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

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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):

![Graph](image)

Yields bound and scattering states.

Kartavtsev and Malykh, JPB 40, 1429 (2007).

Hyperradial coordinate measures the overall size of the system (five angles have been integrated out).
General Formalism: Similar to Born-Oppenheimer Approximation

• Hyperspherical coordinate approach: hyperradius $R$ and hyperangles $\Omega$.

• Idea: $H = T_\Omega + T_R + V_{int} = H_{adia}(R) + T_R$

• Step 1: Solve $H_{adia}(R) \Phi_v(R;\Omega) = U_v(R) \Phi_v(R;\Omega)$ (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 $U_v(R) = \hbar^2[(s_v(R))^2 - \frac{1}{4}] / (2\mu R^2)$
How Do We Solve Hyperangular Schrödinger Equation?

- Use **explicitly correlated Gaussians** to expand hyperangular channel functions [see von Stecher and Greene, PRA (2009) for treatment of $0^+$ states].

$$\Phi_\nu(R;\Omega) = \sum_k c_k \left[f(x, u_{1(k)}, u_{2(k)})\right] \exp\left[-\frac{1}{2} x^T A^{(k)} x\right] |_R$$

- 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 $U_\nu(R)$].
Proof-of-Principle Calculation for Equal-Mass (2,2) System at Unitarity

0⁺ symmetry:

- Red symbols: this work.
- Solid line: fit.

von Stecher and Greene, PRA (2009); HECG approach

1⁻ symmetry:

- Red symbols: this work.
- Solid line: fit.

Rakshit, Daily, Blume, PRA (2012); extracted from trap spectrum

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

$r_0/R = 0.1$

$r_0/R = 0.01$
Potential Curve for (3,1) System with $1^+$ Symmetry and Positive $a_s$

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

mass ratio 9.75

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.


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

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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.

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- Properties are fully determined by $a_s$.
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Under Which Conditions Do Universal States Exist?

- \((T_R + U_v(R) + \Sigma_v \cdot \text{coupling}_{v'v}) F_{vq}(R) = E_{vq} F_{vq}(R)\)

- For finite \(a_s\), small \(R\) and \(r_0=0\):
  - \(U_v(R) + \Sigma_v \cdot \text{coupling}_{v'v} \sim \hbar^2[(s_{0,\text{unit}})^2 - \frac{1}{4}] / (2\mu R^2)\)

- \(S_{0,\text{unit}}>1\) [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 $L^{\Pi=1^+}$

Conclusion: Universal bound states in heavy light mixtures with positive interspecies s-wave scattering 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.
Well known:
Interaction energy (IE) of $N$ bosons $\neq \frac{N(N-1)}{2} \times$ IE of 2 bosons

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 $r_{\text{eff}}$: Effective N-Body Interactions

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

where $U_N$ are effective N-body interactions:

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

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

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

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

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

Harmonically Trapped Five-Boson System: Illustration of Convergence

\[ r_0 = 0.01 a_{ho} \]
\[ a_s = 0.0096 a_{ho} \]

Used energy to benchmark effective field theory Hamiltonian:
Johnson, Blume, Yin, Flynn, Tiesinga, NJP (2012).

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

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

\[
N_0 / N = 1 - 0.420004(N - 1) \left[ \frac{a_s(0)}{a_{HO}} \right]^2 \\
+ \left[ -0.373241(N - 1) \right] \left[ \frac{a_s(0)}{a_{HO}} \right]^3 + \cdots
\]
Condensate Fraction $N/N_0$ of Weakly-Interacting Trapped Bose Gas

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

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

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

Daily, Yin, Blume, PRA 85, 053614 (2012).
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...