

Efimov Scenario In The Presence Of Spin-Orbit Coupling

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Lecture 3



Discussion of one few-body technique:

Stochastic variational approach with explicitly correlated Gaussians.

Overview Of Lecture 3

Efimov scenario of three equal-mass bosons with 1D spin-orbit coupling

Review of Efimov effect for equal-mass bosons with short-range interactions.

What is 1D spin-orbit coupling (system lives in three-dimensional space) and how does it differ from "conventual" situation?

- One-body problem.
- Intermezzo: Numerical approach.
- Two-body problem.
- Three-body problem.

Unlike lectures 1 and 2:

- Consider stationary system (no time dependence).
- No experimental data yet on generalized radial scaling law, even though spin-orbit coupling has been realized in cold atom systems.

Review: 428, 259 (2006). Three-Boson Hamiltonian

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Question: What units do g_2 and g_3 have?

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 g_2 : energy times length³. g_3 : energy times length⁶.

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Follow-up question: Given this answer, what are the most general expressions for g_2 and g_3 ?

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Follow-up question: Given this answer, what are the most general expressions for g_2 and g_3 ?

$$g_2 = \# \frac{\hbar^2 \text{ length}}{m}$$
; $g_3 = \# \frac{\hbar^2 \text{ length}^4}{m}$ (since energy $= \frac{\hbar^2}{m \text{ length}^2}$).

Peculiar Three-Boson Efimov States

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

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

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 ($\lambda_0 \approx 22.7$):

 $t \to \lambda_0^2 t; \vec{r} \to \lambda_0 \vec{r}; a_s \to \lambda_0 a_s; E \to \lambda_0^{-2} E; \kappa_* \to \kappa_*.$

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 ιs_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 $F(\lambda_0 R_{hyper})$ with $\lambda_0 = \exp\left(\frac{\pi}{s_0}\right) = 22.7$... is a solution with energy $\lambda_0^{-2} E_3^{(n)}$.

bound states **E**_3[↑] n+1n

Infinite

of

Finite s-Wave Scattering Length: Universally Linked States



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.

Measurement Of Loss Rate For Non-Degenerate ¹³³Cs Gas



Efimov Scenario In The Presence Of Spin-Orbit Coupling?

If the single-particle dispersion is modified and the s-wave scattering length is large, what happens to the discrete scaling symmetry/Efimov physics?



Conjecture: Should hold for any type of SOC.

Looking Ahead...

$$H = \left(\frac{\vec{p}_{12}^2}{2\mu_{12}} + \frac{\vec{p}_{12,3}^2}{2\mu_{12,3}} + \sum_{j < k} g_2 \delta(\vec{r}_{jk}) + g_3 \delta(\vec{r}_1 - \vec{r}_2) \delta(\vec{r}_2 - \vec{r}_3)\right) I_8$$

+
$$\frac{\hbar k_{so}}{m} (...) + \Omega(...) + \tilde{\delta}(...).$$
 changes and extra terms due to SOC

Continuous scaling symmetry (easy to check)! $t \rightarrow \lambda^2 t$; $\vec{r} \rightarrow \lambda \vec{r}$; $a_s \rightarrow \lambda a_s$; $k_{so} \rightarrow \lambda^{-1} k_{so}$; $\Omega \rightarrow \lambda^{-2} \Omega$; $\tilde{\delta} \rightarrow \lambda^{-2} \tilde{\delta}$; $E \rightarrow \lambda^{-2} E$; $\kappa_* \rightarrow \lambda^{-1} \kappa_*$

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

Start With Single-Particle Dispersion



Now let the spin states have different momenta:

For this to be interesting, must couple states.



Single-Particle Dispersion

For 1D spin-orbit coupling (equal mixture of Rashba and Dresselhaus coupling): $H = \left(\frac{p_x^2 + p_y^2}{2m} + \frac{p_z^2}{2m}\right)I_2 + \frac{\hbar k_{so}}{m}p_z\sigma_z + \Omega\sigma_x$ $E_{\pm} = \frac{p_x^2 + p_y^2}{2m} + \frac{p_z^2}{2m} \pm \sqrt{\left(\frac{\hbar k_{so}p_z}{m}\right)^2 + \frac{\Omega^2}{4}}$

Add detuning δ : $H = \left(\frac{p_x^2 + p_y^2}{2m} + \frac{p_z^2}{2m}\right)I_2 + \frac{\hbar k_{so}}{m}p_z\sigma_z + \delta\sigma_z.$ $E_{\pm} = \frac{p_x^2 + p_y^2}{2m} + \frac{p_z^2}{2m} \pm \sqrt{\left(\frac{\hbar k_{so}p_z}{m} + \frac{\delta}{2}\right)^2}$



Modified Single-Particle Dispersion \rightarrow New Physics

 $|exc\rangle$





Modified Single-Particle Dispersion \rightarrow New Physics



Why is this of interest? Expand E_{-} for large Ω and $\delta \neq 0$ around $p_{z,min}^{-}$:

$$E_{-} = const + \frac{\left(p_{z} - p_{z,min}^{-}\right)^{2}}{2m} + \cdots$$

Like a charged particle in a uniform vector potential \vec{A}^* : $\vec{eA}^* = p_{z,min}^- \vec{e}_z$!

Possibility to simulate physics of charged particles (e.g., fractional quantum Hall effect) with neutral atoms!

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 μ) and center-of-mass coordinates (\vec{R} and \vec{P} with total mass M):

$$\begin{split} H &= H_{rel} + H_{cm} \\ \hline H_{rel}(P_z) \\ &= \frac{p_x^2 + p_y^2 + p_z^2}{2\mu} I_2^{(1)} \otimes I_2^{(2)} + \frac{\hbar k_{so} p_z}{\mu} \left(\sigma_z^{(1)} \otimes I_2^{(2)} - I_2^{(1)} \otimes \sigma_z^{(2)} \right) \\ &+ \Omega \left(\sigma_x^{(1)} \otimes I_2^{(2)} + I_2^{(1)} \otimes \sigma_x^{(2)} \right) + \left(\delta + \frac{\hbar k_{so} P_z}{M} \right) \left(\sigma_z^{(1)} \otimes I_2^{(2)} + I_2^{(1)} \otimes \sigma_z^{(2)} \right) \\ &+ V_{2b}(r) I_2^{(1)} \otimes I_2^{(2)} \\ \hline [H_{rel}, P_z] = 0 \end{split}$$
parametric dependence on CoM momentum (call

Demands On Numerical Method

- Must be...
 - ...able to treat multiple channels.
 - ...able to describe small and large length scales.
 - ...able to describe eigen energies and eigen states that vary by orders of magnitude.
 - ...applicable to two and three particles.

Our method of choice: Stochastic variational approach with explicitly correlated Gaussian basis function (see also contributed talk yesterday by Roy Yaron).

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

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

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

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

Eigenvalues ε_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).

Question: What changes if Φ_j with $j = 0, 1, \dots$ are not orthogonal?

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

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

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

The eigenvalues ε_l of generalized eigen value equation $\overleftrightarrow{H} \overleftrightarrow{C} = \overleftrightarrow{\varepsilon} \overleftrightarrow{O} \overleftrightarrow{C}$, 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).

Take advantage of the fact that the basis functions Φ_j can be "anything".

Pick Φ_i such that integrals have compact analytical expressions.

Pick Φ_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:

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

Require $r_0 \ll$ other scales: Need to resolve multiple scales. Use Φ_i with "different widths." purely repulsive Gaussian (see also talks by Kievsky)

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

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 $\Pi = +1$.

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

 \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 Φ_1 and calculate ε_1 .
- Goal: Add Φ_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 $(j = 1, \dots, p)$.
 - 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 Φ_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.

Spin-Orbit Coupling: 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 .

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parametric dependence on CoM momentum (call

Non-Interacting Relative Dispersion Curves Along *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?

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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 ¹³³Cs. 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: Enhanced losses between $a_s \approx -7,790a_0$ and $a_s \approx -20,190a_0$. Scattering length window!

Summary

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

Application of this approach to bosons in the presence of 1D spin-orbit coupling.

Generalized radial scaling law for three identical bosons.

Many Thanks To Collaborators

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

Qingze Guan: ECG approach and generalized radial scaling law.

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Three-Boson Spectrum in the Presence of 1D Spin-Orbit Coupling: Efimov's Generalized Radial Scaling Law

Q. Guan and D. Blume

PHYSICAL REVIEW A 100, 042708 (2019)

Energetics and structural properties of two- and three-boson systems in the presence of one-dimensional spin-orbit coupling

Q. Guan[®] and D. Blume

Thank You!