The few-boson problem near unitarity: recent theory and experiments Chris Greene, Purdue University

Revisiting the 3-body parameter for van der Waals two-body interactions

The N>3 boson problem near unitarity

•Thanks, NSF, AFOSR, DOE, BSF!

DAMOP thesis prize co-recipient in 2009





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Strategy of the adiabatic hyperspherical representation: FOR ANY NUMBER OF PARTICLES, convert the partial differential Schroedinger equation into an infinite set of coupled ordinary differential equations:

To solve:
$$\left[-\frac{1}{2\mu} \frac{\partial^2}{\partial R^2} + \frac{\Lambda^2}{2\mu R^2} + V(R,\theta,\varphi) \right] \psi_E = E \psi_E$$

First solve the fixed-R Schroedinger equation, for eigenvalues $U_n(R)$:

$$\left[\frac{\Lambda^2}{2\mu R^2} + \frac{15}{8\mu R^2} + V(R,\theta,\varphi)\right] \Phi_{\nu}(R;\Omega) = U_{\nu}(R) \Phi_{\nu}(R;\Omega)$$

Next expand the desired solution into the complete set of eigenfunctions with unknowns F(R)

$$\rightarrow \psi_E(R,\Omega) = \sum_{\nu} F_{\nu E}(R) \Phi_{\nu}(R;\Omega)$$

And the original T.I.S.Eqn. is transformed into the following set which can be truncated on physical grounds, with the eigenvalues interpretable as adiabatic potential curves, in the Born-Oppenheimer sense.

$$\left[-\frac{1}{2\mu}\frac{d^2}{dR^2} + U_{\nu}(R)\right]F_{\nu E}(R) - \frac{1}{2\mu}\sum_{\nu'}\left[2P_{\nu\nu'}(R)\frac{d}{dR} + Q_{\nu\nu'}(R)\right]F_{\nu' E}(R) = EF_{\nu E}(R)$$

Typically, to solve this PDE, one expands in some basis set and diagonalizes:

$$\left[\frac{\Lambda^2}{2\mu R^2} + \frac{15}{8\mu R^2} + V(R,\theta,\varphi)\right] \Phi_{\nu}(R;\Omega) = U_{\nu}(R) \Phi_{\nu}(R;\Omega)$$

- For three particles, we usually use a B-spline basis to directly solve the coupled PDEs in the two hyperangles → essentially exact
- For N>3 particles, the most efficient method we have found is the correlated Gaussian basis set, implemented for hyperspherical studies by Javier von Stecher, later extended by Doerte Blume
- Another method that works well for N>3 particles, especially at small or modest values of the hyperradius R, is the hyperspherical harmonic expansion, especially if augmented by a few basis functions designed to handle the two-body aymptotic channels

Examples

 Macek, J. Phys. B 1, 831 (1968) ← first idea of adiabatic hyperspherical potential curves, for He two-electron excited states



 The Efimov effect for three particles with short range interactions and infinite scattering length. Efimov's → original paper can be viewed as an example of Macek's adiabatic theory in a limit where it becomes exact.





Another example, a system of 2 positrons and 3 electrons, hyperspherical potential curves showing multiple fragmentation pathways.

Kevin Daily and CHG, 2014 Phys. Rev. A 89, 012503 (correlated gaussians)



FIG. 4. (Color online) The lowest adiabatic potential curves with $L^{\pi} = 0^+$ symmetry for the $(+)_2(-)_3$ system in three dimensions. Dashed, dash-dotted, dash-dot-dotted, and dotted lines are for $(S_+, S_-) = (1, 1/2), (0, 1/2), (1, 3/2), \text{ and } (0, 3/2), \text{ respectively. From top to bottom, the solid lines indicate the asymptotic limits of break-up into <math>2\text{Ps} + e^-$, $\text{Ps} + \text{Ps}^-$, and $\text{Ps}_2 + e^-$, respectively.



FIG. 1: (Color online) Adiabatic potential curves for $L^{\pi} = 0^+$ and charge conjugation eigenvalue +1 shown as effective quantum numbers [see Eq. (14)] vs \sqrt{R} . Panels (a) and (b) are for $(S_+, S_-) = (0, 0)$ and (1, 1), respectively. The thin solid lines show the known asymptotic behavior through order R^{-3} . The asymptotically ionic channel in (a) is the dashdash-dotted line. The dimer-dimer asymptotic thresholds labeled by the angular momentum of the excited Ps.

$$n_{\nu}(R) = \left[-4U_{\nu}(R)/E_H - 1\right]^{-1/2}$$

Daily, von Stecher, CHG, arXiv:1409.6518 e+e+e-e- four-body potential curves for singlet-singlet symmetry, even charge-conjugation symmetry, showing interactions between valence-type channels Ps(n=1)+Ps(nl) and ionic channels like Ps⁻ + e⁺

Calculations of 4-body potential curves used the correlated Gaussian hyperspherical method

See PRA 89, 012503 (2014) PRA 80, 022504 (2009)

These "polyelectron" systems have been studied by many over the years, Wheeler, Ceperley, Adhikari, etc.... FIG. 5: (Color online) Charge redistribution probabilities as a function of scattering energy for SS and (a) positive or (b) negative charge conjugation symmetry. All curves are for dimer-dimer to ionic transitions and are labeled by the dimer-dimer threshold. The ionic threshold is $-0.262E_H$.



Progress in 3-body understanding via hyperspherical ideas:

- Understanding the manifestations of Efimov physics in ultracold 3-body recombination (PRLs: *Macek & Nielsen 1999; Burke, CHG, & Esry 1999*)
 → infinite series of Efimov resonances at a<0 (separated by 22.7)
 → infinite series of interference minima at a>0, (separated by 22.7)
- A quasi-universality of the 3-body parameter for van der Waals interactions, (homonuclear) → experiment = Grimm group PRL 2010 (Berninger et al.)

→ first principles interpretation by Wang, D'Incao, Esry, CHG (2012 PRL) that

approximately a_{3b} = -9.7 r(vdW)

→ newest, even stronger evidence (Naidon et al. 2014 PRL)

\rightarrow extended prediction for heteronuclear Efimov systems AAB like ⁶Li-Cs-Cs,

where the parameter space is far more complicated, since a_{3b} is a function of all four of the following parameters: $r(vdW_{AA})$, $r(vdW_{BA})$, m_A/m_B , a(A-A), i.e. a much more complicated version of universality even in the best case scenario *Wang*, *Wang*, *D'Incao*, *CHG* (2012 *PRL*)

3. Multichannel Efimov scenarios in 3D: Macek & Kartavtsev 2002; *Mehta et al 2008 PRA*; For <u>spinor systems</u>, see Bulgac & Efimov 1975; *Colussi, CHG, & D'Incao, 2014 PRL*

Three-body recombination:

$X + X + X \longrightarrow X_2(v, \ell) + X + E_{v\ell}$

Collision energies: 1 $\mu K \approx 100 \text{ peV}$

•This is important for Bose-Einstein condensates, since the loss of atoms goes as:

$$\frac{dn}{dt} = -L_3 n^3 - L_2 n^2$$

The 3-body term is important at high density, or whenever L_3 gets large, $L_3 \propto a^4$

•Large a is also the same regime where meanfield theory breaks down, namely $na^3 \ge 1$ Vitaly Efimov, 1970 - A three-body system, whose dimers each have infinite scattering lengths and no bound states, must have an infinite number of trimer bound states.



$$E_{n+1} = E_n e^{-2\pi/s_0}$$
, where $s_0 = 1.00624...$ is a universal constant.

General features of three-body recombination



"Recombination length" defined as

Predicted dependence of the 3-body recombination rate on the two-body scattering length,

Esry, Greene, Burke, 1999 PRL:

""...the zero-energy rate should be enhanced at an infinite number of Efimovlike shape resonances as A approaches –infinity." See also: Nielsen & Macek 1999 PRL, and later work by Braaten, Hammer, and coworkers, e.g. 2006 Phys Rep, and Macek, Ovchinnikov, and Gasaneo 2006 PRA



Recombination length ρ_3 defined as

$$\rho_3 = \left[\frac{\mu}{\hbar} K_3\right]^{1/2}$$

Numerical results from over 150 different potentials. The scaling coefficient is given by $c_s = 18.8/r'_0$, where r'_0 is a potentialdependent length scale parameter. Slide from 2001 Trento talk, showing early evidence for universality of the 3-body parameter in minima positions! (Burke, Esry, & CHG unpublished)

Empirically we find that the interaction dependent parameter r_0 is related to the "natural" length scale of the two-body potential, i.e. $r_0 \sim (2\mu C_6/\hbar^2)^{1/4}$ for neutral ground state atoms. (Values given in a.u.)

Atom (Model)	$(2\mu C_6/\hbar^2)^{1/4}$	numerical
⁷ Li $(C_{12} - V_{lr})$	65.0	68.0
23 Na $(C_{12} - V_{lr})$	89.6	96.0
$^{87}{ m Rb}~(C_{12}-V_{lr})$	165.2	
23 Na $(lpha C_6)$	16.0	14.4
39 K ($lpha C_6$)	18.4	16.8
87 Rb ($lpha C_6$)	19.9	18.8

But we thought at that time that this was an artifact of our oversimplified model calculations. In fact this universality turned out to be general for van der Waals interactions

Three-body recombination ``length'' versus a 2006 exp. results



And experiments have confirmed (and sometimes led) a great deal of theory concerning 3-body recombination since the late 1990s, so that we now understand:

- Efimov resonances occur at a<0 (an infinite number of these)
- Destructive interference minima occur at a>0
- The K₃ ~ a⁴ scaling really is there and it makes it difficult to imagine exploring the unitary Bose gas where a→infinity



Zaccanti et al. Nature Physics 2009 expt confirms the a⁴ general scaling and also predicted resonance (a<0) and minima (a>0) features

An obvious conclusion: trying to make a BEC at a→ infinity would be <u>bad</u> <u>news</u>, explosive losses, etc.... •Large a is also the same regime where mean-field theory breaks down $\rightarrow na^3 \ge 1$

<u>i.e.</u> an interesting case of the unitary Bose gas was recently explored by Jose D'Incao, in Sykes et al. PRA 89, 021601(R) (2014), where he found that L₃ saturates when $na^3 \ge 1$ at the unitarity limit except with: $36\sqrt{3}\pi^2 (1 - e^{-4\eta})$

$$L_{3}(k_{B}T) = \frac{56\sqrt{5\pi}}{m^{3}} \frac{(1-e^{-t})}{(k_{B}T)^{2}} \hbar^{5}$$

But replace $[k_{B}T] \rightarrow \hbar\omega_{F}$

for the ⁸⁵Rb experiment [22] ($n \approx 5.5 \times 10^{12} \text{ cm}^{-3}$ and $\eta \approx 0.06$ [45]), we find a lifetime of about 0.20 ms.

The Innsbruck experiment generated a flurry of activity from theorists, attempting to understand this apparent near-constancy of the 3-body parameter observed experimentally

Origin of the Three-Body Parameter Universality in Efimov Physics

Jia Wang,¹ J. P. D'Incao,¹ B. D. Esry,² and Chris H. Greene¹

PRL 108, 263001 (2012)

Other relevant theoretical work to interpret this result: Cheng Chin's toy model (arXiv 2011)

And detailed hyperspherical calculations by Naidon, Endo, & Ueda:

``Physical Origin of the Universal Three-body Parameter in Atomic Efimov Physics" *arXiv*:1208.3912 (largely confirms our interpretation), and more recently, PRL 112, 105301 (2014)

> R. Schmidt, S. P. Rath and W. Zwerger, Eur. Phys. J. B 85, 386 (2012).

See also → P. K. Sorensen, D. V. Fedorov, A. S. Jensen, N. T. Zinner, Phys. Rev. A 86, 052516 (2012). The "three-body parameter" controlling the first Efimov resonance location had been thought to be more or less "random", but the new experimental evidence strongly suggests that it must be approximately universal:

- 1) 133 Cs (Berninger et al.) PRL 107, 120401 (2011) : |a-|/ L_{vdW}= 9.4, 11.1, 10.4, and 10.3
- 2) ⁷Li (Hulet) Science 326, 1683 (2009) : $|a-|/ L_{vdW} = 10.0$
- 3) ⁷Li (Khaykovich) PRL 103, 163202 (2009) : $|a-|/ L_{vdW} = 8.9$
- 4) ⁷Li (Khaykovich) PRL 105, 103203 (2010) : |a-|/ L_{vdW}= 9.0
- 5) ³⁹K (Modungno) Nat. Phys. 5, 586 (2009): |a-|/ L_{vdW}= 11.0
- 6) ⁸⁵Rb(Cornell-Jin group at JILA) 2012 PRL: |a-|/ L_{vdW}= 9.7(1)

Also Roy et al for ³⁹K → **PRL 111, 053202 (2013)**

3-body hyperspherical potential curves based on 2-body Lennard-Jones interaction potential with 10 s-wave bound states, around 100 total, including all angular momentum states



Figure 5.12: This figure shows the three-body potentials obtained using the $v_{\lambda}^{a}(\lambda = \lambda_{10}^{*})$ model supporting a total of 100 bound states. Roughly speaking, the potential of Eq. (5.18) [16] (black solid line) can be seen as a diabatic potential since it passes near one of the series of avoided crossings.

PRL 2012 Jia Wang, D'Incao, Esry, CHG



FIG. 4: Values for the three-body parameter (a) κ_* and (b) a_{3b}^- as functions of the number *n* of two-body *s*-wave bound states for each of the potential model studied here. (c) Experimental values for a_{3b}^- for ¹³³Cs [3] (red: \times , +, \square , and *), ³⁹K [4] (magenta: \triangle), ⁷Li [5] (blue: •) and [6, 7] (green: \blacksquare and \circ), ⁶Li [8, 9] (cyan: \blacktriangle and \bigtriangledown) and [10, 11] (brown: \checkmark and \diamondsuit), and ⁸⁵Rb [12] (black: \blacklozenge). The gray region specifies a band where there is a ±15% deviation from the v_{vdW}^{hs} results. The inset of

Another finding: This property of 3-atom states is not expected to hold for nuclear systems, which have no van der Waals tail and few bound states. So this might be re-phrased as a QUASI-Universality of the 3-body parameter

Our study of hyperspherical potentials in the bosonic A+A+A system, showing that any two atoms "go over the van der Waals cliff" when they approach within their vdW radius, and this rise in kinetic energy produces a repulsive hyperspherical potential barrier



Even more convincing is a study of the broad resonance limit of the 3-body parameter for homonuclear A+A+A systems, and its dependence on different 2-body interactions, **PRL 112, 105301 (2014):**

Microscopic Origin and Universality Classes of the Efimov Three-Body Parameter



"...In the particular case of a van der Waals tail, we obtain a_=-10.86(1) r6, and kappa = 0.187(1)/r6 in good agreement with **Ref.25(Wang et al)** and experimental observations."

Note: Their excellent numerics are based on a separable potential model Next, what can theory PREDICT for the heteronuclear Efimov

Universal three-body parameter in heteronuclear atomic systems

Yujun Wang, Jia Wang, J. P. D'Incao, & CHG PRL 109, 243201 (2012)

<u>Main result</u>: we see that the Efimov physics is also universal for the case of 2 identical bosonic atoms (AA) and 1 distinguishable atom (X), but the parameter space is larger and more complicated. This is because the universality values predicted depend on the mass ratio, M_A/M_X , and on the background A-A scattering length, and on TWO different vdW radii (A-X and A-A).

(also online at arXiv:1207.6439)

The Efimov effect: universality



For three particles with two or three resonant interactions (scattering length $a \to \infty$), an infinite series of three-body bound states emerge with $E_n = E_0 e^{-2n\pi/s_0}$ [1].

Heteronuclear system *AAX*: *Efimov-favored* when $m_A/m_X \gg 1$ such that $s_0 > 1$; *Efimov-unfavored* when $m_A/m_X \lesssim 1$ 1 such that $s_0 < 1$.

Three-body parameter can be expressed in three-body recombination observables a_{-}^{*} (first Efimov resonance) or a_{0}^{*} (first interference minimum).

For identical bosonic atoms, $a_{-}^* \approx -9.1 r_{vdW} [r_{vdW} = (2\mu_2 C_6)^{1/4}/2]$.

Universal three-body parameter for AAX?

Key finding: Our numerical evidence suggests that the 3-body parameter is UNIVERSAL for heteronuclear AAX systems also, but this universality depends on the AA scattering length, the mass ratio, and the two van der Waals lengths, and must be mapped out

Efimov-favored AAX systems — universal three-body parameter



Predictions of first Efimov resonance (negative a) and destructive interference Stueckelberg minimum (positive a)

	s_0	s_0^*	$a_{AA,bg}$ (a.u.)	a_0^* (a.u.)	a_{-}^{*} (a.u.)	<u>Exp[π/s₀]</u>
¹⁷⁴ Yb ₂ ⁶ Li	2.246	2.382	104 [32, 33]	1.3×10^3	-8.4×10^2	4.050 -
$^{133}\mathrm{Cs_2}^6\mathrm{Li}$	1.983	2.155	2000 [34]	9.6×10^2	-1.4×10^3	4.876
$\mathrm{^{87}Rb_2{^6}Li}$	1.633	1.860	100 [35]	3.8×10^2	-1.6×10^3	6.847
$\rm ^{41}K_2{}^6Li$	1.154	1.477	62 [<mark>36</mark>]	3.7×10^2	-2.4×10^3	15.2
$^{23}\mathrm{Na_2}^6\mathrm{Li}$	0.875	1.269	100 [37]	1.5×10^3	-1.3×10^4	36.2
${}^{87}\mathrm{Rb_2}{}^{40}\mathrm{K}$	0.653	1.125	100	2.8×10^3	$<-3\times10^4$	123
$^{133}\mathrm{Cs_2}^{87}\mathrm{Rb}$	0.535	1.060	2000	2.3×10^3	$<-4\times10^4$	355
${}^{41}\mathrm{K_2}{}^{87}\mathrm{Rb}$	0.246	0.961	62	$> 7 \times 10^3$	$< -1 \times 10^{6}$	3.52x10⁵

TABLE I: The universal Efimov scaling constants s_0 , s_0^* and the 3BPs $a_{AX} = a_0^*$ and $a_{AX} = a_-^*$ obtained by keeping a_{AA} fixed at its background value $(a_{AA,bg})$.

Our prediction from this 2012 PRL was that the first Cs-Cs-Li resonance should appear at either a = -1400 or else -1400/4.88 = -287 a.u. The new Chicago experiment observes a_(expt)= -337(9) a.u.

And the other big piece of excitement comes from the 6Li-Cs-Cs experiment of Cheng Chin, Shi-Kuang Tung, and collaborators at the University of Chicago, who have observed 3 Efimov trimers with approximately the expected Efimov 4.87 geometric scaling factor between them: arXiv:1402.5943v1

Observation of geometric scaling of Efimov states in a Fermi-Bose Li-Cs mixture



FIG. 3. Observation of three Li-Cs-Cs Efimov resonances. a. Scaled Li number versus magnetic field showing

Observation of Efimov Resonances in a Mixture with Extreme Mass Imbalance

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The first resonance is detected at a scattering length of $a_{-}^{(0)} = -320(10)a_{0}$.

Theory prediction from our 2012 PRL was that the first Cs-Cs-Li resonance should appear at either a= -1400 or else -1400/4.88 = -287 a.u. The Chicago experiment observes a_(expt)= -337(9) a.u.

The second resonance appears at $5.8(1.0)a_{-}^{(0)}$, close to the unitaritylimited regime at the sample temperature of 450 nK. Indication of a third resonance is found in the atom loss spectra. The scaling of the resonance positions is close to the predicted universal scaling value of 4.9 for zero temperature. Deviations from universality might be caused by finite-range and temperature effects, as well as magnetic field-dependent Cs-Cs interactions.

Spinor systems in few-body and many-body physics

Most early dilute gas BECs were make of atoms in only one hyperfine spin substate. But within a few years of experimental BEC progress, spinor systems were investigated, in which the number of atoms in different spin substates is not individually conserved.

e.g. there are collisions between two atoms $|f_1,m_1\rangle$ and $|f_2,m_2\rangle$ that can change m1 and m2, processes like:

 $|1,0> + |1,0> \rightarrow |1,1> + |1,-1>$

These are controlled by two rotationally-invariant scattering lengths, a_0 and a_2 for a system of f=1 atoms. Instead for a system of f=2 atoms, there are four invariant scattering lengths controlling the nature of the BEC, namely a_0 , a_2 , a_4 .

Review D. M. Stamper-Kurn and M. Ueda, Rev. Mod. Phys. 85, article: 1191 (2013)

Three-Body Physics in Strongly Correlated Spinor Condensates

The idea: when bosonic atoms have a spin degeneracy, the different spin substates can combine in different ways at large scattering lengths, producing multiple Efimov families with different universal exponents.

$$\hat{v}(r) = \frac{4\pi\hat{A}}{m}\delta^3(\vec{r})\frac{\partial}{\partial r}r$$

$$\hat{A} = \sum_{F_{2b}M_{F_{2b}}} a_{F_{2b}} |F_{2b}M_{F_{2b}}\rangle \langle F_{2b}M_{F_{2b}}|$$

TABLE I. Values of s_{ν} relevant for f = 1 and 2 spinor condensates covering all possible regions of R for the different L ranges of the relevant scattering lengths. For f = 1, we list the lowest few values of s_{ν} for each F_{3b} while for f = 2 we only list the values of s_{ν} and their multiplicity (superscript), instead of the specific value of F_{3b} where they occur.

$$(f=1)$$
 $F_{3b} = 1$ $F_{3b} = 2$ $F_{3b} = 3$ $R \ll |a_{\{0,2\}}|$ 1.0062i, 2.16622.16621.0062i, 4.4653 $|a_0| \ll R \ll |a_2|$ 0.74292.16621.0062i, 4.4653 $|a_2| \ll R \ll |a_0|$ 0.409742 $R \gg |a_{\{0,2\}}|$ 242

PRL 113, 045302 (2014)

Colussi, CHG, and D'Incao

$$J_{\nu}(R) = \frac{s_{\nu}(R)^2 - 1/4}{2\mu R^2}$$

$$U_{\nu}(R) = \frac{s_{\nu}(R)^2 - 1/4}{2\mu R^2}$$



Thus one could in principle observe multiple Efimov families in spinor few-body systems, having different characteristic Efimov exponent parameter s_0 . This effect has not yet been observed in experiment.



FIG. 1 (color online). $F_{3b} = 1$ (red solid line), 2 (green dashed line), and 3 (blue dash-dotted line) hyperspherical adiabatic potentials for f = 1 spinors with $a_0 = 10^2 r_{vdW}$ and $a_2 = 10^5 r_{vdW}$. (a) For $R \le \{a_0, a_2\}$ (shaded region) two attractive potentials exist (both with $s_0 \approx 1.0062i$), allowing for two families of Efimov states, and for $R > a_0$, one of these potentials turns into an atom-dimer channel $|F_{2b} = 0, M_{F_{2b}} = 0\rangle + |m_f = 0\rangle$

Example of multiple Efimov families for a spinor 3-boson system, homonuclear Efimov states embedded in the three-body continuum

Mehta, Rittenhouse, D'Incao, CHG

PHYSICAL REVIEW A 78, 020701(R) (2008)



Efimov physics beyond scale invariance and universality: The reality for most atomic systems is that there will be multiple two-body channel thresholds, and also therefore multiple 3-body breakup thresholds, as in the example above.

Summary

- For atomic few-body systems (but probably not for nuclear systems), two body physics can predict the three-body parameter to about 15% or better accuracy
- 2. For heteronuclear AAB systems there is a more complicated universality that depends on 4 parameters, but need more experiments/theories
- 3. Going beyond 4 or 5 particles is challenging, especially for the description of N-body scattering observables such as recombination or breakup rates