Challenges ahead in atomic, molecular, and nuclear few-body physics Chris H Greene, Purdue University

Few-body reactive processes, bound states, and resonances

- Develop an analytic zero-range interaction solution to the four-body problem, analogous to the well-known exact solution to the zero-range 3body problem
- Push numerical and/or analytical methods to treat more than 5 particles (e.g. atoms or nucleons), with or without spin, in their full Hilbert space including collisions

Challenges in the atomic realm

- Can the disastrously bad N⁷ scaling of all-electron methods ever be overcome?
- Bring electron-atom (or ion) scattering theory to spectroscopic accuracy, comparable to the best treatments of bound state correlations?
- Compute electron-atom scattering lengths for any atom in the periodic table to within 10-20%?

Challenges in the molecular realm (diatomics & triatomics)

- Developing a theory and/or computational method that can determine the FULL electron-molecule scattering matrix including ALL fragmentation channels (e.g. in H₂: e + H₂+, H(n₁ l₁)+H(n₂ l₂), p + H⁻, etc.)
- Formulate a quantitatively accurate theory that can calculate the Born-Oppenheimer potential curves for two heavy open shell atoms, and their scattering lengths versus magnetic field

https://arxiv.org/a/greene_c_1.html





Here are some of the theory directions stimulated by sensing the power of an unconventional idea/toolkit, and exploring where it might yield valuable insights.

In this case, it is the adiabatic toolkit, broadly interpreted



Many Big Goals have been formulated for the field of ultracold atoms over the past 3 decades, such as:

- Realize the BCS-BEC crossover, by using tunable Fano-Feshbach resonances (accomplished!)
- Create a cold atom system that simulates high-Tc superconductivity, and helps to understand it. (not yet?)
- Realize the Fractional Quantum Hall effect with trapped atoms (perhaps only partially, in a sense)
- Simulate nuclear reactive processes, except with ultracold fermionic atoms instead of nucleons (not yet)

Challenges in the Realm of Few-Body Physics

**Current progress in the full treatment of N particles with short-range interactions has largely stalled at around 4 or 5 particles. Let's push this to more complex systems.

Limited bound state calculations for highly simplified Hamiltonians (e.g. Gaussian interactions) have occasionally treated more, e.g. up to around 8 or 10 particles. Many more particles than that have been treated by a variety of Monte Carlo methods, but usually only the ground state.

Treatments of collision/reactive processes for 5 particles are highly limited (examples shown below), and for 6 particles even fewer, and usually with extreme approximations.

Why is this a hard problem? The N-body Schroedinger equation with no external forces has dimension 3N-3, e.g. for 6 particles it is a 15-dimensional PDE.

Monte Carlo methods exist to solve for ground states in high dimensional problems, but those methods have difficulty to describe collision processes, especially reactive ones One of our long-time goals has been to improve our ability to understand <u>reactivity</u> of all kinds for systems having more and more particles, e.g. in <u>chemical or nuclear or cold atom</u> physics, reactions like:

 A_2 +BCD \rightarrow AB+AC+D or \rightarrow A_2D+BC, etc.

This is the famous "N-body problem" in quantum mechanics

In FEW BODY PHYSICS, N might be 2 or 3 or 4 or 5 or

We have pursued this goal primarily by improving what we call the

"Adiabatic Hyperspherical Coordinate Toolkit",

both a mathematical technique and a way to gain intuition

One Key Idea: From Enrico Fermi – understanding the energy content of a single scattering event at low energies, i.e., what we now call

THE FERMI PSEUDOPOTENTIAL (models short range interactions at very low energy)



$$U(\vec{r}) = \frac{2\pi a\hbar^2}{m_{\rm red}} \delta(\vec{r} - \vec{R})$$

$$a = -\mathrm{Lim}_{k\to 0} \tan \delta_0(k)/k$$

In the low energy limit of a particle colliding with another particle through only the S-wave, the energy of interaction is controlled by the <u>scattering length a</u> and can be represented by *U*.

From left to right: Oscar D'Agostino, Emilio Segrè, Edoardo Amaldi, Franco Rasetti and Enrico Fermi, from Wikipedia, the "Panispera Boys" The following discussion addresses a simple but fundamental question, for bosonic atoms:

We know that in 3D a certain minimum strength of attraction is needed in order to just barely bind two atoms into a stable molecular bound state.

molecules get formed in a gas of trapped free atoms?

Extensions of Universal Physics to N>3 bosonic particles in 3D ----Schroedinger's equation with pair-wise additive forces:



FAST TRACK COMMUNICATION

Weakly bound cluster states of Efimov character MORE THAN 4 BOSONS: von Stecher's J. Phys. B article in 2010: combined study using correlate

MORE THAN 4 BOSONS: von Stecher's J. Phys. B article in 2010: combined study using correlated Gaussians, and diffusion Monte Carlo

Javier von Stecher



Clusters predicted up to N=13. The idea of hyperspherical coordinates: replace the N independent-particle coordinates, namely:

 $\{x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, ...\}$

by a representation in hyperspherical coordinates, which

look like:

 $\{R, \theta_1, \theta_2, \theta_3, \theta_4, \dots\}$

where now there is only ONE length-dimension coordinate, the hyperradius R, plus (N-1) hyperangles.

And now, treat *R* as an adiabatic coordinate, implementing the very same math as in the Born-Oppenheimer approximation of physical chemistry, and calculate energy levels versus the hyperradius, $U_v(R)$, which gives us similar interpretive power as when we look at a diatomic molecule's potential energy curve.



To a mathematician, this would be called an "n-ball", i.e. a sphere in ndimensions How to tackle 5-body recombination for 5 free bosonic atoms with pairwise additive forces?

i.e. the reaction A+A+A+A+A \rightarrow A₃+A₂ or A₄+A or...

Start with the time-independent Schroedinger equation:

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{p_3^2}{2m_3} + \frac{p_4^2}{2m_4} + \frac{p_5^2}{2m_5}$$

 $+ V(r_{12}) + V(r_{13}) + V(r_{14}) + V(r_{15}) + V(r_{23}) + V(r_{24}) + V(r_{25}) + V(r_{34}) + V(r_{35}) + V(r_{45})$

After eliminating the center-of-mass degree of freedom, we're left with a 12-dimensional PDE to solve, which can be reduced to **a mere 9 dimensions** for J=0 states after going to the body frame.

So we go to hyperspherical coordinates with only one distance **R** and 3N-4 hyperangles to represent the remainder

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):

Γ.

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

Next expand the desired solution into the complete set of hyperangle = 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

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

This is a divide-and-conquer strategy: how to leverage bound state calculations to solve collision problems

Our group has advanced this approach to solving the manyparticle Schroedinger equation in diverse contexts, from chemical physics to Bose-Einstein condensates in ultracold science to the fractional quantum Hall effect, the 4-neutron problem, and very recently, to the 5-boson problem

Hyperspherical Potential Energy Curve Examples

Simplest triatomic molecule (dissociative recombination of $\rm H_{3}{}^{+}$)



Integer and fractional quantum Hall effect (2D electron gas in a B-field)



Short history of the Efimov effect for three identical bosons:

In 1970, Efimov considered the problem of 3 particles with a scattering length "a" tuned to infinity. In this scenario, NO 2-body bound states exist in 3D. Nevertheless, Efimov predicted that an **infinite number** of 3-BODY bound states must exist.

This was not observed experimentally for several decades, until the possibility to CONTROLLABLY CHANGE the atom-atom scattering length **'a'** became possible in an ultracold atomic gas, thanks to magnetic Feshbach resonances.

The spark that allowed the Efimov states to be observed in an ultracold gas came in a theory study that was studying something else, the 3-body recombination process in the gas, namely:

 $A + A + A \rightarrow A_2 + A$... in late 1990s

which is the dominant loss process in a Bose-Einstein condensate (usually)

By 1999, our goal was to study 3-body recombination in an ultracold Bose gas, and find the systematics as well as possible ideas that might enable control of this dastardly loss process that was limiting the lifetime of BECs: Esry, CHG, Burke, PRL 83, 1751 (1999), $A+A+A \rightarrow A_2+A$



Three-body recombination rate plotted as a "recombination length", versus the atom-atom scattering length A, showing a prominent Efimov resonance in agreement with 3-body theory at A=-850 Bohr radii

Figure 2 | Observation of the Efimov resonance in measurements of three-body recombination. The recombination length $\rho_3 \propto L_3^{1/4}$ is plotted as a function of the scattering length *a*. The dots and the filled triangles show

Qualitative pictures of the 2-different quantum mechanisms for 3-body recombination

QUANTUM PHYSICS

A ménage à trois laid bare

After the 3-particle Efimov effect was proved correct, our attention turned to the 4-body problem next, as we realized that our divide-and-conquer hyperspherical strategy should work there too.

It took a major effort and a development of better ways to solve for the potential energy curves and nonadiabatic couplings, but we succeeded and were able to calculate 4-body recombination resonances, which had physics connected to Efimov states.

A very talented PhD student in my group, Javier von Stecher, spearheaded the treatment that solved the 4-body problem, and he was co-recipient of the DAMOP thesis award for that work.

Other theorists (especially Deltuva) have since confirmed that work and have carried out even much more accurate calculations of 4-boson recombination.

But there have been almost no calculations of 5-body recombination, until very recently.

How Efimov physics extends to more than 3 particles. This figure shows the schematic entrance channel potential curve expected for N particles at negative 2-body scattering length, From Mehta et al., 2009 PRL

FIG. 1 (color online). A schematic representation of the N-boson hyperradial potential curves is shown. When a meta-stable N-boson state crosses the collision energy threshold at E = 0, N-body recombination into a lower channel with N - 1 atoms bound plus one free atom is resonantly enhanced.

Before we could actually calculate the rate of 4-body recombination in an ultracold gas, we had to develop some scattering theory:

PRL 103, 153201 (2009)

A general theoretical description of N-body recombination

N. P. Mehta,^{1,2} Seth T. Rittenhouse,¹ J. P. D'Incao,¹ J. von Stecher,¹ and Chris H. Greene¹

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We present a formula for the cross section and event rate constant describing recombination of N particles in terms of general S-matrix elements. Our result immediately yields the generalized Wigner threshold scaling for the recombination of N bosons. We find that four-boson recombination is resonantly enhanced by the presence of metastable states in the entrance channel. Hence, recombination into a trimer-atom channel could be an effective mechanism for the formation of Efimov trimers.

And here it is, THE FORMULA for N-boson recombination, i.e. for the process: A+A+A+....+..A \rightarrow A_{N-1}+A or A_{N-2}+A+A +...etc.

$$K_N^{0^+} = \frac{2\pi\hbar}{\mu_N} N! \left(\frac{2\pi}{k}\right)^{(3N-5)} \frac{\Gamma\left((3N-3)/2\right)}{2\pi^{(3N-3)/2}} \left|S_{f0}^{0^+}\right|^2$$

Since 2006 – We initiated a concerted effort on the 4body problem using hyperspherical coordinates

Resulting 2009 papers:

Correlated Gaussian Hyperspherical Method for Few-Body Systems

PRA 80, 022504, (2009)

Javier von Stecher and Chris H. Greene

Universal Four-Boson States in Ultracold Molecular Gases: Resonant Effects in Dimer-Dimer Collisions PRL 103, 033004, 2009

J. P. D'Incao,^{1,2} J. von Stecher,¹ and Chris H. Greene¹

A general theoretical description of N-body recombination (2009).

N. P. Mehta,^{1,2} Seth T. Rittenhouse,¹ J. P. D'Incao,^{1,3} J. von Stecher,¹ and Chris H. Greene¹

Signatures of universal four-body phenomena and their relation to the Efimov effect Nature Phys. 5, 417 (2009)

J. von Stecher, J. P. D'Incao and Chris H. Greene*

Dimer-dimer collisions at finite energies in two-component Fermi gasesPhys. Rev. A 79,J. P. D'Incao, Seth T. Rittenhouse, N. P. Mehta,* and Chris H. Greene030501(R), (2009)

Technical Point: How to solve this high-dimensional PDE at many different values of the hyperradius, in order to determine the potential energy curves U(R) and their couplings: the correlated Gaussian hyperspherical method

$$\Phi_{\nu}(R,\Omega) = \hat{S} \sum_{j} c_{j} e^{-\frac{1}{2}x^{T}} \underline{A}_{j} x [\Theta_{L}^{K}(\boldsymbol{u},\boldsymbol{x}) \times \chi_{S}]_{JM_{J}}$$

This basis set has been the decisive tool, developed in Javier von Stecher's thesis work. Note that the Gaussian parameters in the basis set are determined stochastically.

The main difference from other Gaussian expansion calculations, e.g. by Suzuki and Varga, is that we have to perform all integrals at fixed hyperradius R, in the matrix elements of the fixed-R Hamiltonian. But we have found a way to do those integrals for an arbitrary number of particles and dimensions analytically, except for one final 1D integral in the complex plane that still must be done numerically.

Key finding:

Two four-body states are found to lie between each successive pair of Efimov trimers - von Stecher et al. Nature Phys. 2009 – which confirms insightful work by <u>Platter and Hammer (</u>Eur. Phys. J. A. 2007), and extends it

Figure from Ferlaino & Grimm. See also Ferlaino et al., PRL 102, 140401 (2009) for experimental confirmation, and later theoretical extensions by Deltuva. Extended Efimov plot showing universal dimer, trimer, and tetramer states of four identical bosons with short-range interactions.

Tetramer states predicted to hit zero energy at a=0.43 a(Efimov) and a=0.90 a(Efimov)

And, after our four-body recombination resonance predictions were verified experimentally, we felt that one should try eventually to tackle 5-atom recombination The amount of attention to the 5-body problem in collision physics has not been very extensive. Here is one early reference.

Example of 5-body scattering theory (formalism only):

Tatuya SASAKAWAFive-Body EquationSupplement of the Progress of Theoretical Physics, No. 61, 1977

→ Formulated the Fadeev-Yakubovsky coupled equations that would need to be solved.

Citations to date: 3 (all by Lazauskas and/or Carbonell)

Fig. 91.1 Jacobi coordinate sets proper to 5-body Faddeev-Yakubovsky components. From left to right components $\mathcal{K}_{12,3}^4$, \mathcal{H}_{12}^{34} , $\mathcal{T}_{12,3}$, \mathcal{S}_{12}^{34} and \mathcal{F}_{12}^{34} are represented

$$\begin{cases} \mathcal{K}_{ij,k}^{l} = G_{ij}V_{ij}\left(\mathcal{K}_{ik,j}^{l} + K_{jk,i}^{l} + \psi_{ik}^{ikl} + \psi_{jk}^{jkl} + \psi_{ik}^{ik,jl} + \psi_{jk}^{jk,il}\right), \\ \mathcal{H}_{ij}^{kl} = G_{ij}V_{ij}\left(\mathcal{H}_{kl}^{ij} + \psi_{kl}^{jkl} + \psi_{kl}^{ikl}\right), \\ \mathcal{T}_{ij,k} = G_{ij}V_{ij}\left(\mathcal{T}_{ik,j} + \mathcal{T}_{jk,i} + \psi_{ik}^{lm} + \psi_{jk}^{lm}\right), \\ \mathcal{S}_{ij}^{lm} = G_{ij}V_{ij}\left(\mathcal{F}_{lm}^{ij} + \psi_{lm}^{jk} + \psi_{lm}^{ik}\right), \\ \mathcal{F}_{ij}^{lm} = G_{ij}V_{ij}\left(\mathcal{S}_{lm}^{ij} + \psi_{lm}^{klm}\right). \end{cases}$$
(91.3)

This has only been applied to solve the simplest 5-body scattering problem, namely neutron+ ⁴He elastic scattering

FIGURE 10 Apparent correlation between the calculated ⁴He binding energies and n-⁴He scattering length. Calculated values are compared with those adapted from the experiment by NIST [100], Atlas n-res [99], and TUNL [25]. Interesting result, a correlation between the ⁴He binding energy and the n-⁴He elastic scattering length Example calculation: Probably THE most impressive and IMPORTANT 5-body reaction computed to date is the $d+t \rightarrow \alpha + n$ nuclear fusion reaction, accomplished using the no-core shell model approach, plus huge computational resources (i.e. from the Lawrence Livermore National Laboratory (LLNL) institutional Computing Grand Challenge program) As far as I am aware, this is probably the ONLY realistic computation of this 5-nucleon reaction carried out to date, and the reference below is the latest study, showing that by polarizing the colliding fragments, a large increase in efficiency results

https://doi.org/10.1038/s41467-018-08052-6

OPEN

Ab initio predictions for polarized deuteriumtritium thermonuclear fusion

Guillaume Hupin^{1,2,3}, Sofia Quaglioni ³ & Petr Navrátil⁴

Why is there ONLY ONE full 5-nucleon calculation to date that includes 3-nucleon interactions? It is a high dimensional Hilbert space AND it is a problem in the scattering continuum.

Fig. 1 Unpolarized DT cross sections. **a** Astrophysical S-factor as a function of the energy in the center-of-mass (c.m.) frame, $E_{c.m.}$, compared to

Our very recent article on a 5-atom reactive process

PNAS 2025 Vol. 122 No. 18 e2503390122

Five-body recombination of identical bosons

Michael D. Higgins^{a,1} and Chris H. Greene^{a,b,1,2}

Adiabatic hyperspherical potential curves for 5 cesium atoms, showing the entrance 5body continuum channels at W>0, and a bound 4+1 recombination channel that is negative beyond about $R = 2 r_0$.

Fig. 1. Conceptual picture of a 5-body recombination event, where 5 free atoms collide and exchange energy, resulting in 4 of those atoms bound together as a tetramer and the fifth atom flying away with the majority of the kinetic energy released.

Five-body recombination rate coefficient versus twobody scattering length, showing a resonance in Cs_5^* Comparison of 3, 4, and 5-body recombination loss rates, expressed as effective 3-body rates, for a realistic experimental cold Cs atom density.

Somewhat surprisingly, there are clear regions of the twobody scattering length **a** where the dominant loss process is actually 5-body recombination

Note: there are three 5-body recombination resonances per Efimov cycle

Fig. 7. Effective 3-body loss rates, displayed as L_3 , n_0L_4 , and $n_0^2L_5$ for a

Our article with the Innsbruck group in 2013. The first and only experimental observation of 5-body recombination (as far as I'm aware).

Resonant Five-Body Recombination in an Ultracold Gas

A. Zenesini, B. Huang, M. Berninger, S. Besler, H.-C. Nägerl, F. Ferlaino, and R. Grimm

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Chris H. Greene and J. von Stecher*

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New Journal of Physics 15 (2013) 043040

FIG. 1. (color online) *N*-body scenario in the region of negative twobody scattering length *a*. The lower panel shows the *N*-body binding energies as a function of the inverse scattering length. $E_3^U = (\bar{h}\kappa)^2/m$ is the trimer binding energy for resonant interaction. The dotted,

The most attractive hyperspherical potential curves for the 4n and 3n systems, obtained using realistic n-n interaction potentials

Nuclear physics: Does the tetraneutron exist? Controversy!

Totally repulsive potential energy curves we computed for the 3-neutron and 4neutron systems, that we argue are a DISPROOF of any possible existence of a tri-neutron or a tetraneutron bound state or resonance.

The converged potentials are clearly totally repulsive, with <u>no sign of a local maximum</u> that can trap probability in a resonance.

ρ (fm) Higgins, CHG, Kievsky, Viviani PHYSICAL REVIEW LETTERS 125, 052501 (2020) PHYSICAL REVIEW C 111, 014001 (2025), Michael Higgins & CHG **Resonances and collisional properties of neutron-rich helium isotopes in the adiabatic hyperspherical representation** Our first 5-body calculation in nuclear physics: the ⁸He nucleus

FIG. 9. The lowest few Born-Oppenheimer potential curves for the ⁴He +4*n* system in the $(L^{\pi}, S)J^{\pi} = (0, 0)0^+$ symmetry. The solid curves are the Born-Oppenheimer potentials and the dashed curves are the adiabatic potentials, which includes the diagonal secondderivative coupling term. Only the lowest two adiabatic potentials are shown here. Adiabatic hyperspherical potential energy curves, energy versus hyperradius, for the 0+ symmetry of the ⁸He nucleus.

A goal for the future is to compute such potential energy graphs for the lowest few symmetries, for all nuclei up to A=8, as a way to visualize and compute reaction pathways in energy and position.

Future 6-body challenges for theory:

- Collision between two Efimov trimers at ultracold temperature (the best to date is a very approximate treatment by Naidon, Endo, and Garcia-Garcia 2016)
- Triton-Triton fusion reaction, t+t $\rightarrow \alpha$ + n + n
- Note that there is a fully analytical solution of the 3body hyperangular problem with zero-range (S-wave) interactions, but <u>a similar analytical solution has</u> <u>never been found for the 4-body problem</u>. This would be a desirable goal for theory to solve, if possible.

Conclusion:

Progress is underway to extend the predictive and analysis power of the adiabatic hyperspherical representation to handle more particles and more complex few-particle scenarios in both nuclear and atomic systems.

But these are hard problems and each bit of progress is hard-earned....

Thanks for listening!