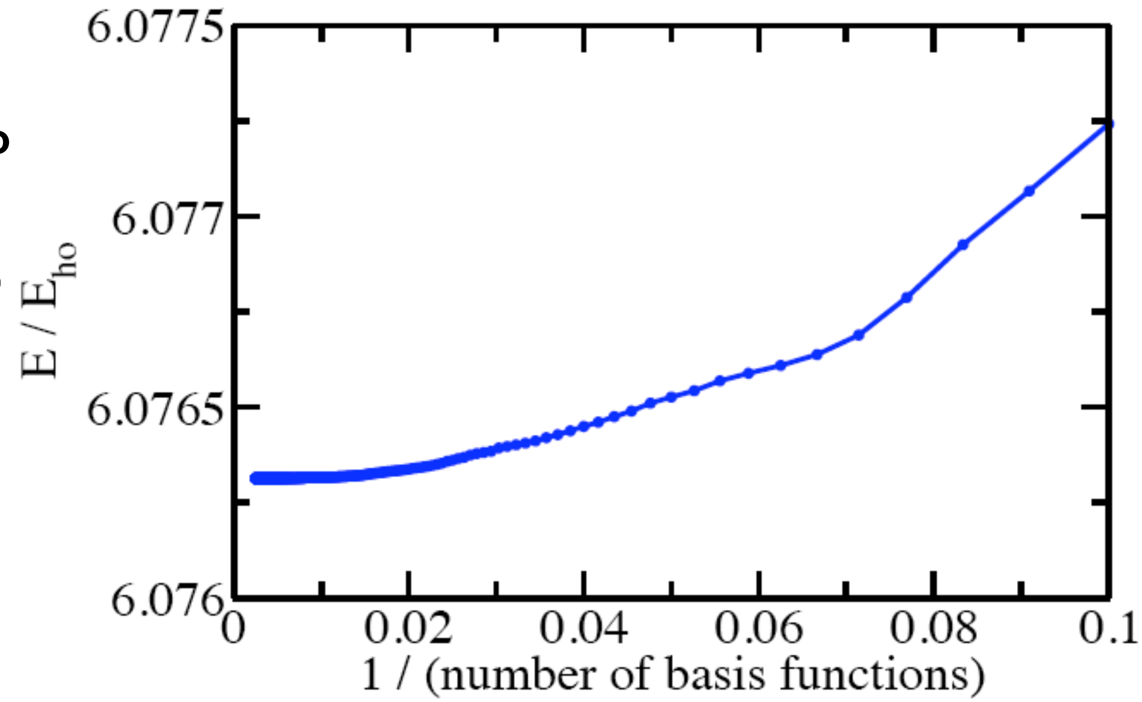
- Goal: Add φ_3.
- Procedure: As above.

- Once basis set is complete, calculate structural properties.

Five-Boson System: Illustration of Convergence

Purely repulsive 2-body potential with $r_0 = 0.01a_{ho}$ and $a_s = 0.0096a_{ho}$





Accuracy we can obtain: $\Delta E \sim 2x10^{-8} h\nu$. $(a_s/a_{ho})^4 \sim 10^{-8}$.

Trapped BBB System with Pairwise δ-Function Interactions ($x=a_s/a_{ho}$)

$E(3) =$

$E_{NI}(3) + [3a_1(2)x + [3a_2(2)+a_2(3)]x^2 + \ldots$

$\sqrt{2/\pi}$ $2[1-\ln(2)]/\pi>0$ $-0.8557583\ldots$

$=-0.2697125\ldots$

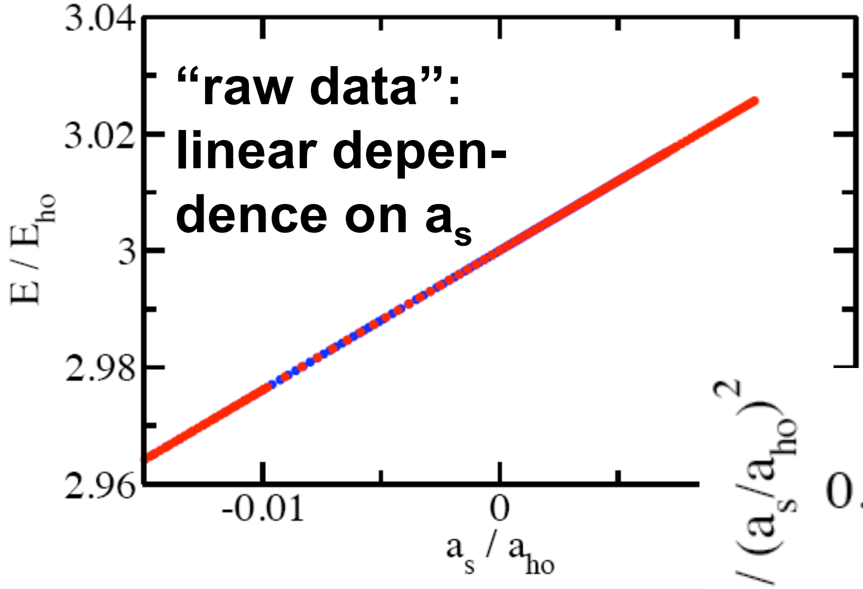
See also Jonsell et al., PRL (2002).

[Johnson, Tiesinga, et al., NJP 11, 093022 (2009): Effective field theory approach (regularization)]
$a_2(3)$ term is interpreted as leading order
Effective *attractive* three-body interaction.

Higher order terms should additionally depend on three-body parameter.

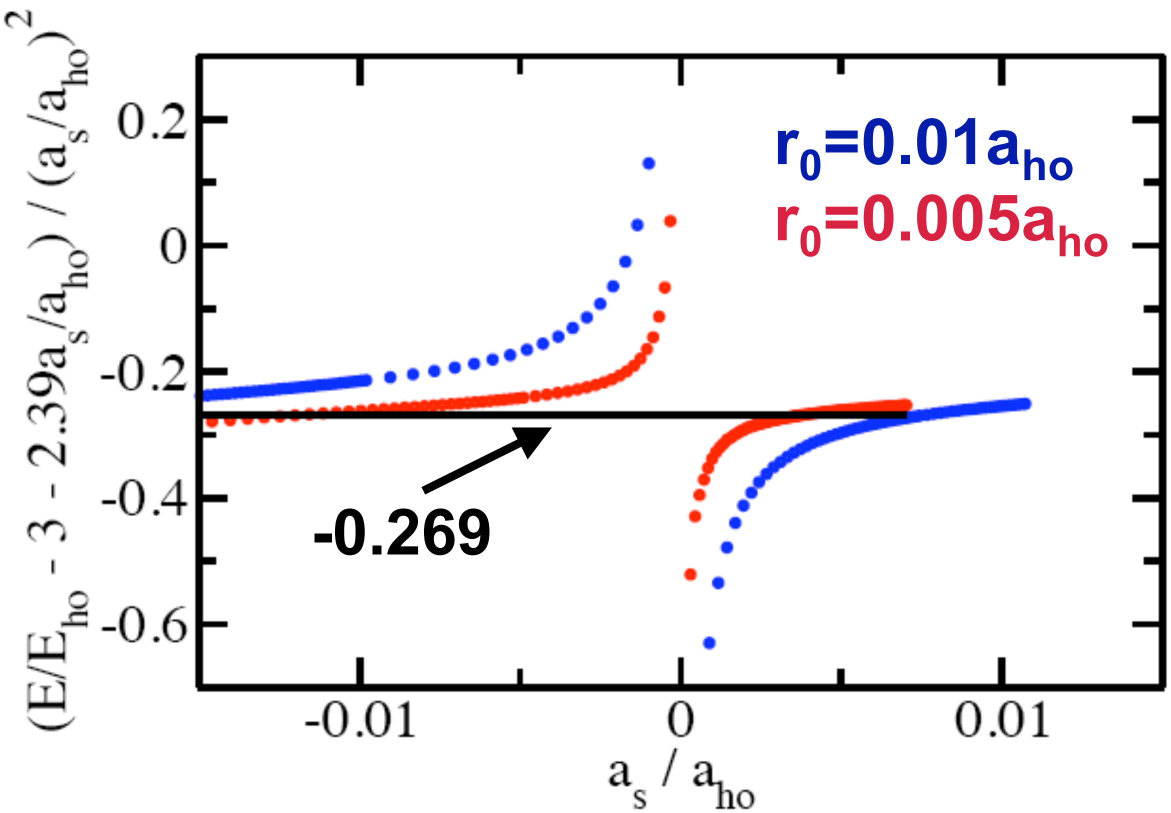
Last summer, Eite Tiesinga asked if their analytical prediction can be checked numerically…

Analysis of BBB Energies for Finite-Range Gaussian Interaction Potential

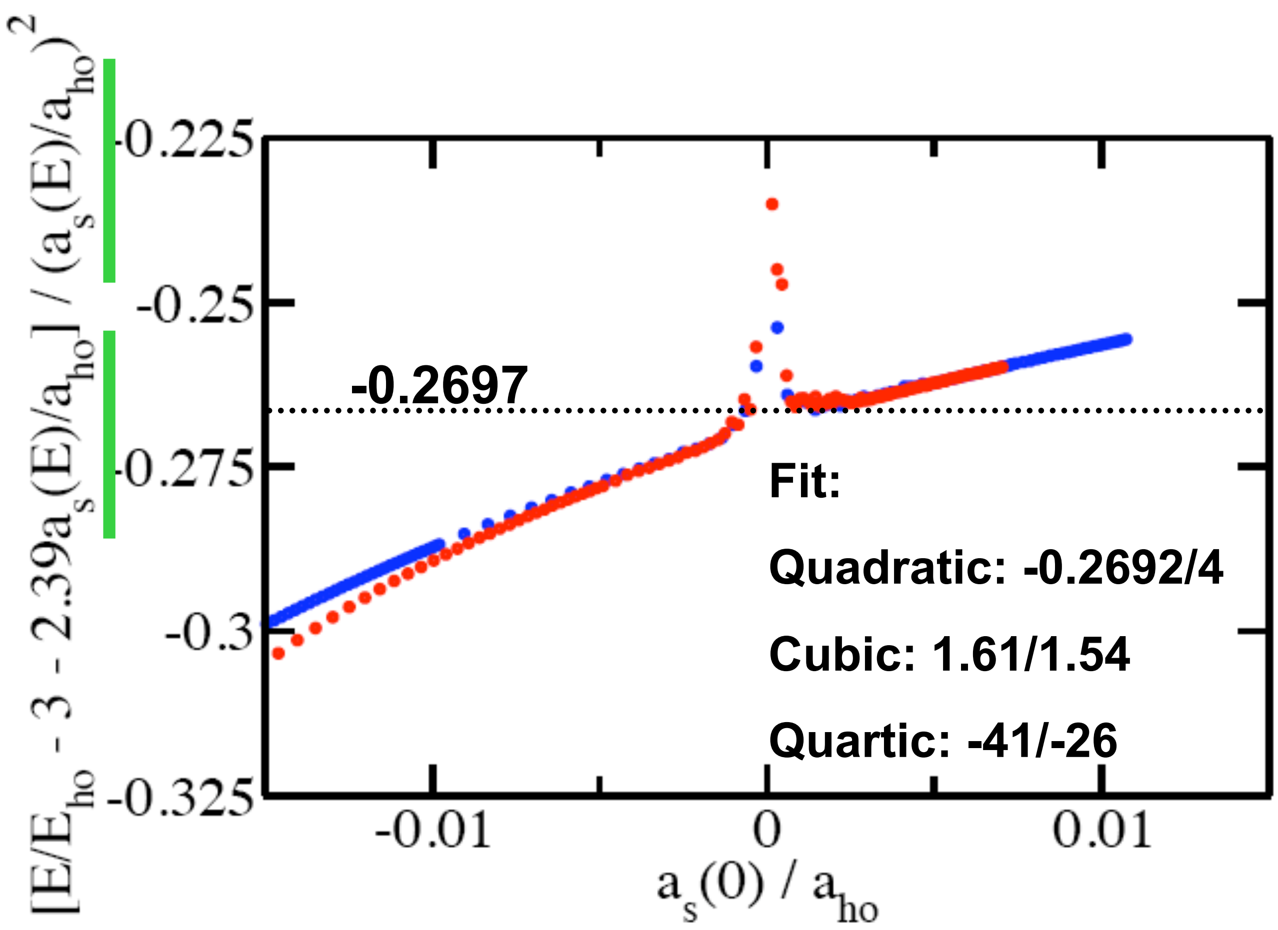


Prediction:
E(3) =
$E_{NI}(3)$ + [2.394x - 0.269x^2 +...]hν

Expectation:
Series expansion works best for small a_s, not large a_s.
But: We do have FR dependence...



BBB: Accounting for FR Effects through Energy-Dep. Scattering Length



- E-dependence leads to collapse to single curve (almost).
- Analytical prediction fulfilled: Effectively attractive three-body interaction.
- Fit: $|a_s|<0.01a_{ho}$.
- Next steps:
  - Include r_{eff}.
  - Go to larger N.

Energy-dependent scattering length: Blume and Greene, PRA 65, 043613 (2002); Bolda et al., PRA 66, 013403 (2002).

Two-Component Fermi Gas under Spherically Symmetric Confinement

- (1,1) system: “Gound state” (I.e., energetically lowest lying low-energy state) has 0^+ symmetry throughout entire “crossover”/for all a_s.
- (2,1) system: Ground state has 1^- symmetry for $a_s=0^-$ and 0^+ symmetry for $a_s=0^+$.
- (2,2) system: Ground state has 0^+ symmetry for all a_s.
- (3,1) system: Ground state has 1^+ symmetry for $a_s=0^-$.
- (4,1) system: Ground state has 0^- symmetry for $a_s=0^-$.

Natural parity: $\Pi=(-1)^L$. Unnatural parity: $\Pi=(-1)^{L+1}$.

Universal Relations for ZR Interactions throughout Crossover due to Tan

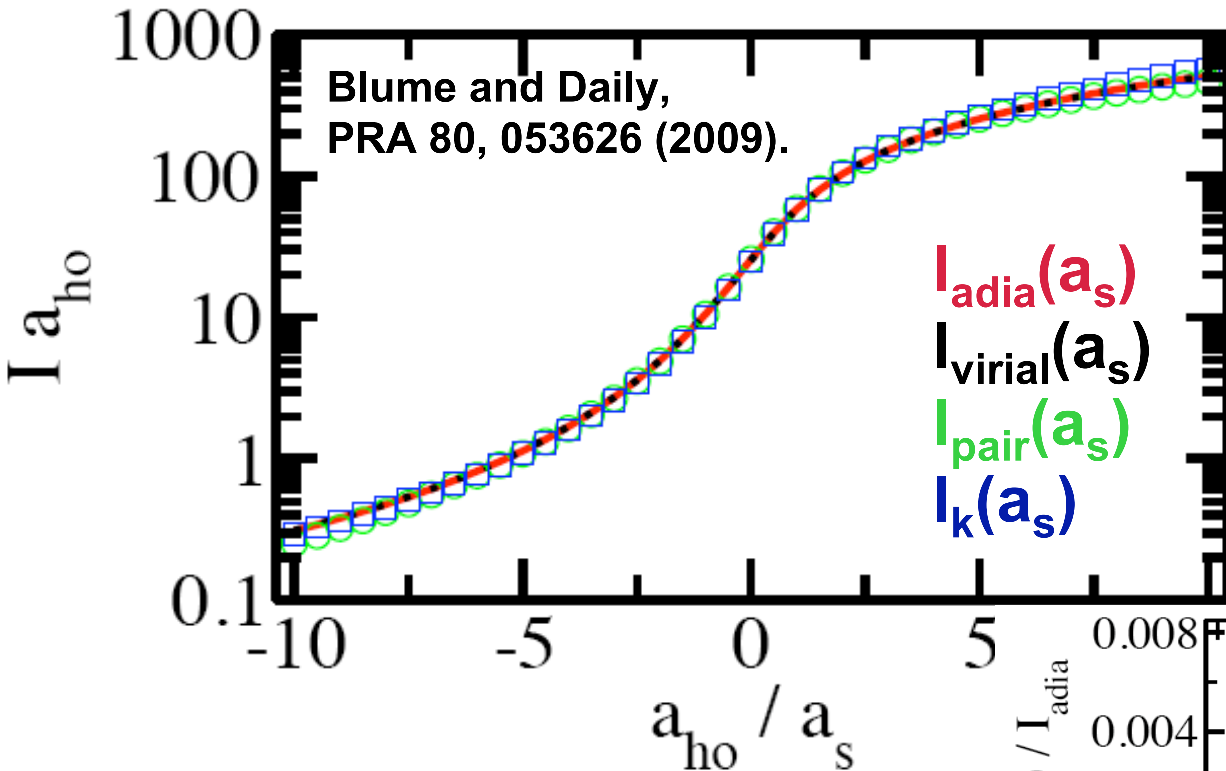
Quantitative relation between distinctly different quantities such as change of energy, trap energy, pair distribution function and momentum distribution, inelastic two-body loss rate,...

"Integrated contact intensity" $I(a_s)$ defined through momentum relation [Tan, Annals of Physics ('08)]: $I_k(a_s) = \lim_{K\to\infty} \pi^2 K N_{atom}(k>K)$.

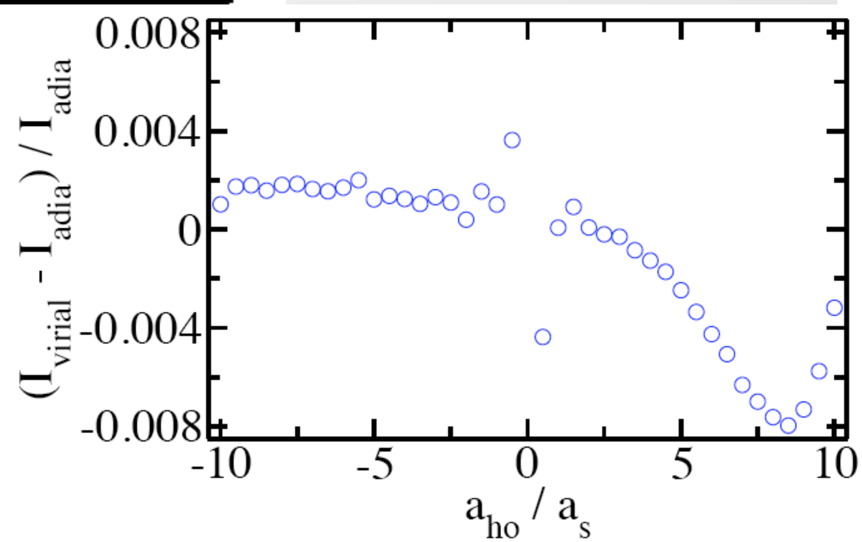
- It then follows:
  - Adiabatic relation: $\partial E(a_s,0)/\partial a_s = h^2/(16\pi^3 m a_s^2)\, I_{adia}(a_s)$.
  - Virial theorem: $E(a_s,0) = 2 \langle V_{trap}(a_s,0)\rangle - h^2/(32\pi^3 m a_s)\, I_{virial}(a_s)$.
  - Pair relation: $I_{pair}(a_s) = \lim_{s\to 0} 4\pi\, N_{pair}(r<s) / s$.

As a check, use all four relations to obtain $I(a_s)$ and compare.

Integrated Contact for Energetically Lowest Gas-Like State of (2,2) System

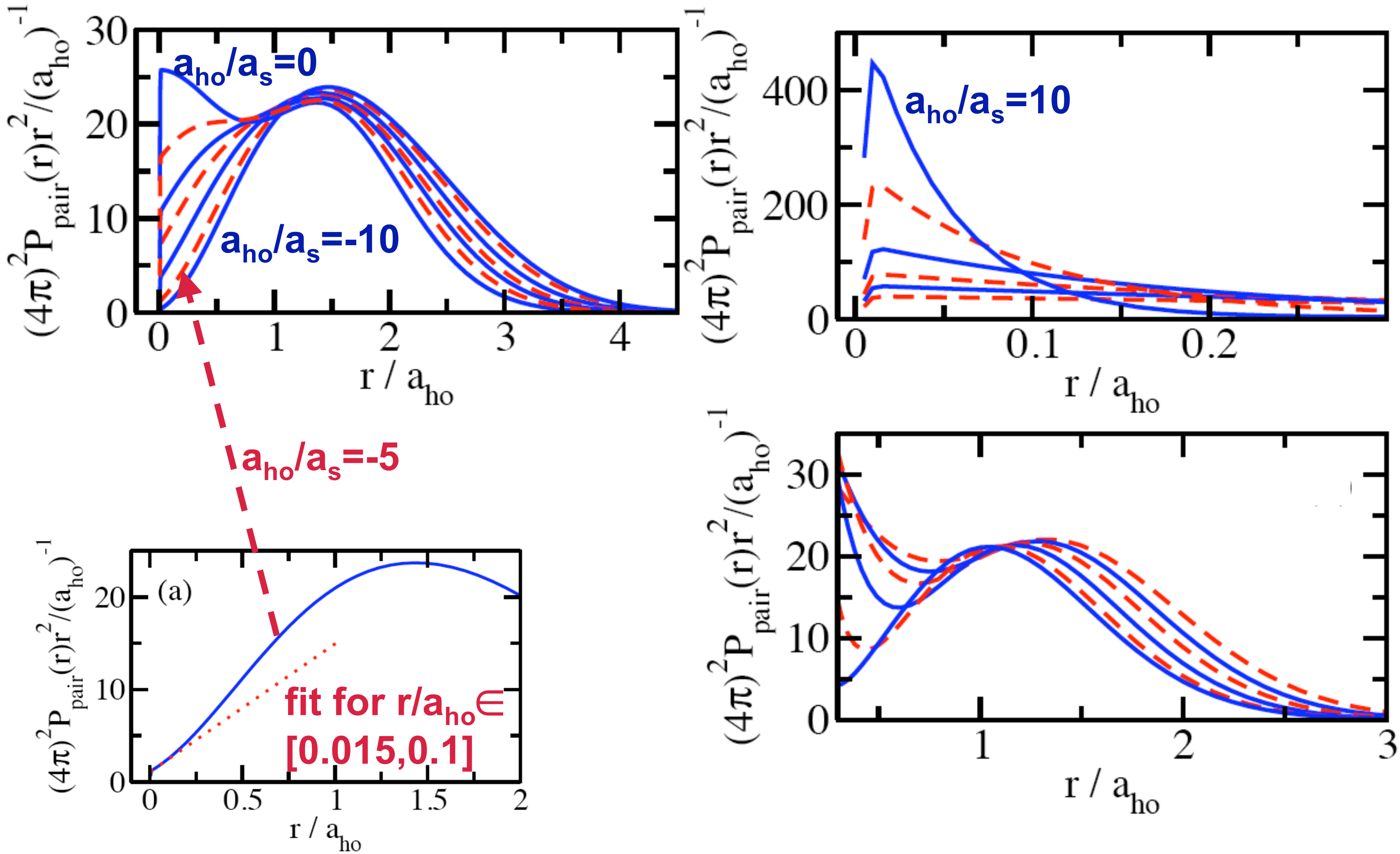


Recent experiments:
Hu et al., arXiv:1001.3200.
Stewart et al., PRL 2010.
Earlier work:
Partridge et al., PRL 95, 020404 (2005). Re-interpretation by Castin and coworkers.



$I(a_s)$ changes by about three orders of magnitude throughout crossover.
Very good agreement among the four “different” $I(a_s)$.

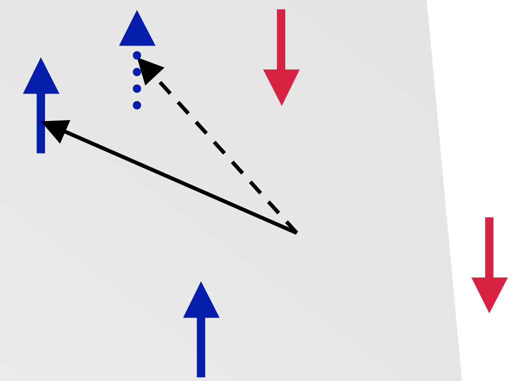
Pair Distribution Functions for N=4 ($r_0=0.005a_{ho}$)



Momentum Distribution from One-Body Density Matrix

- **One-body density matrix:**
  $\rho(\underline{r}',\underline{r}) = \int\ldots\int\Psi^*(\underline{r}',\underline{r}_2,\ldots,\underline{r}_N)\Psi(\underline{r},\underline{r}_2,\ldots,\underline{r}_N)d\underline{r}_2\ldots d\underline{r}_N$

- **Alternatively:**
  $\rho(\underline{r}',\underline{r}) = \langle\psi^+(\underline{r}')\psi(\underline{r})\rangle$, **where** $\psi^+(\underline{r}')$ **and** $\psi(\underline{r})$ **are field operators that create and destroy a particle at position** $\underline{r}$ **and** $\underline{r}'$**.**



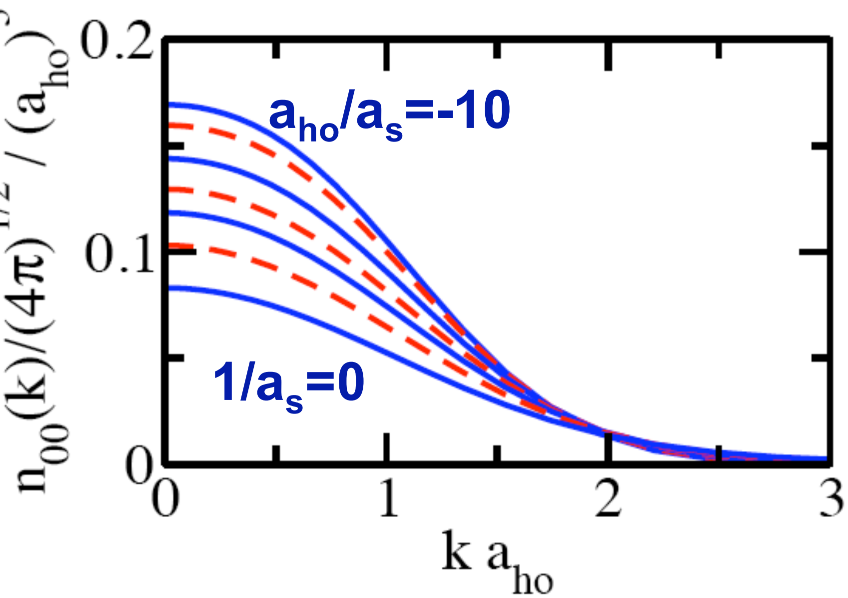
- **It follows:** $n(\underline{k}) = (2\pi)^{-3}\iint \exp[i\underline{k}\cdot(\underline{r}-\underline{r}')]\rho(\underline{r}',\underline{r})\, d\underline{r}d\underline{r}'$.

- **Partial wave decomposition:**
  $n(\underline{k}) = \Sigma_{lm}\, n_l(k)\, Y_{lm}(\theta_k,\varphi_k)$.

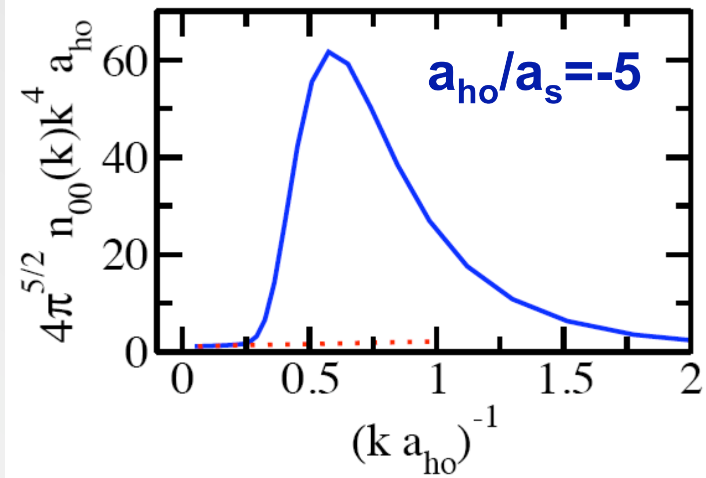
- **Then:** $\int n(\underline{k})d\Omega_k = (4\pi)^{1/2}\, n_0(k)$

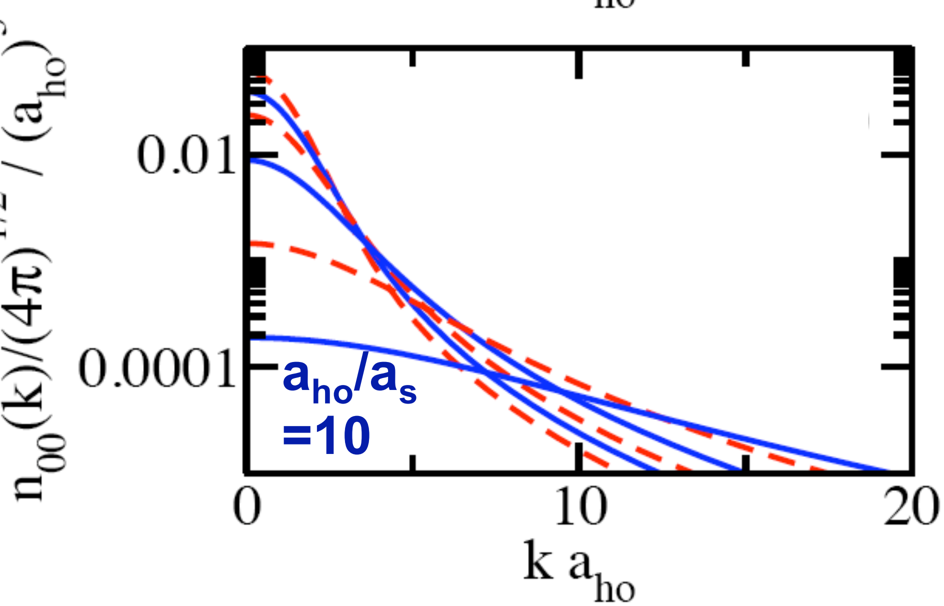
Shown on next slide for N=4

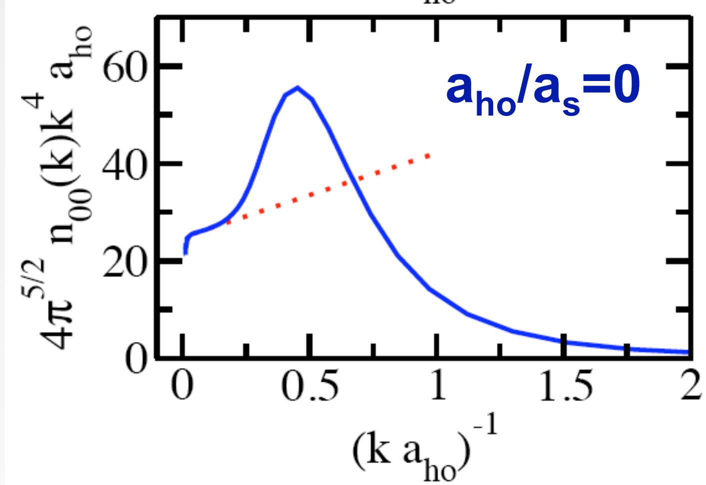
Lowest Partial Wave Projection of Momentum Distribution: (2,2) System



$I_{k,\uparrow}(a_s) = \lim_{1/k\to 0} 4\pi^{5/2} n_{00,\uparrow}(k) k^4$







Condensate Fraction on BEC Side

Astrakharchik et al., PRL 230405 (2005).

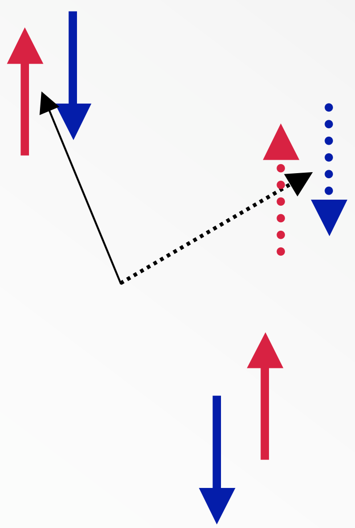
- Number of pairs: $<\Psi^{+}(\underline{r}_1')\Psi^{+}(\underline{r}_2')\Psi(\underline{r}_1)\Psi(\underline{r}_2)>$

up-down position vectors

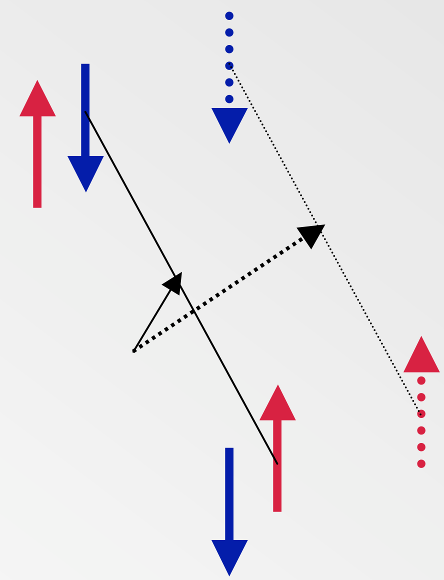
- Pair density matrix:

$\rho(\underline{R}',\underline{R}) = \int\ldots\int\Psi^{*}(\underline{R}',\underline{r}_{12},\ldots,\underline{r}_N)\Psi(\underline{R},\underline{r}_{12},\ldots,\underline{r}_N)d\underline{r}_{12}d_3\ldots d\underline{r}_N$

CM of up-down pair



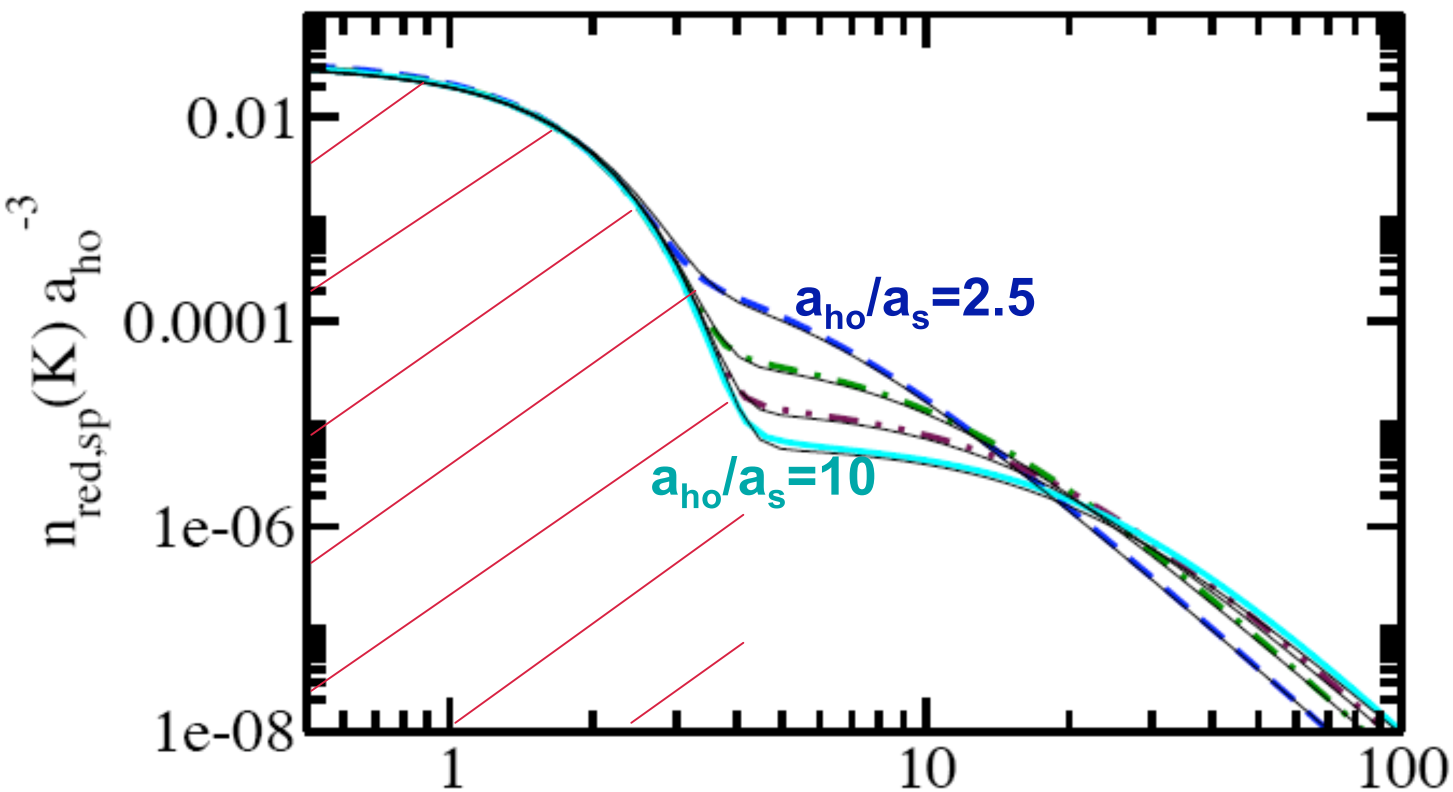
Pair remains "in tact": "good CM vector".

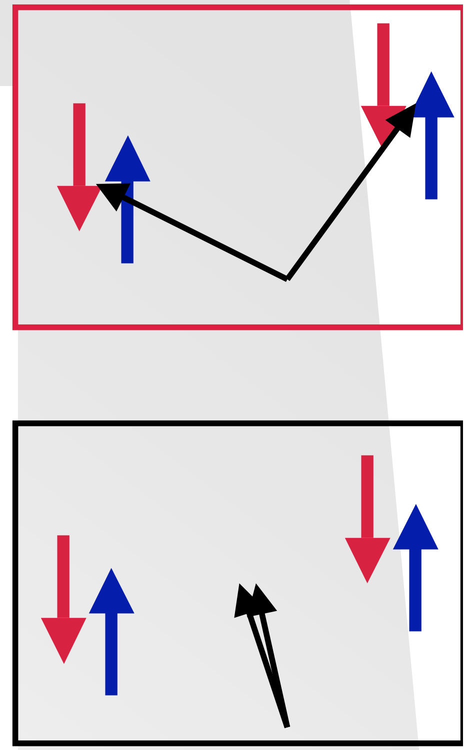


Pair "destroyed": "bad CM vector".

Molecular Condensate Fraction and Momentum Distribution: (2,2) System

Color: numerics; thin black line: analytical.

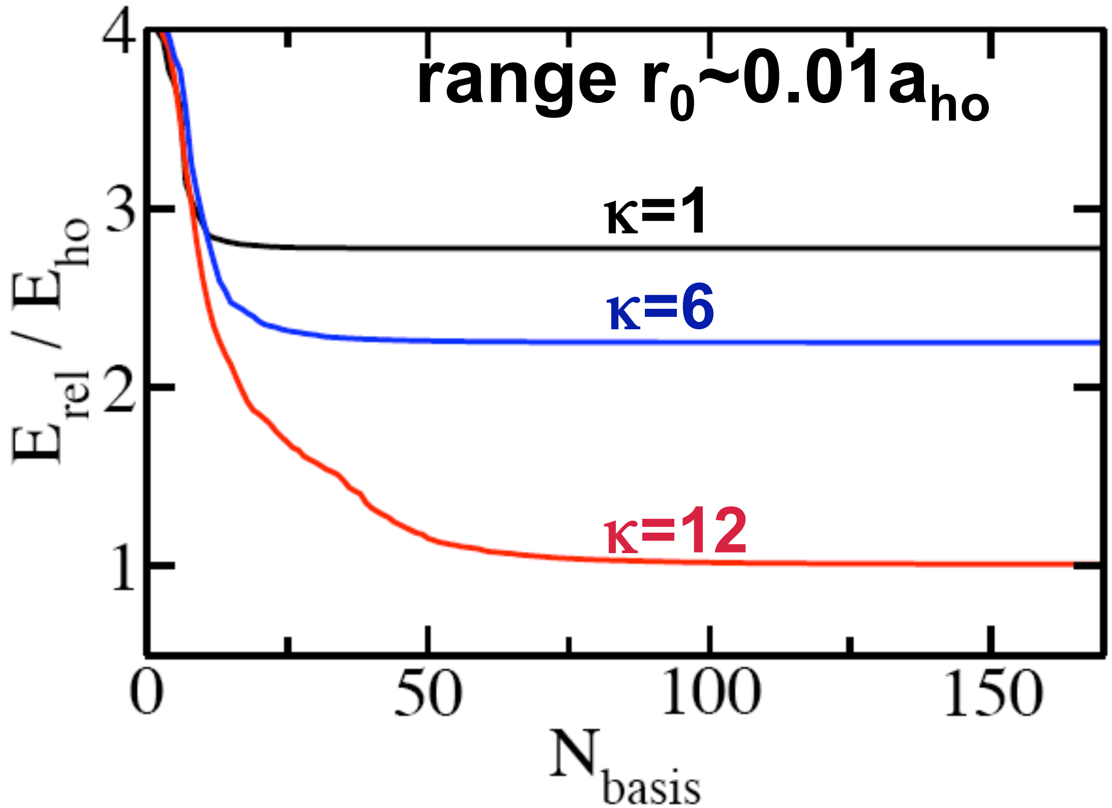




Condensation of pairs!

Blume and Daily, C. R. Physique 12, 86 (2011).

Convergence for Different Mass Ratios: FFX System with 1^- Symmetry ($1/a_s=0$)



Typically between 120 and 650 basis functions.
Each basis function selected from about 1000.

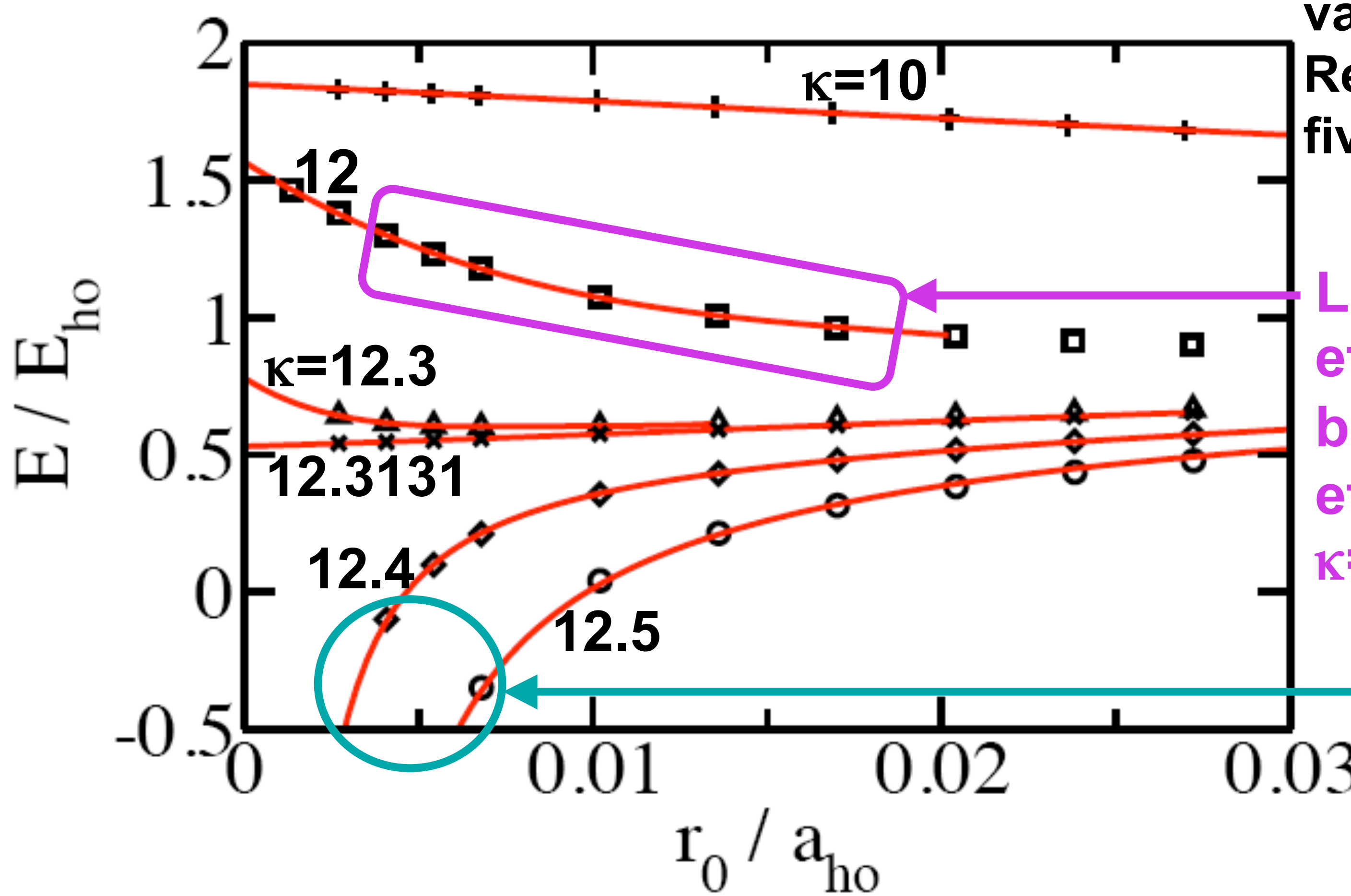
$$\vec{v}^{(k)} = \sum_{j=1}^{N-1} u_j^{(k)} \vec{\rho}_j$$

Angular momentum distributed among all Jacobi vectors.

$$\varphi_k(\vec{x}) = |\vec{v}^{(k)}|^L Y_{L0}(\hat{v}^{(k)}) \exp\left[-\sum_{i<j}^{N}\left(\frac{r_{ij}}{\sqrt{2}d_{ij}^{(k)}}\right)^2\right]$$

Finite Range Effects: Trapped FFX System with $L^{\Pi}=1^{-}$ at Unitarity

Symbols: Stochastic variational energies. Red lines: Four to five parameter fits.

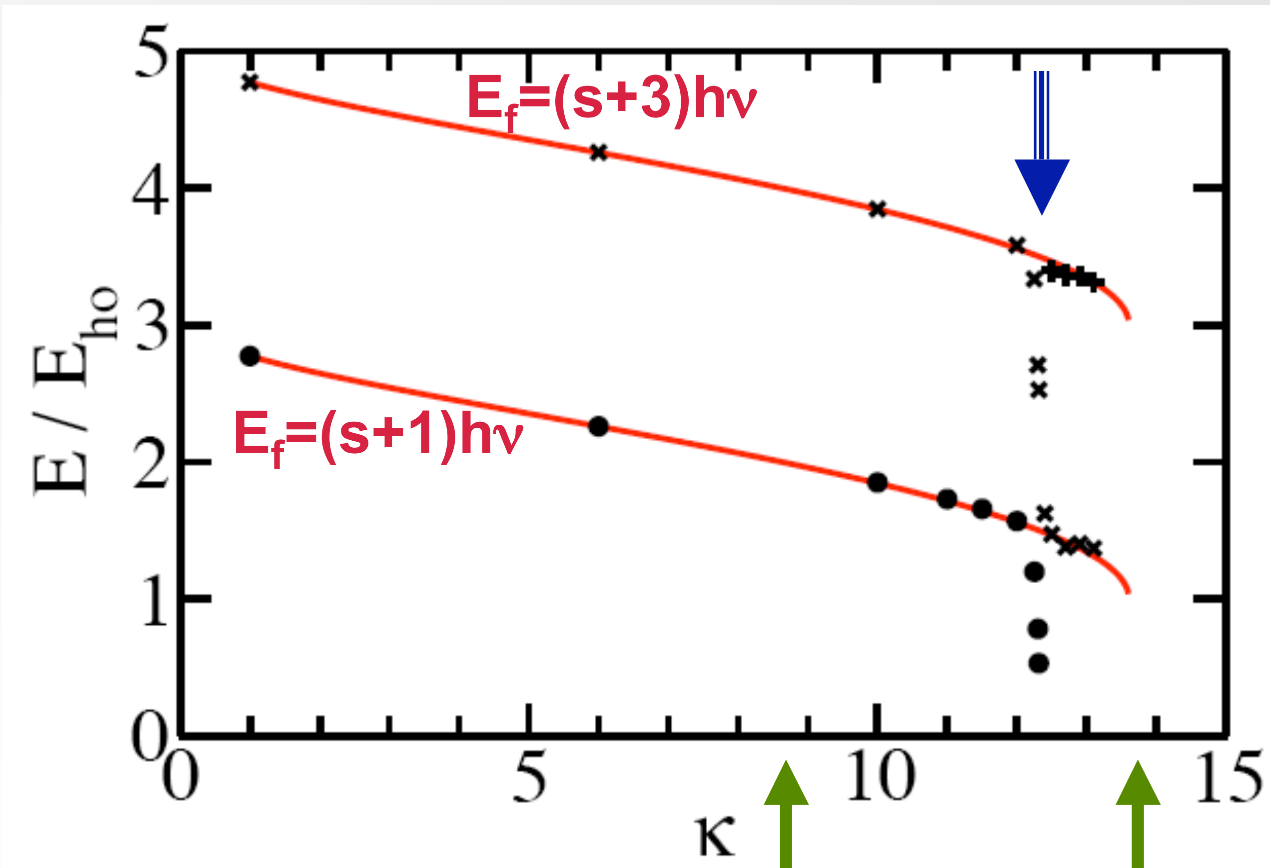


Large FR effects for κ=12; but small FR effects for κ=12.313!

Bound states! Diverge as r_0^{-2}.

Calculations employ a purely attractive Gaussian potential between FX pairs with range r_0. See Blume and Daily, PRL 105, 170403; PRA 82, 063612.

Energies for Trapped FFX System with $L^{\Pi}=1^{-}$ at Unitarity



κ=8.619 κ=13.606

Black symbols: Stochastic variational energies for finite-range Gaussian extra-polated to $r_0=0$.

Away from κ≈12.313 (or s≈1/2), extra-polated FR energies agree well with E_f.

E_f: energy within universal theory.

We interpret the dropping of the 3-body energies around κ≈12.313 as a "3-body (atom+atom+atom) resonance"!

Hyperradial Solution for "Generic" Effective $1/R^2$ Potential

Radial SE [$s=l+1/2$: $s^2-1/4=l(l+1)$]:

$$\left(\frac{-\hbar^2}{2\mu}\frac{\partial^2}{\partial R^2}+V_{\nu,\text{eff}}(R)\right)F_{\nu q}(R)=E_{\nu q}F_{\nu q}(R)$$

$$V_{\nu,\text{eff}}(R)=\frac{\hbar^2(s_\nu^2-1/4)}{2\mu R^2}+\frac{1}{2}\mu\omega^2R^2$$

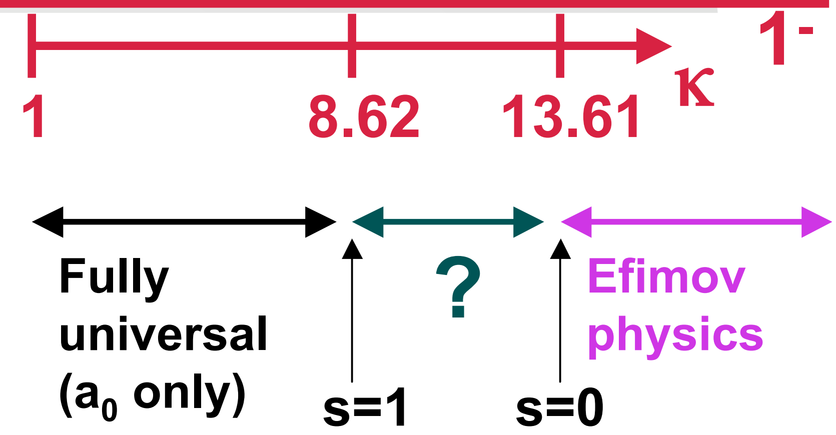
Write $E=(2q+s_\nu+1)h\nu$.

Two linearly indep. solutions ($s_\nu>0$):

$f(R)\rightarrow R^{s+1/2}$ as $R\rightarrow 0$.

$g(R)\rightarrow R^{-s+1/2}$ as $R\rightarrow 0$.

For $s_\nu>1$, g not normalizable. Eliminate.

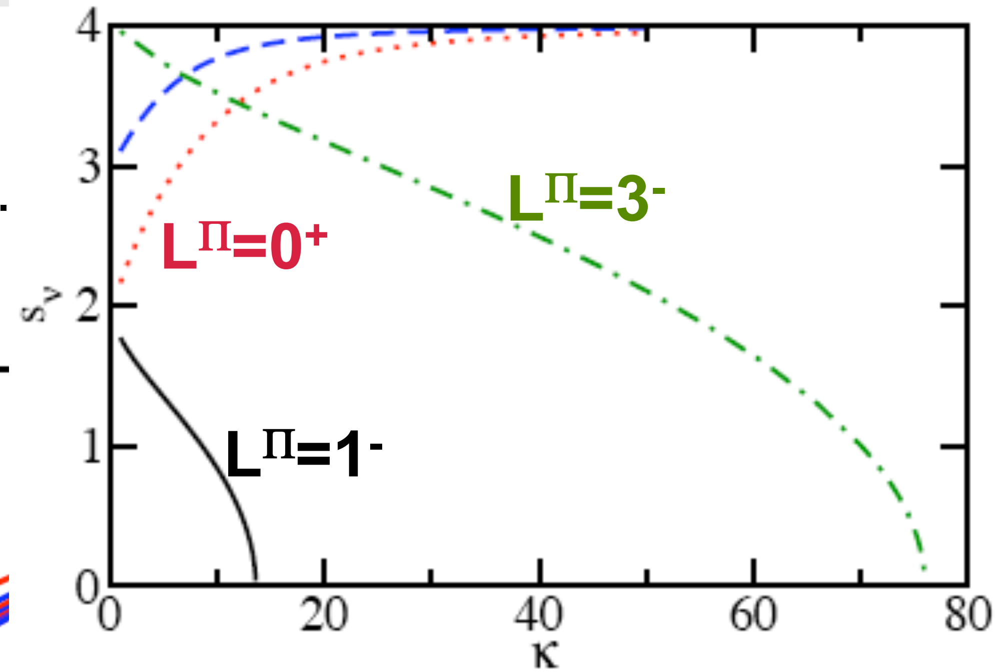


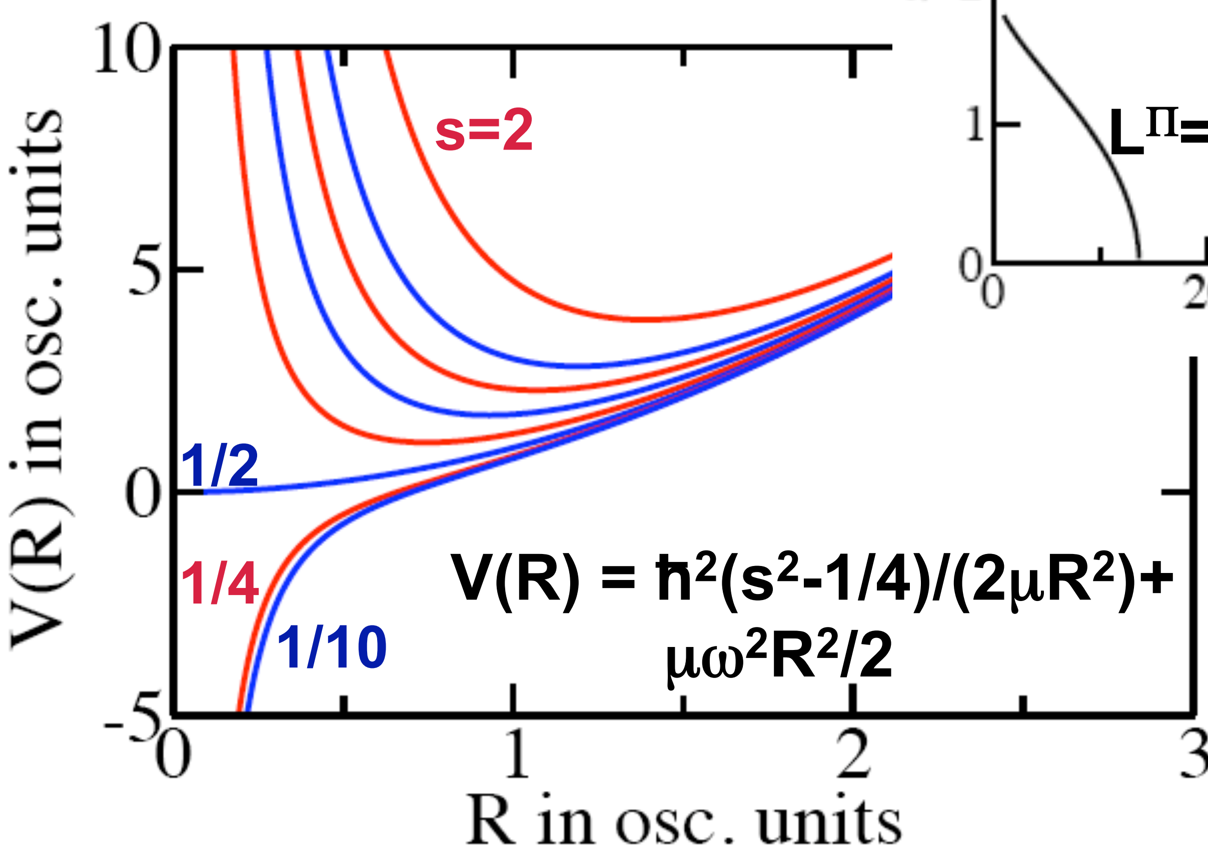
Efimov, Yad. Fiz. 12, 1080 (1970); Nucl. Phys. A 210, 157 (1973). D'Incao and Esry, PRA 73, 030702 (2006) and follow-up work. Petrov, PRA 67, 010703(R) (2003). Nishida, Tan, Son, PRL 100, 090405 (2008). Werner and Castin, PRA 74, 053604 (2006). Kartavtsev and Malykh, JPB 40, 1429 (2007).

s_ν real, $s_\nu>1$	$q=0,1,\cdots$
➡ s_ν real, $1>s_\nu>0$	➡ q depends on hyperradial BC
s_ν imaginary	q depends on hyperradial BC (Efimov physics)

Hyperradial Potentials for FFX System with Infinitely Large Scattering Length

s_0 obtained using formalism developed in Ph.D. thesis of Seth Rittenhouse, CU Boulder. See PRA 82, 022706.





$$V(R) = \hbar^2(s^2-1/4)/(2\mu R^2)+ \mu\omega^2R^2/2$$

Effective three-body interaction:
$F(R) \sim f(R) - \tan[\delta_{3b}(k)]g(R)$.
3-body resonance= phase shift of $\pi/2$.

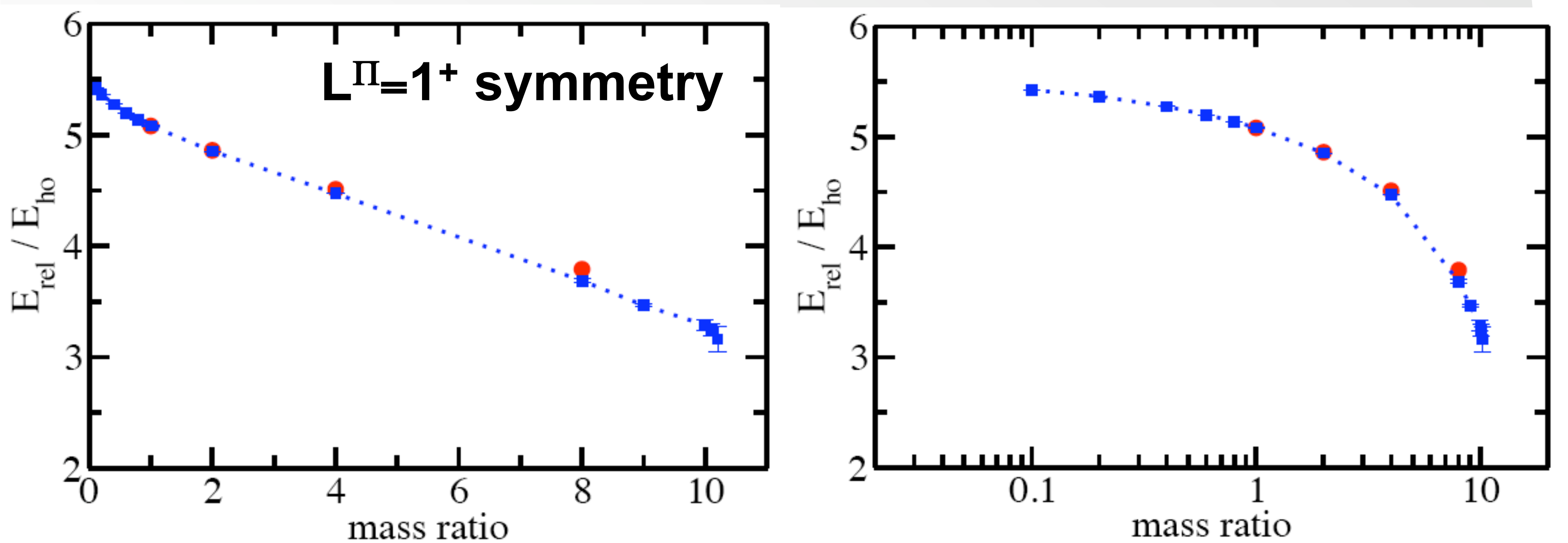
What about FFFX System at Unitarity?

$$\varphi_k(\vec{x}) = \exp\left[-\sum_{i<j}^{N}\left(\frac{r_{ij}}{\sqrt{2}d_{ij}^{(k)}}\right)^2 + (\vec{s}^{(k)})^T\vec{x}\right]$$

No good angular momentum or parity.

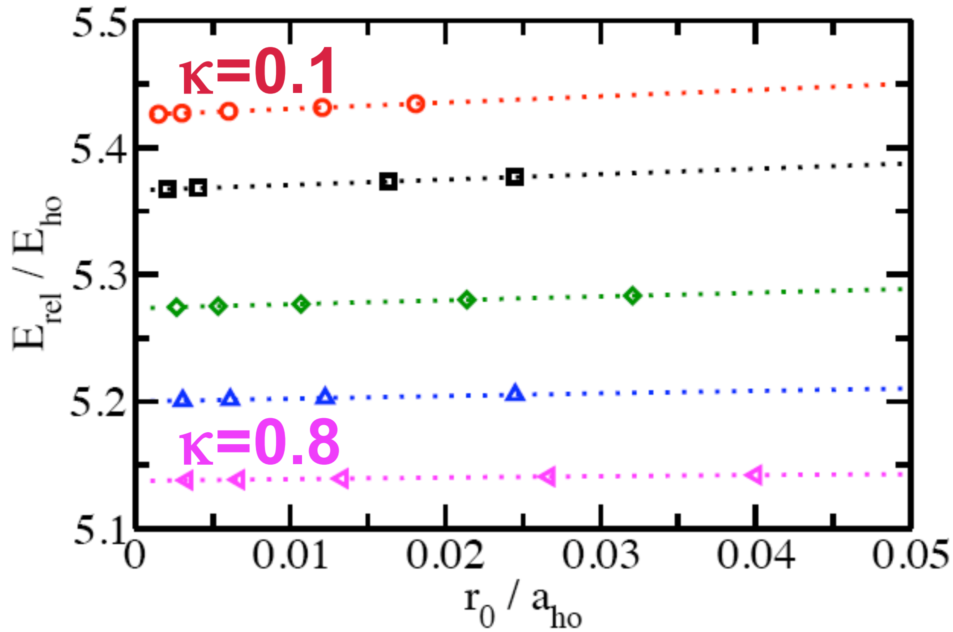
$$\varphi_k(\vec{x}) = \left[Y_{10}(\hat{v}_1^{(k)}) \times Y_{10}(\hat{v}_2^{(k)})\right]_{10} \exp\left[-\sum_{i<j}^{N}\left(\frac{r_{ij}}{\sqrt{2}d_{ij}^{(k)}}\right)^2\right]$$

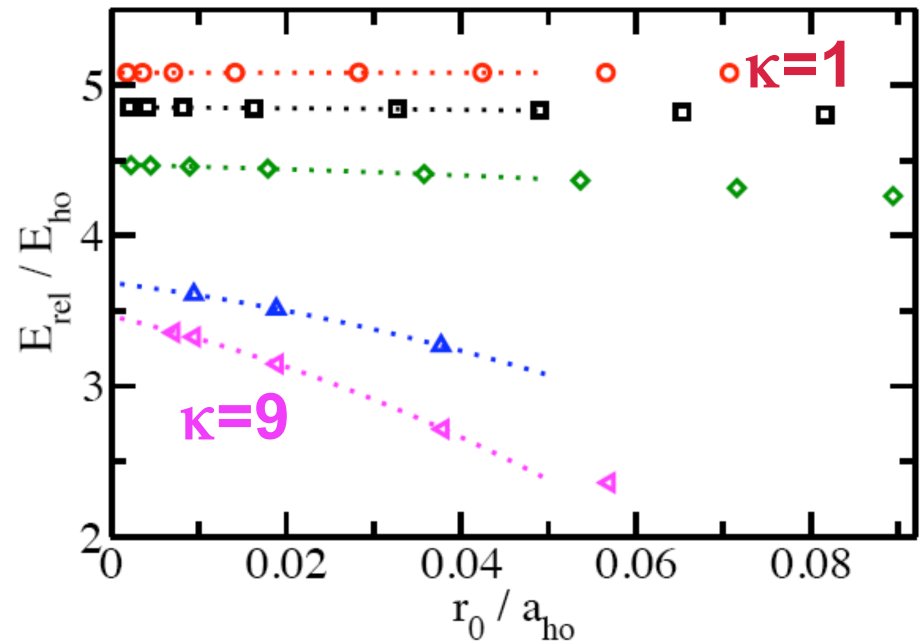
$L^{\Pi}=1^{+}$ symmetry

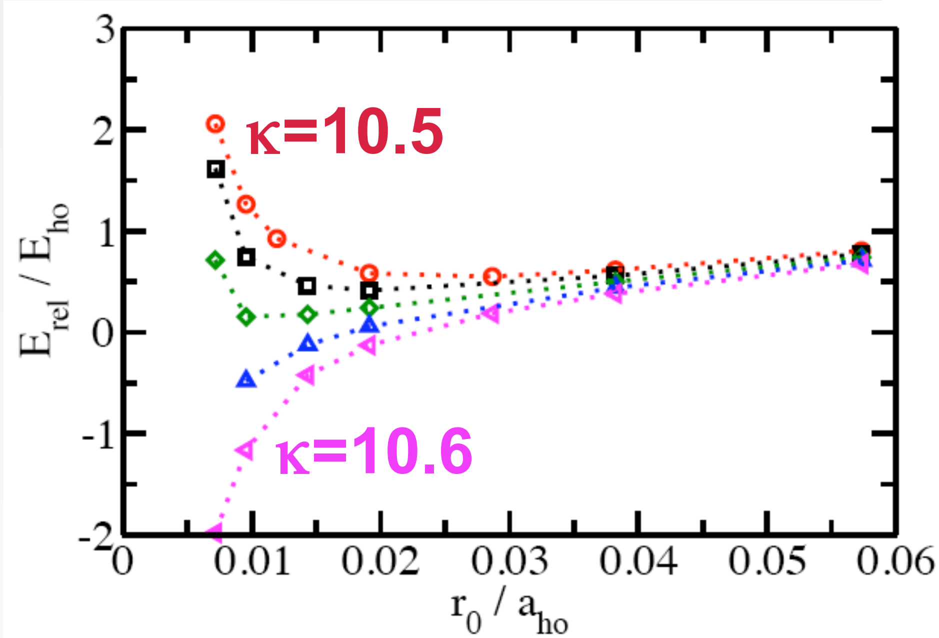


Range-Dependence FFFX System

$L^{\Pi}=1^{+}$ symmetry.







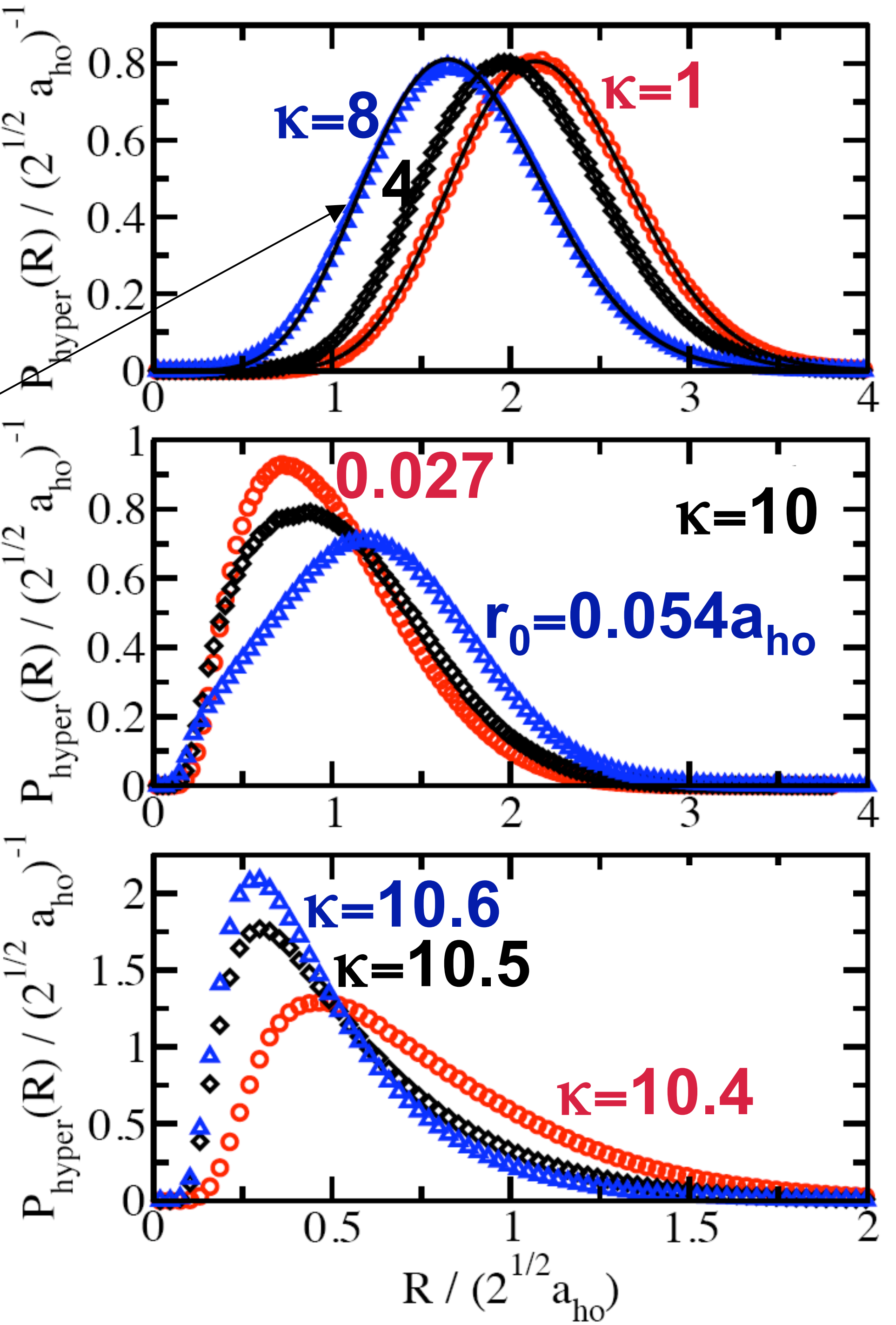
Calculations are performed for 2-body Gaussian potential.

Work by Gandolfi and Carlson (arXiv:1006.5186): 3-, 4-, 5-body resonance but no (N>5)-resonance.

FFFX: Hyperradial Densities

Solid lines obtained by assuming universal state and fitting density to expected density (treating s as fitting parameter)

Densities are obtained through Metropolis sampling of wave function obtained by stochastic variational approach (VMC method).



Next Steps

- Extend the calculations to fixed-R:
  - Gives hyperangular eigenvalue directly.
  - Allows for scattering calculations.

- For $L^{\Pi}=0^{+}$ symmetry: See von Stecher and Greene, PRA 80, 022504 (2010).
  - Application to four-boson system (Greene group).
  - Application to (2,2) fermion system (Greene group).

- For $L^{\Pi}=1^{-}$:
  - We have worked out and tested integrals for N=3 and 4.

- For $L^{\Pi}=1^{+}$:
  - We have worked out and tested integrals for N=3.

Summary

- Motivated the importance of few-body studies, also in view of benchmarking the many-body problem.

- Introduced stochastic variational approach and its application to small Bose and Fermi systems:
  - Bose gas.
  - Equal-mass fermions.
  - Unequal-mass fermions.