### Quantum Mechanical Few-Body Systems

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Supported by the NSF.

# **Outline Of This Lecture**

### Why are few-body systems interesting? Understanding transition from few to many.

Neat systems on their own.

#### **Discussion of one few-body technique:**

Stochastic variational approach with explicitly correlated Gaussians.

Application of this approach to...

...spinless bosons under external harmonic confinement.

...bosons in the presence of 1D spin-orbit coupling.

# Going From Few To Many...

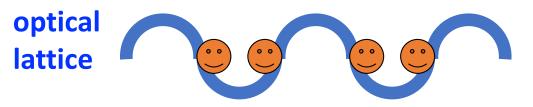
Figure from Toennies et al., Physics Today 54, 31 (2001).

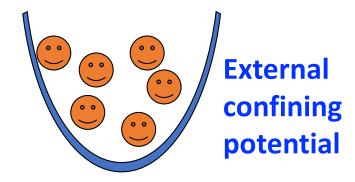
Microscopic to macroscopic:



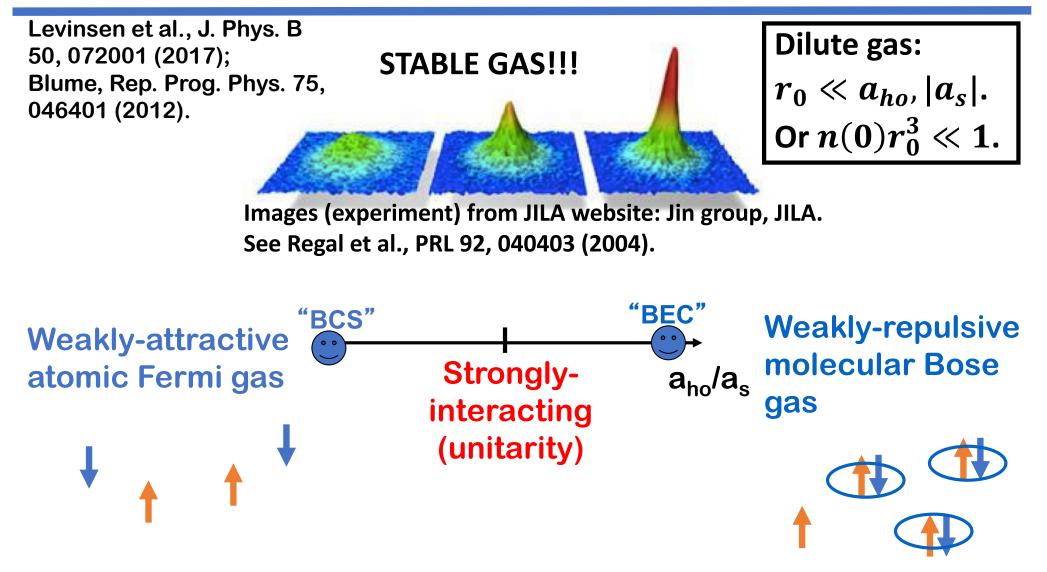
#### **Examples:**

- Doped helium clusters: Molecular rotations, microscopic superfluidity,...
- Metal clusters: conductivity, designing materials,...
- What is special about cold atomic Bose and Fermi systems?
  - Universal behavior.
  - Much experimental progress!

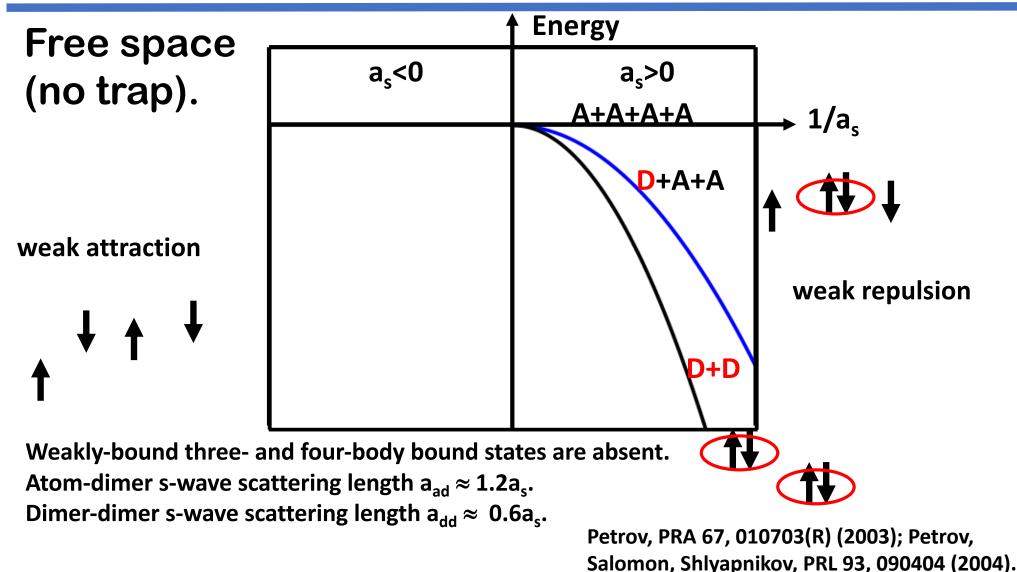




### Use Few-Body System To Understand BCS-BEC Crossover



### Dimer Bound State But No Up-Up-Down Trimer Or Tetramer



Borromean rings: The blue ring lies under the green ring (the "blue-green dimer" is unbound). If the red ring is cut open, the trimer flies apart.

### **BBB: Let s-Wave Scattering Length Be Infinitely Large**

Hyperradial and hyperangular motion separate exactly:  $\Psi = F(R_{hyper})\Phi(\vec{\Omega}); R^2_{hyper} \propto r^2_{12} + r^2_{13} + r^2_{23}.$ 

 $L^{\Pi} = 0^+$  hyperangular equation yields eigenvalue  $\iota s_0$ , where  $s_0 = 1.006...$ 

Hyperangular eigenvalue enters into Schroedinger-like hyperradial equation:  $H_{radial}F(R_{hyper}) = E_3F(R_{hyper})$ , where  $H_{radial}(R_{hyper}) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial R_{hyper}^2} + \frac{\hbar^2((\iota s_0)^2 - \frac{1}{4})}{2mR_{hyper}^2}$ .

If  $F(R_{hyper})$  is a solution with energy  $E_3^{(n)}$ , then  $F(\lambda R_{hyper})$ with  $\lambda = \exp\left(\frac{\pi}{s_0}\right) = 22.7 \dots$  is a solution with energy  $\lambda^{-2}E_3^{(n)}$ .

bound states  $E_3$  n+1 n

<u>n – 1</u>

Infinite

# of

#### Braaten, Hammer, Physics Reports 428, 259 (2006).

### Peculiar Three-Boson Efimov States

$$H = \frac{\vec{p}_{12}^2}{2\mu_{12}} + \frac{\vec{p}_{12,3}^2}{2\mu_{12,3}} + \sum_{j < k} g_2 \delta(\vec{r}_{jk}) + g_3 \delta(\vec{r}_1 - \vec{r}_2) \delta(\vec{r}_2 - \vec{r}_3).$$
$$g_2 = \frac{4\pi\hbar^2 a_s}{m} \text{ and } g_3 = \frac{\#\hbar^2 \kappa_*^{-4}}{m}, \text{ where } E_{unit} = \frac{\hbar^2 \kappa_*^2}{m}.$$

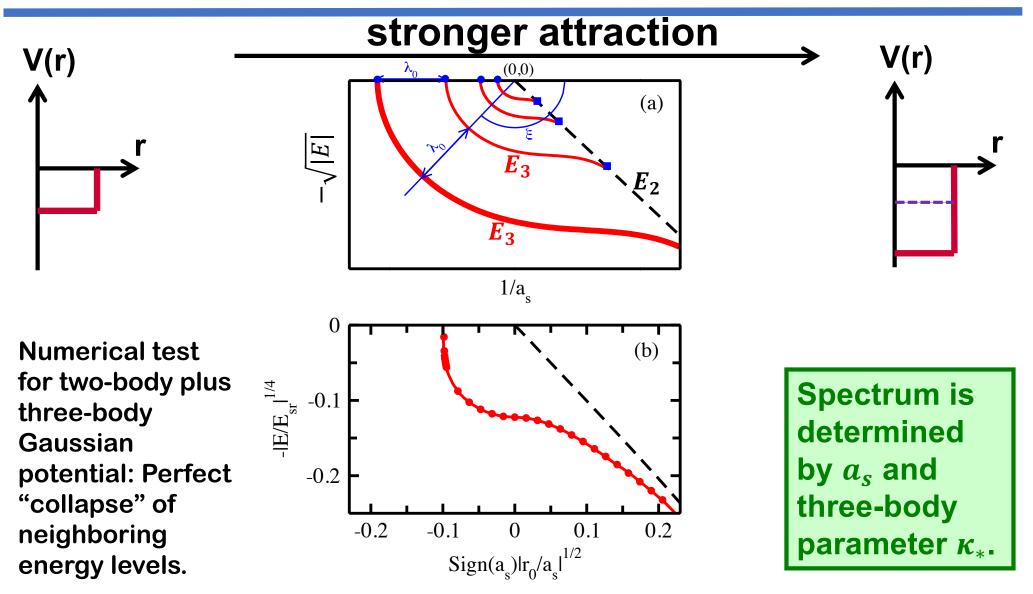
Time-dependent SE for *H* possesses continuous scaling symmetry:

$$t \to \lambda^2 t; \vec{r} \to \lambda \vec{r}; a_s \to \lambda a_s; E \to \lambda^{-2} E; \kappa_* \to \lambda^{-1} \kappa_*$$

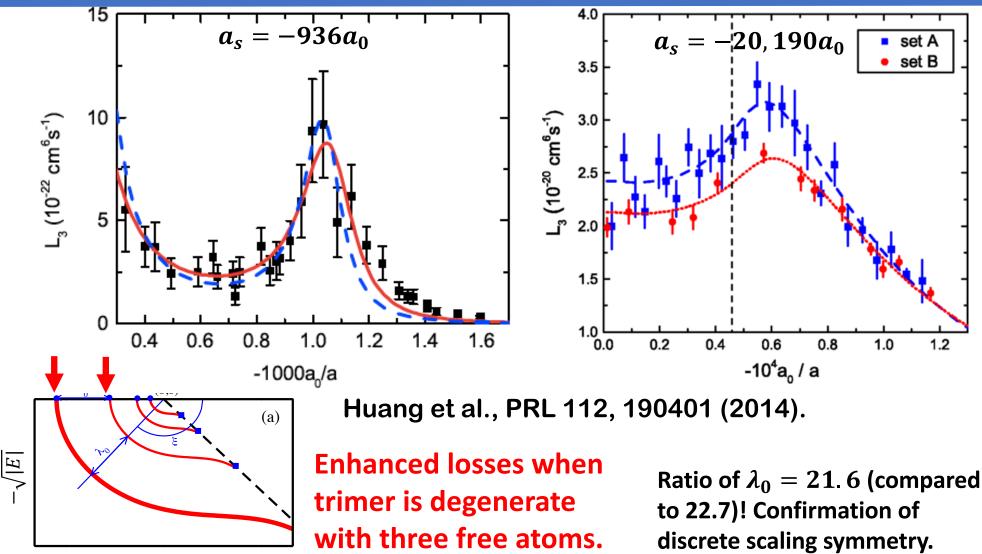
Time-dependent SE for *H* also possesses discrete scaling symmetry:

$$t \rightarrow \lambda_0^2 t; \vec{r} \rightarrow \lambda_0 \vec{r} a_s \rightarrow \lambda_0 a_s; E \rightarrow \lambda_0^{-2} E; \kappa_* \rightarrow \kappa_*; \lambda_0 \approx 22.7$$

### Finite s-Wave Scattering Length: Universally Linked States



### Measurement Of Loss Rate For Non-Degenerate <sup>133</sup>Cs Gas



1/a

### **Basis Set Expansion:** Variational Approach

Let  $\Phi_j$  with  $j = 0, 1, \cdots$  be an orthonormal complete set.

Any eigen state  $\varphi_l$  with energy  $E_l$  of H can be expanded as  $\varphi_l = \sum_{j=0}^{\infty} c_j^{(l)} \Phi_j.$ 

In reality:  $\phi_l = \sum_{j=0}^{N_b} c_j^{(l)} \Phi_j$  ( $N_b < \infty$ ;  $\phi_l$  is an approximation to  $\varphi_l$ ).

Form matrix  $\overleftarrow{C}$  with matrix elements  $C_{jl} = c_j^{(l)}$ .

Eigenvalues  $\varepsilon_l$  of matrix equation  $\overleftrightarrow{H} \overleftrightarrow{C} = \overleftrightarrow{\varepsilon} \overleftrightarrow{C}$  have the following property:

 $E_0 \leq \varepsilon_0$ ,  $E_1 \leq \varepsilon_1$ ,  $\cdots$  (variational upper bounds).

### **Basis Set Expansion:** Variational Approach

Now: Allow  $\Phi_j$  with  $j = 0, 1, \cdots$  to be linearly dependent (but not too much).

Expand  $\phi_l = \sum_{j=0}^{N_b} c_j^{(l)} \Phi_j$  ( $N_b < \infty$ ;  $\phi_l$  is an approximation to exact eigen state  $\phi_l$ ).

Form matrix  $\overleftarrow{C}$  with matrix elements  $C_{jl} = c_j^{(l)}$ .

The eigenvalues  $\varepsilon_l$  of generalized eigen value equation  $\widehat{H} \ \widehat{C} = \widehat{\varepsilon} \ \widehat{O} \ \widehat{C}$ , where  $O_{jl} = \langle \Phi_j | \Phi_l \rangle$ , have the following property:

 $E_0 \leq \varepsilon_0, E_1 \leq \varepsilon_1, \cdots$  (variational upper bounds).

### Basis Set Expansion: Variational Approach

Take advantage of the fact that the basis functions  $\Phi_j$  can be "anything".

Pick  $\Phi_i$  such that integrals have compact analytical expressions.

Pick  $\Phi_i$  such that the different length scales of the system are covered.

Take advantage of the fact that low-energy Hamiltonian can be constructed using different functional forms for interaction potential:

$$H = \sum_{j} T_{j} + V_{trap,j} + V_{soc,j} + \sum_{j < k} V_{2b,jk} + \sum_{j < k < l} V_{3b,jkl}$$

Usually,  $r_0 \ll a_{ho}$  (100 $a_0 \ll$  10000 $a_0$ ): Need to resolve multiple scales. Use  $\Phi_j$  with different widths.

$$V_{2b,jk} = v_0 exp\left(-\frac{r_{jk}^2}{2r_0^2}\right)$$

### Basis Set Expansion: Stochastic Variational Approach

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).

#### Idea:

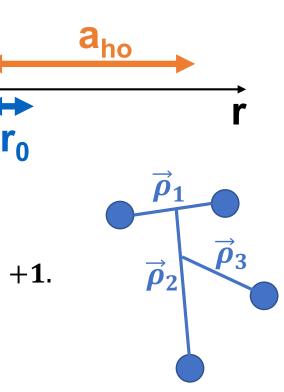
Use basis functions that involve Gaussians with different widths in interparticle distances (correlations).

Large number of non-linear parameters that are being optimized semi-stochastically.

Simplest case: Basis functions with L = 0 and  $\Pi = +1$ .

$$\boldsymbol{\Phi}_{j} = \exp\left(-\sum_{s < t}^{N} \frac{r_{st}^{2}}{2d_{j,st}^{2}}\right) = \exp\left(-\frac{1}{2} \vec{x}^{T} \stackrel{\leftrightarrow}{A} \vec{x}\right).$$

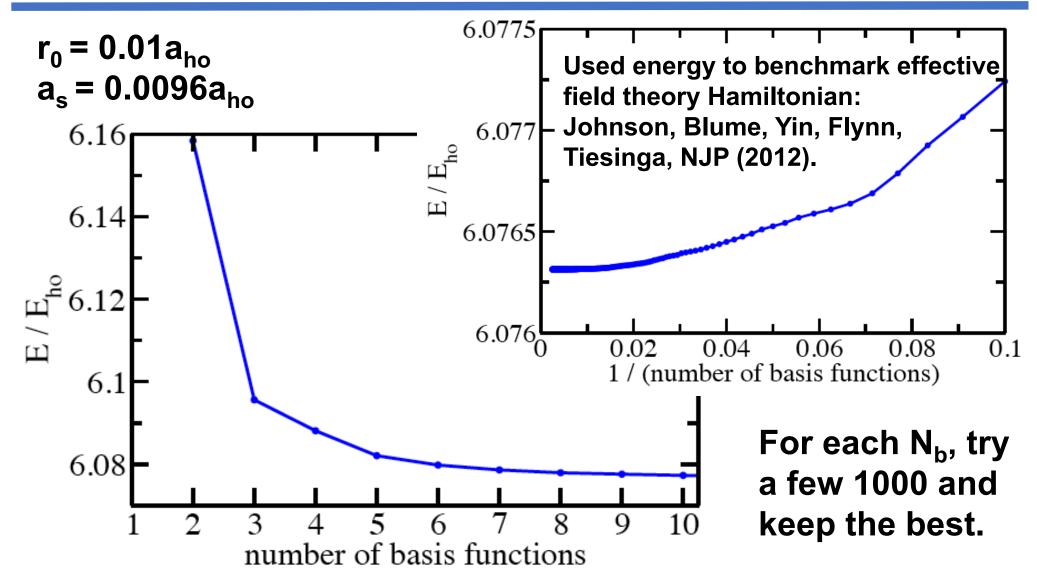
 $\vec{x}$ : Denotes Jacobi vectors  $\vec{\rho}_1$ ,  $\vec{\rho}_2$ , ....  $\vec{A}$ :  $(N-1) \times (N-1)$  matrix with N(N-1)/2 independent parameters.



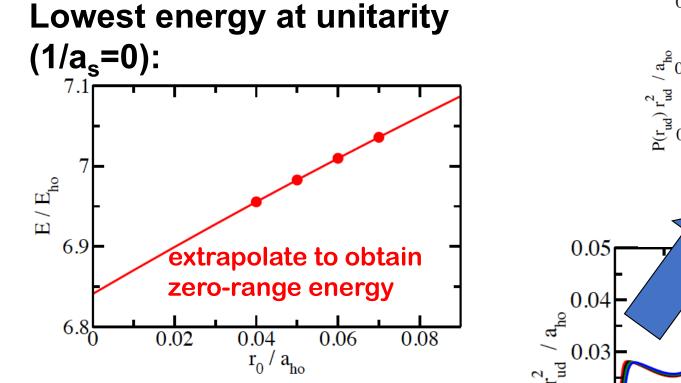
### Stochastic Variational Approach: Outline of Algorithm

- Pick basis function  $\Phi_1$  and calculate  $\varepsilon_1$ .
- Goal: Add  $\Phi_2$ .
- Procedure:
  - Pick  $\Phi_{2,1},...,\Phi_{2,p}$  ( $p \sim 1 10000$ ).
  - Calculate  $\varepsilon_{2,1}, \dots, \varepsilon_{2,p}$ .  $\varepsilon_{2,j}$  is eigen value of target state if basis function  $\Phi_{2,j}$  is added to basis.
  - Determine  $\Phi_2 = \Phi_{2,j}$  such that  $\varepsilon_2 = \varepsilon_{2,j} = \min(\varepsilon_{2,1},...,\varepsilon_{2,p})$ .
  - Diagonalize Hamiltonian matrix to obtain eigenvalues and eigenvectors.
- To add  $\Phi_3$ , proceed as above.
- Once basis set is "complete", calculate structural properties.
- Can optimize ground or excited state.
- Can optimize multiple states simultaneously.

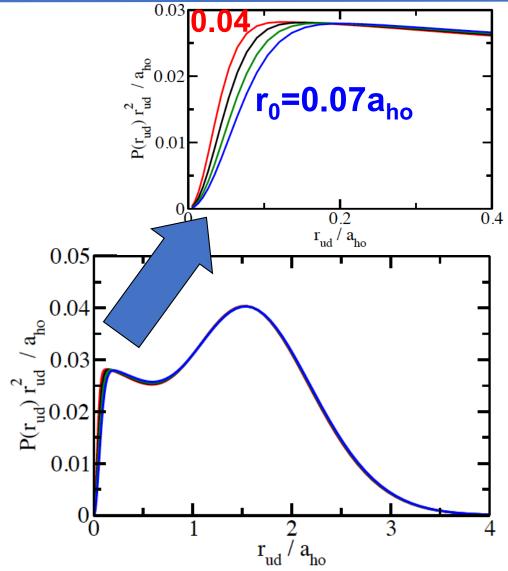
### Harmonically Trapped Five-Boson System: Convergence



### **Trapped (3,3) System: Energy And Pair Distribution Function**



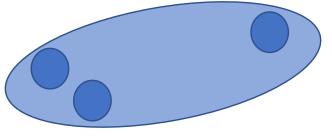
Two-peak structure of updown pair distribution function: Small  $r_{ud}$  peak: pair formation. Large  $r_{ud}$  peak: unpaired.



# A Few More Comments

Basis functions need to be symmetrized: Five identical bosons implies 5!=120 permutations.

Use physical insight to choose  $d_{j,st}$  efficiently: E.g., "2+1" or "1+1+1" configuration.



If parameter windows for non-linear variational parameters are not set properly, a non-converged energy may appear converged...

Basis sets tend to be small (a few 1000); but we work hard to select the basis functions we want.

Beyond  $L^{\Pi} = 0^+$  states? Many possibilities... Global vector approach is quite convenient.

### Application: Four Harmonically Confined Bosons

#### Want to know:

If we start in the non-interacting state and slowly increase the s-wave scattering length to an infinitely large value, what type of state do we end up in? State that is dependent on  $a_s$  only? Or state that depends on three-body parameter  $\kappa_*$  as well?

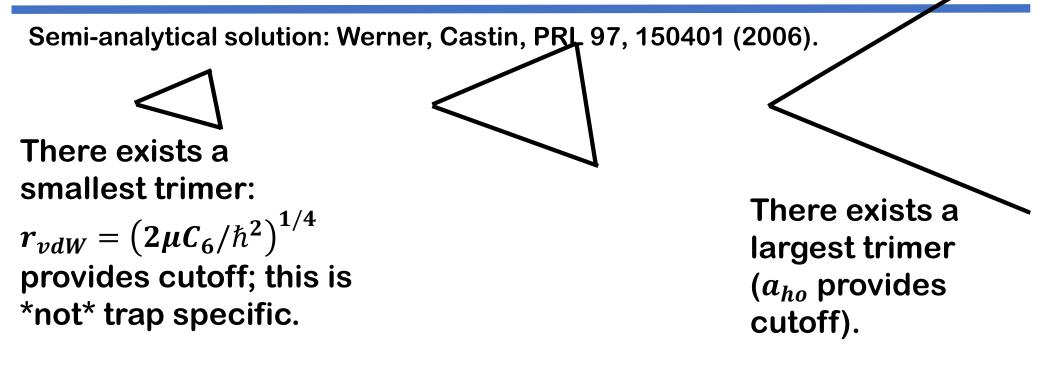
#### Why do we want to know this?

Recent experiments on Bose gases in unitary regime (Cornell/Jin, Hadzibabic, Salomon): many-body treatment of these systems is hard. Attempts to gain insight based on two- and three-body problem. Go a step further and look at N = 4 bosons.

#### Approach:

Calculate and analyze four-body spectrum.

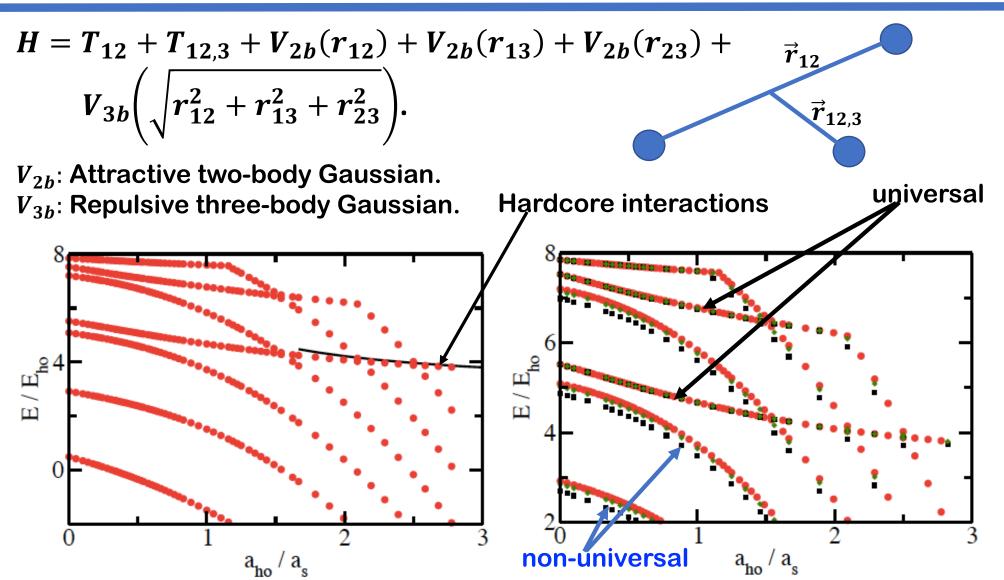
### First: Think About Three Harmonically Confined Bosons



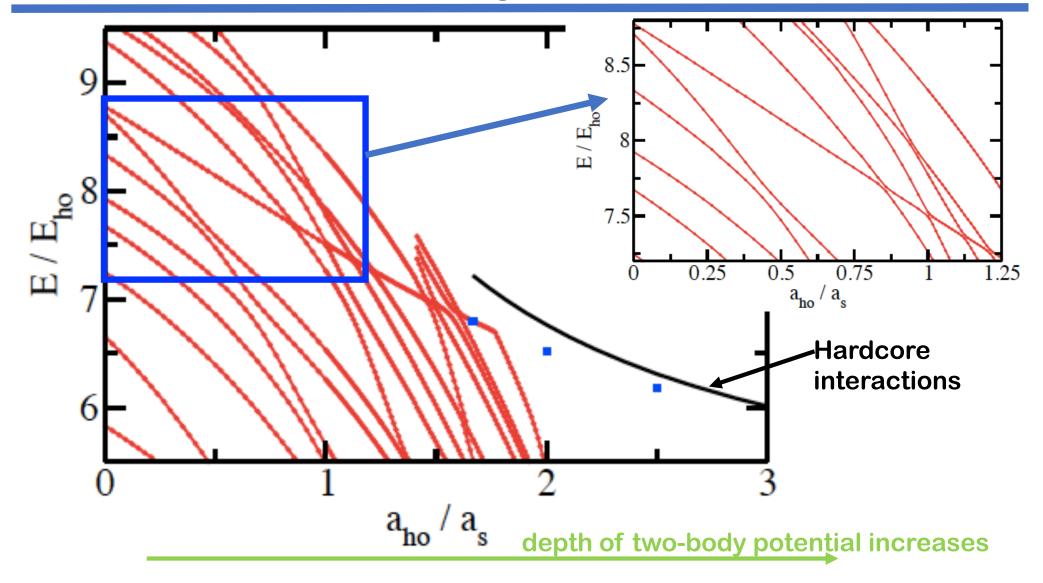
 $L^{\Pi} = 0^+$  trap states that depend on three-body parameter ("squished" version of free-space trimers).

There also exist  $L^{\Pi} = 0^+$  trap states that are largely independent of three-body parameter (eigenvalues  $s_1$ , ... are real).

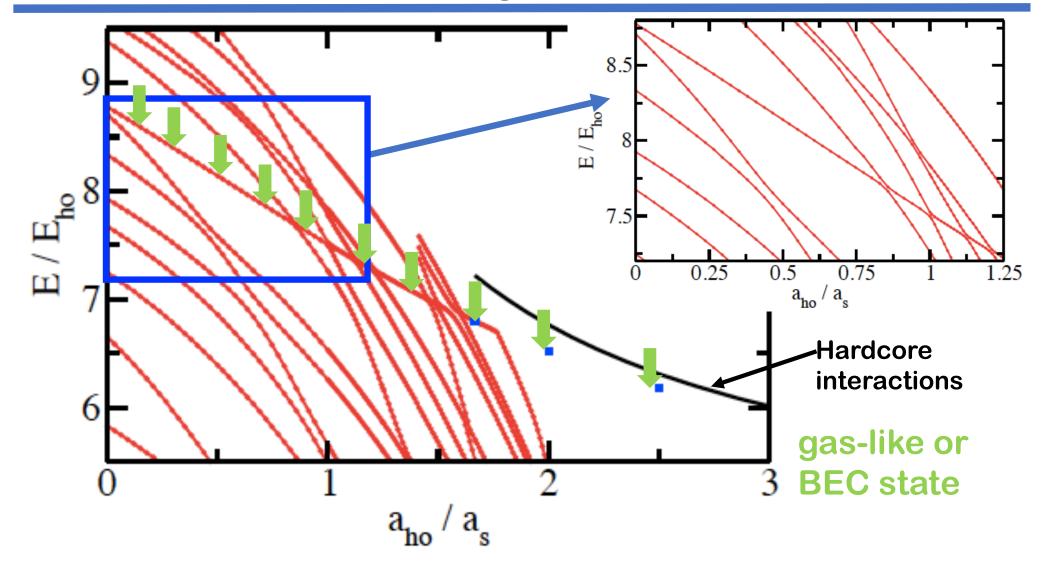
### **Energy Spectrum For Trapped Three-Boson System**



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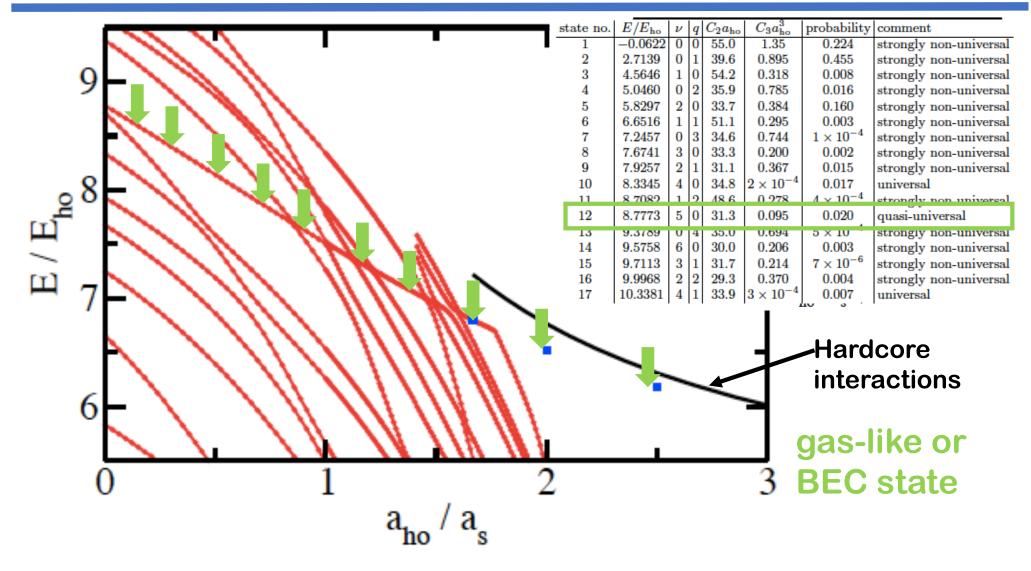


### Classification Of States At Unitarity

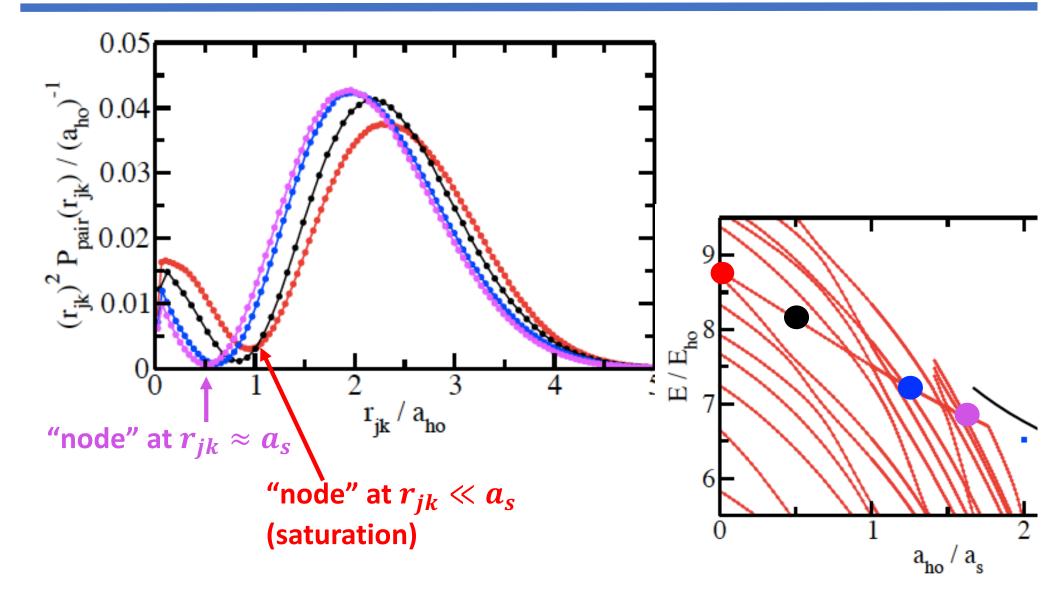
state no.	$E/E_{\rm ho}$	ν	q	$C_2 a_{ m ho}$	$C_3 a_{ m ho}^3$	probability	comment	
1	-0.0622	0	0	55.0	1.35	0.224	strongly non-universal	
2	2.7139	0	1	39.6	0.895	0.455	strongly non-universal	Two-body contact:
3	4.5646	1	0	54.2	0.318	0.008	strongly non-universal	Two-body contact.
4	5.0460	0	2	35.9	0.785	0.016	strongly non-universal	$C = 8\pi m \partial E$
5	5.8297	2	0	33.7	0.384	0.160	strongly non-universal	$C_2 = -\frac{8\pi m}{\hbar^2} \frac{\partial E}{\partial (a_s^{-1})}$
6	6.6516	1	1	51.1	0.295	0.003	strongly non-universal	- (3 )
7	7.2457	0	3	34.6	0.744	$1 \times 10^{-4}$	strongly non-universal	
8	7.6741	3	0	33.3	0.200	0.002	strongly non-universal	Three-body
9	7.9257	2	1	31.1	0.367	0.015	strongly non-universal	contact:
10	8.3345	4	0	34.8	$2 \times 10^{-4}$	0.017	universal	
11	8.7082	1	2	48.6	0.278	$4 \times 10^{-4}$	strongly non-universal	$C_3 = -\frac{m\kappa_{fs}}{2\hbar^2} \frac{\partial E}{\partial \kappa_{fs}}$
12	8.7773	5	0	31.3	0.095	0.020	quasi-universal	$2\hbar^2 \partial \kappa_{\rm fs}$
13	9.3789	0	4	35.0	0.694	$5 \times 10^{-4}$	strongly non-universal	
14	9.5758	6	0	30.0	0.206	0.003	strongly non-universal	Seminal work by
15	9.7113	3	1	31.7	0.214	$7 \times 10^{-6}$	strongly non-universal	Tan.
16	9.9968	2	2	29.3	0.370	0.004	strongly non-universal	Smith et al., PRL
17	10.3381	4	1	33.9	$3 \times 10^{-4}$	0.007	universal	112, 110402 (2014).

Universal states at unitarity:  $E = (s_v + 2q + 1)\hbar\omega$ Wave function is product state:  $\Psi = \Phi(\vec{\Omega})F(R_{hyper})$ ;  $R_{hyper}$  hyperradius.

### **Energy Spectrum For Trapped Four-Boson System**



### Pair Distribution Function For Various s-Wave Scattering Lengths



### Four Harmonically Trapped Bosons: What Did We Learn?

Explicitly Correlated Gaussian basis can be used to map out good portion of eigen energies.

BEC state at unitarity seems to be quasi-universal (weak dependence on three-body parameter).

Saturation of "near zero crossing" of pair distribution function.

Blume, Sze, Bohn, PRA 97, 033621 (2018) Sze, Sykes, Blume, Bohn, PRA 97, 033608 (2018)

**Future:** 

Like to calculate four-body dynamics...

# Three Bosons With 1D Spin-Orbit Coupling

Effects of modified single-particle dispersion on three identical bosons with large s-wave scattering length: What happens to discrete scaling symmetry/Efimov physics?

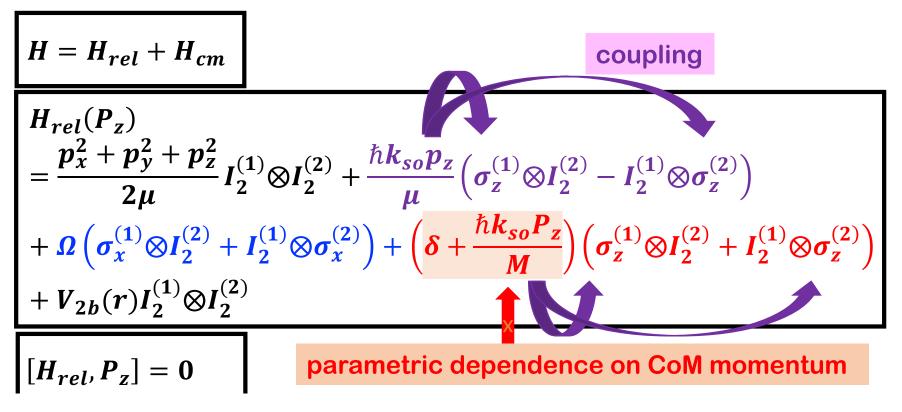
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Fermions with 3D SOC:
Shi et al., PRL 112, 013201 (2014); PRA 91, 023618 (2015).
discrete scaling
symmetry
does not survive does survive
```

We find for BBB with 1D SOC: Discrete scaling symmetry does survive. Conjecture: Should hold for any type of SOC.

### Two Bosons With One-Dimensional Spin-Orbit Coupling

3D system with 1D SOC (spin-orbit coupling + Raman coupling + detuning)  $\rightarrow$  Two-body bound state or not?

Rewrite Hamiltonian in relative coordinates ( $\vec{r}$  and  $\vec{p}$  with reduced mass  $\mu$ ) and center-of-mass coordinates ( $\vec{R}$  and  $\vec{P}$  with total mass M):



### Basis Functions: Need To Account For Spin...

$$\boldsymbol{\Phi}_{j} = \exp\left(-\sum_{s < t}^{N} \frac{r_{st}^{2}}{2d_{j,st}^{2}} + \sum_{t=1}^{N-1} \iota \vec{s}_{j,t} \cdot \vec{\rho}_{t}\right)$$

Spatial two-body correlations

Correlation between spin and spatial degrees of freedom. Can be rewritten as

 $\sum_{t=1}^{N} \iota \vec{S}_{j,t} \cdot \vec{r}_t$ 

$$\Psi_{rel} = \sum_{j=1}^{N_b} c_j \psi_j$$
 and  $\psi_j = \mathcal{S}(\Phi_j(\vec{\rho}_1, \dots, \vec{\rho}_{N-1})\chi_j)$ 

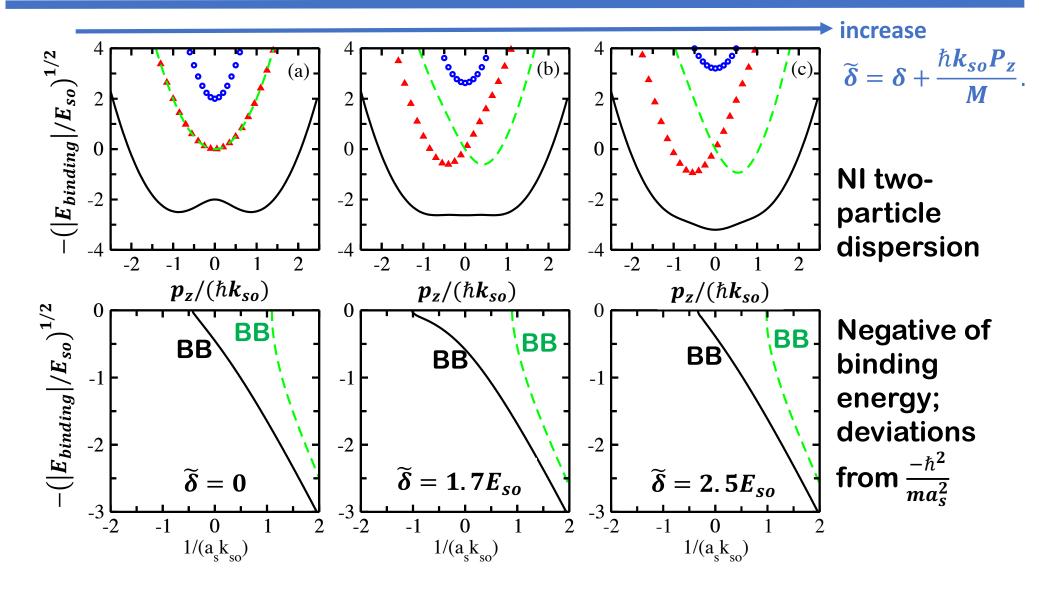
Matrix elements have compact analytical expressions.

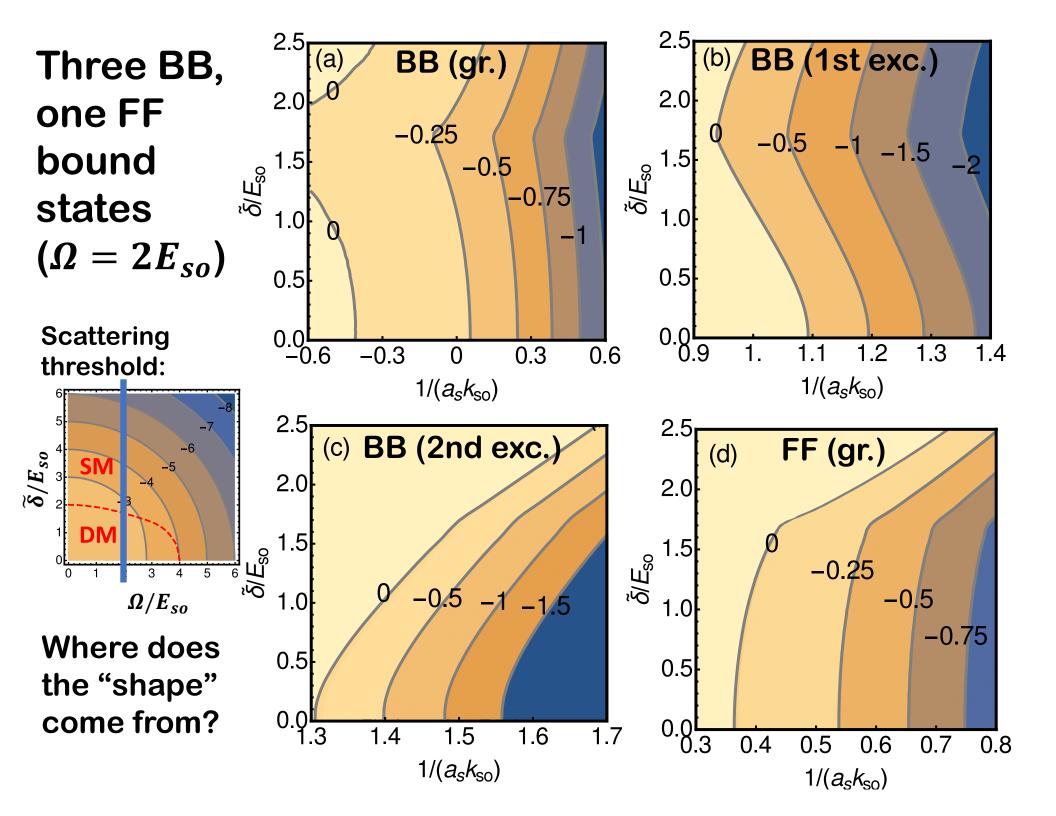
**Bound state:** 

Energy of dimer with CM momentum  $P_z$  is more negative than that of two free atoms with the same  $P_z$ .

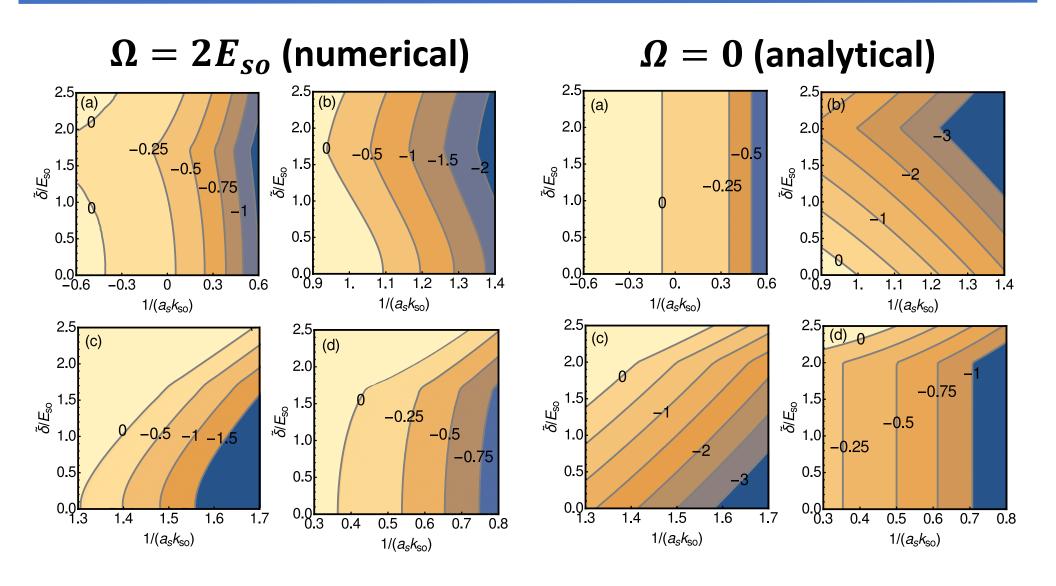
Energy of trimer with CM momentum  $P_z$  is more negative than that of three free atoms with the same  $P_z$  and that of a dimer and an atom with the same  $P_z$ .

### Two Identical Bosons: $\Omega = 2E_{so}; \, \widetilde{\delta} \ge 0 \ (a_{\uparrow\uparrow} = a_{\uparrow\downarrow} = a_{\downarrow\uparrow} = a_{\downarrow\downarrow})$

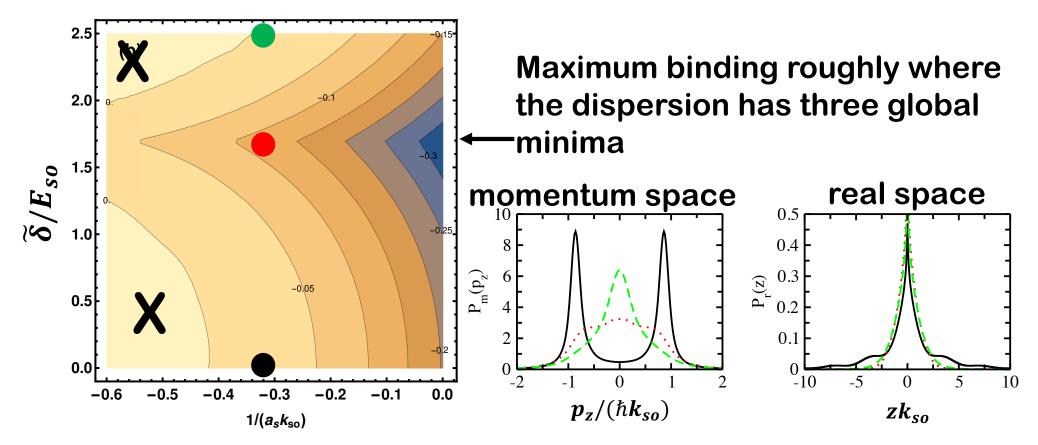




### "Shape"? Simple Qualitative Picture



### Binding Energy for $\Omega = 2E_{so}$ : Lowest BB State



Weakly-bound state for certain negative free-space s-wave scattering lengths.

For FF, see: Shenoy, PRA 88, 033609 (2013). Dong et al., PRA 87, 043616 (2013).

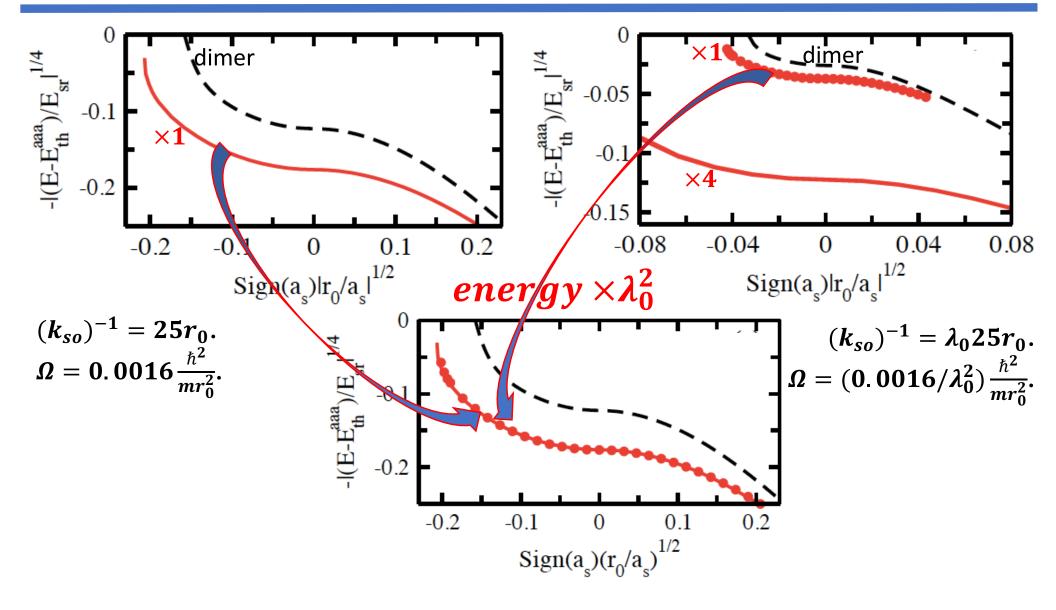
### With SOC: Fate Of Three-Boson Efimov States?

$$\begin{split} H &= (\frac{\vec{p}_{12}^2}{2\mu_{12}} + \frac{\vec{p}_{12,3}^2}{2\mu_{12,3}} + \sum_{j < k} g_2 \delta(\vec{r}_{jk}) + g_3 \delta(\vec{r}_1 - \vec{r}_2) \delta(\vec{r}_2 - \vec{r}_3)) I_8 \\ &+ \frac{\hbar k_{so}}{m} (\dots) + \Omega(\dots) + \widetilde{\delta}(\dots). \end{split}$$

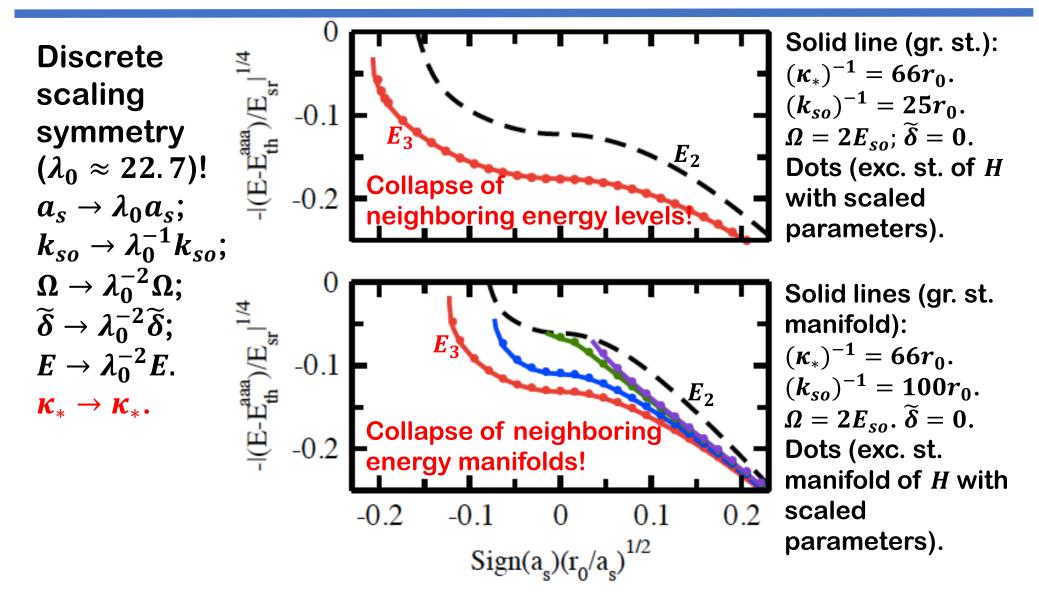
### Continuous scaling symmetry! $t \rightarrow \lambda^2 t; \vec{r} \rightarrow \lambda \vec{r}; a_s \rightarrow \lambda a_s; k_{so} \rightarrow \lambda^{-1} k_{so}; \Omega \rightarrow \lambda^{-2} \Omega;$ $\widetilde{\delta} \rightarrow \lambda^{-2} \widetilde{\delta}; E \rightarrow \lambda^{-2} E; \kappa_* \rightarrow \lambda^{-1} \kappa_*$

Discrete scaling symmetry?  $t \rightarrow \lambda_0^2 t; \vec{r} \rightarrow \lambda_0 \vec{r} a_s \rightarrow \lambda_0 a_s; k_{so} \rightarrow \lambda_0^{-1} k_{so}; \Omega \rightarrow \lambda_0^{-2} \Omega;$  $\tilde{\delta} \rightarrow \lambda_0^{-2} \tilde{\delta}; E \rightarrow \lambda_0^{-2} E; \kappa_* \rightarrow \kappa_*; \lambda_0 \approx 22.7$ 

### Generalized Radial Scaling Law? $\tilde{\delta} = 0 \text{ And } (\kappa_*)^{-1} = 66r_0$



# Generalized Radial Scaling Law (Five Instead Of Two Axes)

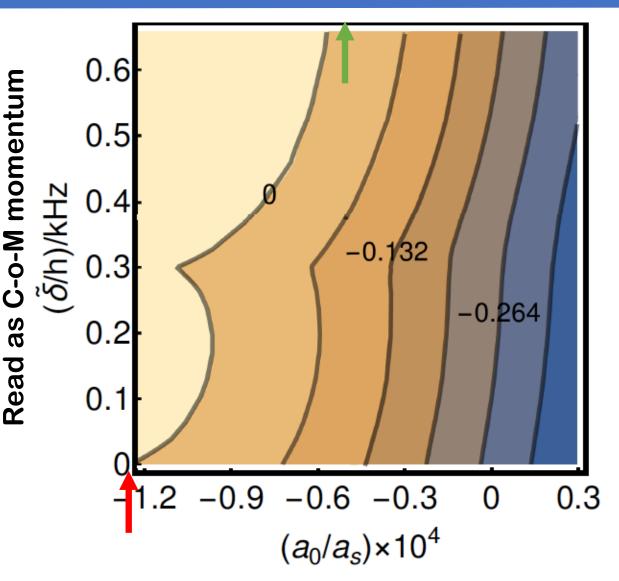


### Proposal: Experimental Observability

Using three-body parameter for <sup>133</sup>Cs. Lowest state in excited state manifold.  $(k_{so})^{-1} \approx 10,160a_0.$  $\frac{k_{so}}{\kappa_*} \approx 1.32$  (exc. state).  $\Omega = 2E_{so}.$ 

Ground state resonance mostly unchanged.

Excited state resonance: C Enhanced losses between  $a_s \approx -7,790a_0$  and  $a_s \approx -20,190a_0$ . Scattering length window!



### Summary

Why are few-body systems interesting?

Discussion of one few-body technique: Stochastic variational approach with explicitly correlated Gaussians.

Application of this approach to...

... spinless bosons under external harmonic confinement.

...bosons in the presence of 1D spin-orbit coupling.

# **Thanks To Collaborators**

Lecture 1:

Chris Greene: Scattering physics.

Brian Granger: Effective odd-z coupling constant, frame transformation.

Krittika Kanjilal: p-wave and odd-z pseudopotentials.

Grigori Astrakharchik, Stefano Giorgini: Quasi-1D Bose and Fermi gases.

Su-Ju Wang, Qingze Guan: Waveguide + SOC. Lecture 2:

Debraj Rakshit, Xiangyu (Desmond) Yin: ECG approach.

John Bohn, Michelle Sze: Trapped bosons.

Qingze Guan: Generalized radial scaling law, ECG approach.

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