EFIMOV EFFECT AND RESONANCES IN ATOMIC AND MOLECULAR PHYSICS

Hiroya Suno
Advanced Institute for Computational Science and Nishina Center, RIKEN
12 December 2012,
YITP Workshop:
Resonances and non-Hermitian systems in quantum mechanics

About myself

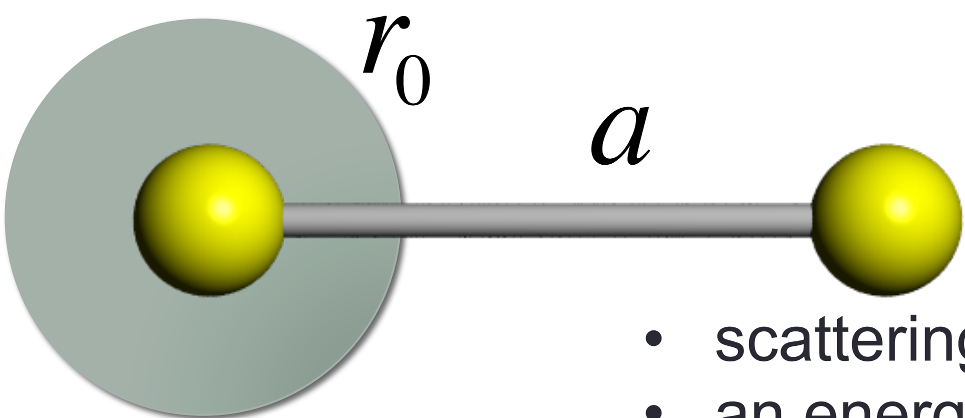
- My research specialty: theoretical atomic & molecular physics
- RIKEN Advanced Institute for Computational Science (K computer, Lattice QCD)

- RIKEN Nishina Center, working in collaboration with Dr. E. Hiyama (Few-body problem)

What is the “Efimov effect”?

- An effect in **quantum few-body systems** predicted by the Soviet theoretical physist **Vitaly Efimov.**

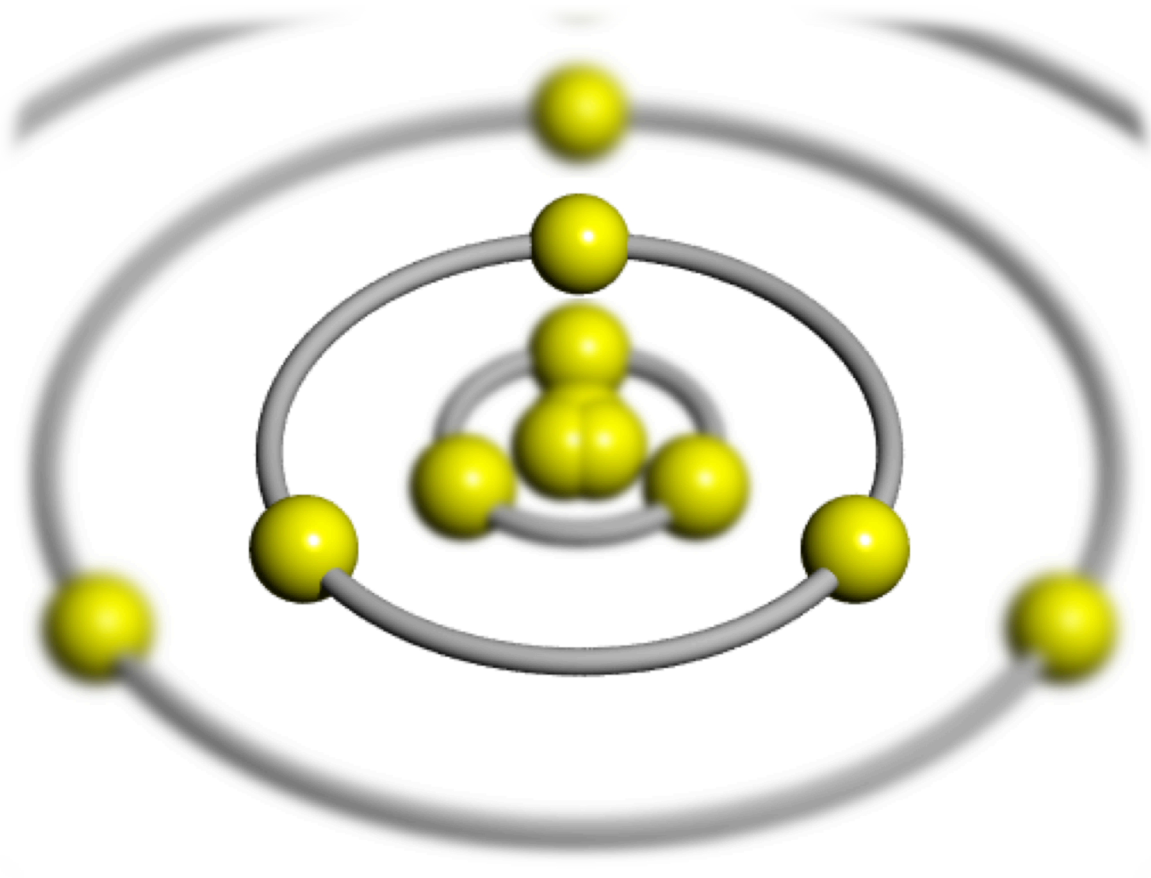
He considered **2 particles interacting with resonant forces.**



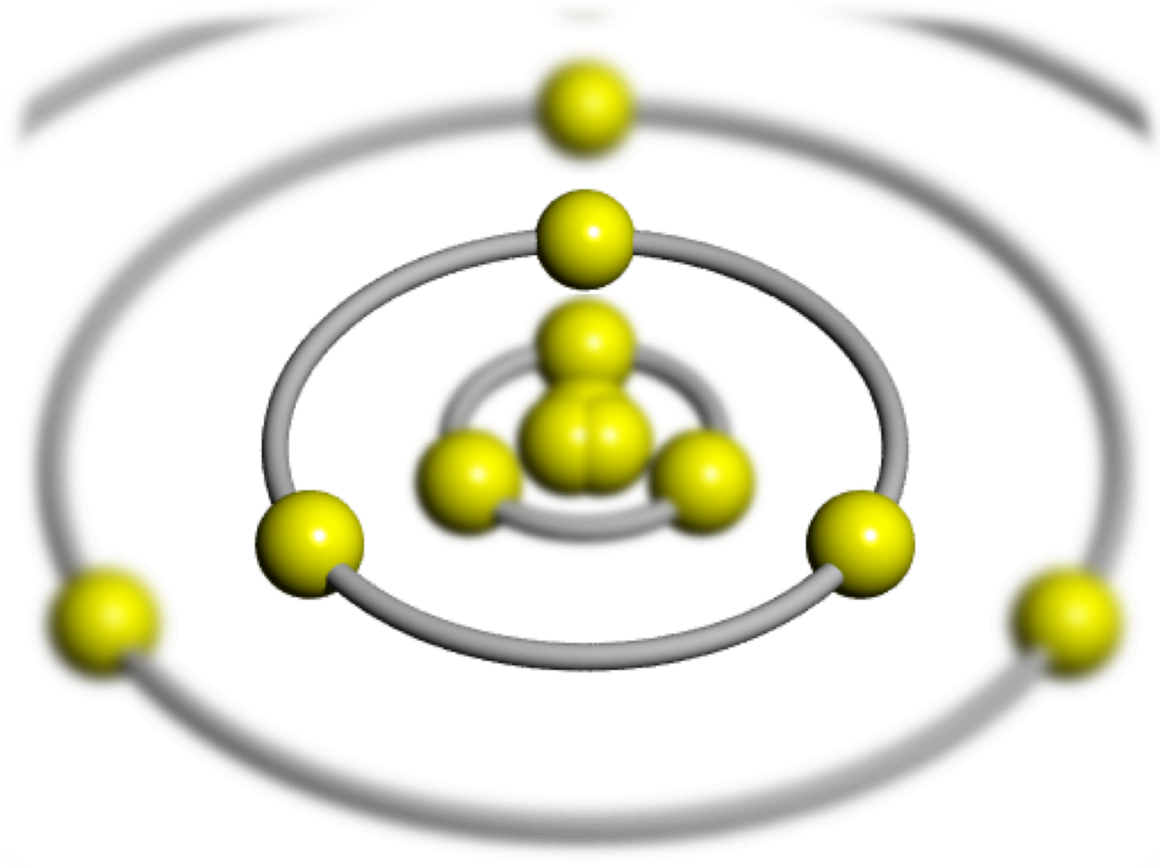
$$a >> r_0$$

- scattering length >> potential range
- an energy level at the threshold

If we put one more particle to this,
an infinite number of bound states will appear…



… even if its subsystems don't bind!



These are "Efimov states" and possess a universal character --- don't depend on the form of the potential.

Efimov’s paper in 1970

Volume 33B, number 8 PHYSICS LETTERS 21 December 1970

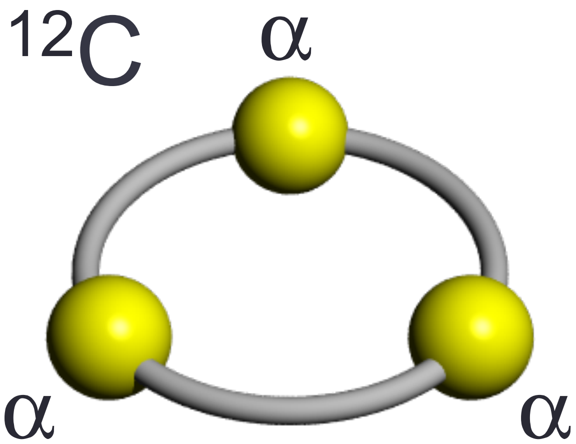
ENERGY LEVELS ARISING FROM RESONANT TWO-BODY FORCES IN A THREE-BODY SYSTEM

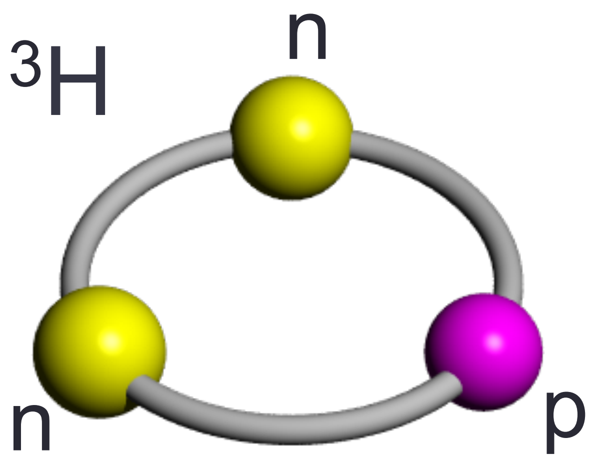
V. EFIMOV

A.F.Ioffe Physico-Technical Institute, Leningrad, USSR

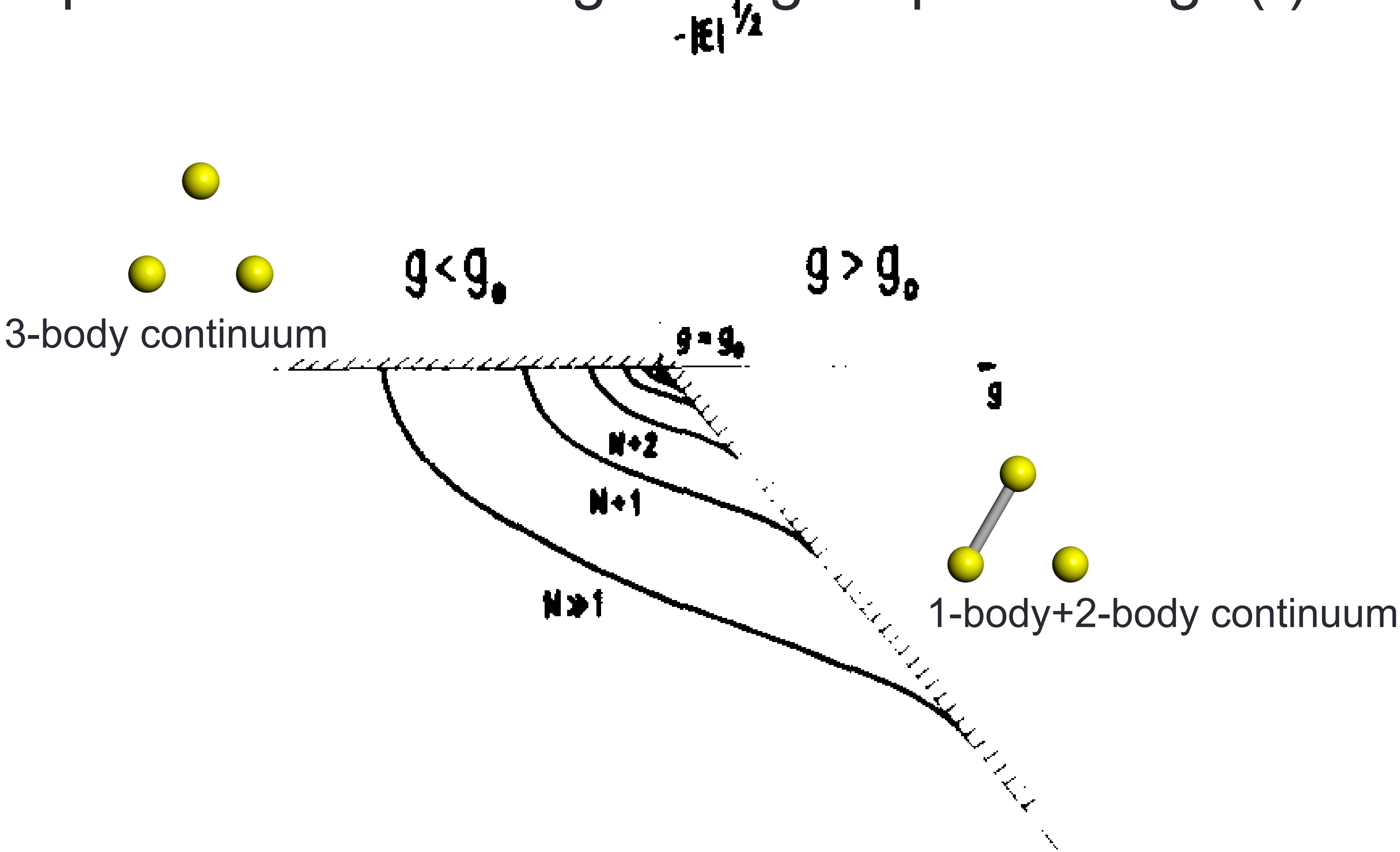
Received 20 October 1970

Resonant two-body forces are shown to give rise to a series of levels in three-particle systems. The number of such levels may be very large. Possibility of the existence of such levels in systems of three α-particles (^{12}C nucleus) and three nucleons (^{3}H) is discussed.





3 particles interacting through a potential gV(r)

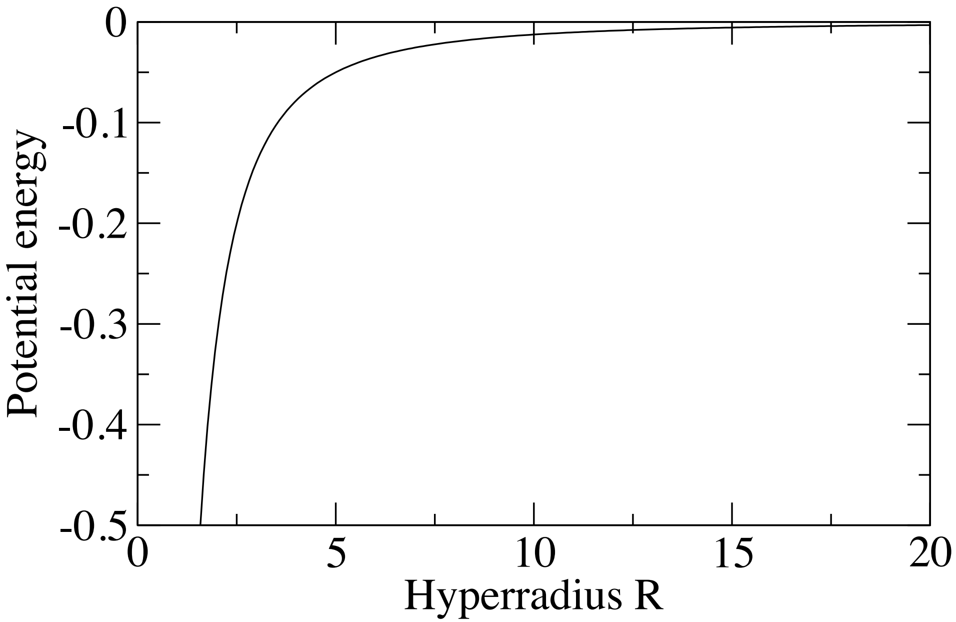


The level spectrum of three neutral spinless particles. The scale is not indicative.

Physical cause of the Efimov effect

The hyperradius: $R^2 \propto r_{12}^2 + r_{23}^2 + r_{31}^2$

R describes the SIZE of the 3-particle triangle, while the shape is measured 2 hyperangles (θ,φ).

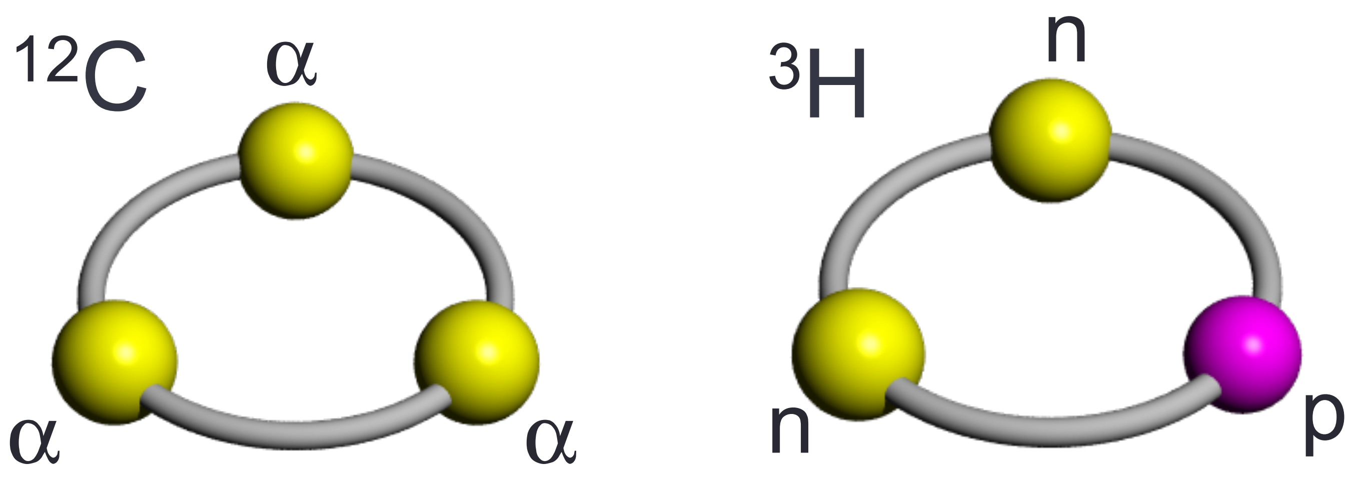


The effective potential curve varies like:

$$-\frac{1.25\ldots}{2mR^2}$$

Dipole potential

$$E_{n+1} = E_n e^{-2\pi/s_0}, s_0 = 1.00624\ldots \text{(universal constant)}$$



Unfortunately, in nuclear systems there's the Coulomb force $-e^2/r$, and the Efimov effect has not been observed so far…

Kraemer *et al.*’s experiment in 2005

Vol 440|16 March 2006|**doi:10.1038/nature04626**

nature

LETTERS

Evidence for Efimov quantum states in an ultracold gas of caesium atoms

T. Kraemer[1], M. Mark[1], P. Waldburger[1], J. G. Danzl[1], C. Chin[1,2], B. Engeser[1], A. D. Lange[1], K. Pilch[1], A. Jaakkola[1], H.-C. Nägerl[1] & R. Grimm[1,3]

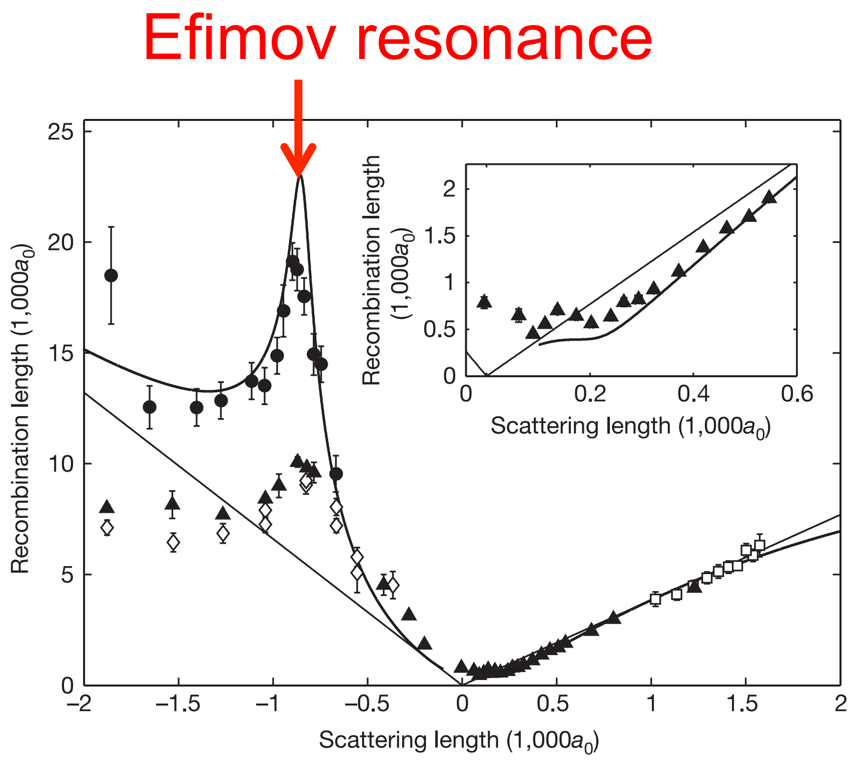
- Evidence for Efimov states observed in an ultracold gas of Cs atoms, where magnetic field induced Feshbach resonances are used to control the scattering length a.
- “Efimov resonaces” were observed in the three-body recombination rate as functions of *a*.

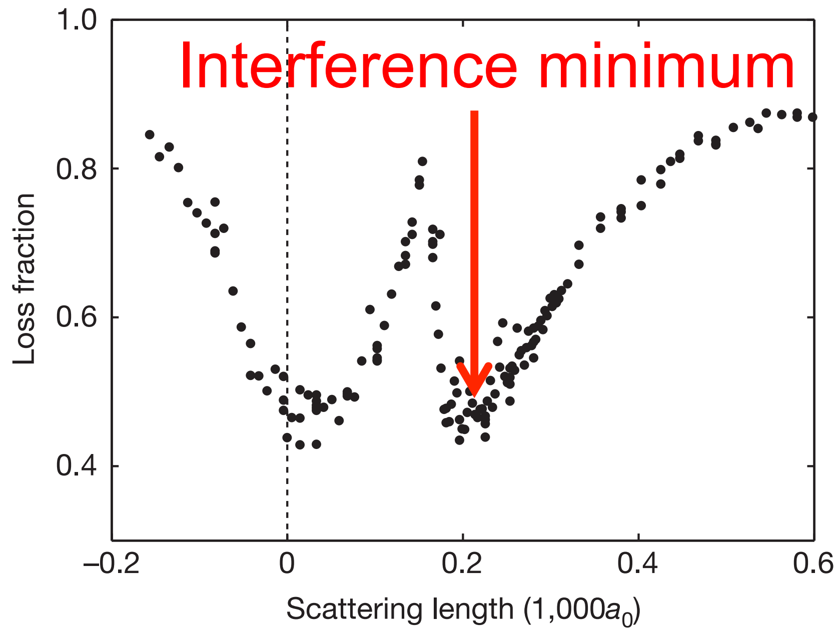
Three-body recombination

$$X + X + X \rightarrow X_2 + X + E_{vl}$$

- Important loss mechanism for trapped ultracold atoms.
- Three-body recombination is enhanced when 3 atoms couple with an Efimov trimer for negative scattering lengths.
- For positive scattering lengths, minima should be detected due to destructive interference.

Kraemer *et al.*'s experiment in 2005





Energy spectrum vs scattering length

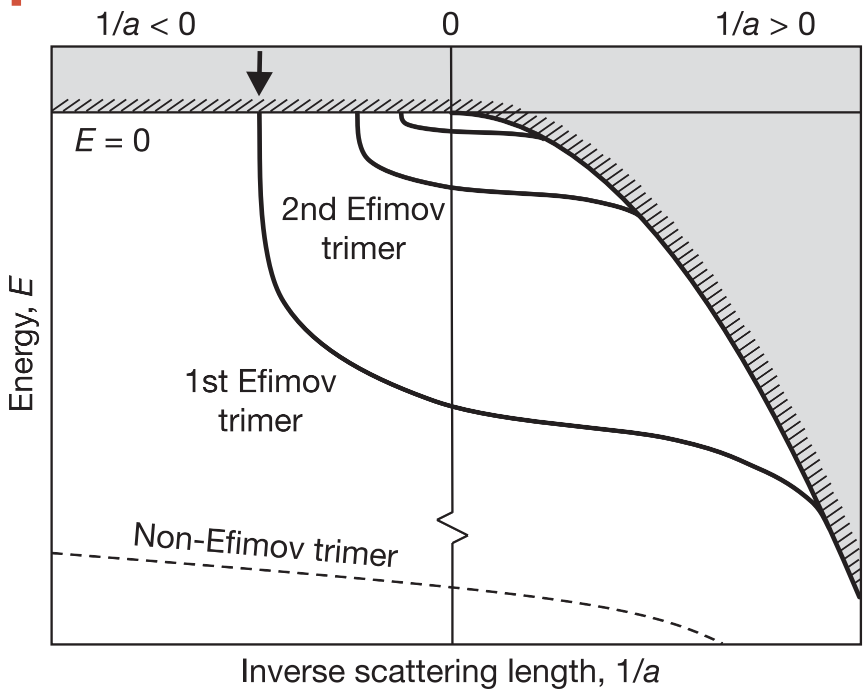
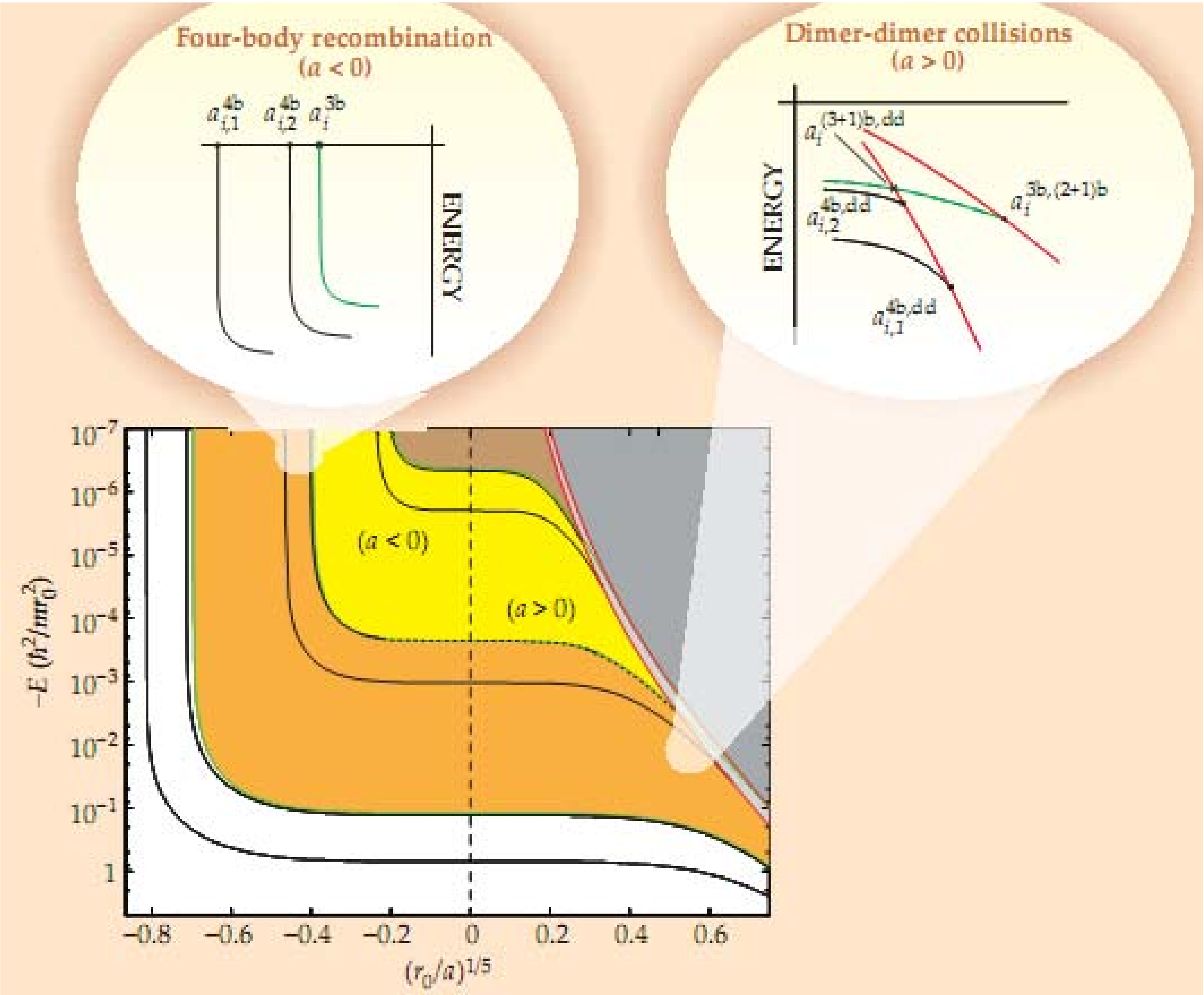


Figure 1 | Efimov's scenario. Appearance of an infinite series of weakly bound Efimov trimer states for resonant two-body interaction. The binding energy is plotted as a function of the inverse two-body scattering length $1/a$. The shaded region indicates the scattering continuum for three atoms ($a < 0$) and for an atom and a dimer ($a > 0$). The arrow marks the intersection of the first Efimov trimer with the three-atom threshold. To illustrate the series of Efimov states, we have artificially reduced the universal scaling factor from 22.7 to 2. For comparison, the dashed line indicates a tightly bound non-Efimov trimer[30], which does not interact with the scattering continuum.

Efimov effect

- There exist an infinite number of 3-body (3B) bound states if the 2-body (2B) scattering length is much larger than the range of the 2B interaction: $a \gg r_0$.
- This occurs even when there's no bound state for the 2B subsystems.
- Theory formulated in nuclear physics in 1970, but experimentally confirmed only in 2006 in an ultracold gas of Cs.
- Evidence of Efimov physics seen measuring the three-body recombination rates.

Extended energy spectrum



Efimov effect in atomic and molecular physics

- Helium has long been considered to be a candidate for seeing the Efimov effect.
- The ^{4}He dimer has a scattering length ($\approx 200a_0$) much larger than the potential range ($\approx 10a_0$).
- Mostly, $^4He_3$ is predicted to have an excited state with Efimov character, but this state has not yet been observed experimentally.
- Numerous theoretical investigations have been carried out so far on the helium trimer $^4He_3$ and its isotope $^4He_2{}^3He$.
- These investigations have been extended to mixed systems $^4He_2H$, $^4He_2H^-$, $^4He_2Li$, …, $^4He_2Cs$ or other rare gas trimers Ne_3 and Ar_3.

Hiyama & other's extension to the ^{4}He tetramer

- The work has been extended to 4-body systems by Lazauskas&Carbonell and Hiyama&Kamimura…

PHYSICAL REVIEW A **85**, 022502 (2012)

Variational calculation of ^{4}He tetramer ground and excited states using a realistic pair potential

E. Hiyama*
RIKEN Nishina Center, RIKEN, Wako 351-0198, Japan

M. Kamimura†
Department of Physics, Kyushu University, Fukuoka 812-8581, Japan and RIKEN Nishina Center, RIKEN, Wako 351-0198, Japan
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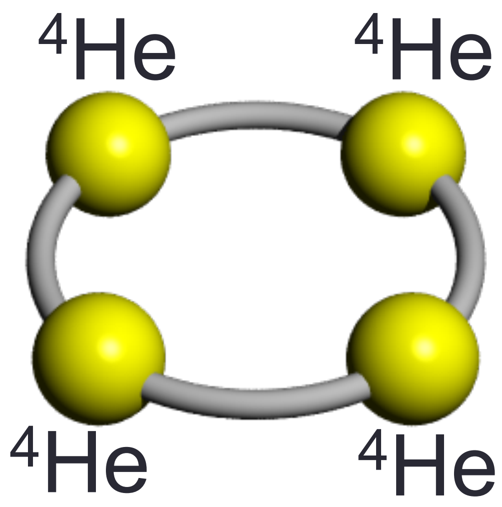
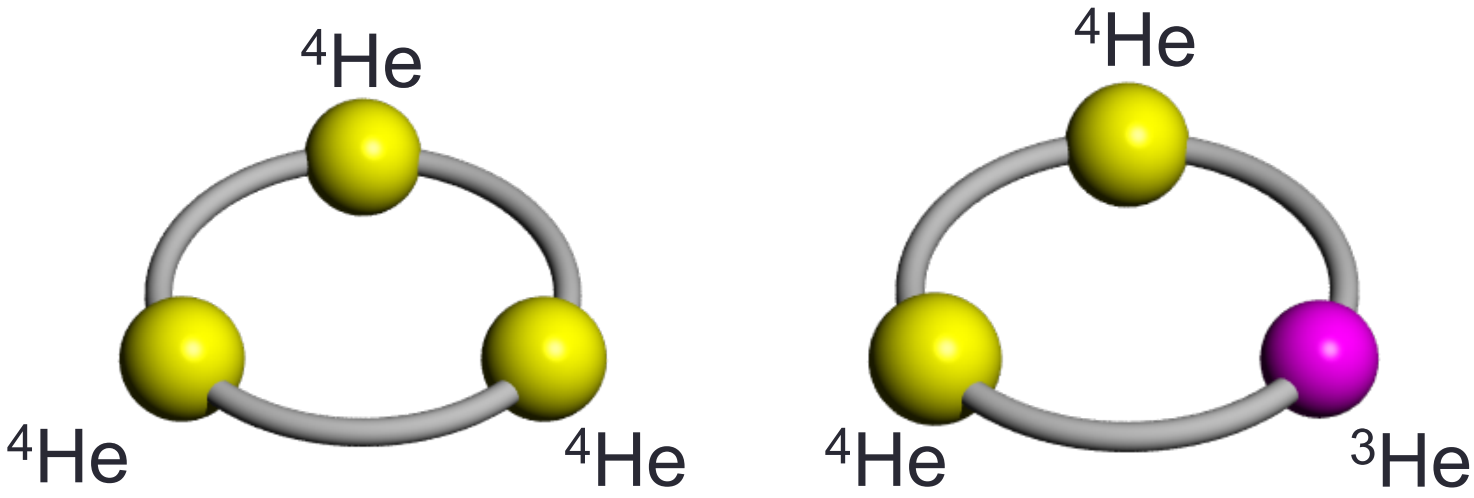
We calculated the ^{4}He trimer and tetramer ground and excited states with the LM2M2 potential using our Gaussian expansion method for *ab initio* variational calculations of few-body systems. The method has been extensively used for a variety of three-, four-, and five-body systems in nuclear physics and exotic atomic and molecular physics. The trimer (tetramer) wave function is expanded in terms of symmetric three- (four-) body Gaussian basis functions, ranging from very compact to very diffuse, without assumption of any pair correlation function. The calculated results for the trimer ground and excited states are in excellent agreement with values reported in the literature. The binding energies of the tetramer ground and excited states are obtained as 558.98 and 127.33 mK (0.93 mK below the trimer ground state), respectively. We found that precisely the same shape of the short-range correlation ($r_{ij} \lesssim 4$ Å) in the dimer appears in the ground and excited states of the trimer and tetramer. The overlap function between the trimer excited state and the dimer ground state and that between the tetramer excited state and the trimer ground state are almost proportional to the dimer wave function in the asymptotic region (up to ∼1000 Å). Also, the pair correlation functions of trimer and tetramer excited states are almost proportional to the squared dimer wave function. We then propose a model which predicts the binding energy of the first excited state of $^4\mathrm{He}_N$ ($N \geqslant 3$) measured from the $^4\mathrm{He}_{N-1}$ ground state to be nearly $\frac{N}{2(N-1)} B_2$ where B_2 is the dimer binding energy.



Triatomic helium systems



- Weakly bound systems: binding energy about 1mK≈100neV.
- $^4He_3$ has been a candidate for seeing "Efimov states", since $^4He_2$ has a large scattering length $a \approx 200a_0$.
- Theoretical treatment simple since $^4He_2$ has only 1 bound state with l=0.
- Experimentally, $^4He_2$ (ground state) observed by Luo et *al*., and Schöllkopf and Toennies, $^4He_3$ and $^4He_4$ also observed.

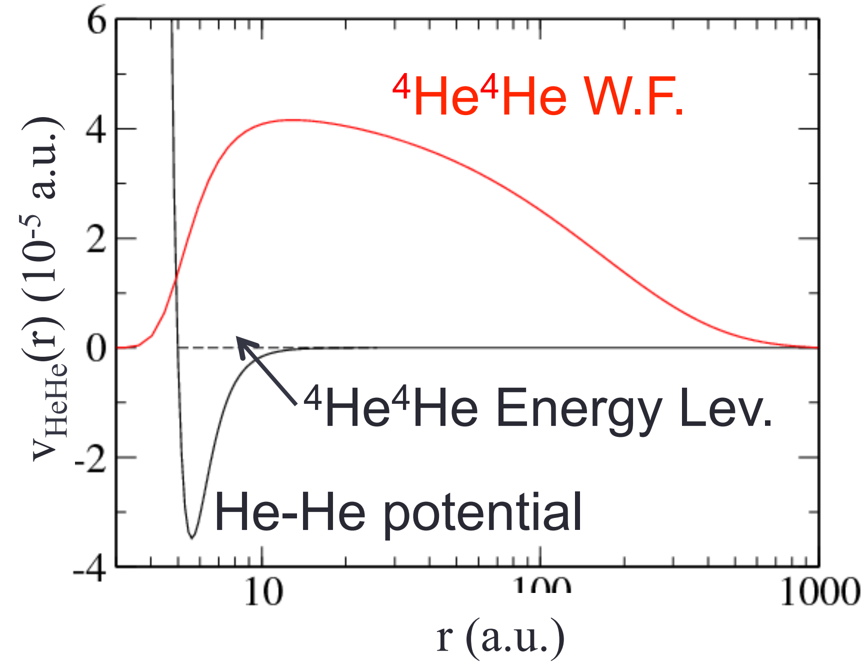
Three-body recombination

$$\mathrm{He} + \mathrm{He} + \mathrm{He} \rightarrow \mathrm{He}_2 + \mathrm{He} + E_{v=0,l=0}$$

- We calculate the recombination rate up to 10mK.
- Relatively simple and an interesting benchmark.
- I and my collaborators in U.S. are among the first to carry out such calculations.

He-He systems: bound state properties

- Use the dimer potential developed by Jeziorska *et al*.
- We can also include retardation: change from $1/r^6$ to $1/r^7$, for details see the quantum field theory book by Itzykson & Zuber!
- $^4He^4He$: one bound state.
- $^4He^3He$, $^3He^3He$: no bound state

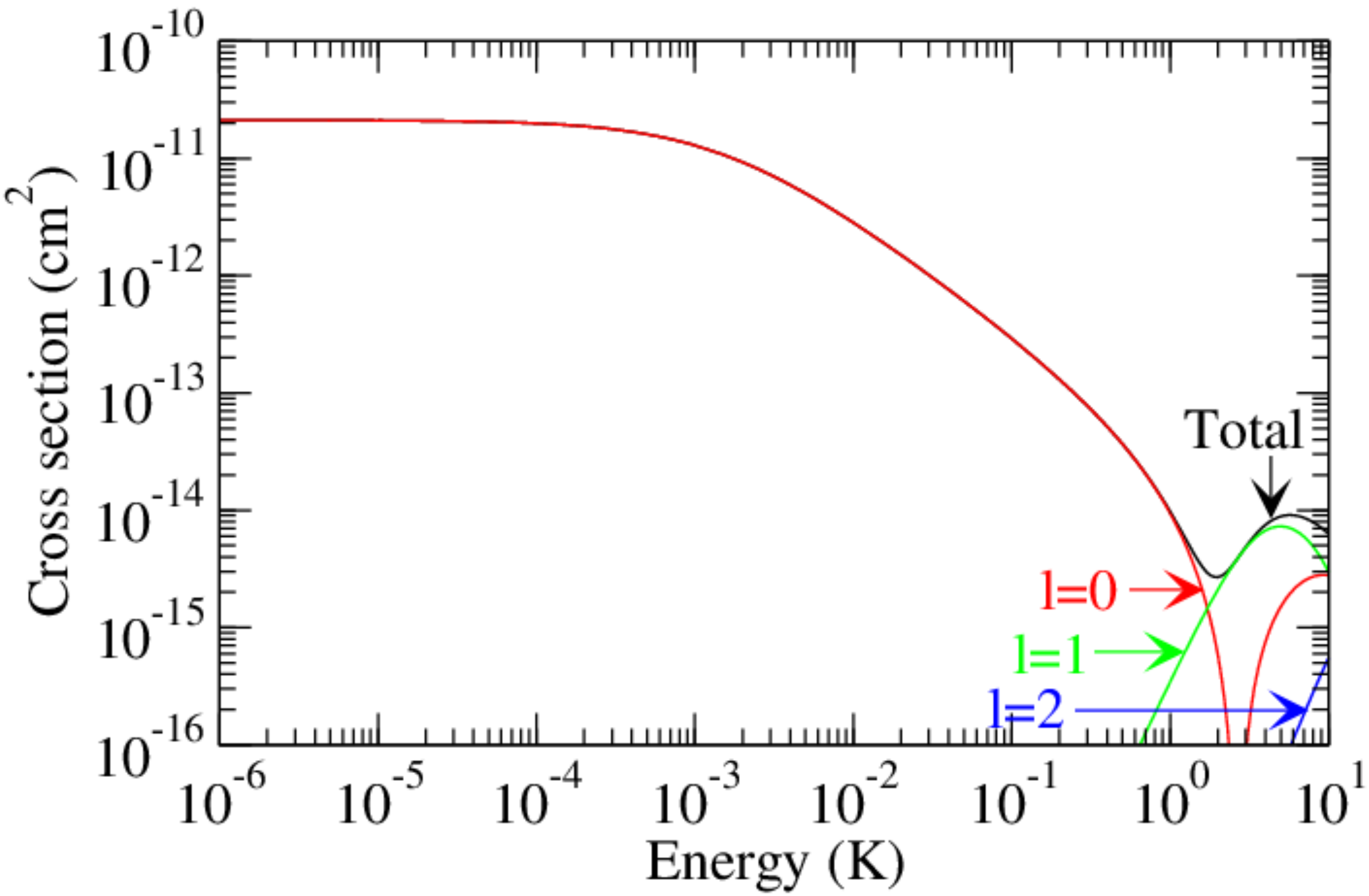


E_{ret}=-4.95x10^{-9} a.u.=-1.56mK

E_{unret}=-5.47x10^{-9} a.u.=-1.73mK

Elastic scattering cross section for $^4He+^4He$

$$\sigma \rightarrow 8\pi a^2 \text{ as } E \rightarrow 0$$



Numeriacal method: Adiabatic hyperspherical method

- Use Whitten-Smith's hyperspherical coordinates
  - Consist of 1 hyperradius, 5 hyperangles
  - Simplify imposing the permutation symmetry
- Adiabatic expansion method
  - First calculate eigenfunctions and eigenvalues of the fixed-hyperradius Hamiltonian
  - Construct a set of coupled radial equations
- R-matrix method
  - Extract the scattering S-matrix from the coupled radial equations.

Whitten-Smith's hyperspherical coordinates

$$(R, \Omega) \equiv (R, \theta, \varphi, \alpha, \beta, \gamma)$$

- The hyperradius R
  measures the SIZE of the molecular triagle.
- The hyperradius (θ,φ)
  measure its SHAPE.
- The Euler angles (α,β,γ)
  describes the orientation of the body-fixed frame in space.

Schrödinger equation

$$\left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial R^2}+\frac{\hat{\Lambda}^2+\frac{15}{4}\hbar^2}{2\mu R^2}+V(R,\theta,\varphi)\right]\psi=E\psi$$

- Λ^2 is the squared "grand angular momentum operator".
- Interaction potential:

$$V(R,\theta,\varphi)=v(r_{12})+v(r_{23})+v(r_{31})+w(r_{12},r_{23},r_{31}),$$

- Good quantum numbers:
  J(total angular momentum), M(projection),and Π (parity)

Adiabatic expansion method

- We first solve the R-fixed Schrödinger equation:

$$\left[\frac{\Lambda^2+\frac{15}{4}\hbar^2}{2\mu R^2}+V(R,\theta,\varphi)\right]\Phi_\nu(R;\Omega)=U_\nu(R)\Phi_\nu(R;\Omega).$$

to obtain $U_v(R)$(potential curves) & $\Phi_v(R;\Omega)$(channel functions)

- The total wave function is expanded as

$$\psi(R,\Omega)=\sum_{\nu=0}^{\nu_{\max}}F_\nu(R)\Phi_\nu(R;\Omega).$$

We then obtain a set of coupled radial equations:

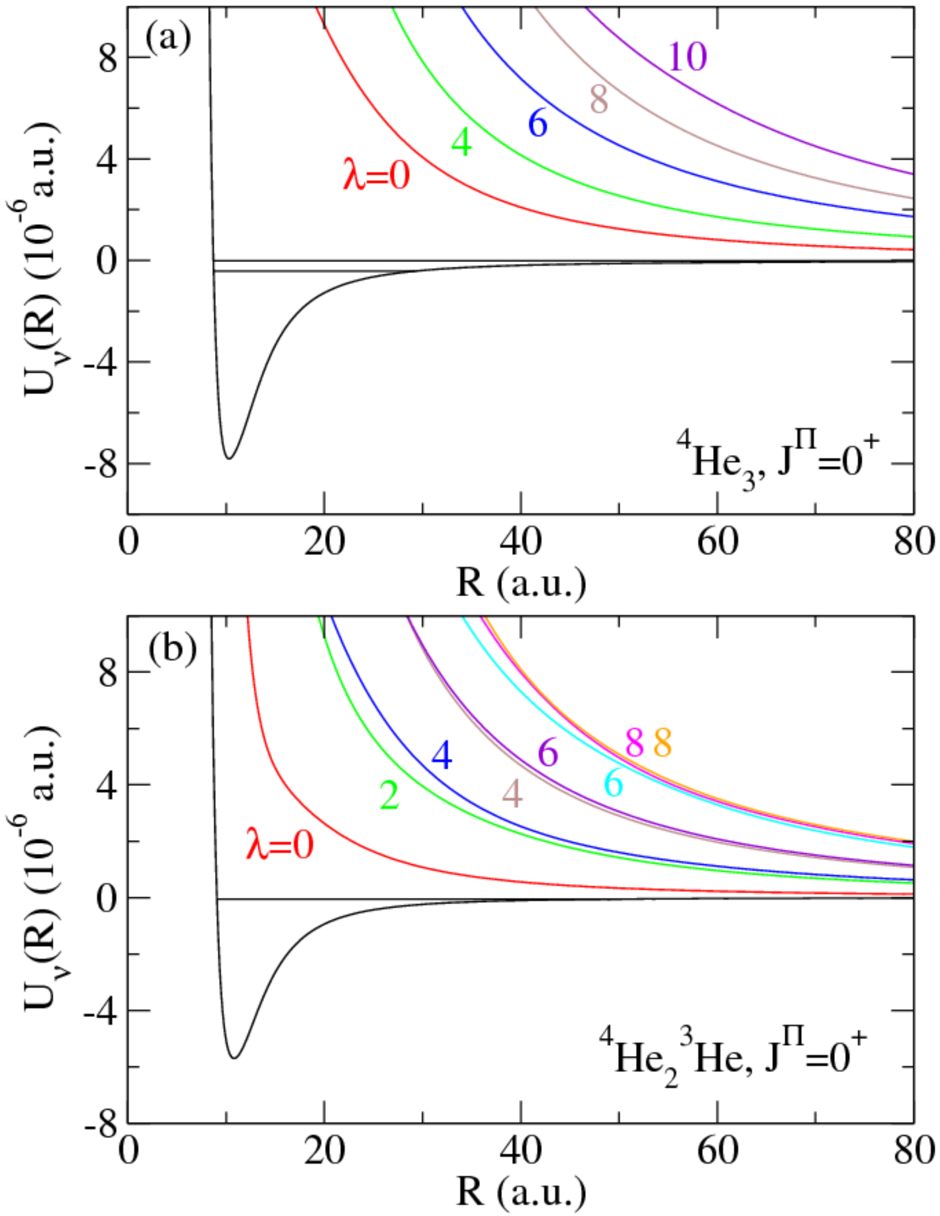
$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dR^2}+U_\nu(R)\right]F_{\nu E}(R)-\frac{\hbar^2}{2\mu}\sum_{\nu'}\left[P_{\nu\nu'}(R)\frac{d}{dR}+Q_{\nu\nu'}(R)\right]F_{\nu' E}(R)=EF_{\nu E}(R),$$

with the nonadiabatic couplings:

$$P_{\nu\nu'}(R)=\left\langle\left\langle\Phi_\nu(R;\Omega)\left|\frac{\partial}{\partial R}\right|\Phi_{\nu'}(R;\Omega)\right\rangle\right\rangle,\ Q_{\nu\nu'}(R)=\left\langle\left\langle\Phi_\nu(R;\Omega)\left|\frac{\partial^2}{\partial R^2}\right|\Phi_{\nu'}(R,\Omega)\right\rangle\right\rangle.$$

Adiabatic hyperspherical potential curves

- The lowest potential curve: $^4He^2$+$^{4,3}He$
- The higher potential curves: 3B continuum states.



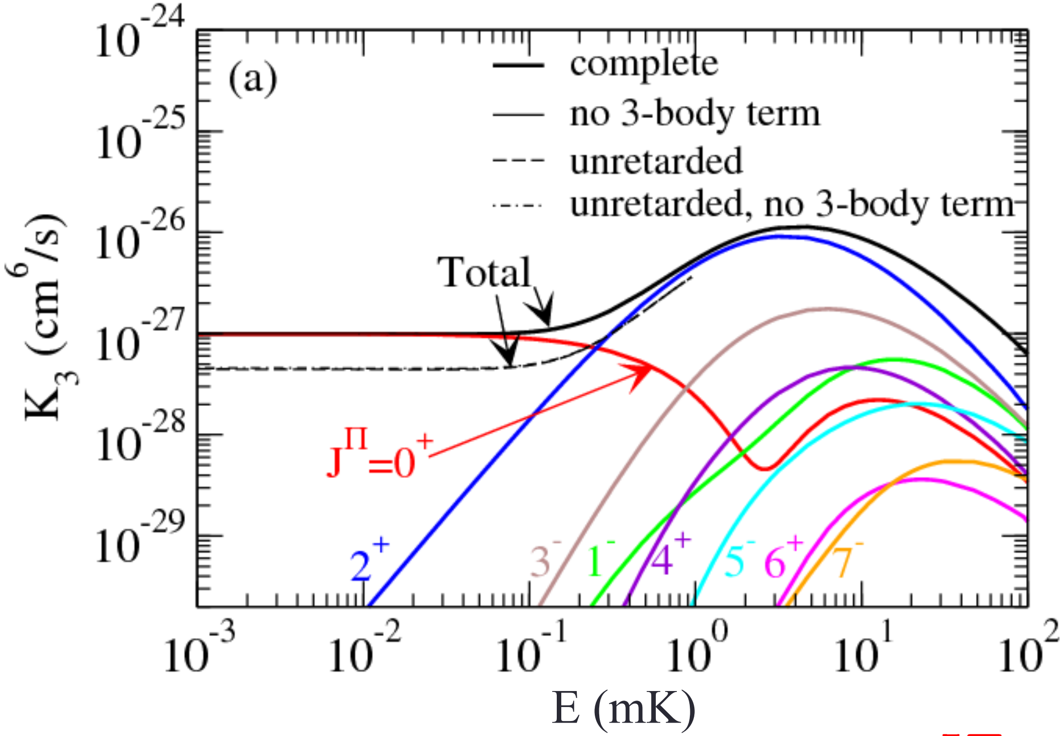
$^4He_3$ and $^4He_2{}^3He$ bound state energies

- We have found 2 bound states for $^4He_3$(J^Π=0$^+$), one bound state for $^4He_2{}^3He$ (J^Π=0$^+$) and none for J>0.
- The effect of retardation is found to be more significant than the 3B term.

Bound state energies in mK

retardation	yes	yes	no	no
3-body term	yes	no	yes	no
$^4He_3$				
$n = 0$	−130.86	−131.12	−133.44	−133.70
$n = 1$	−2.5882	−2.5900	−2.7838	−2.7856
$^4He_2^3He$				
$n = 0$	−16.237	−16.293	−17.346	−17.405

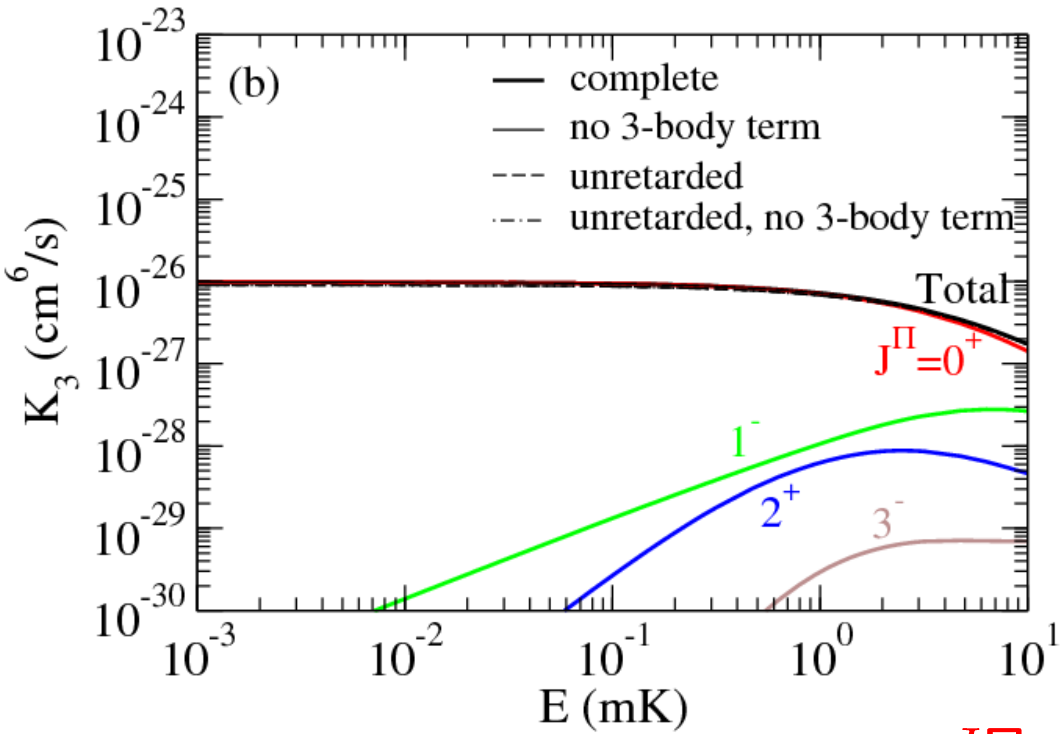
Recombination rates for $^4He+^4He+^4He \rightarrow ^4He_2+^4He$



•Threshold law: at ultracold energies, $K_3^{J\Pi} \propto E^{\lambda_{\min}}$,

$\lambda_{\min} = 0, 3, 2, 3, 4, \ldots$ for $J^{\Pi} = 0^+, 1^-, 2^+, 3^-, 4^+, \ldots$

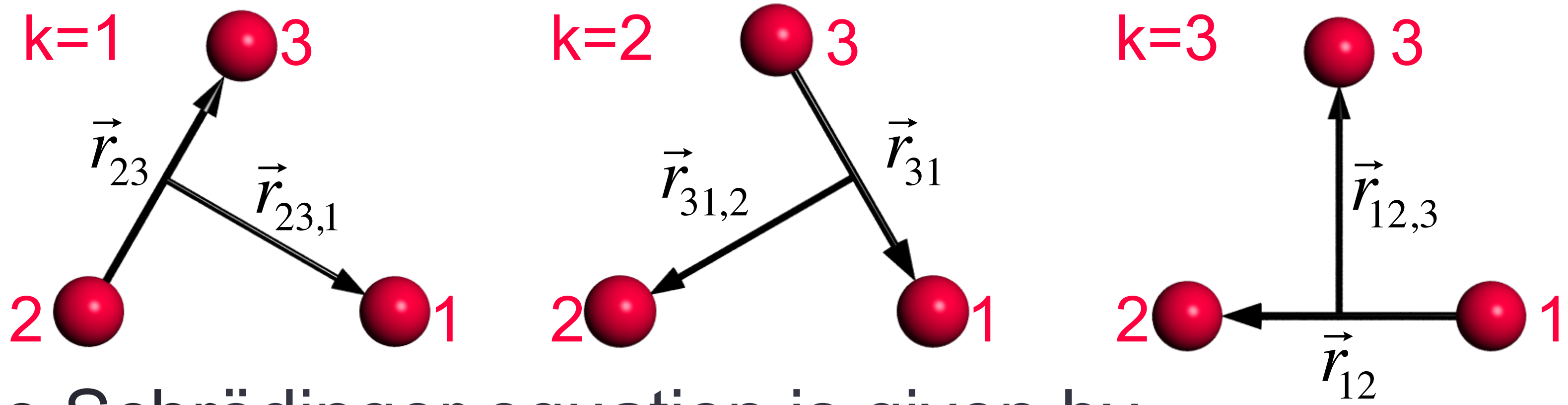
Recombination rates for $^4He+^4He+^3He \rightarrow ^4He_2+^3He$



- Threshold law: at ultracold collision energies, $K_3^{J\Pi} \propto E^{\lambda_{\min}}$, $\lambda_{\min} = 0, 1, 2, 3,$ for $J^{\Pi} = 0^+, 1^-, 2^+, 3^-$.

Gaussian Expansion Method (GEM)

In terms of Jacobi coordinates:



the Schrödinger equation is given by

$$\left[-\frac{\hbar^2}{2\mu_{23}}\nabla^2_{23}-\frac{\hbar^2}{2\mu_{23,1}}\nabla^2_{23,1}+\sum_{1=i<j}^{3}v(r_{ij})\right]\Psi=E\Psi.$$

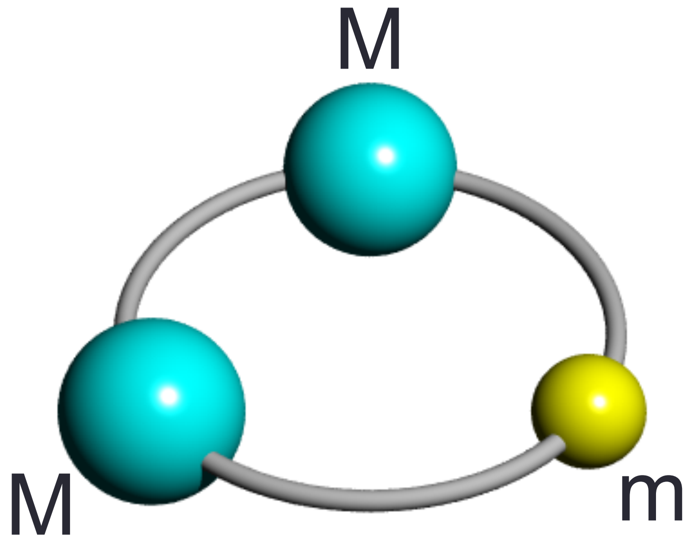
We express the wave function in the form

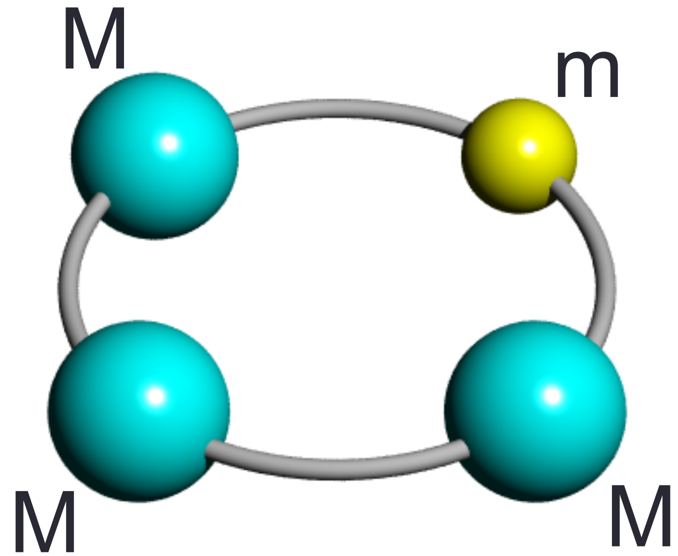
$$\Psi_{JM}=\sum_{k=1}^{3}\sum_{n_k,l_k,n'_k,l'_k}A^{(k)}_{n_kl_kn'_kl_k}\left[\phi_{n_kl_k}(\vec{r}_{ij})\psi_{n'_kl'_k}(\vec{r}_{ij,k})\right]_{JM},$$

with

$$\phi_{nl}(\vec{r})=N_{nl}r^le^{-\nu_nr^2}Y_{lm}(\hat{r}),\ \psi_{n'l'}(\vec{r})=N'_{n'l'}r^{l'}e^{-\nu'_{n'}r^2}Y_{l'm'}(\hat{r}).$$

Efimov states in mixed 3-body and 4-body systems





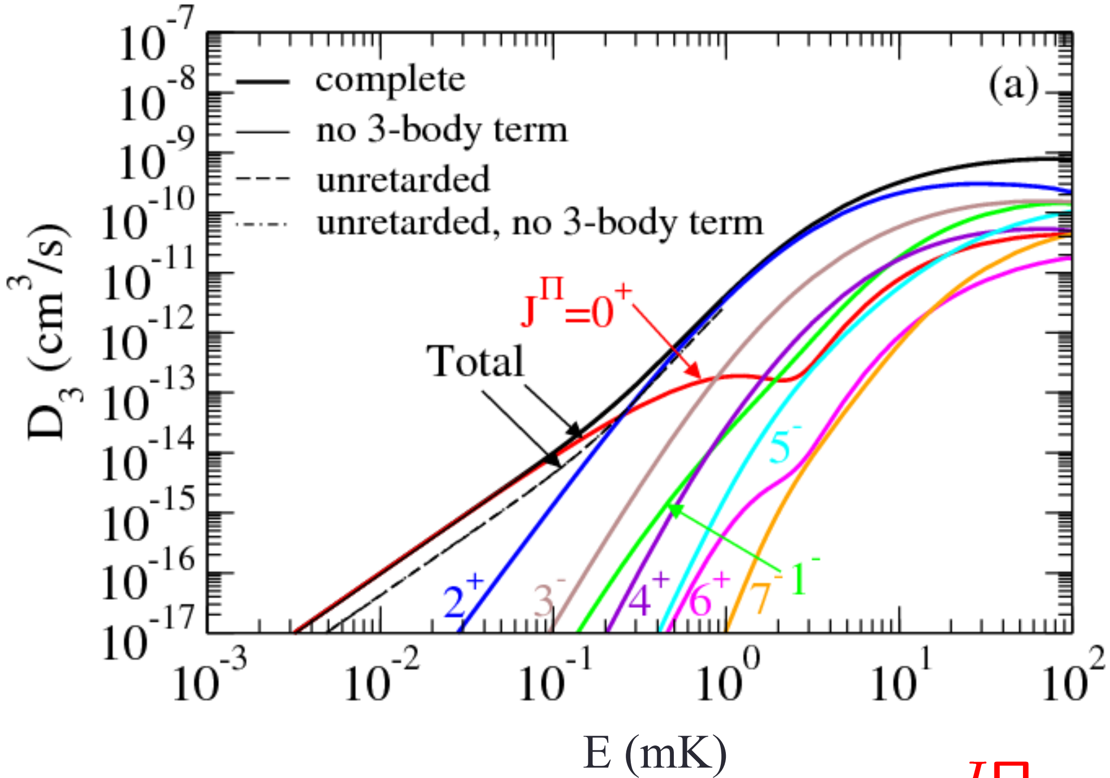
M=Fermion, m=Light atom

Efimov states are predicted to exist in (2+1) and (3+1) systems for certain range of the mass ratio M/m.

Summary

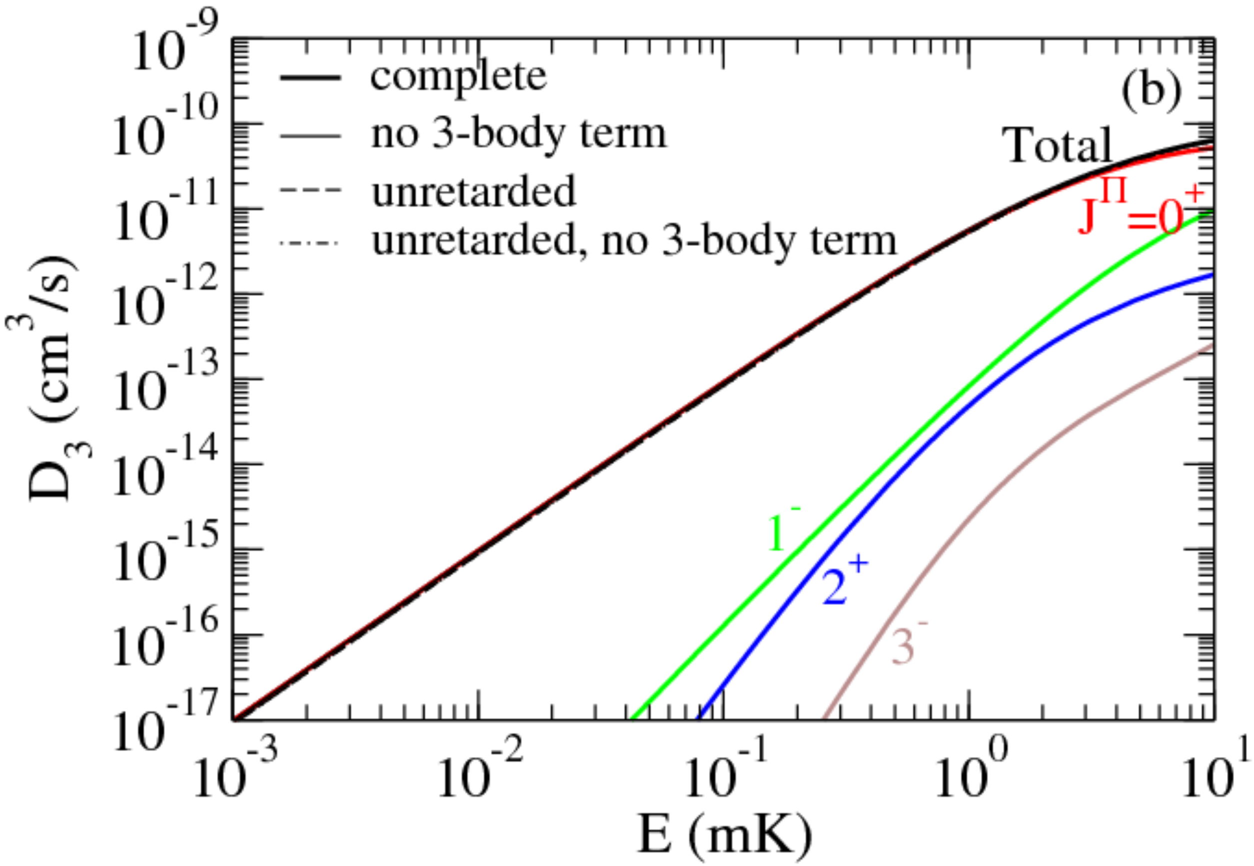
- Presented a theoretical description of Efimov physics and discussed applications in atomic and molecular physics.
- Studied triatomic helium systems $^4He_3$ and $^4He_2{}^3He$ using the most realistic helium interaction potential.
- Ongoing and future work: search for Efimov states or other novel quantum states in mixed triatomic and tetraatomic systems using the Gaussian expansion method.

Collision induced dissociation rates for $^4He_2 + ^4He \rightarrow ^4He + ^4He + ^4He$



- Threshold law: at ultracold collision energies, $D_3^{J\Pi} \propto E^{\lambda_{\min}+2}$.

Collision induced dissociation rates for $^4He_2 + ^3He \rightarrow ^4He + ^4He + ^3He$



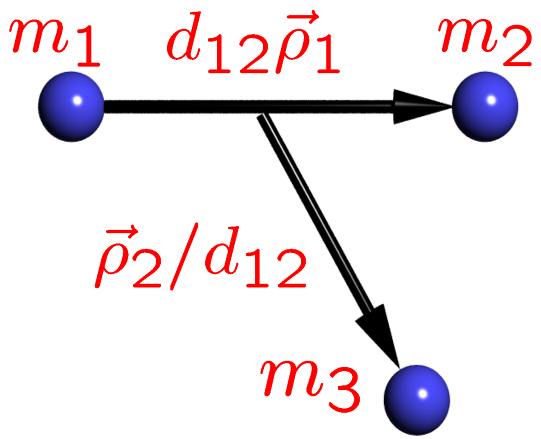
Whitten-Smith's hyperspherical coordinates

$$(R,\Omega) \equiv (\underbrace{R}_{\text{Hyperradius}}, \underbrace{\theta,\varphi,\alpha,\beta,\gamma}_{\text{Hyperangles}})$$

$$\vec{\rho}_1 = \vec{\xi}_1/d_{12}, \quad \vec{\rho}_2 = d_{12}\vec{\xi}_2$$

$$d_{12} = \frac{(m_3/\mu)(m_1+m_2)}{m_1+m_2+m_3}$$

$$\mu^2 = \frac{m_1 m_2 m_3}{m_1+m_2+m_3}$$

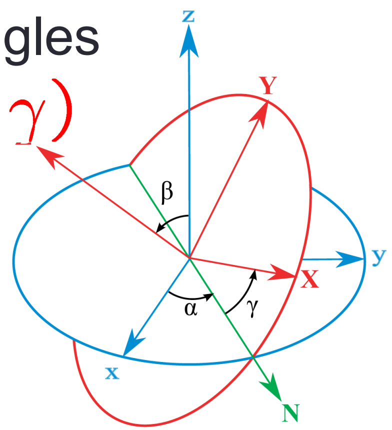


$$R^2 = \rho_1^2 + \rho_2^2, R \in [0,\infty)$$

$$\begin{cases} (\vec{\rho}_1)_x = R\cos(\pi/4-\theta/2)\cos(\varphi/2+\varphi_{12}/2) \\ (\vec{\rho}_1)_y = R\sin(\pi/4-\theta/2)\sin(\varphi/2+\varphi_{12}/2) \\ (\vec{\rho}_1)_z = 0 \\ (\vec{\rho}_2)_x = -R\cos(\pi/4-\theta/2)\sin(\varphi/2+\varphi_{12}/2) \\ (\vec{\rho}_2)_y = R\sin(\pi/4-\theta/2)\cos(\varphi/2+\varphi_{12}/2) \\ (\vec{\rho}_2)_z = 0 \end{cases}$$

$$\varphi_{12} = 2\tan^{-1}(m_2/\mu)$$
$$0 \le R < \infty, 0 \le \theta \le \pi/2, 0 \le \varphi \le 2\pi$$

Euler angles (α,β,γ)



Schrödinger equation

$$\left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial R^2}+\frac{\hat{\Lambda}^2+\frac{15}{4}\hbar^2}{2\mu R^2}+V(R,\theta,\varphi)\right]\psi=E\psi$$

- Λ^2 is the squared "grand angular momentum operator":

$$\begin{aligned}\frac{\hat{\Lambda}^2}{2\mu R^2} &= -\frac{2\hbar^2}{\mu R^2\sin 2\theta}\frac{\partial}{\partial\theta}\sin 2\theta\frac{\partial}{\partial\theta}\\ &+\frac{\hbar^2}{\mu R^2\sin^2\theta}\left(i\hbar\frac{\partial}{\partial\varphi}-\cos\theta\frac{J_z}{2}\right)^2\\ &+\frac{J_x^2}{\mu R^2(1-\sin\theta)}+\frac{J_y^2}{\mu R^2(1+\sin\theta)}+\frac{J_z^2}{2\mu R^2}.\end{aligned}$$

- Λ^2 has eigenvalues $\lambda(\lambda+4)\hbar^2$
- Interaction potential:

$$V(R,\theta,\varphi)=v(r_{12})+v(r_{23})+v(r_{31})+w(r_{12},r_{23},r_{31}),$$

- Good quantum numbers: *J*(total angular momentum), *M*(projecztion),and Π(parity)

Adiabatic hyperspherical potential curves

- The lowest potential curve corresponds asymptotically to $^4He_2 + ^{4,3}He$:

$$U_0(R) - \frac{1}{2\mu} Q_{00}(R) \to E_{00} + \frac{l_{1,23}(l_{1,23}+1)}{2\mu R^2}, \text{ for } R \to \infty.$$

- The higher potential curves correspond to the 3B continuum states:

$$U_\nu(R) \to \frac{\lambda(\lambda+4) + \frac{15}{4}}{2\mu R^2}, \text{ for } R \to \infty.$$

- By symmetry requirement, the atom-diatom channel exists only for the parity-favored cases: $\Pi=(-1)^J$.
- We have also calculated the potential curves for $J^\Pi=1^-, 2^+, \ldots$

Three-body recombination rates

- The event rate constant for 3B recombination X+X+X→X_2+X: $$K_3 = \sum_{J,\Pi} K_3^{J\Pi} = 3! \sum_{J,\Pi} \sum_{\nu=1}^{\nu_{max}} \frac{32(2J+1)\pi^2}{\mu k^4} |S_{0\leftarrow\nu}^{J\Pi}|^2.$$
- The event rate constant for 3B recombination X+X+Y→X_2+Y or X+X+Y→XY+X : $$K_3 = \sum_{J,\Pi} K_3^{J\Pi} = 2! \sum_{J,\Pi} \sum_{\nu=1}^{\nu_{max}} \frac{32(2J+1)\pi^2}{\mu k^4} |S_{0\leftarrow\nu}^{J\Pi}|^2.$$
- $k=(2\mu E)^{1/2}$ is the hyperradial wave number, $S^{J\Pi}_{0<-v}$ the scattering matrix element.
- Collision induced dissociation rate:

$$D_3 = \sum_{J,\Pi} D_3^{J\Pi} = \sum_{J,\Pi} \sum_{\nu=1}^{\nu_{max}} \frac{(2J+1)\pi}{\mu_{1,23} k_{1,23}} |S_{\nu\leftarrow 0}^{J\Pi}|^2,$$

$$\mu_{1,23} = \frac{m_1(m_2+m_3)}{m_1+m_2+m_3},\ k_{1,23} = [2\mu_{1,23}(E-E_{00})]^{1/2}.$$