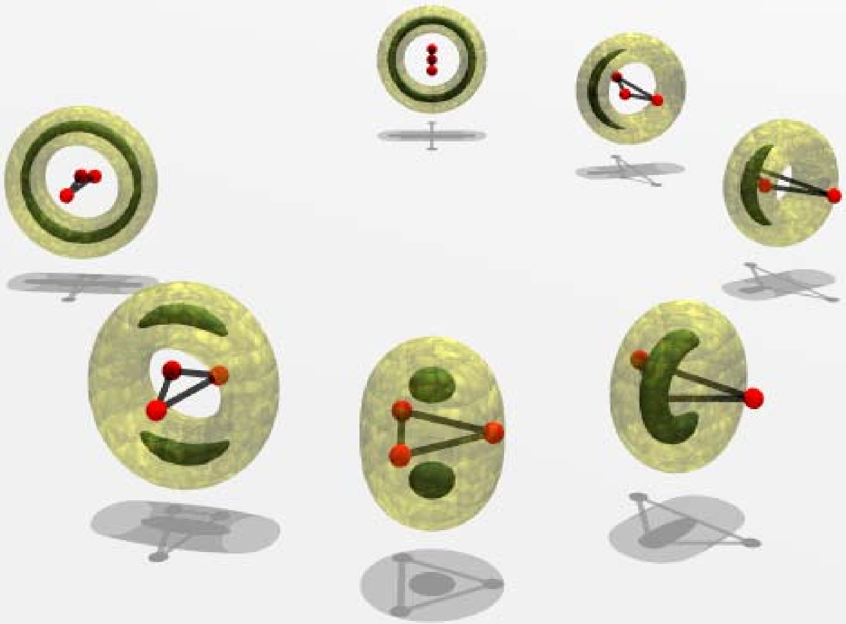
Few-Body Physics with Correlated Gaussian Methods

Javier von Stecher

Department of Physics and JILA
University of Colorado

In collaboration with
Chris H. Greene
Jose P. D'Incao



Acknowledgments:
Doerte Blume
Seth Rittenhouse
Nirav Mehta

Support

Probable configurations of a weakly-bound four-boson state.

Outline:

- ***Correlated Gaussian Method***
  - ***Implementation***
  - ***Connection with other methods***
- ***How does Efimov physics and universality extends beyond three bodies?***

- ***Universality in four-boson systems***
- ***Extension to larger systems***

Outline:

- ***Correlated Gaussian Method***
  - ***Implementation***
  - *Connection with other methods*
- ***How does Efimov physics and universality extends beyond three bodies?***

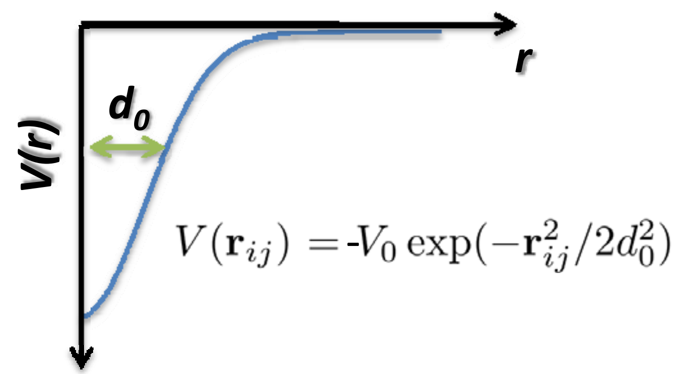
- *Universality in four-boson systems*
- *Extension to larger systems*

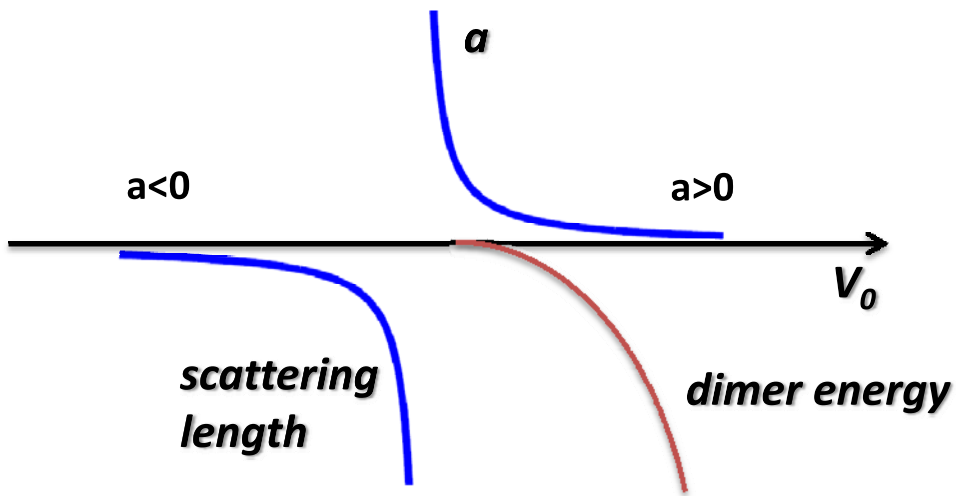
Solving the Schrödinger equation

Hamiltonian:

$$\mathcal{H} = \sum_i^4 \left(-\frac{\hbar^2}{2m}\nabla_i^2 + \frac{1}{2} m\omega_0^2 \mathbf{r}_i^2 \right) + \sum_{i<j} V(\mathbf{r}_{ij})$$

model interactions:





Gaussian,
Combination of Gaussians,
Sech^2
Square well,
…

zero bound state

one bound state

Correlated Gaussian basis set expansion:

$$\mathcal{H}\Psi = E\Psi$$

S. F. Boys and K. Singer (1960)
K. Varga and Y. Suzuki ... (1990)
Sorensen, Federov and Jensen (2002)

Expand in a basis and diagonalize a matrix

explicitly correlated:
build correlations in the basis function

$$\tilde{\Phi} = \exp\left(-\sum_{ij} a_{ij}\mathbf{r}_i.\mathbf{r}_j\right)$$

- *Analytical form of matrix elements (accurate and fast).*
- *Efficient Optimization: Stochastical variational method*
- *Good for bound/trapped states.*
- *Difficult to describe scattering properties*

J. Mitroy, K Varga and coworkers (2008)

Four-body Formulation

Correlated Gaussian basis set expansion:

- *expansion for L=0 and positive parity*

$$\Psi_T(\mathbf{r}_1, ..., \mathbf{r}_N) = \sum_n C_n \Phi_n(\mathbf{r}_1, ..., \mathbf{r}_N)$$

- *basis functions:*

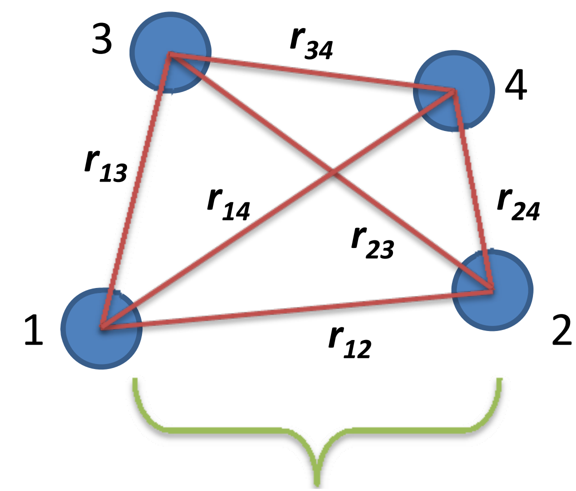
$$\Phi_n(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) = \mathcal{S}\{\tilde{\Phi}_n(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4)\}$$

$$\mathcal{S} = \sum_p \mathrm{sign}(p)\hat{p}$$

Symmetrization: spin statistic

- *remove CM:*

$$\tilde{\Phi}_n(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4)\} = \prod_{i>j} \phi_{d^n_{ij}}(r_{ij})$$



$$\Phi_{d_{12}}(r_{12}) = e^{-r_{12}^2/2d_{12}^2}$$

Correlated Gaussian basis set expansion:

- *expansion for L=0 and positive parity*

$$\Psi_T(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \sum_n C_n \Phi_n(\mathbf{r}_1, \ldots, \mathbf{r}_N)$$

- *basis functions:*

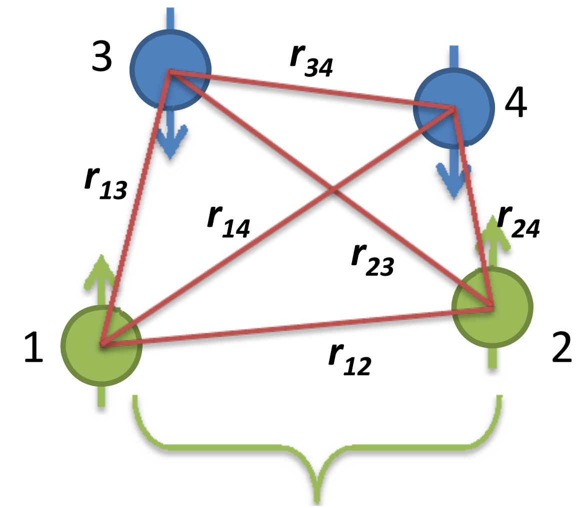
$$\Phi_n(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) = \mathcal{S}\{\tilde{\Phi}_n(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4)\}$$

$$\mathcal{S} = \sum_p \mathrm{sign}(p)\hat{p}$$

Symmetrization: spin statistic

- *remove CM:*

$$\tilde{\Phi}_n(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4)\} = \prod_{i>j} \phi_{d_{ij}^n}(r_{ij})$$



$$\Phi_{d_{12}}(r_{12}) = e^{-r_{12}^2/2d_{12}^2}$$

Symmetrization of two-component Fermi system:

$$\Phi_n(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) = \tilde{\Phi}_n(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) - \tilde{\Phi}_n(\mathbf{r}_2, \mathbf{r}_1, \mathbf{r}_3, \mathbf{r}_4) - \tilde{\Phi}_n(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_4, \mathbf{r}_3) + \tilde{\Phi}_n(\mathbf{r}_2, \mathbf{r}_1, \mathbf{r}_4, \mathbf{r}_3)$$

Stochastical variational method:

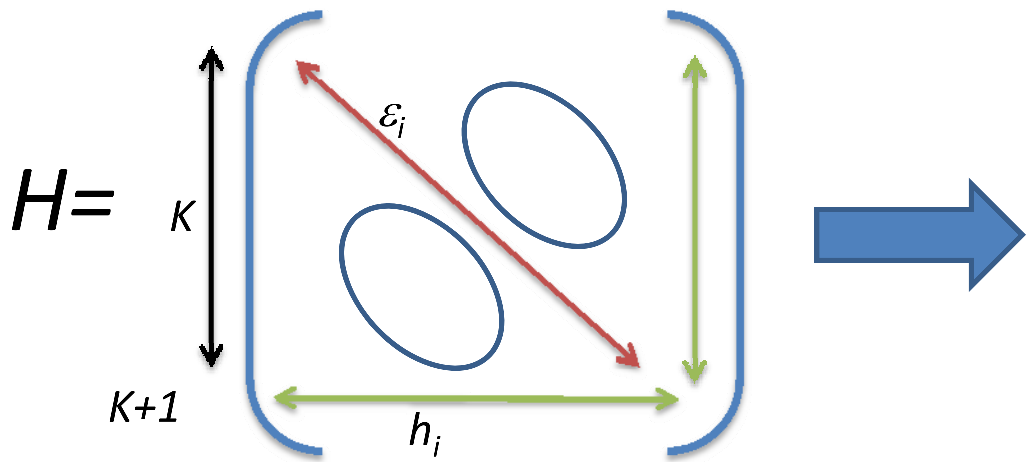
Add one optimized basis function at a time

Iterate:

1. *Select the parameters randomly*

$$\tilde{\Phi}_n(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4)\} = \prod_{i>j} \phi_{d^n_{ij}}(r_{ij})$$

2. *Gram-Schmidt diagonalization*



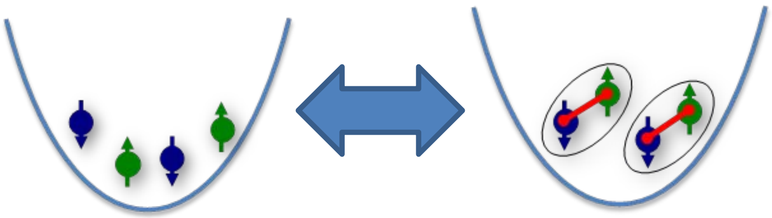
Roots of a transcendental equation

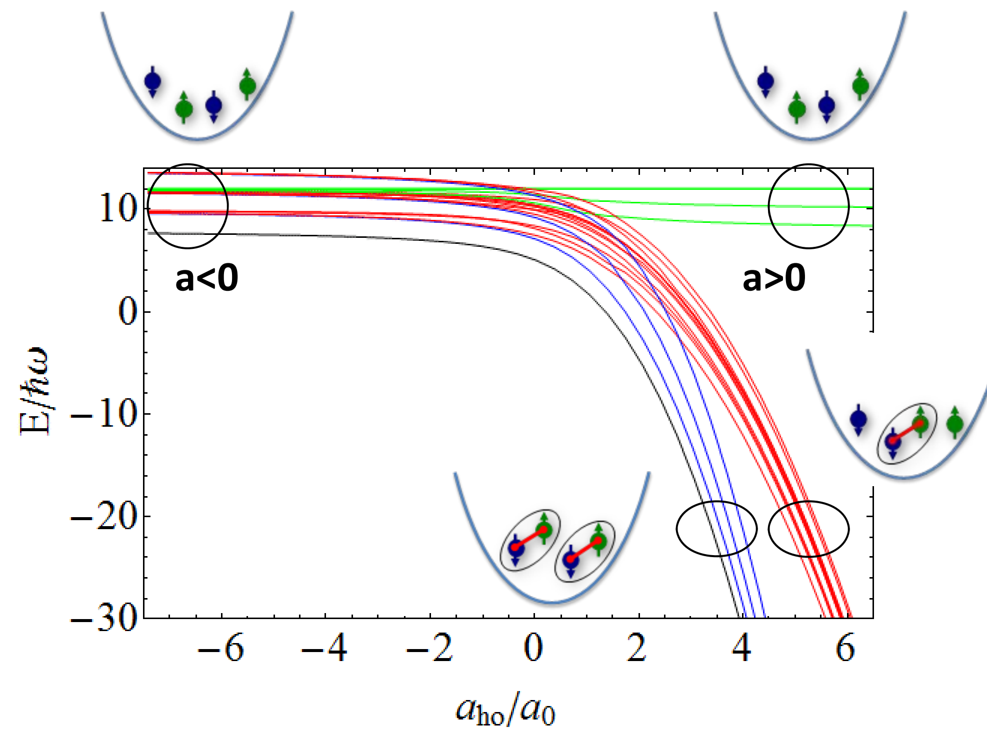
$$D(\lambda) = \sum_{i=1}^{K} \frac{|h_i|^2}{(\epsilon_i - \lambda)} - \lambda + h_{K+1}$$

3. *Test improvement*

Four-body Formulation

Example: Four fermions in a trap.





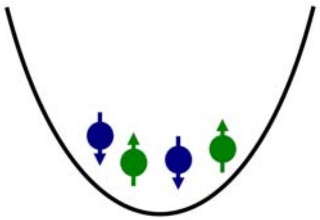
Outline:

- ***Correlated Gaussian Method***
  - *Implementation*
  - ***Connection with other methods***
- ***How does Efimov physics and universality extends beyond three bodies?***

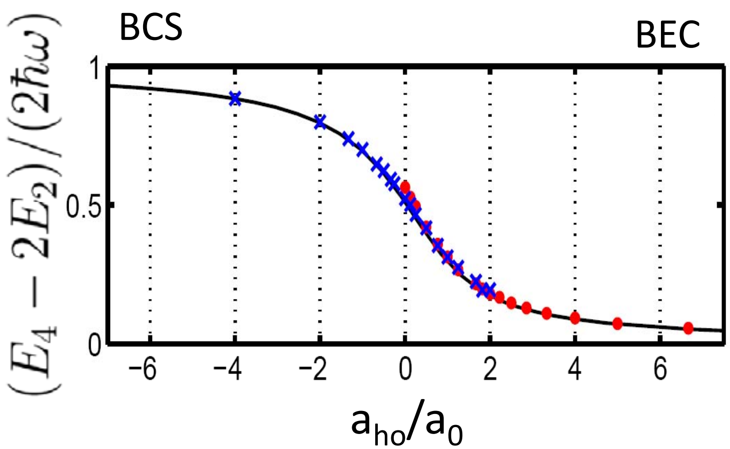
- ***Universality in four-boson systems***
- ***Extension to larger systems***

Correlated Gaussians and Monte Carlo methods

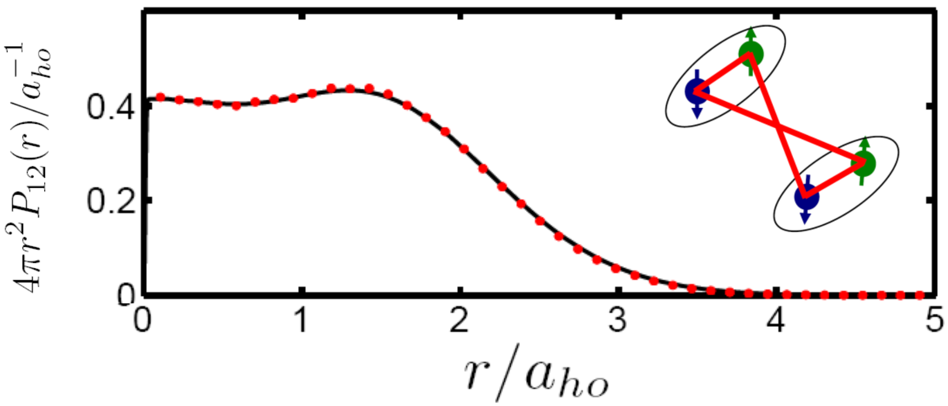
- ***Verify the accuracy of these methods***
- ***Construct better trial wave functions for diffusion Monte Carlo method***
- ***Extend calculations to larger systems***



Four fermion system



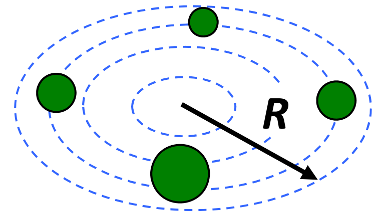
Pair correlation at unitarity



Four-body Formulation

J. von Stecher, C. H. Greene PRA (2009)

Review of hyperspherical representation:



***R**: overall size*

(collective motion)

Divide and conquer:

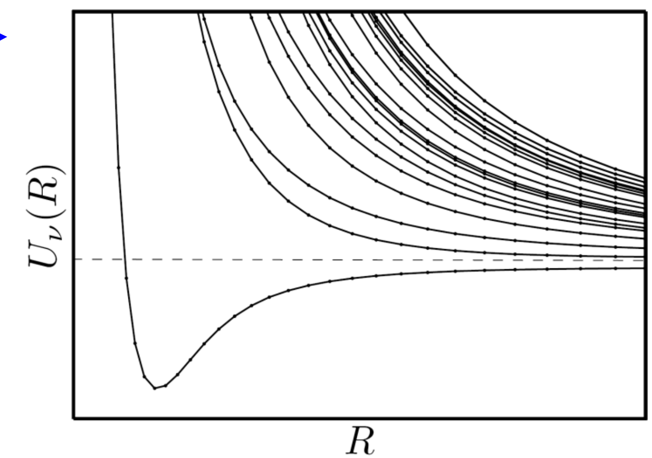
$$\Psi_E(R,\Omega) = \sum_\nu F_{\nu E}(R)\Phi_\nu(R;\Omega)$$

$$\mathcal{H}(R;\Omega)\Phi_\nu(R;\Omega) = U_\nu(R)\Phi_\nu(R;\Omega)$$

…solved at fixed R.

Coupled 1D equations

typical potential curves



Use correlated Gaussian to expand channel functions

$$\Phi_\nu(R;\Omega) = \sum_k C_{\nu,k}(R)\ \mathcal{S}\left[e^{-\sum_{ij} r_{ij}^2/2d_{ij,k}^2}\right]$$

Find efficient way to evaluate matrix elements

- ***Accurate description of four-body systems!!***

Correlated Gaussian Hyperspherical

… from five dimensions to one dimension

Adiabatic Hamiltonian:

$$\mathcal{H}(R;\Omega)\Phi_\nu(R;\Omega) = U_\nu(R)\Phi_\nu(R;\Omega)$$

How to calculate matrix elements?

Idea: select set of coordinates that simplify ME evaluation

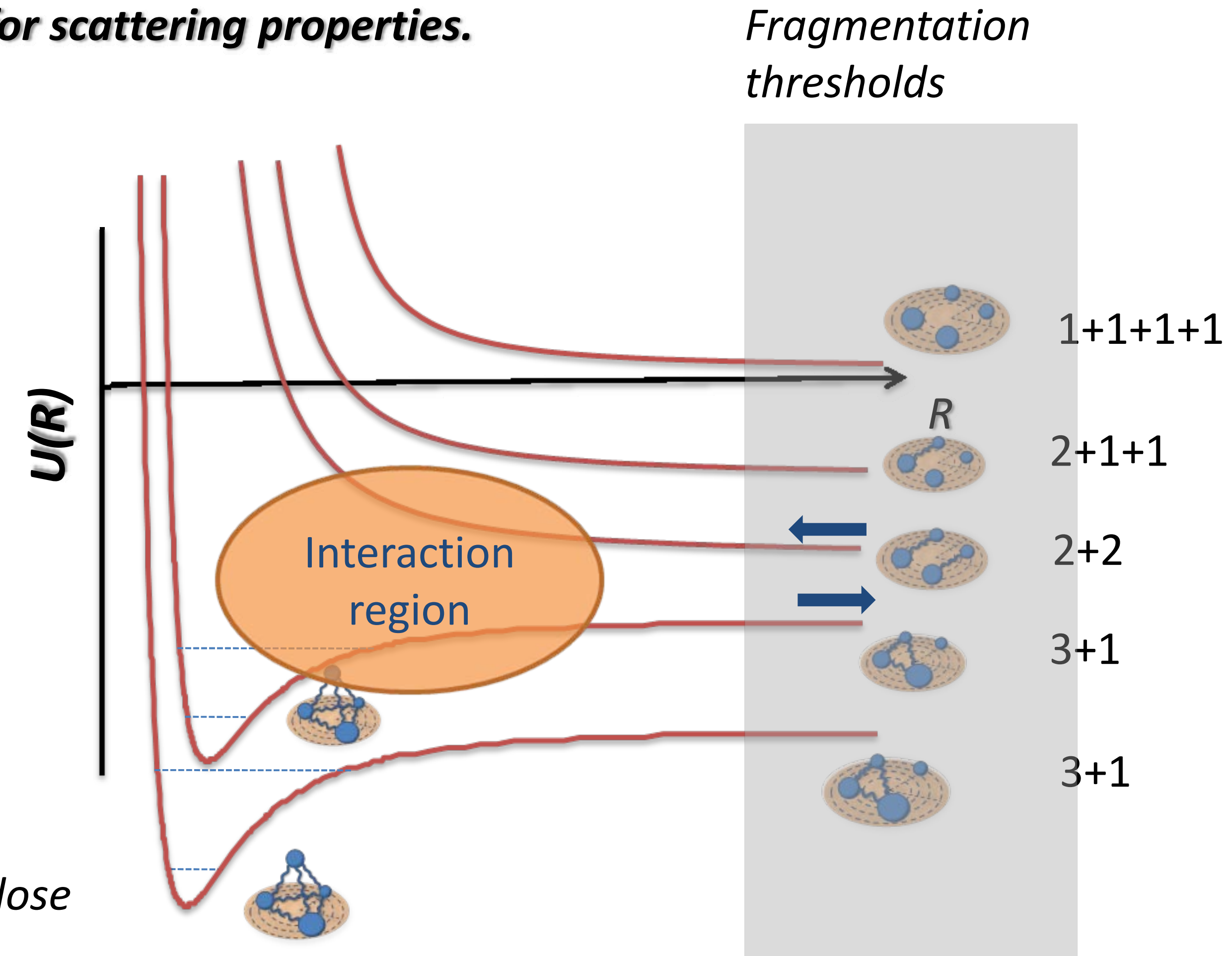
$$\int d\Omega \exp\left(-\sum_{ij} a_{ij}\mathbf{r}_i.\mathbf{r}_j\right) = \int d\Omega \exp\left(-\sum_{ij} \alpha_i \rho_i^2\right)$$

- Integration over $\boldsymbol{r}_i$ angles is trivial (for Gaussian interactions).
- Another integration can be done analytically .

- *For each ME evaluation, a new set of coordinates.*
- *Very accurate, suitable for SVM.*

Hyperspherical Picture

...for scattering properties.



All particles close together:
Bound and quasi-bound states

Hyperspherical Picture

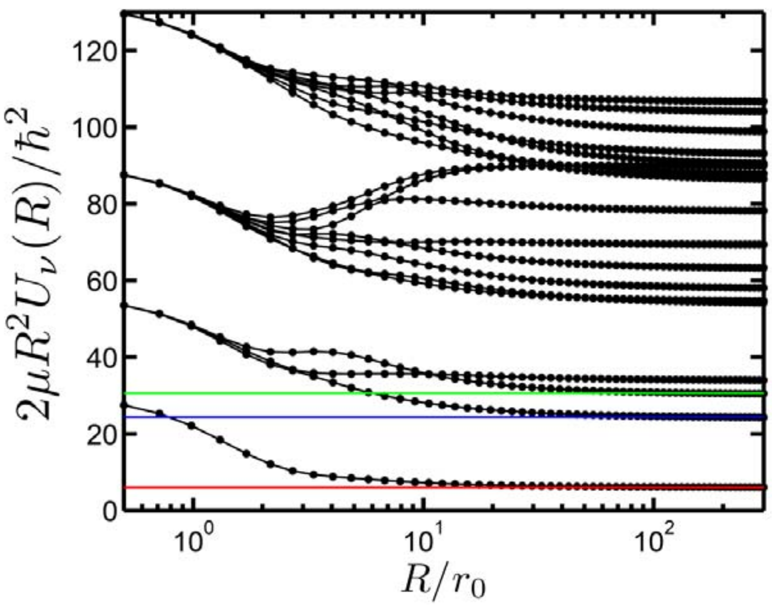
…for studying universality

D.S. Petrov, C. Salomon, G.V. Shlyapnikov PRL (2004)

Four fermion system at unitarity

➢ *Universality arguments predict that the hyperspherical potential curves are of the type (Tan, Werner & Castin, …):*

$$U_\nu(R) = \frac{\hbar^2 s_\nu(s_\nu+1)}{2\mu R^2}$$



Connection to trapped system:

$$E_0 = (s_0 + 3)\hbar\omega$$ → *trap frequency*

Trap system predictions:

J. von Stecher, D. Blume, C. H. Greene PRL 2007, PRA 2007, 2008

S.Y. Chang, and G. F. Bertsch PRA (R) (2007)

I. Stetcu, B. Barrett, U. van Kolck, J. Vary. PRA (2007)

Y. Alhassid, G. F. Bertsch, and L. Fang PRL (2008)

…..

Predictions:

s_0=2.0096 (CG) **s_0=2.0092 (CGH)**

➢ *Appropriate framework to analyze universality*

See also: J. P. D'Incao et al PRA (2009)

Outline:

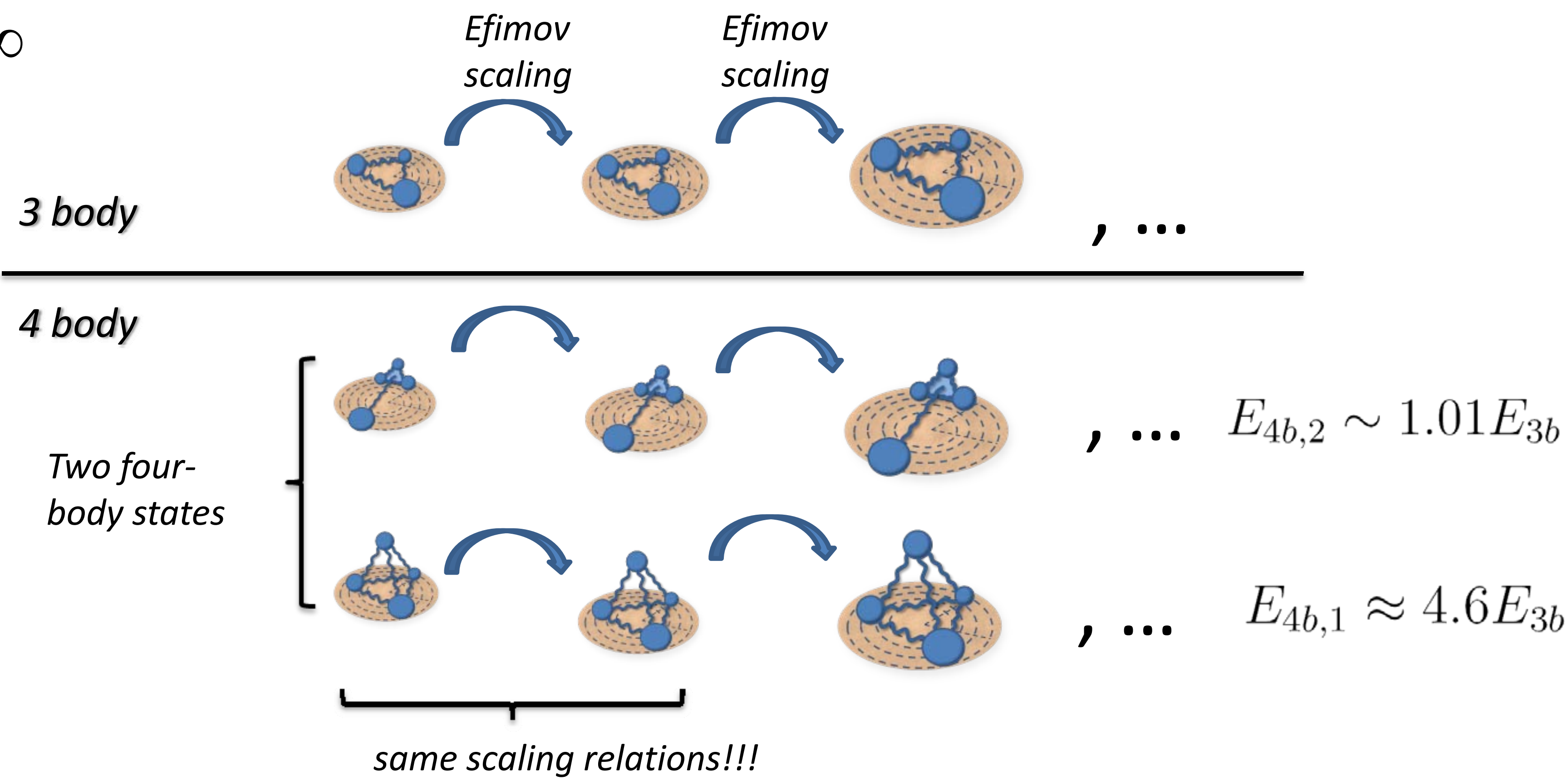
- *Correlated Gaussian Method*
  - *Implementation*
  - *Connection with other methods*
- ***How does Efimov physics and universality extends beyond three bodies?***

- ***Universality in four-boson systems***
- *Extension to larger systems*

J. von Stecher, J. P. D'Incao and C. H. Greene, Nat. Phys. (2009)

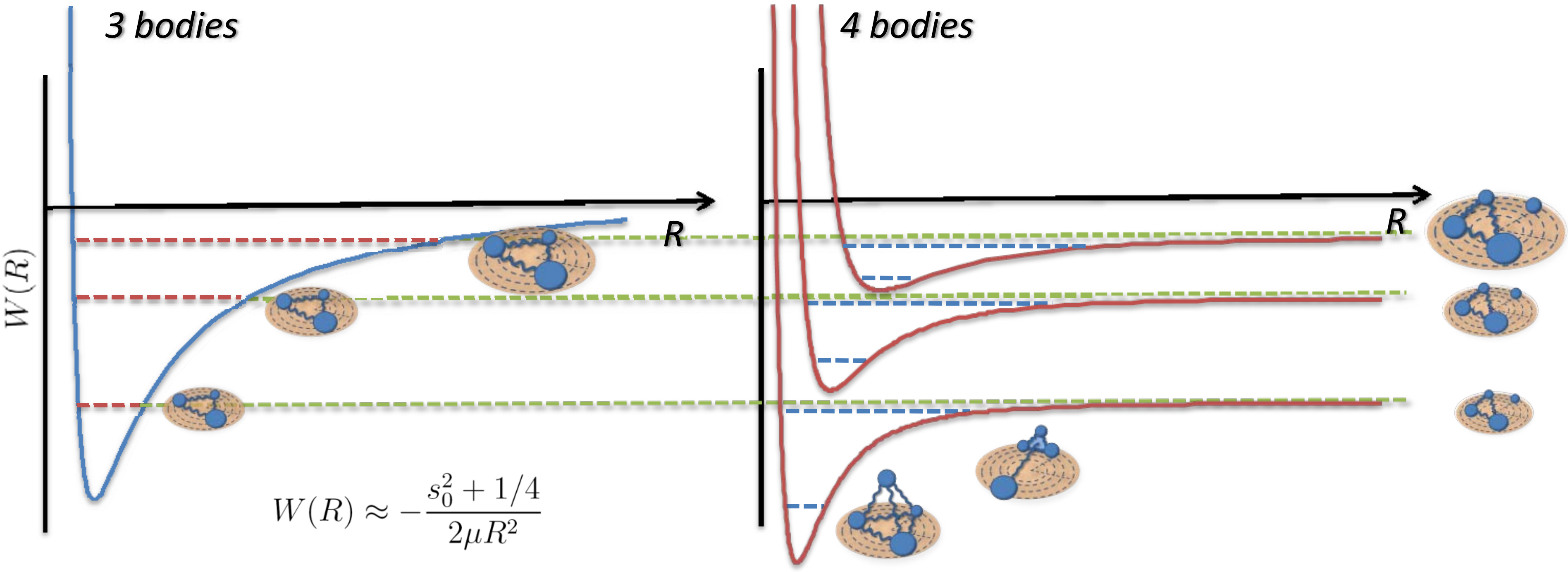
Universality in four bosons

a=∞



In agreement with Hammer & Platter EJPA (2007)

Hyperspherical Picture (a=∞)



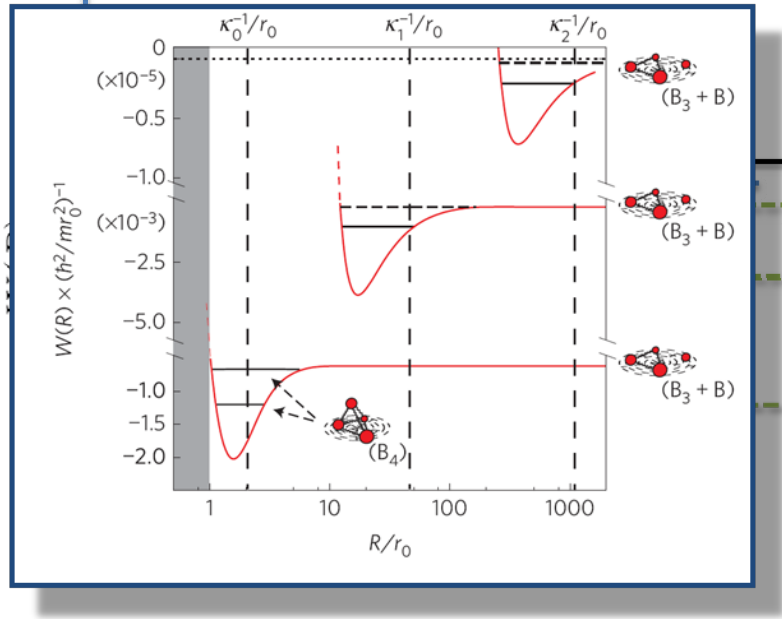
$$W(R) \approx -\frac{s_0^2 + 1/4}{2\mu R^2}$$

Four-body potential curves follow the same scaling of the Efimov states !!!

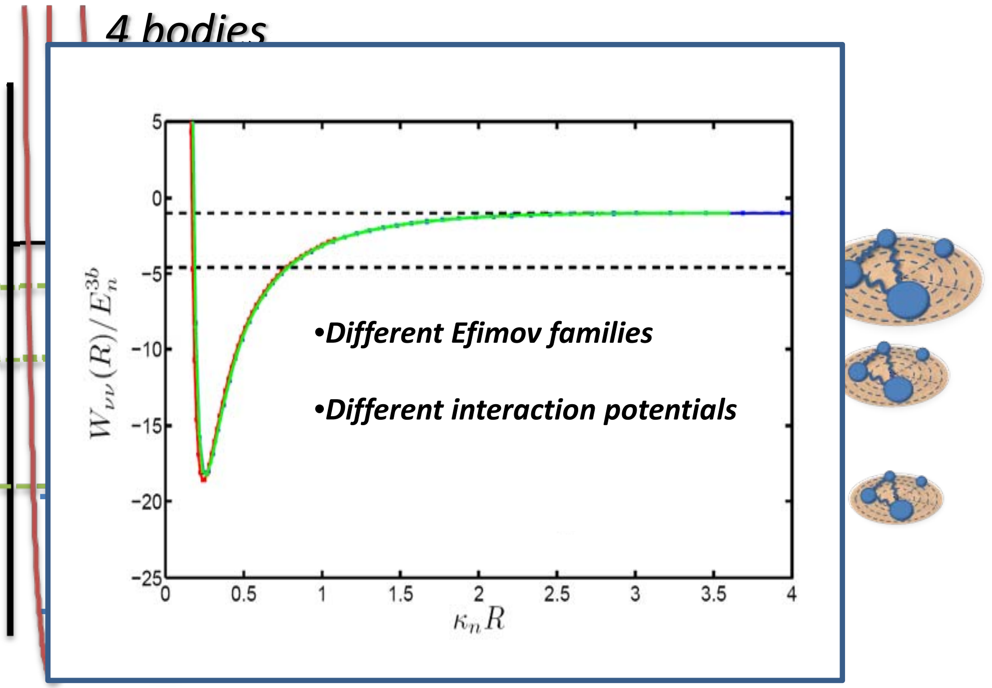
Four-body physics is universal!!

Hyperspherical Picture (a=∞)

3 bodies



4 bodies



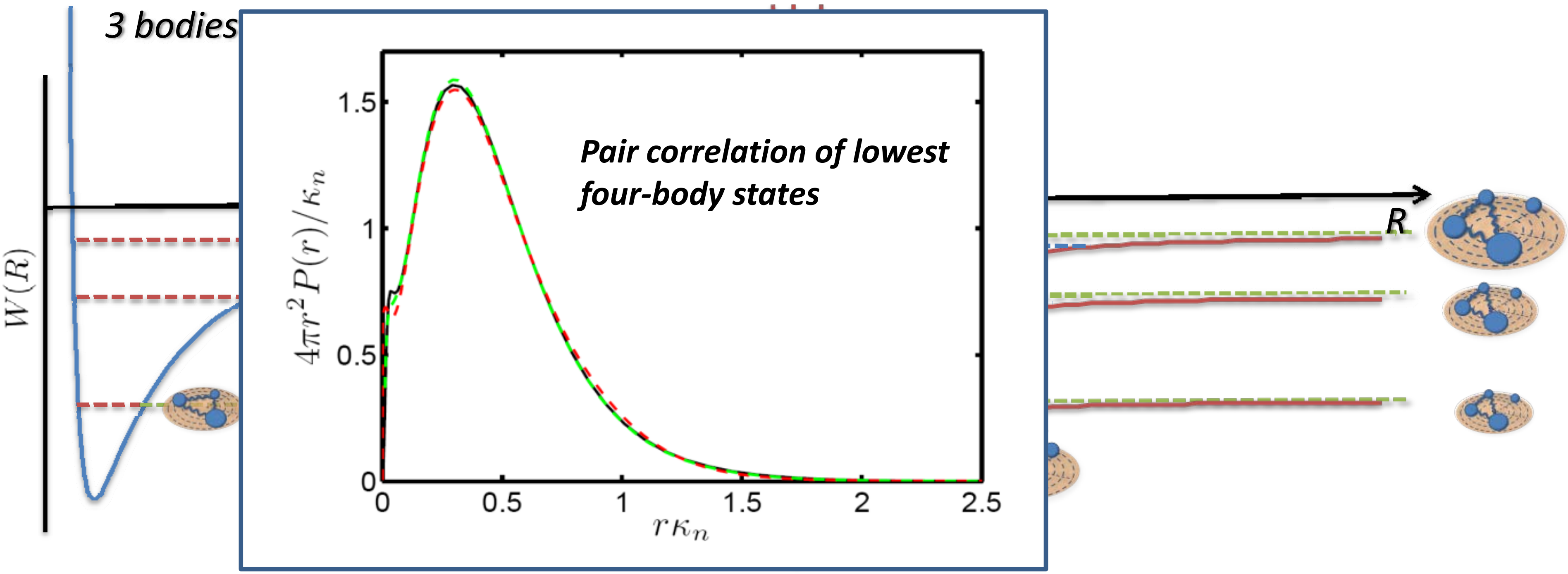
Four-body potential curves follow the same scaling of the Efimov states !!!

Three-body parameter:

$$\kappa_n = \sqrt{mE_{3b}^{(n)}/\hbar}$$

Four-body physics is universal!!

Hyperspherical Picture (a=∞)



Four-body potential curves follow the same scaling of the Efimov states !!!

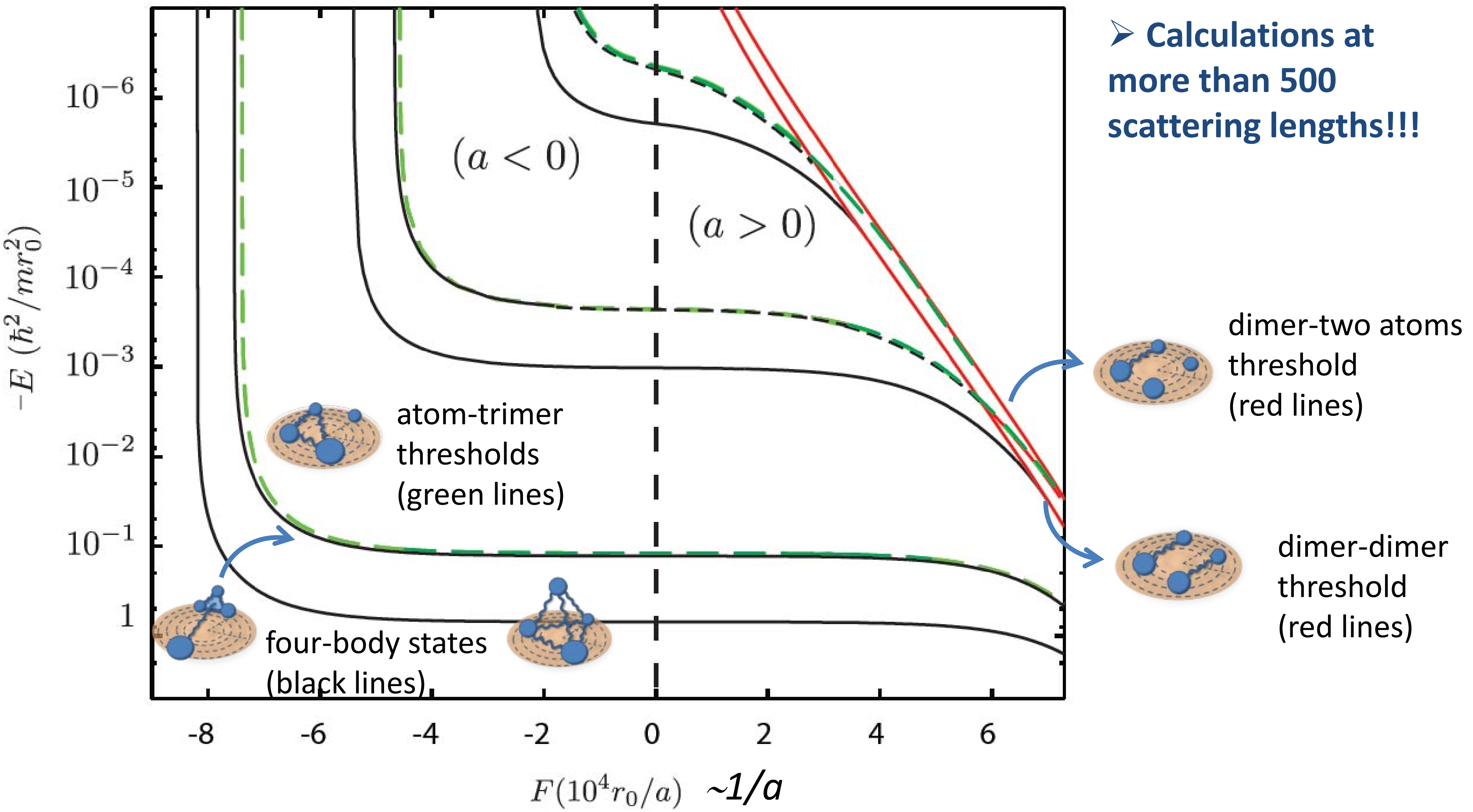
Three-body parameter:

$$\kappa_n = \sqrt{mE_{3b}^{(n)}/\hbar}$$

Four-body physics is universal!!

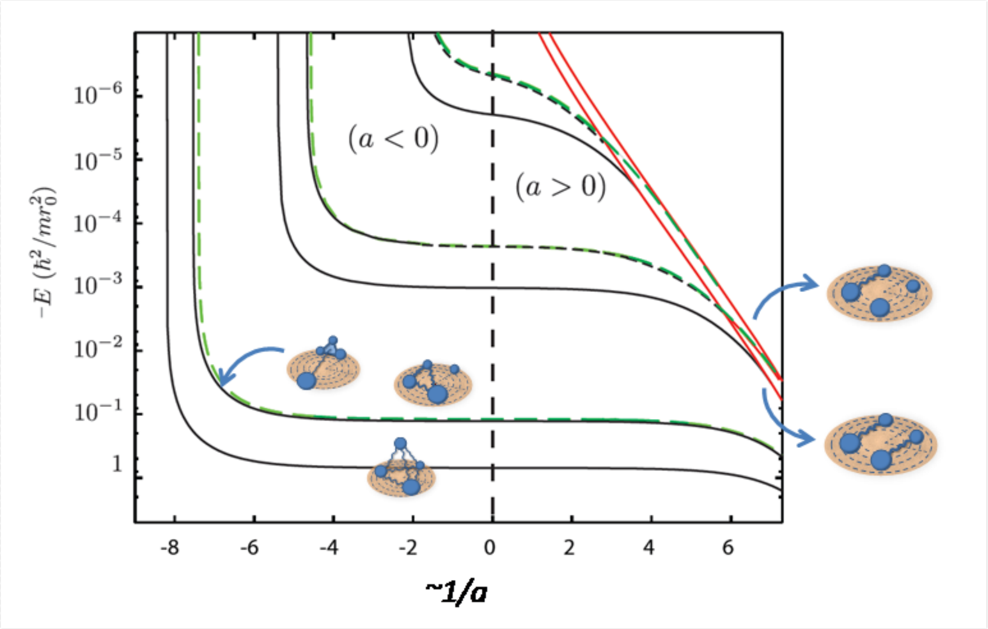
J. von Stecher, J. P. D'Incao and C. H. Greene, Nat. Phys. (2009)

Spectrum: Extended Efimov plot

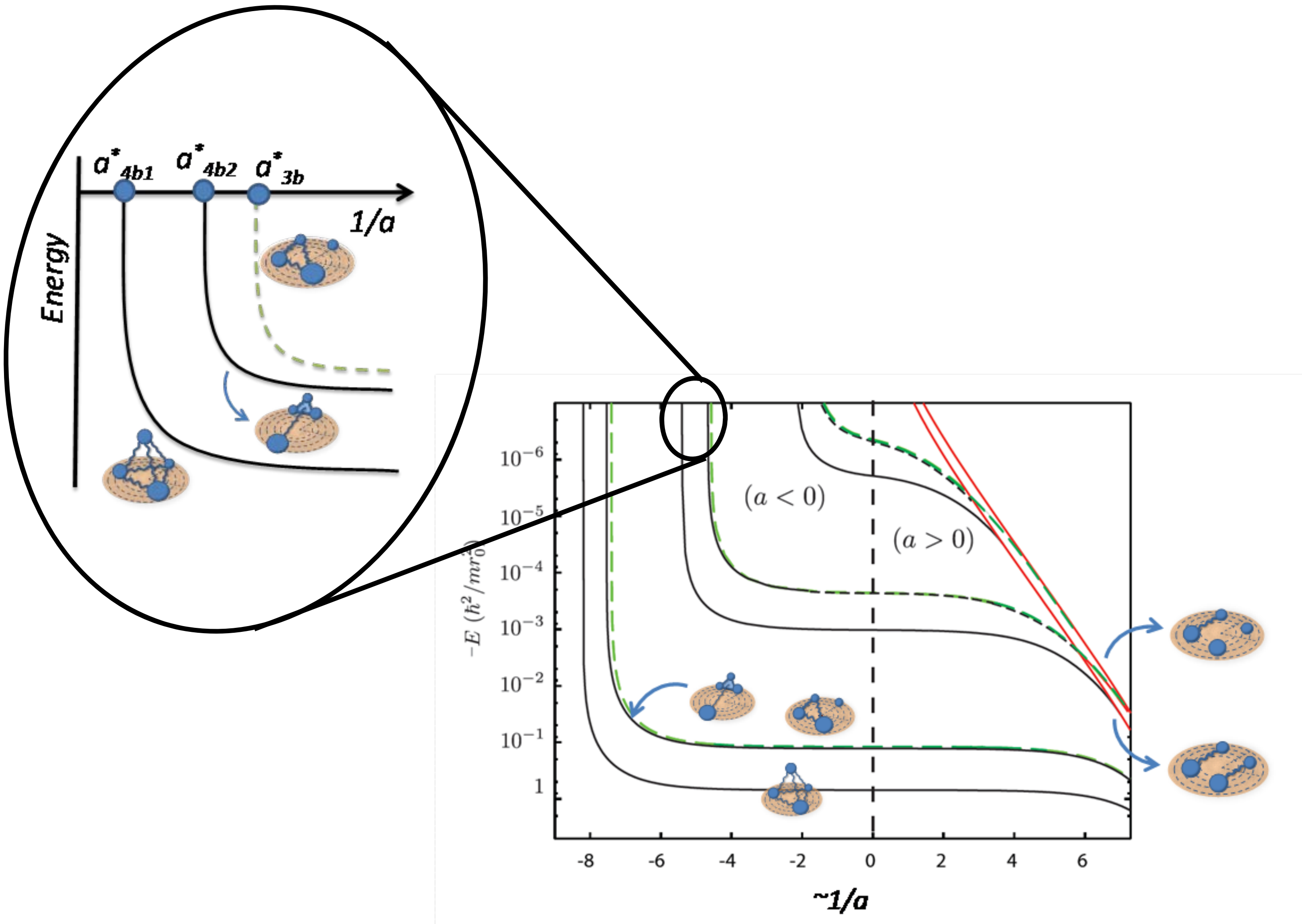


- **Calculations at more than 500 scattering lengths!!!**

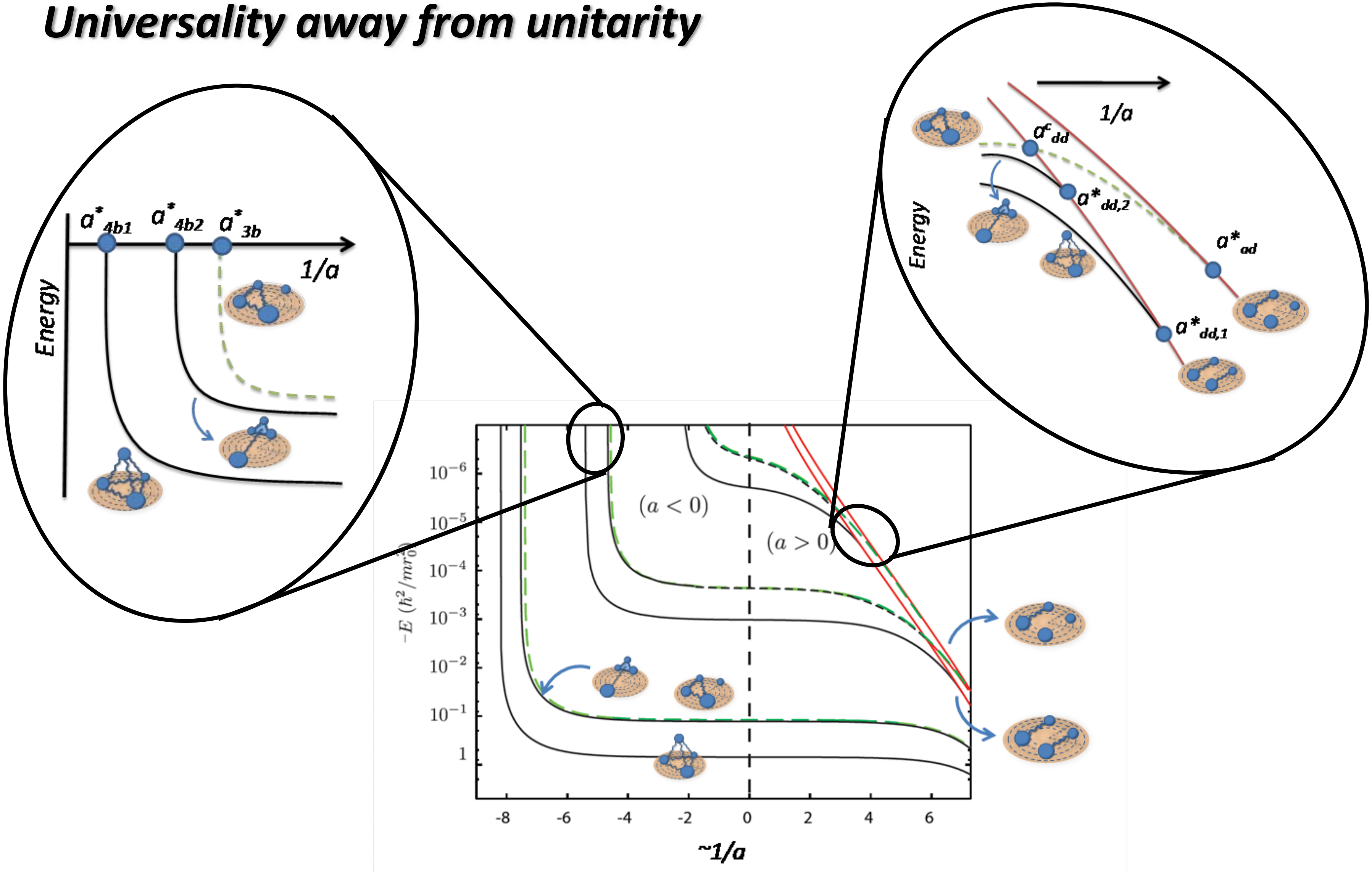
Universality away from unitarity



Universality away from unitarity

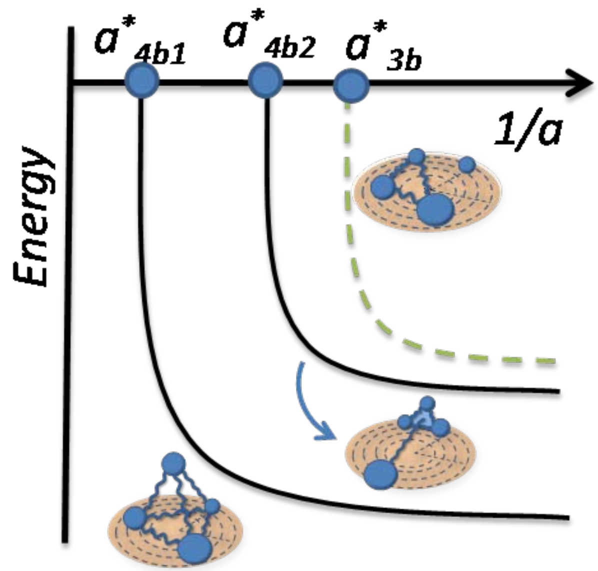


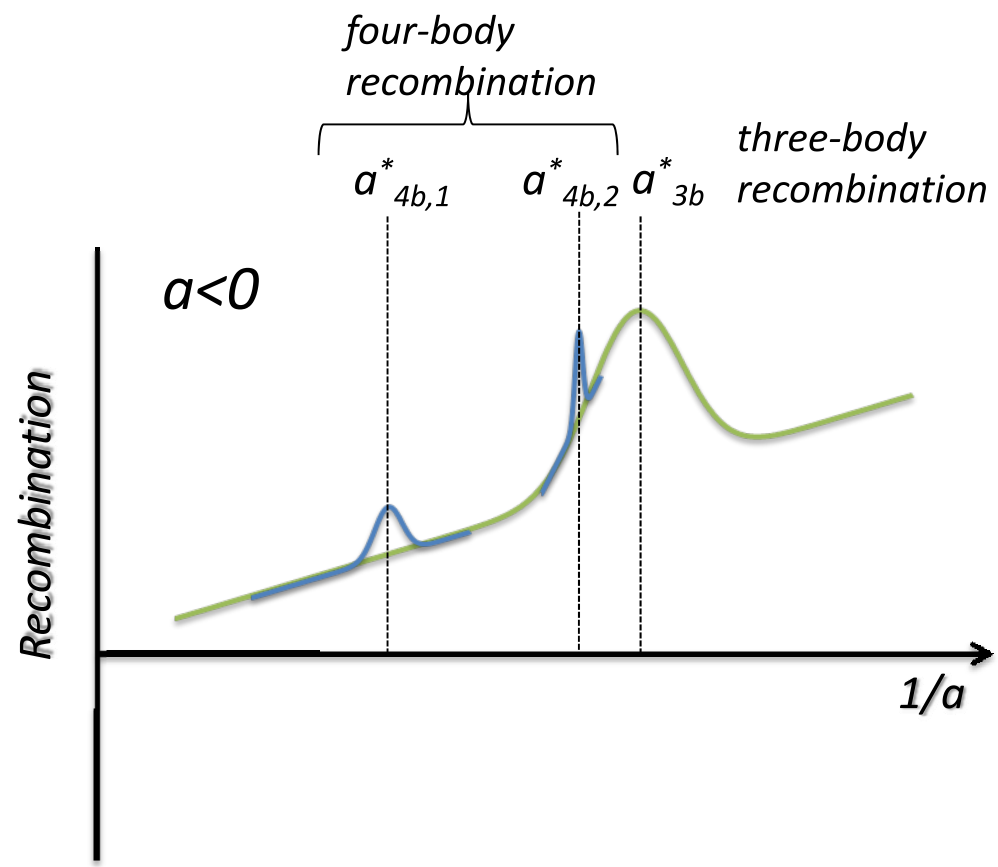
Universality away from unitarity



Universality away from unitarity

a<0



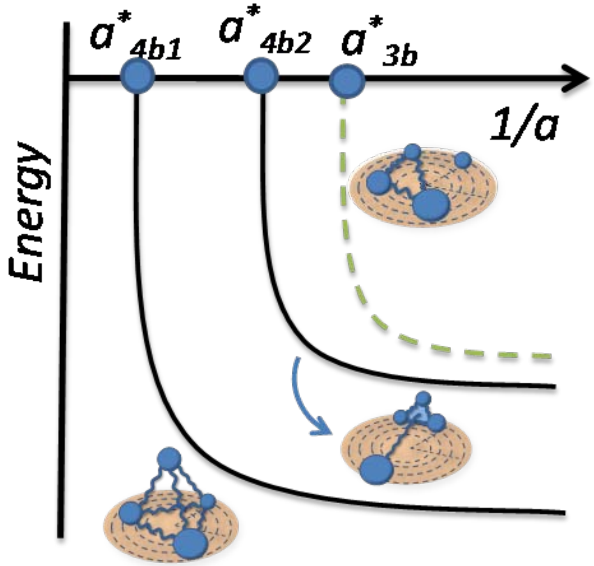


$$a^*_{4b,1} \approx 0.43 a^*_{3b}$$

$$a^*_{4b,2} \approx 0.90 a^*_{3b}$$

Universality away from unitarity

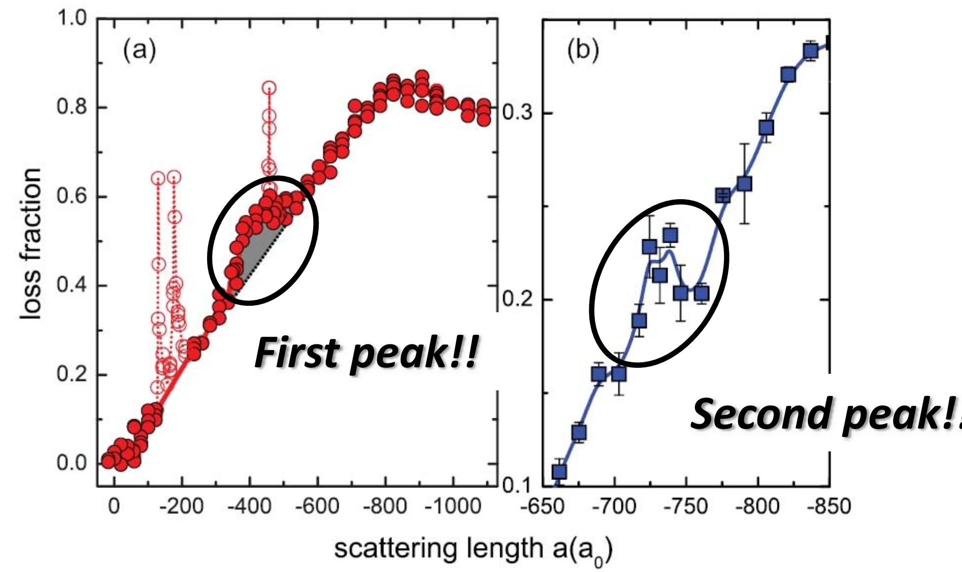
a<0



$$a^*_{4b,1} \approx 0.43 a^*_{3b}$$

$$a^*_{4b,2} \approx 0.90 a^*_{3b}$$

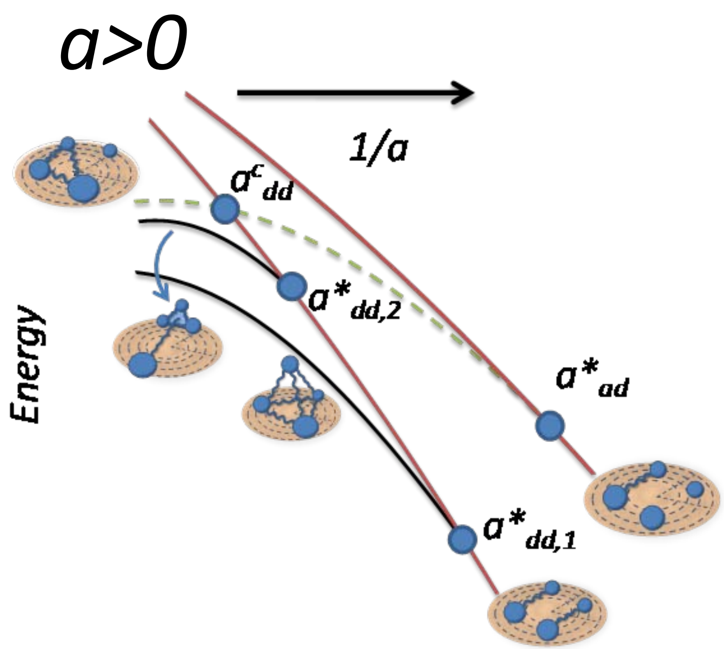
Experimental observation



Ferlaino, et al. (2009)

More experimental evidence:
Lens, Rice

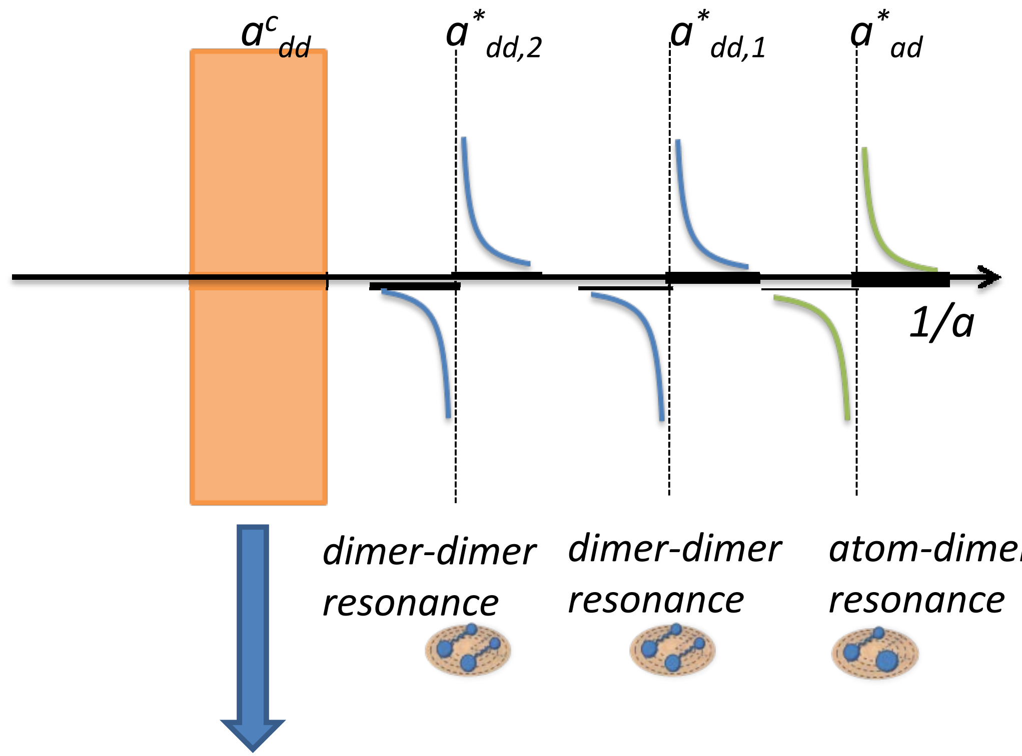
Universality away from unitarity



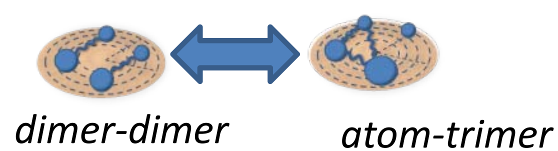
$$a^*_{dd,1} \approx 2.37 a^*_{ad}$$

$$a^*_{dd,2} \sim 6.6 a^*_{ad}$$

$$a^c_{dd} \approx 6.73 a^*_{ad}$$



Efficient conversion:



Outline:

- Correlated Gaussian Method
  - Implementation
  - Connection with other methods
- **How does Efimov physics and universality extends beyond three bodies?**

- Universality in four-boson systems
- Extension to larger systems

- ***How to extend the analysis of universality to larger systems?***

Extension to larger systems

- ***How many parameters are needed to describe N-boson systems?***

Hanna & Blume, PRA (2006):

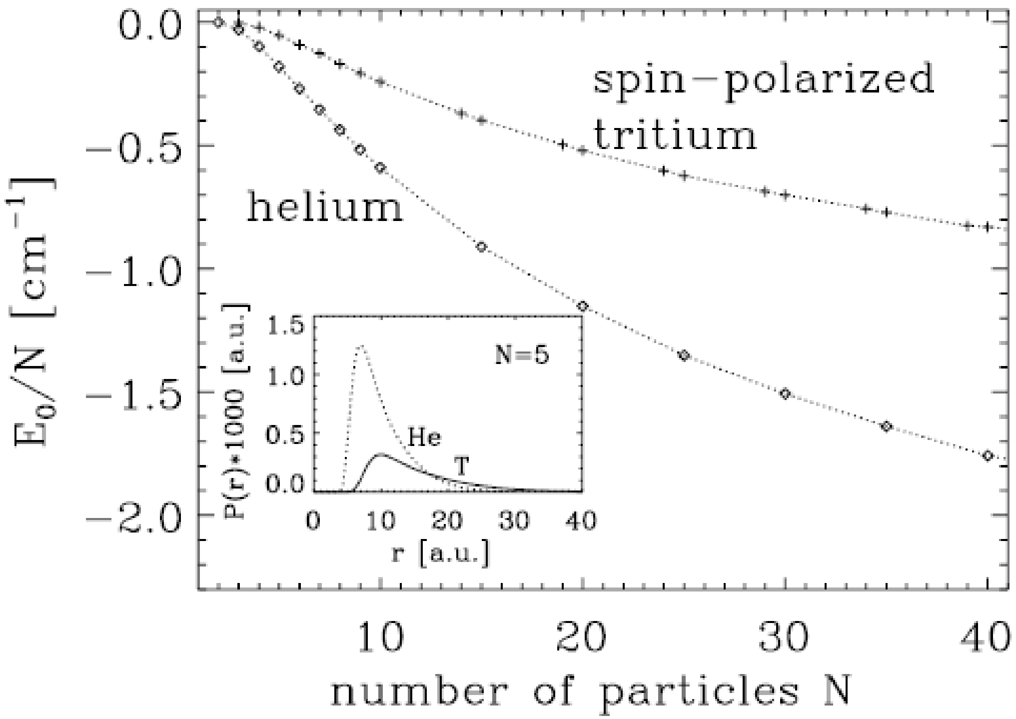
- *Linear correlations between cluster energies (like Tjon lines)*

Other studies:

Lewerenz, JCP (1997).
Blume & Greene, JCP(2000).
Hanna & Blume, PRA (2006).
…

Hammer & Platter, EPJA (2007).

Helium and spin-polarized tritium: similar behavior



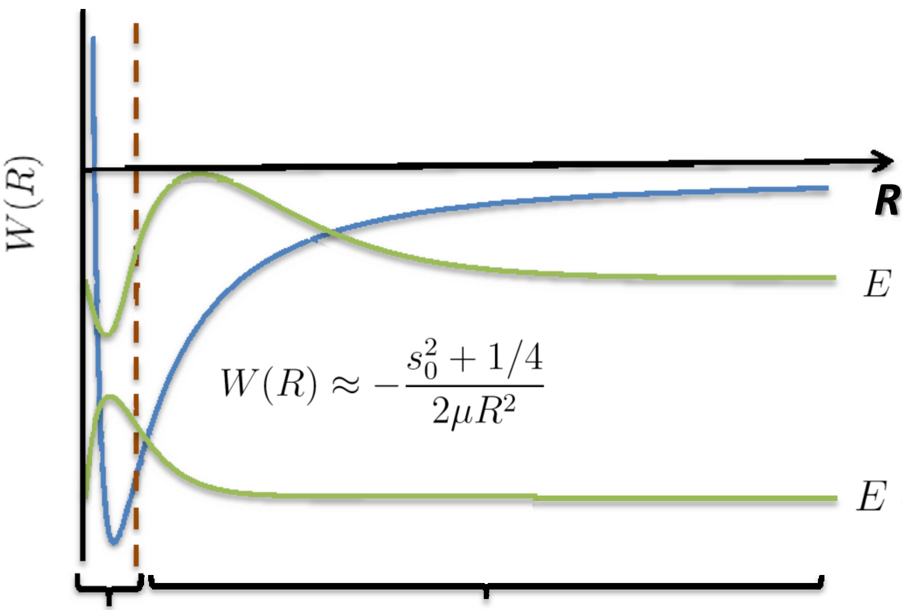
Blume et al., PRL(2002)

Model Hamiltonian

Hypersperical potential at unitatity

3 bodies

➢ ***Goal: construct a minimal Hamiltonian that would lead to a "universal ground state".***



$E \ll \hbar^2/mr_0^2$ *dilute and weakly bound ~ universal*

$E \sim \hbar^2/mr_0^2$ *controlled by short-range physics*

short-range physics $R \lesssim r_0$

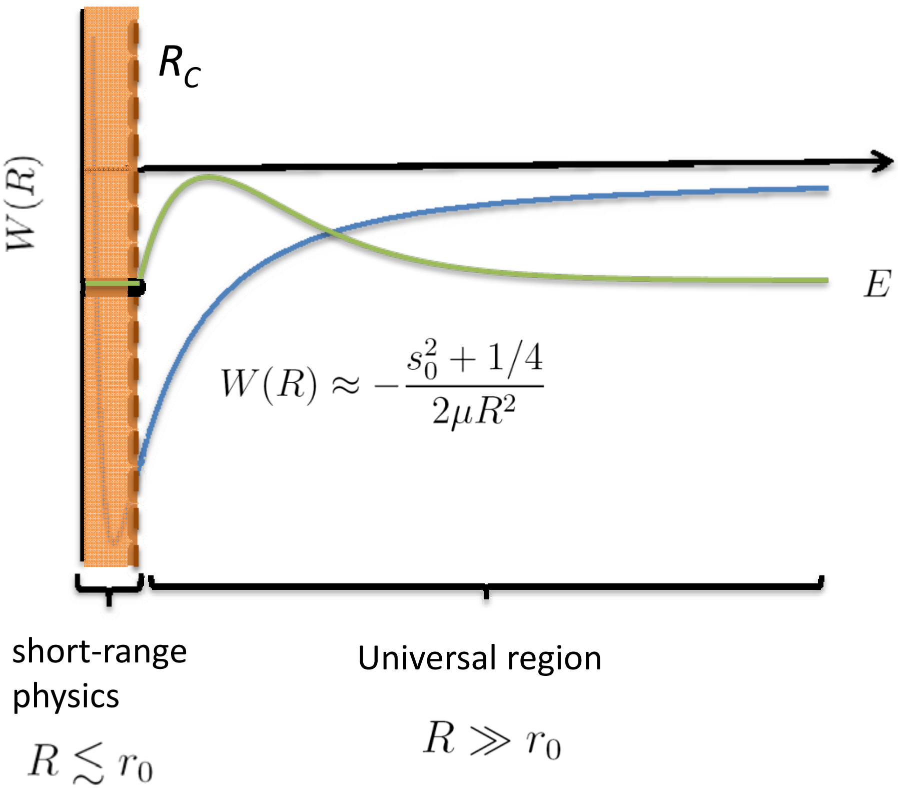
Universal region $R \gg r_0$

J. von Stecher arXiv:0909.4056 (2009)

Model Hamiltonian

Hypersperical potential at unitatity

3 bodies



$E \ll \hbar^2/mr_0^2$

dilute and weakly bound
~ universal !!

> ➢ ***Goal: construct a minimal Hamiltonian that would lead to a "universal ground state".***

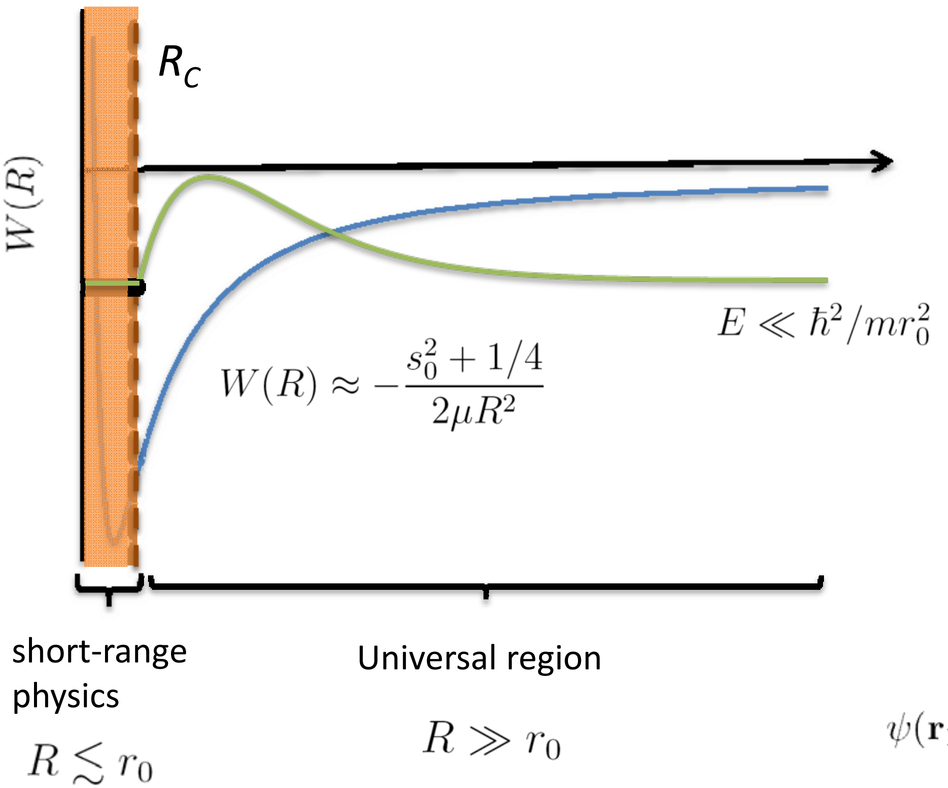
J. von Stecher arXiv:0909.4056 (2009)

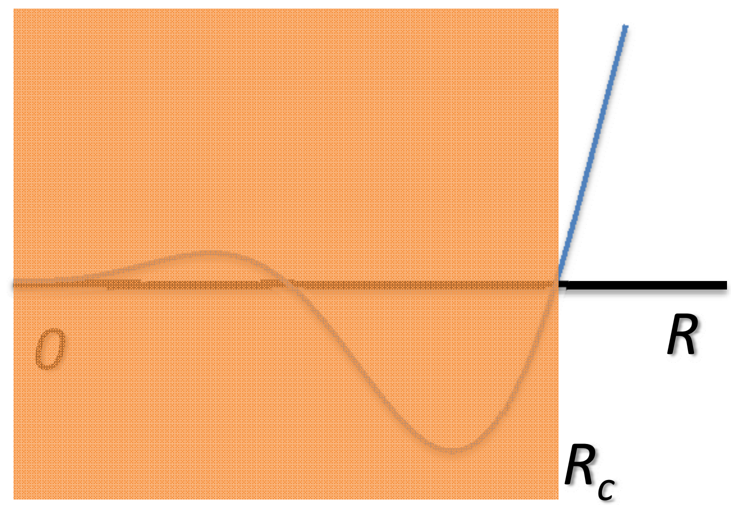
Model Hamiltonian

Hyperspherical potential at unitatity

3 bodies

➢ ***Goal: construct a minimal Hamiltonian that would lead to a "universal ground state".***





$$\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) \underset{R\to 0}{\sim} \frac{1}{R^2}\sin\left[|s_0|\ln\frac{R}{R_c}\right]\Phi(\mathbf{\Omega})\,B(\mathbf{C},\mathbf{r}_4,\ldots,\mathbf{r}_N).$$

F. Werner & Y Castin

J. von Stecher arXiv:0909.4056 (2009)

Model Hamiltonian

Many-body Hamiltonian:

$$H = \sum_i \frac{-\hbar^2}{2m}\nabla_i^2 + \sum_{i,j} V_2(r_{ij}) + \sum_{i,j,k} V_3(R_{ijk})$$

$$R_{ijk} = \sqrt{(r_{ij}^2 + r_{ik}^2 + r_{jk}^2)/3}$$

controls two-body physics: scattering length

controls three-body physics: 3-body parameter

Model Hamiltonian

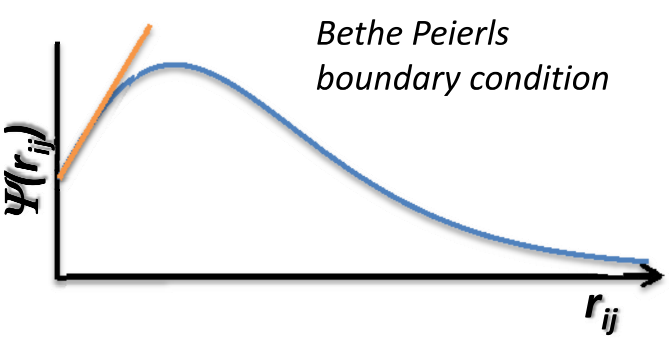
- ***Two parameters (a and R_c) to independently control two and three-body physics.***

Many-body Hamiltonian:

$$H = \sum_i \frac{-\hbar^2}{2m}\nabla_i^2 + \sum_{i,j} V_2(r_{ij}) + \sum_{i,j,k} V_3(R_{ijk})$$

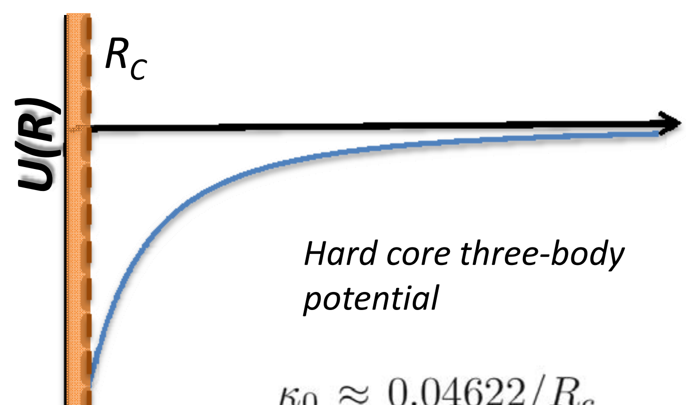
$$R_{ijk} = \sqrt{(r_{ij}^2 + r_{ik}^2 + r_{jk}^2)/3}$$

2 bodies



$$V_2(\mathbf{r}) \;=\; 4\pi a\hbar^2/m\,\delta(\mathbf{r})\frac{\partial}{\partial r}r$$

3 bodies



$$\kappa_0 \approx 0.04622/R_c$$

J. von Stecher arXiv:0909.4056 (2009)

Numerical methods

- ***Correlated Gaussian basis set expansion up to N=6.***
  - *Gaussian potential for two and three-body interactions*

- ***Diffusion Monte Carlo simulations up to N=13.***
  - *Hard Wall 3-body potential and an attractive square 2-body potential*
  - *Trial wave function:* $$\Psi_T(\mathbf{r}_1, ..., \mathbf{r}_n) = \Phi(R_T) \prod_{i,j,k} g(R_{i,j,k}) \prod_{i,j} f(r_{i,j})$$

HR correlations | **3-body correlations** | **2-body correlations**

J. von Stecher arXiv:0909.4056 (2009)

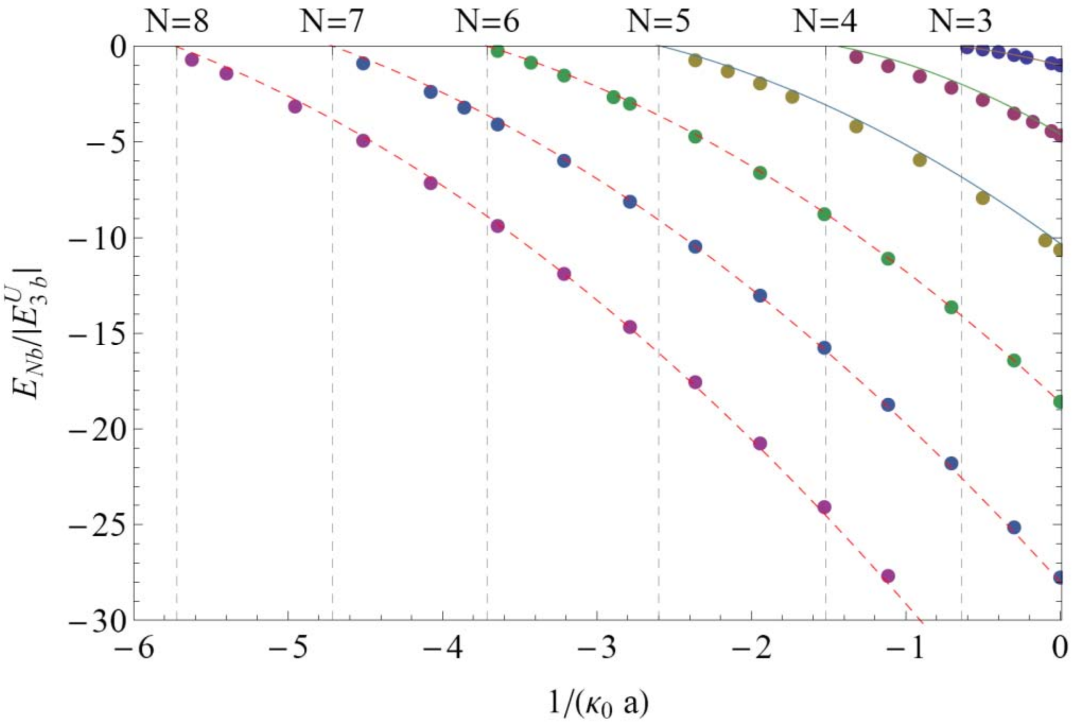
Weakly-bound Clusters

$\sim 10^{-5}\hbar^2/(mr_0^2)$

Universal description: $E_{Nb} = |E^U_{3b}|\epsilon_N[1/(\kappa_0 a)]$ $\quad (E^U_{3b} = -\kappa_0^2\hbar^2/m)$ ***(just from dimensional analysis)***

Universal function

Numerical predictions:



Comparison with other predictions

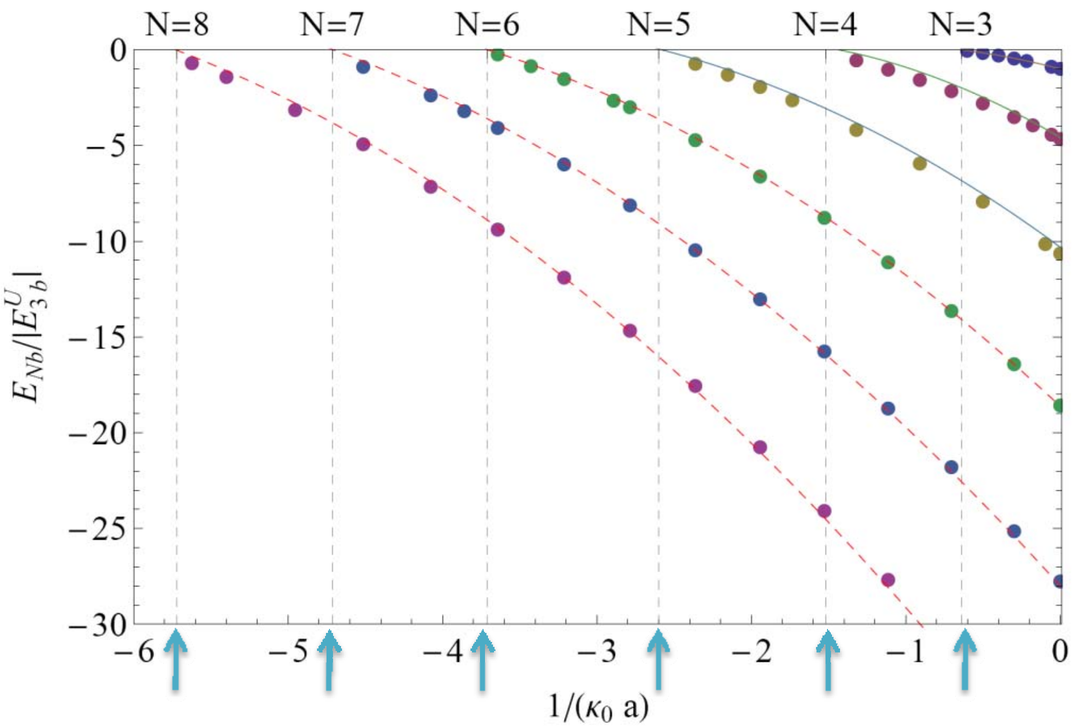
$E_{4b,1} \approx 4.65(4)E_{3b}$

$a^*_{4b,1} \approx 0.42(1)a^*_{3b}$

Comparison between CG and DMC

➢ ***At least one N-body cluster state for each Efimov trimer!!***

Weakly-bound Clusters



Positions of resonances

Properties:

- *"Super" Borromean states*
- *Linear Correlations (Tjon lines):*

$$E_{4b} \approx 2.66 E^U_{3b} + 2.0\, E_{3b}$$

- *N-body resonant enhancement of losses:*

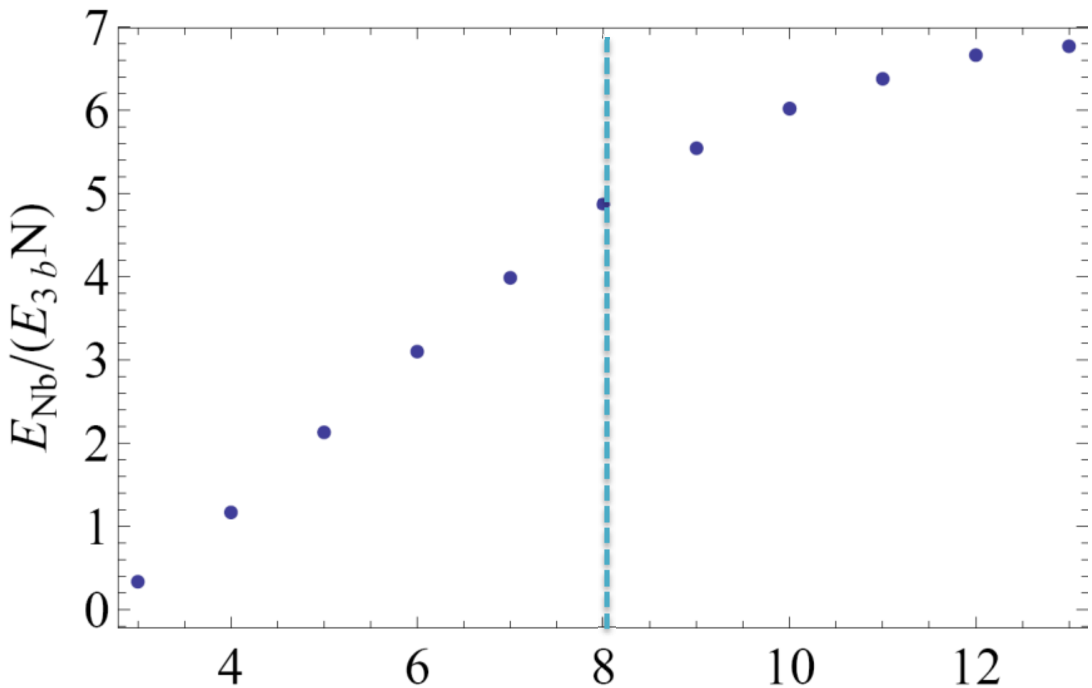
$$1/(\kappa_0 a^*_{Nb}) \approx 2.3(1) - N$$

Position of five-body resonance: $a^*_{5b} \approx 0.6 a^*_{4b}$

J. von Stecher arXiv:0909.4056 (2009)

Weakly-bound Clusters

Energy per particle at unitarity

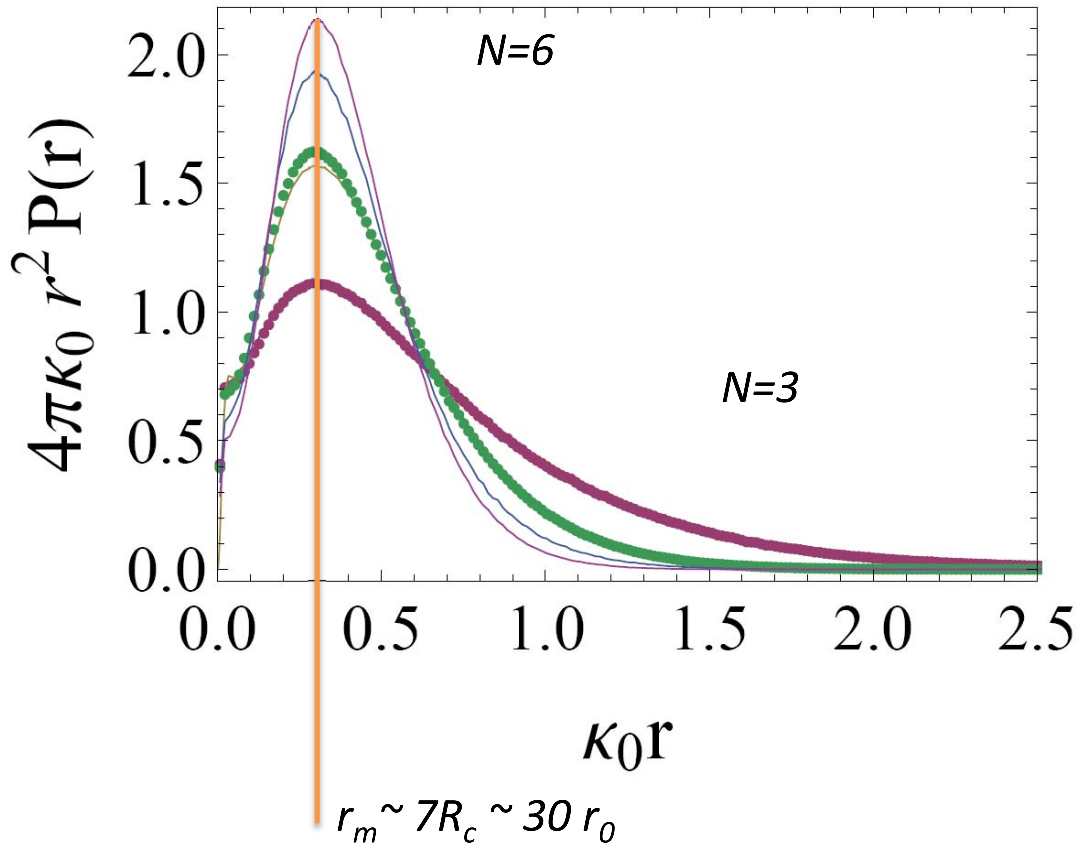


$E_{Nb} \propto N^2$ N $E_{Nb} \propto N$?

J. von Stecher arXiv:0909.4056 (2009)

Dilute Clusters

Pair correlation function

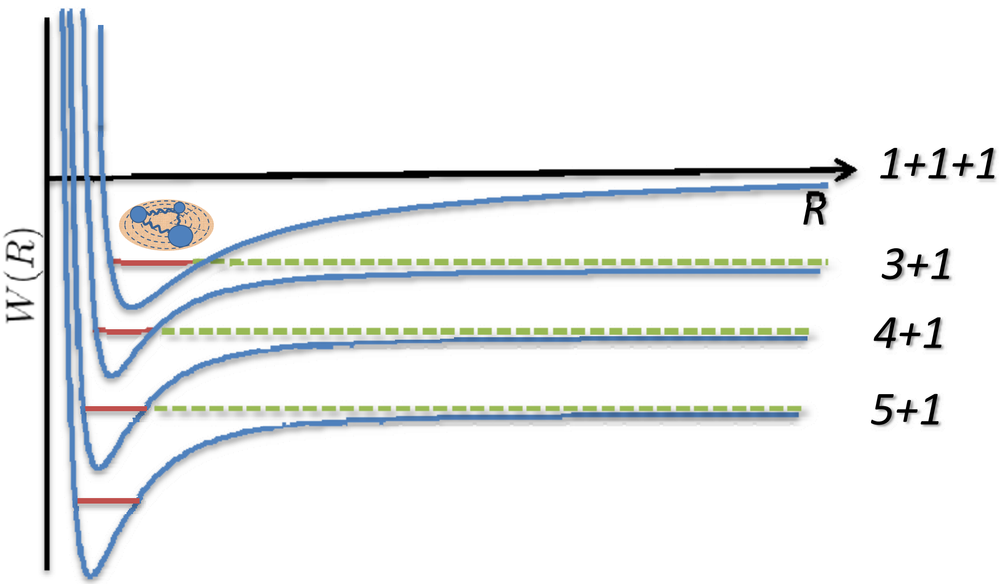


J. von Stecher arXiv:0909.4056 (2009)

Hyperspherical Picture

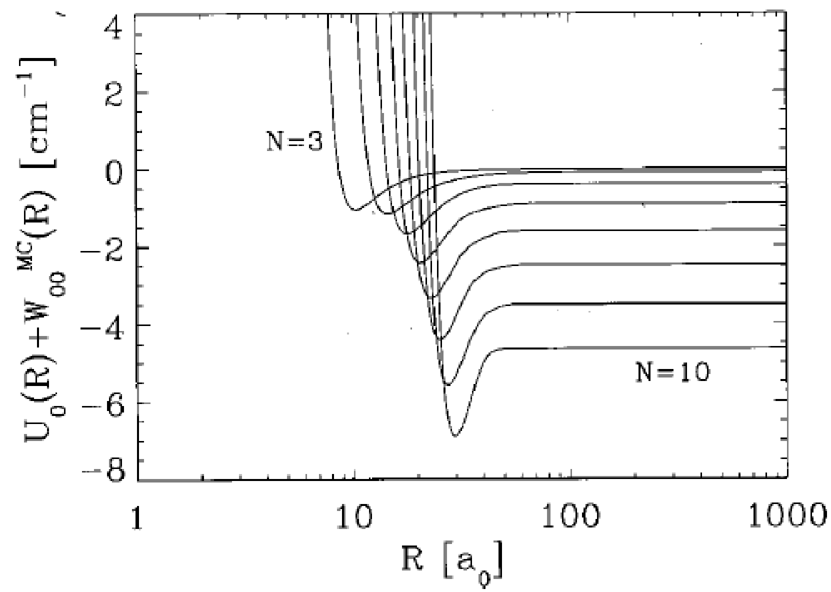
…sketching potentials

N bodies



Helium clusters

Monte Carlo + Hyperspherical



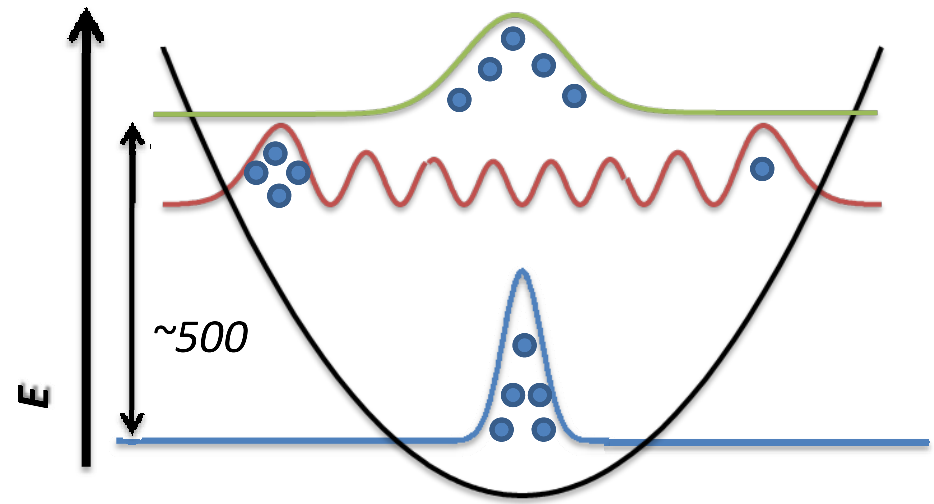
D. Blume & C. H. Greene, JCP 2001

- *Potential curves scale with size and energy of cluster states*
- *All clusters follow Efimov scaling relations*

Testing predictions

Five-body states:

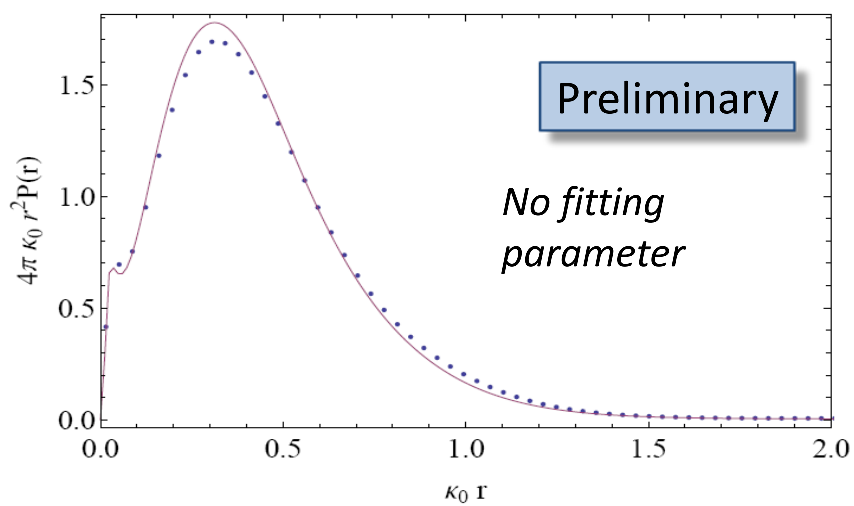
- *Search for states attached to excited Efimov states.*
- *Test universality (change two-body interaction)*



Comparison of predictions for two different model interactions

$$E_{5B} \approx 10\ E_{3B}$$

(good agreement with model $E_{5B} \approx 10.6\ E_{3B}$)



The universal five-body state is there!

Conclusions:

- *Correlated Gaussians for atomic systems (N>3)*
- *CG+QMC and Hyperspherical methods for studying universality*

Outlook:

- *Different species or/and spin statistic?*
  - *Universality?*
  - *Four-body states?*
- *Model Hamiltonian*
  - *with Quantum Monte Carlo*
- *Cluster states*
  - *Large N limit*