Few-body problem

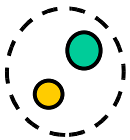
Dmitry Petrov

Laboratoire Physique Théorique et Modèles Statistiques (Orsay)

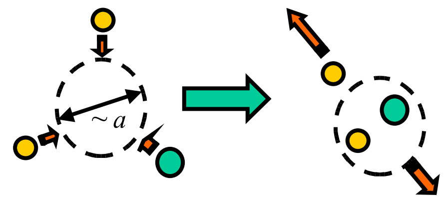
Few-body problem in ultracold gases?

Microscopic level

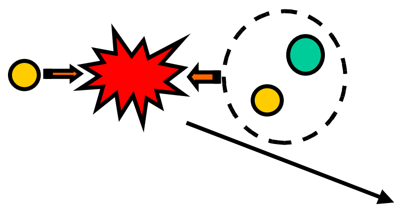
Structure of molecules



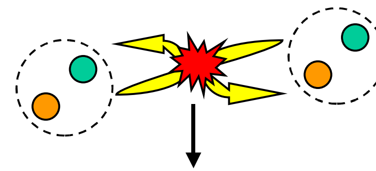
Three-body recombination



Atom-dimer scattering

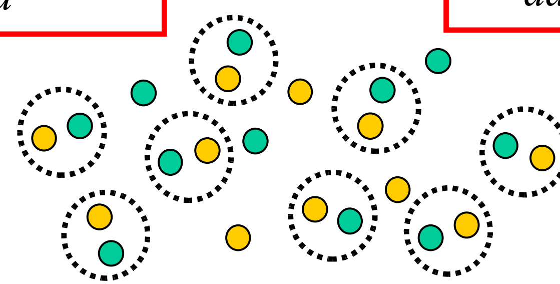


Dimer-dimer scattering



$$a_{ad} = ?$$

$$a_{dd} = ?$$



Macroscopic level

- compressibility, analysis of collapse or phase separation?
- equation of state and test for Monte-Carlo calculations

Path towards many-body case

Exact account of few-body correlations, cluster expansion, virial coefficients…

Size of configuration space

N-body problem in 3D → 3N (degrees of freedom)

- 3 (translational invariance)

- 3(2) (rotational invariance)

= 3N-6(5)

2-body → Single coordinate. Radial Schrödinger equation. Not enough accuracy for realistic potentials

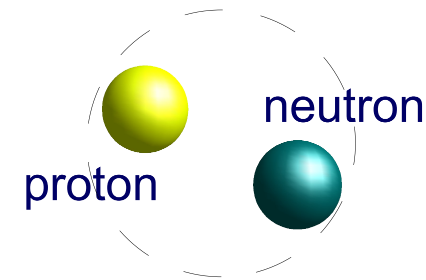
3-body → 3 coordinates. Involved numerics with simple model potentials.

4-body → 6 coordinates. Reliable solution impossible even for simple model potentials

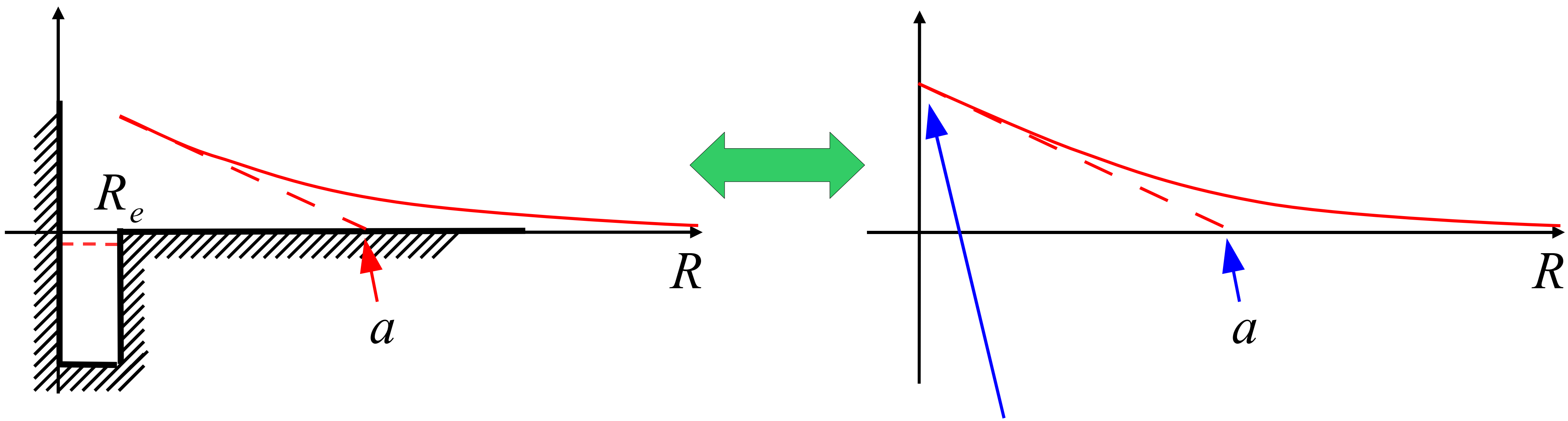
Fortunately, many interesting few-body problems can be solved in an elegant way by using the short-range character of interparticle forces

Bethe – Peierls boundary conditions

Bethe and Peierls (1934), “Quantum theory of the diplon”



Diplon (deutron) is a weakly bound dimer with $R_e \approx 10^{-13}\,\mathrm{cm}$, $a \approx 4.5 \cdot 10^{-13}\,\mathrm{cm}$

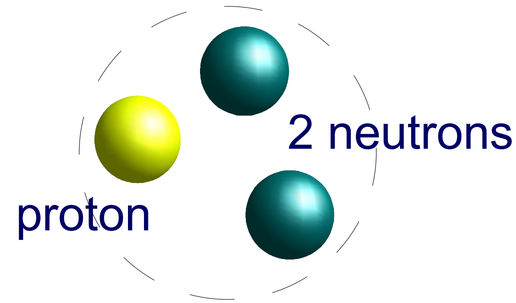


Bethe-Peierls boundary condition

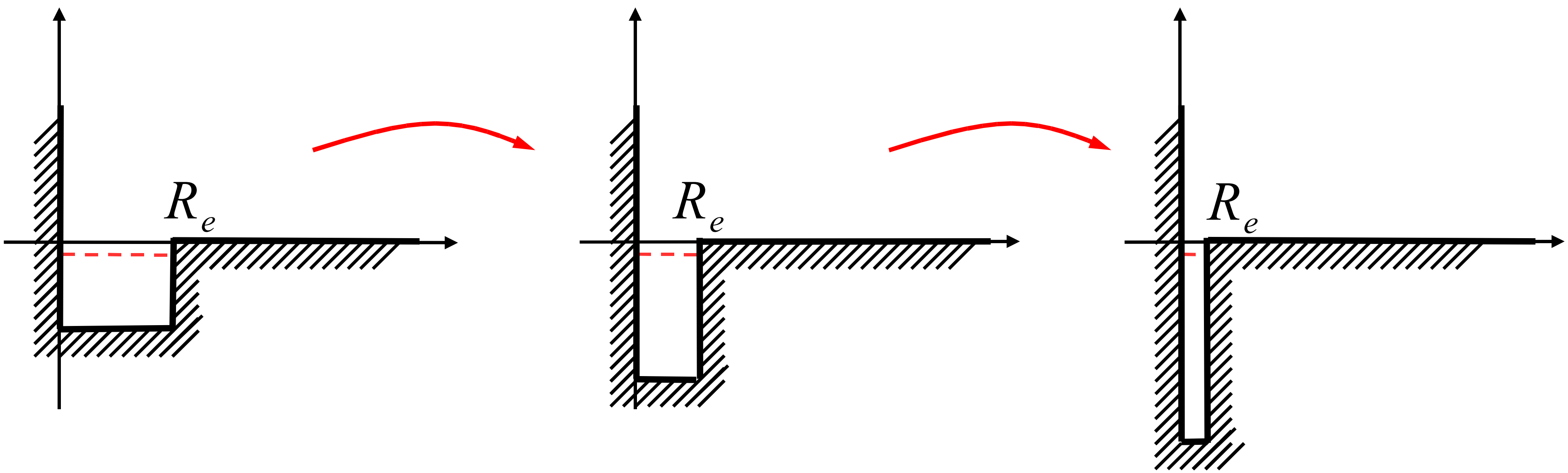
$$\frac{(R\psi(R))'}{R\psi(R)} = -\frac{1}{a} \quad \Longleftrightarrow \quad \psi(R) \underset{R\to 0}{\to} \frac{1}{R} - \frac{1}{a}$$

Thomas effect

Thomas (1935), “The interaction between a neutron and a proton and the structure of ^3H”



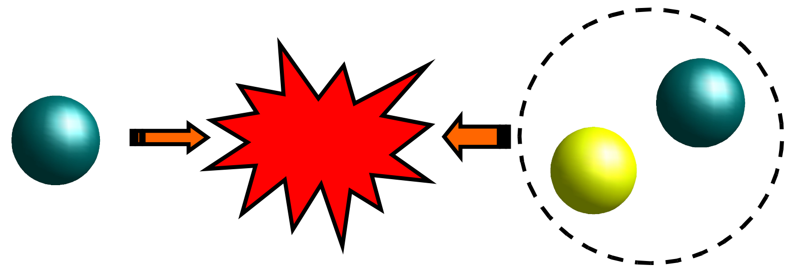
Decrease the range of the proton-neutron potential keeping their binding energy constant



The trimer binding energy tends to infinity! → Thomas effect or Thomas collapse

Example: three ^4He atoms form much deeper bound molecule than two ^4He atoms

Neutron-deuteron scattering



Skorniakov and Ter-Martirosian (1957) derived an integral equation for the neutron-neutron-proton 3-body problem in the zero-range approximation. They calculated the neutron - deuteron scattering length.

Exact in the limit $R_e \ll a$

This results are more applicable for the field of ultracold gases because

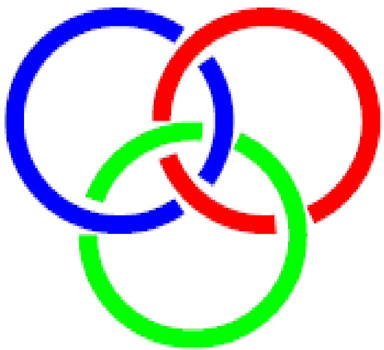
Nuclear matter:

$$R_e \approx 10^{-13}\,\mathrm{cm}\,,\;\; a \approx 4.5 \cdot 10^{-13}\,\mathrm{cm}$$

Ultracold atoms:

$$R_e \sim 0.5 \cdot 10^{-6}\,\mathrm{cm}\,,\;\; a > 10^{-5}\,\mathrm{cm}$$

Borromean binding

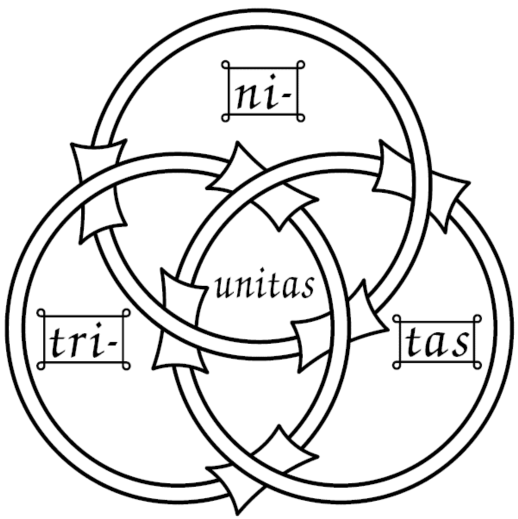


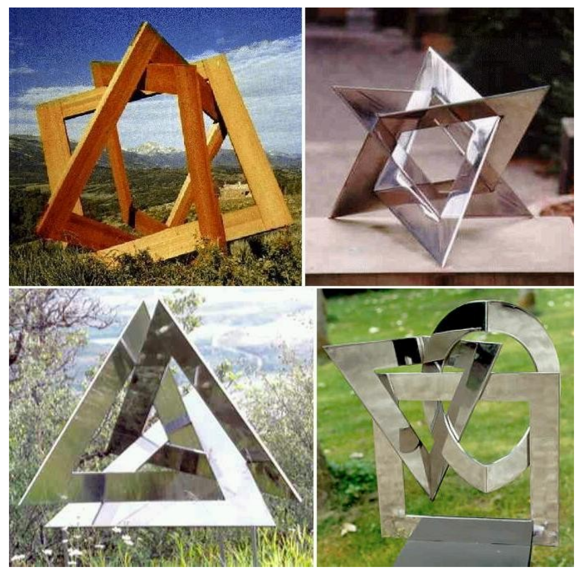
Borromean rings – symbol of strength in unity.
Remove one ring and the other two fall apart

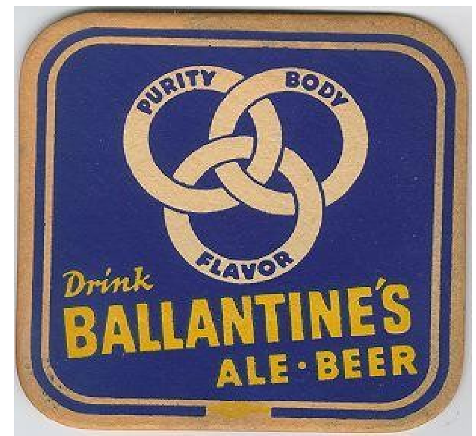
The symbol is used in a number of other applications

Borromean sculptures (John Robinson)

Christian Trinity



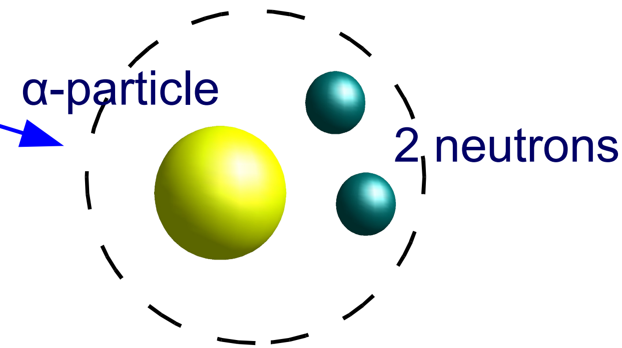


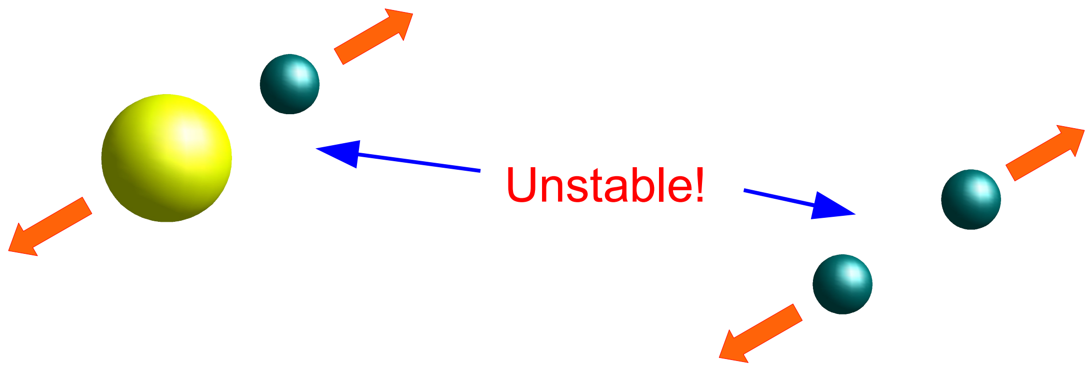


Borromean binding

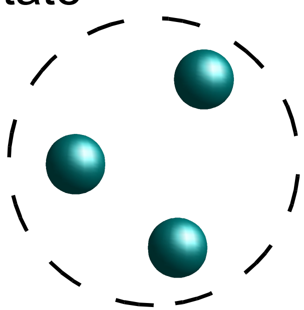
... in nuclear physics to represent halo nuclei

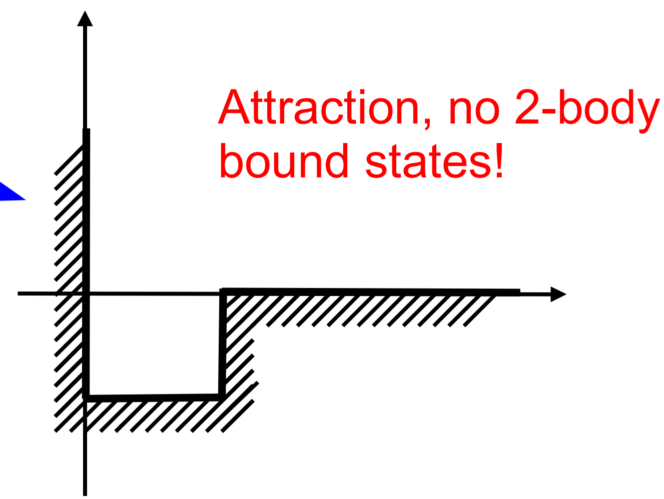
Example: stable ^{6}He nucleus



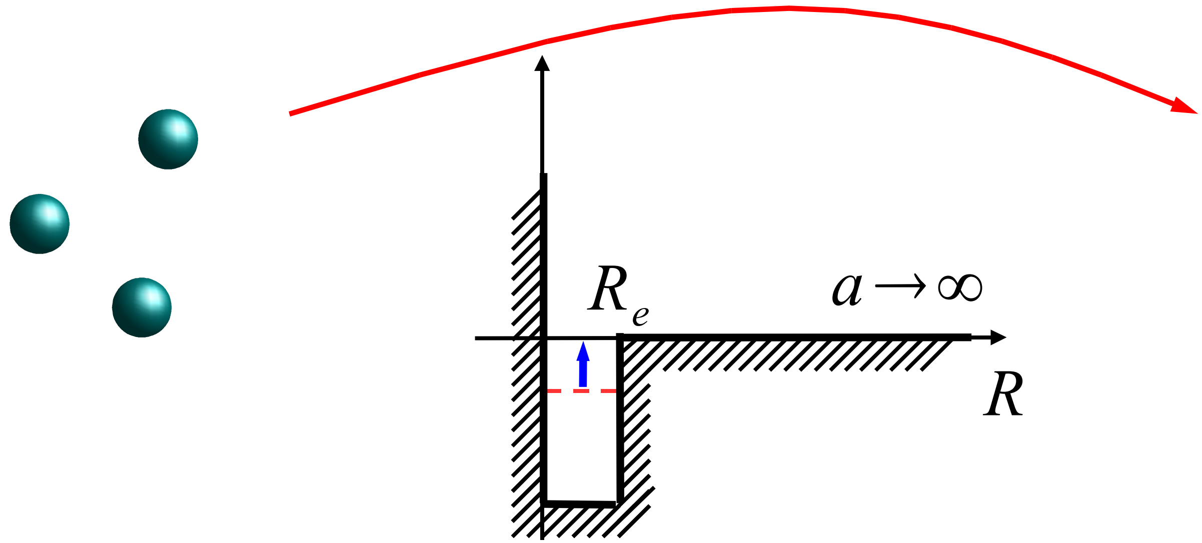


Not a big surprise. Three bosons attracting each other via this potential could form a trimer state





Efimov effect



Efimov (1970) found that the number of trimer states

$$N_{tr} \sim \frac{s_0}{\pi} \log(|a|/R_e) \to \infty$$

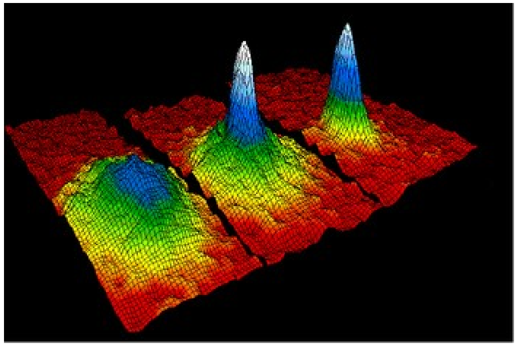
with the accumulation point at $E=0$

Efimov state – weakly bound trimer state

Discrete scaling symmetry: three-body observables depend on R_e, but if $R'_e = R_e \exp(\pm\pi/s_0)$, they do not change

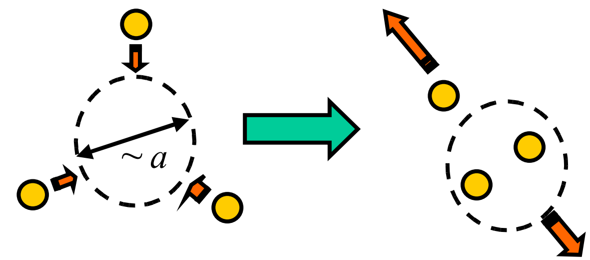
For three identical bosons $s_0 \approx 1.00624$. This number depends on the symmetry (Fermi, Bose) and on the masses of particles

Few-ultracold-atom physics after 1995



BEC of atoms is metastable. Increasing density leads to enhanced 3-body recombination

3-body recombination to a weakly bound state
Theoretical papers:
Fedichev, Reynolds, and Shlyapnikov (1996)
Nielsen and Macek (1999)
Esry, Greene, and Burke (1999)
Bedaque, Braaten, and Hammer (2000)



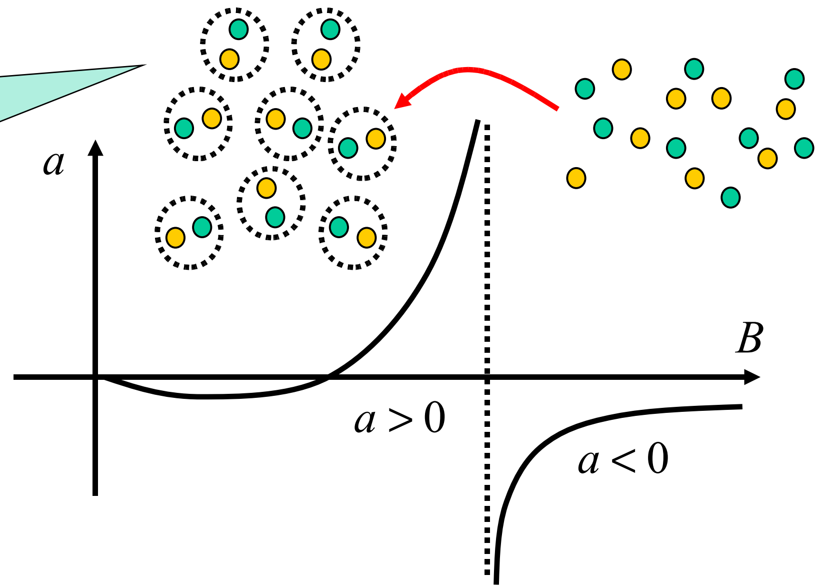
$$\alpha_{rec} \sim \hbar a^4 / m$$

MIT (1999) BEC + Feshbach resonance ⇒ Strong losses

Difficult to reach strongly interacting regime with bosons! Efimov states are not stable because of the relaxation to deep molecular states

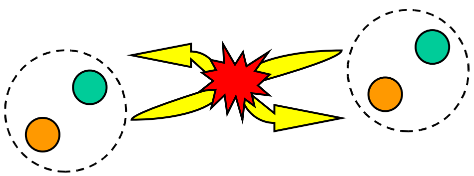
New era: BCS-BEC crossover, molecules

Bose gas of dimers ("BEC side" of the resonance)



Two-component Fermi gas ("BCS side" of the resonance)

Interaction between molecules:

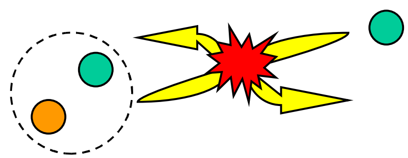


$$a_{dd}=0.6\,a$$

DSP, Salomon,

Shlyapnikov (2003)

Atom-molecule scattering:

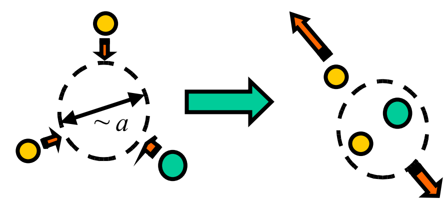


$$a_{ad}=1.2\,a$$

Skorniakov,

Ter-Martirosian (1957)

3-body recombination to the dimer state:

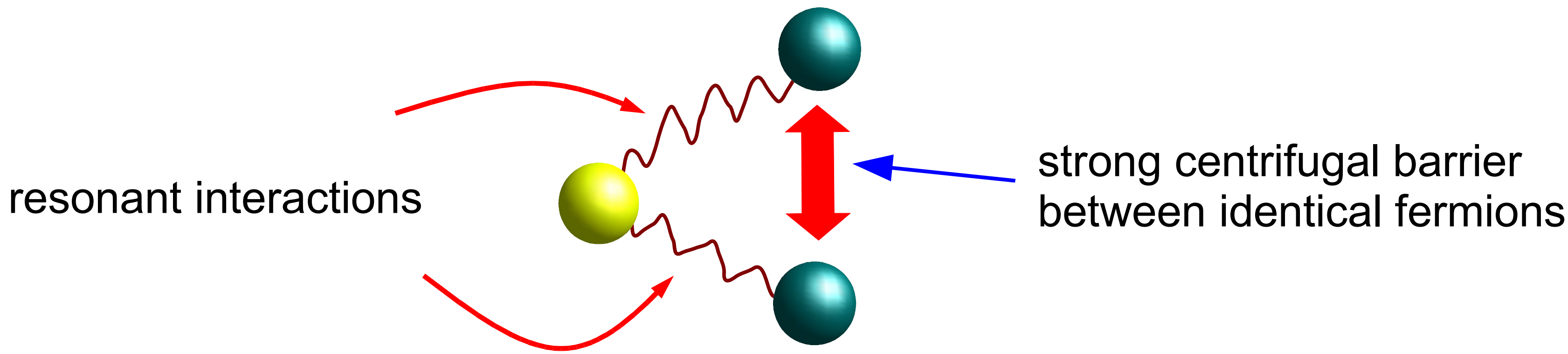


$$\alpha_{rec}=148\,\frac{\hbar a^4}{m}\cdot\frac{\bar{\epsilon}}{\epsilon_0}$$

DSP (2003)

Need Efimov physics in a stable system?

Fermionic Li and K mixtures are stable, but there are no weakly bound trimer (Efimov) states. Reason – Fermi statistics:



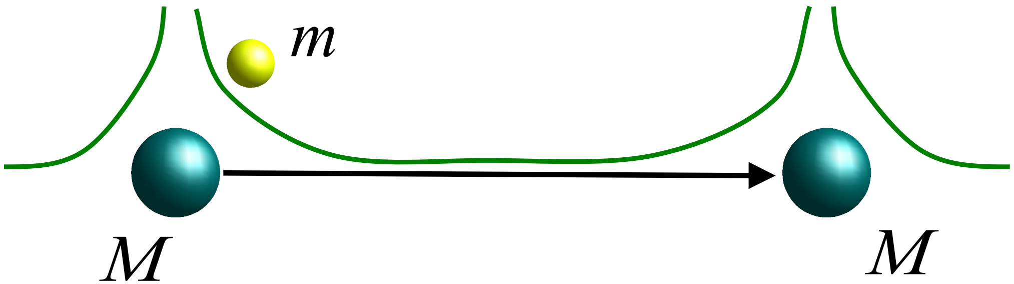
Can we have Efimov states and stability? Yes

We need:

- protective fermionic statistics at short distances (high energies)
- resonant interactions at large distances (low energies)

Consider fermionic heteronuclear mixtures with large mass ratio

Born-Oppenheimer approximation



Effective interaction between heavy fermions is provided by exchange of the fast light particle. Born-Oppenheimer approximation.

Light atom wavefunction: $$\psi(\boldsymbol{r}) = \frac{\exp(-\kappa|\boldsymbol{r}-\boldsymbol{R}/2|)}{|\boldsymbol{r}-\boldsymbol{R}/2|} + \frac{\exp(-\kappa|\boldsymbol{r}+\boldsymbol{R}/2|)}{|\boldsymbol{r}+\boldsymbol{R}/2|}$$

Bethe-Peierls boundary condition gives: $$\frac{1}{a} - \kappa + \frac{\exp(-\kappa R)}{R} = 0$$

$R \ll a \Rightarrow \kappa \approx \frac{0.567}{R}$

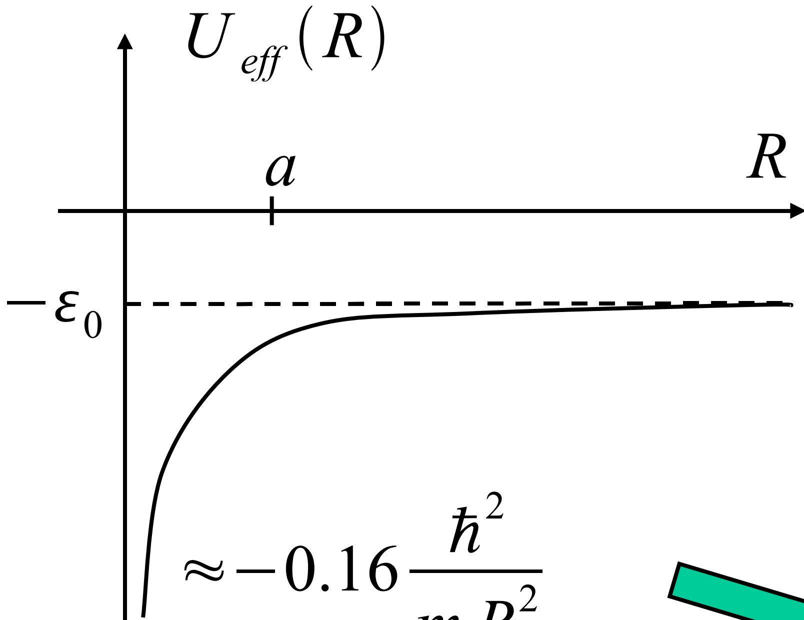
$$U_{eff}(R) = -\frac{\hbar^2\kappa^2}{2m} \approx -0.16\frac{\hbar^2}{mR^2}$$

$R \gg a \Rightarrow \kappa \approx \frac{1}{a}$

$$U_{eff}(R) \approx -\frac{\hbar^2}{2ma^2} = -|\epsilon_0|$$

$$\left[-\frac{\hbar^2}{M}\frac{\partial^2}{\partial R^2}+\tilde{U}_{eff}(R)\right]\chi(R)=E\,\chi(R)$$

Solving the Schrödinger equation for the heavy atoms we take into account their fermionic statistics:



$$\approx -0.16\frac{\hbar^2}{mR^2}$$

$$\tilde{U}_{eff}(R)\approx U_{eff}+\frac{\hbar^2 l(l+1)}{MR^2}$$

Symmetry $\Rightarrow$ $l=1,2,3\ldots$

$$\tilde{U}_{eff}(R)\approx\frac{\hbar^2}{MR^2}\underbrace{\left(l(l+1)-0.16\frac{M}{m}\right)}_{\beta}$$

$R\ll a,\ E=0$ $\Rightarrow$ $\left(-\partial^2/\partial R^2+\beta/R^2\right)\chi(R)=0$

$\chi(R)=R^{\nu}$ $\qquad \nu_{\pm}=1/2\pm\sqrt{\beta+1/4}$

Critical mass ratio

$$R \ll a,\ E=0 \ \Rightarrow\ \left(-\partial^2/\partial R^2 + \beta/R^2\right)\chi(R) = 0$$

$$\chi(R) \propto R^{\nu} \qquad \nu_{\pm} = 1/2 \pm \sqrt{\beta + 1/4}$$

$$\beta = l(l+1) - 0.16\frac{M}{m}$$

$$M/m < 13.6 \ \Rightarrow\ \beta > -1/4$$

$$\chi(R) \propto R^{\nu_+}$$

Unique wavefunction without zeros ⇒ no trimer states. Centrifugal barrier is stronger than the induced attraction

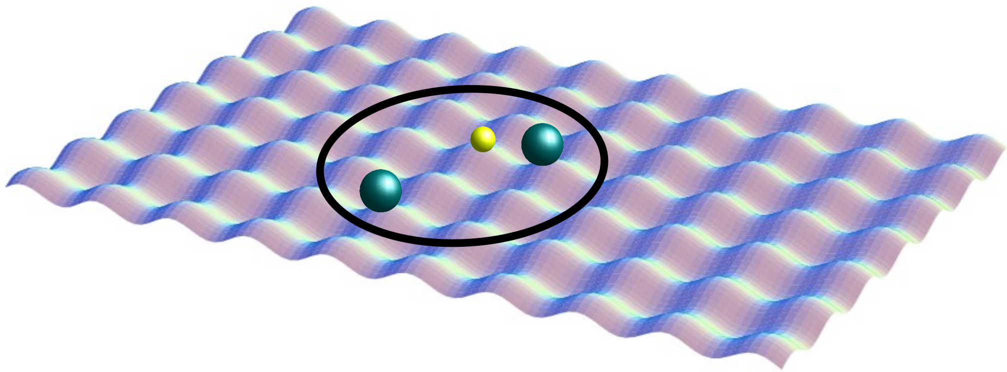
$$M/m > 13.6 \ \Rightarrow\ \beta < -1/4$$

$$\chi(R) \propto \sqrt{R}\cos\left(s_0 \log R/r_0\right),\ s_0 = \sqrt{-1/4 - \beta}$$

"Fall of a particle to the center in R^{-2} potential". Infinite number of zeros of the wavefunction. Infinite number of trimer states. Efimov effect

Li-Li, K-K and K-Li mixtures are stable, since the mass ratio is smaller than the critical one. No Efimov states as well

K-Li mixture in an optical lattice



Optical lattice increases the effective mass of K atoms. We need only a factor of 2

Efimov trimer states

Exactly what we want:

Efimov physics in a stable system

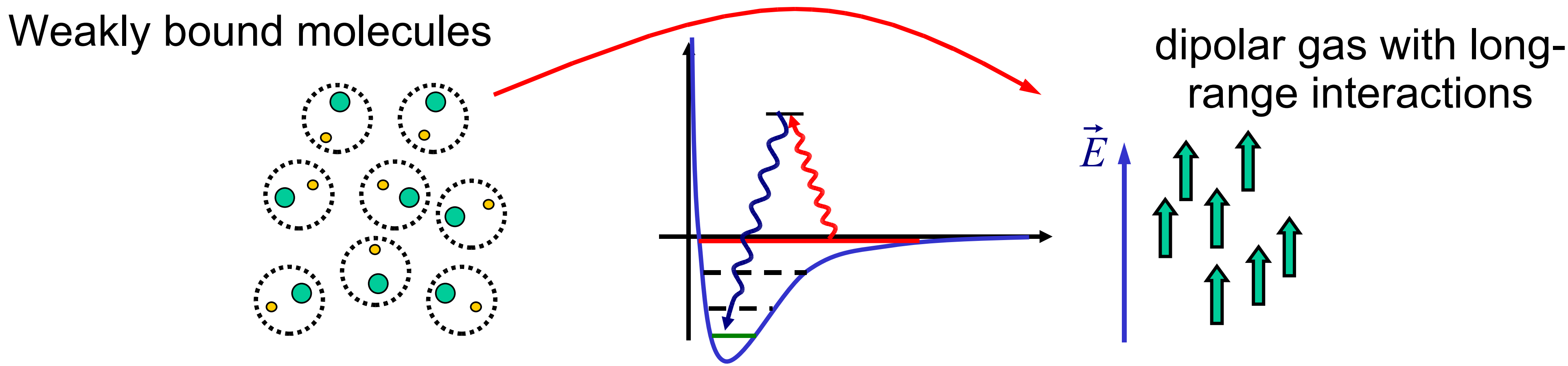
On the other hand, the relaxation to deeply bound molecular states is a local processes and it is insensitive to the lattice potential

At distances smaller than the optical lattice constant the atoms "remember" their natural mass ratio (6.7<13.6)

Interaction of heteronuclear molecules

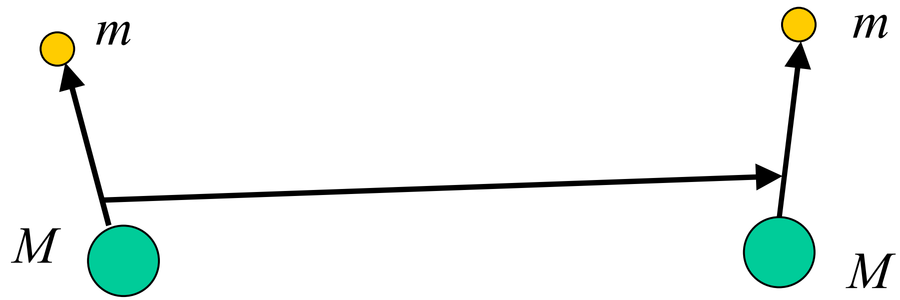
Why different isotopes?

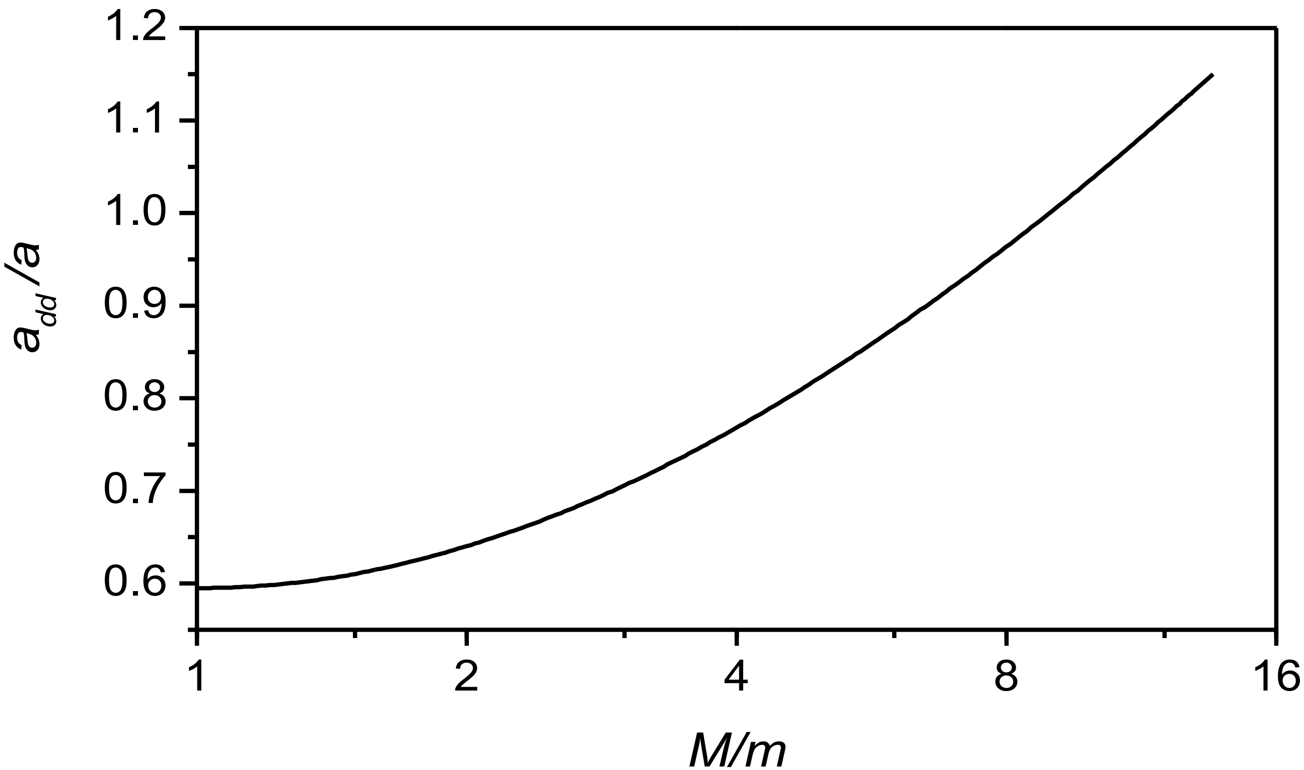
- Way toward dipolar gases



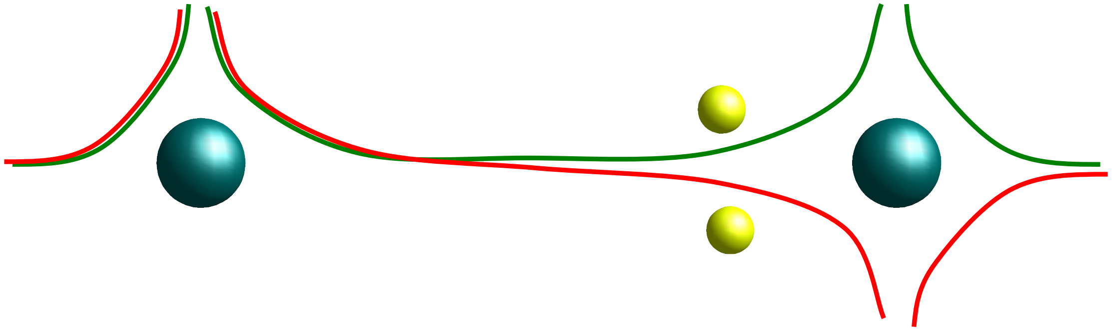
- For fermionic mixtures qualitatively different physics of the BCS-BEC crossover for large *M/m*, gas-crystal transition

Scattering length for Fermi-Fermi molecules

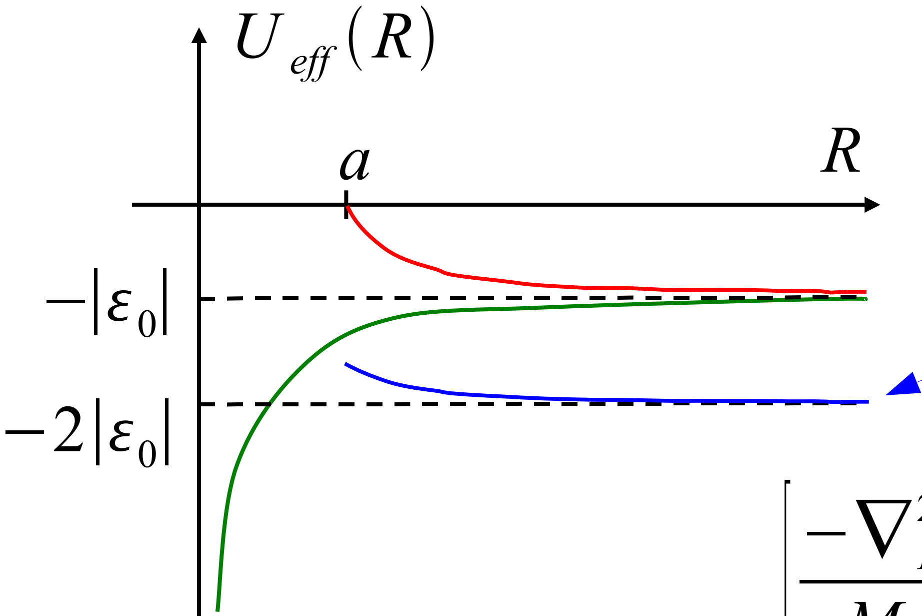




Born-Oppenheimer approximation



Effective interaction is the sum of the energies of light fermions in "gerade" and "ungerade" states.



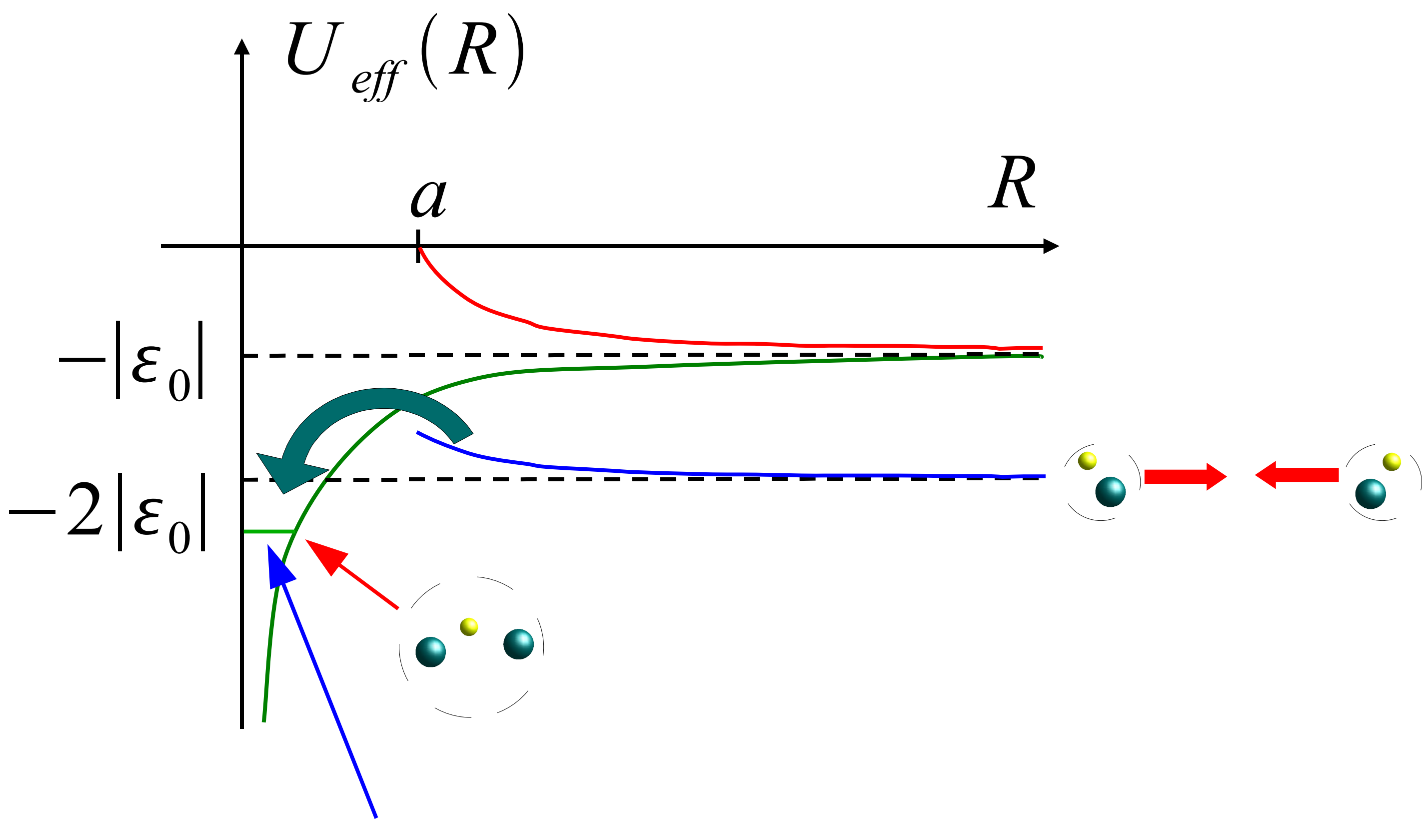
$$R \gg a$$

$$U_{eff}(R) \approx -2\varepsilon_0 + \frac{2\hbar^2}{maR}\exp(-2R/a)$$

$$\left[\frac{-\nabla_{\boldsymbol{R}}^2}{M} + \frac{1}{m}\frac{2}{aR}\exp(-2R/a)\right]\Psi(\boldsymbol{R}) = E\,\Psi(\boldsymbol{R})$$

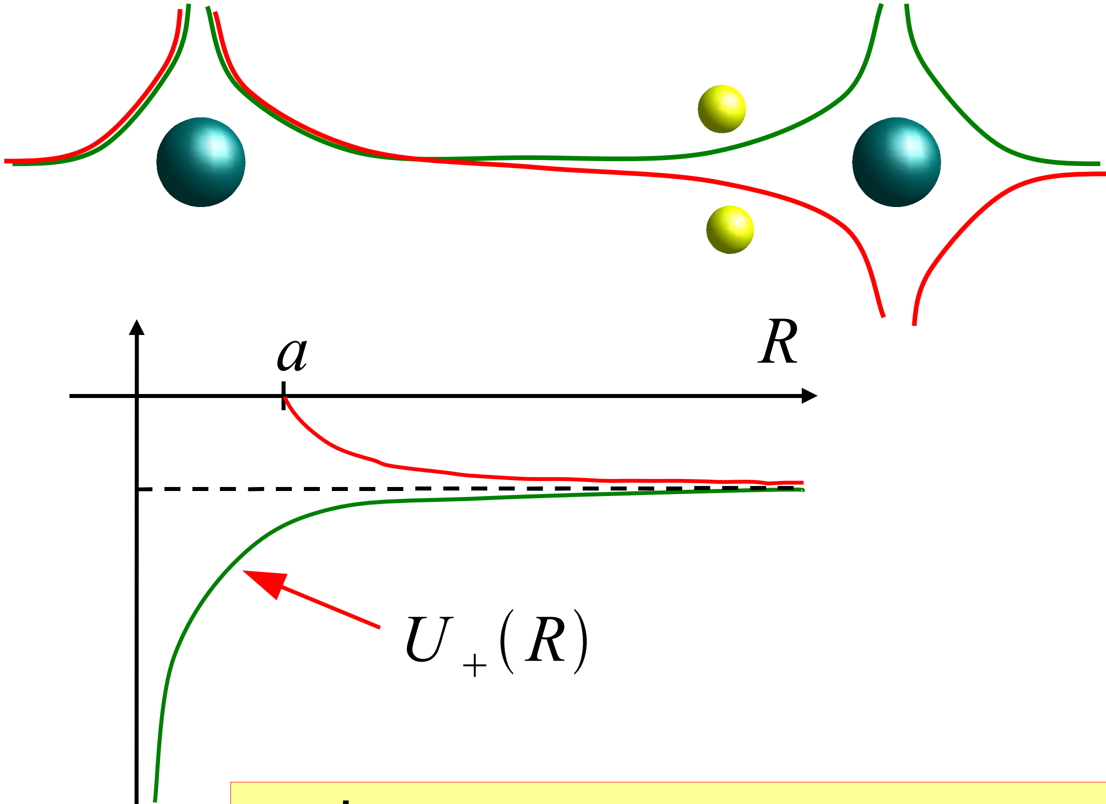
Tunneling probability $P \propto \exp\left(-\text{const}\sqrt{M/m}\right)$ can be completely neglected for M/m>100

Formation of trimers



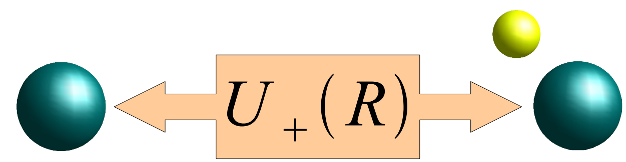
“Dangerous” trimer state

Hybrid Born-Oppenheimer approximation



- Exact solution is technically difficult for $M/m > 20$
- BO does not work for $R < a$

Solution - Hybrid BO:
Integrate out the "gerade" fermion



$$\Bigg[\underbrace{-\frac{\hbar^2\nabla_{\boldsymbol{R}}^2}{M}+U_+(R)}_{H_0}-\frac{\hbar^2\nabla_{\boldsymbol{r}}^2}{2\text{m}}-E\Bigg]\Psi(\boldsymbol{R},\boldsymbol{r})=0$$

+

Bethe-Peierls boundary conditions for $\boldsymbol{r}\to\pm\boldsymbol{R}/2$

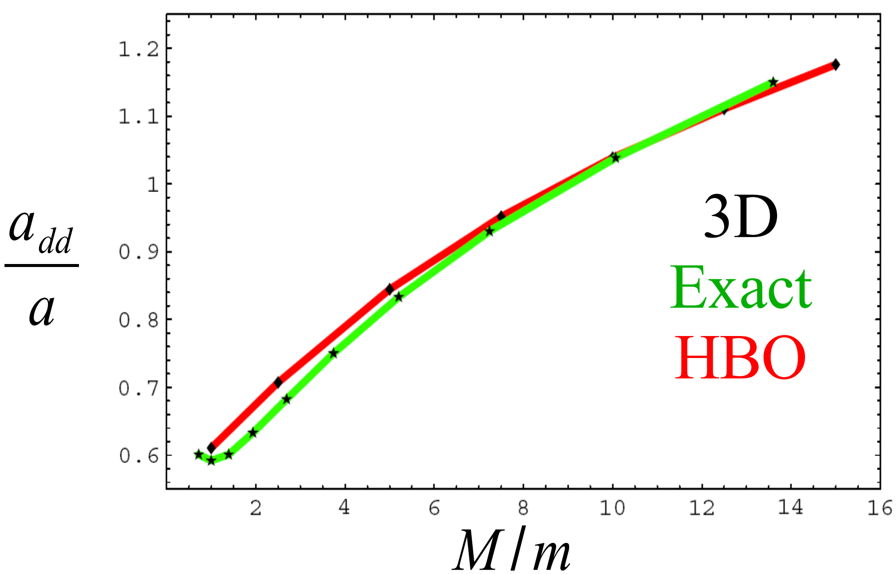
$$\Psi(\boldsymbol{R},\boldsymbol{r})=\sum_{\boldsymbol{R}',\mu} f_\mu(\boldsymbol{R})\, f_\mu^*(\boldsymbol{R}')\, f(R')\left[\frac{\exp(-\kappa_\mu|\boldsymbol{r}-\boldsymbol{R}'/2|)}{4\pi|\boldsymbol{r}-\boldsymbol{R}'/2|}-\frac{\exp(-\kappa_\mu|\boldsymbol{r}+\boldsymbol{R}'/2|)}{4\pi|\boldsymbol{r}+\boldsymbol{R}'/2|}\right]$$

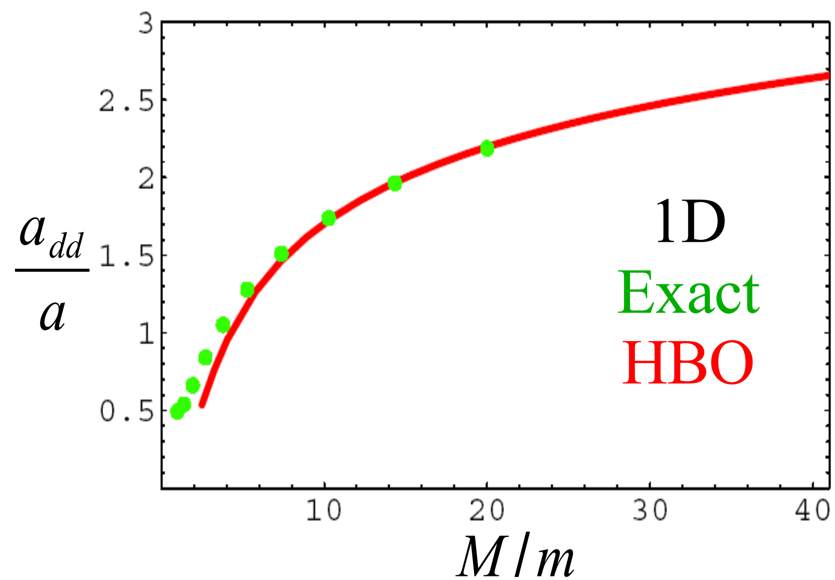
$$H_0 f_\mu(\boldsymbol{R})=\epsilon_\mu f_\mu(\boldsymbol{R})$$

$$\kappa_\mu=\sqrt{2\mathrm{m}(\epsilon_\mu-E)/\hbar^2}$$

Bethe-Peierls conditions

Integral equation for *f*





Summary

- Efimov effect in ultracold gases is difficult to observe due to the relaxation to deeply bound states

- It might be possible with fermionic mixtures in an optical lattice. One can also study the mass dependence of few-body observables

- In this respect Li-K mixture is promising

- Hybrid Born-Oppenheimer approach simplifies life in the case of large mass ratios

<u>Collaboration with:</u>
Bout Marcelis (TUE, Netherlands)
Gora Shlyapnikov (LPTMS, Orsay)
Christophe Salomon (LKB, ENS)
Servaas Kokkelmans (TUE, Netherlands)