

# The few-atom problem

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# Few-body problem in ultracold gases?

## Microscopic level

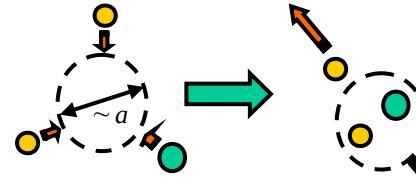
Structure of molecules



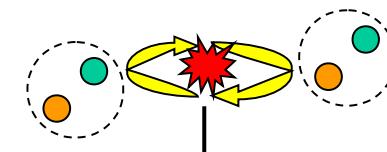
Atom-dimer scattering



Three-body recombination



Dimer-dimer scattering

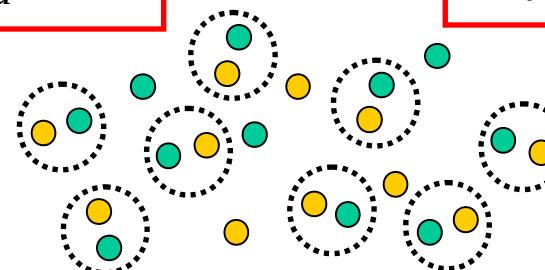


## Macroscopic level

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

$$a_{ad} = ?$$

$$a_{dd} = ?$$



## Path towards many-body case

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

# Size of configuration space

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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.  
Calculations possible for realistic potentials

3-body



3 coordinates. Involved numerics with simple model  
potentials.

4-body



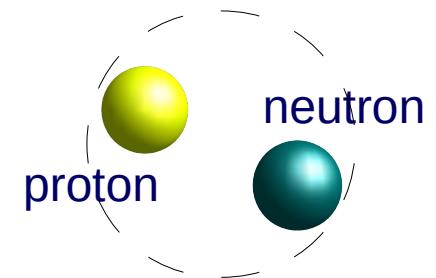
6 coordinates. Reliable solution very difficult even  
for simple model potentials

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

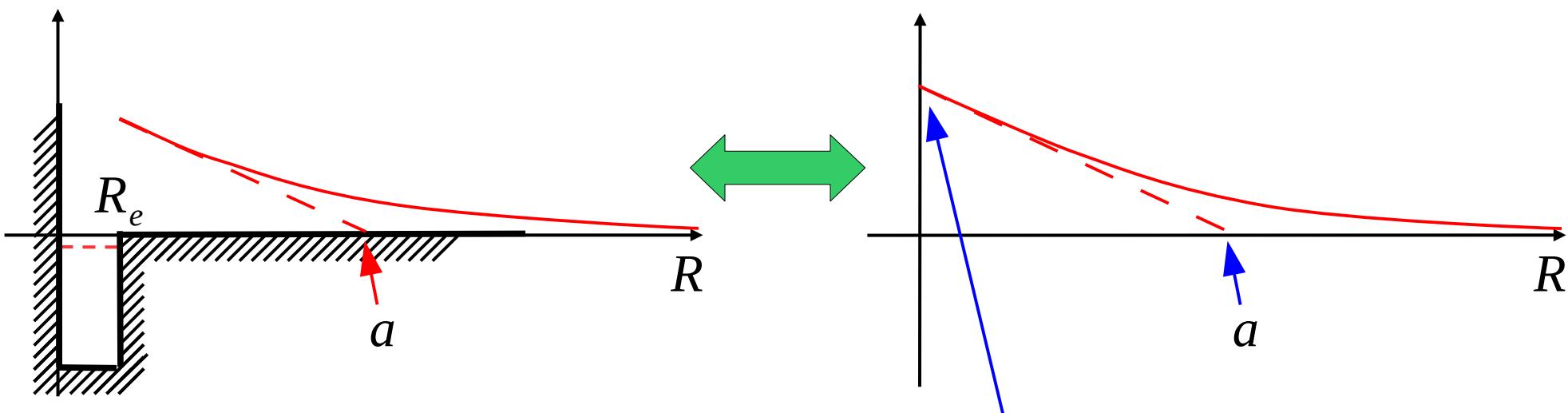
Some history  
(of the zero-range approach)

# Bethe – Peierls boundary conditions

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



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



Bethe-Peierls boundary condition

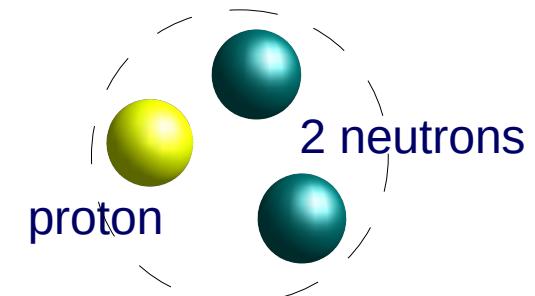
$$\frac{(R\psi(R))'}{R\psi(R)} = -\frac{1}{a}$$



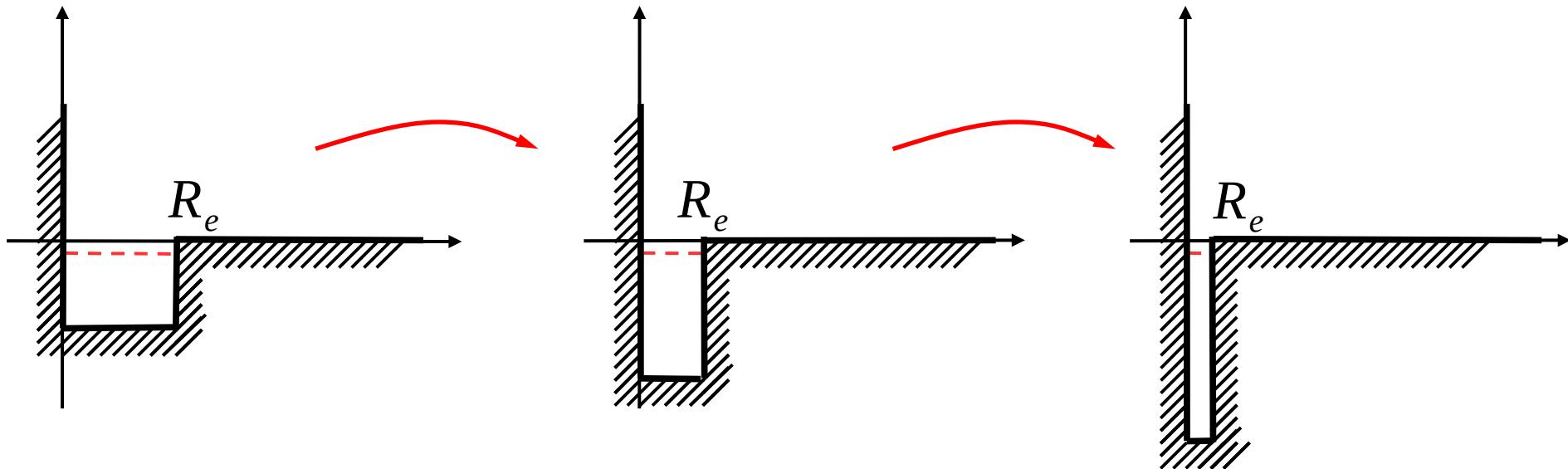
$$\psi(R) \xrightarrow[R \rightarrow 0]{} \frac{1}{R} - \frac{1}{a}$$

# Thomas effect

Thomas (1935), "The interaction between a neutron and a proton and the structure of  ${}^3\text{H}$ "



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



The trimer binding energy tends to infinity!

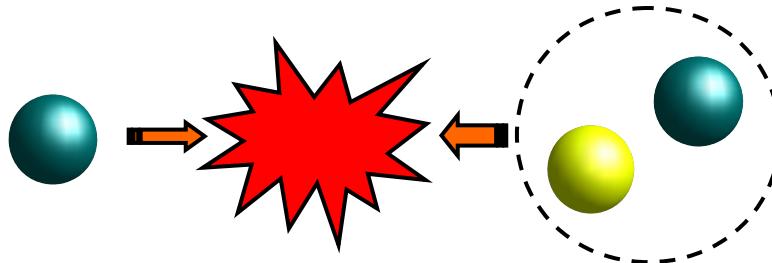


Thomas effect or Thomas collapse

Example: three  ${}^4\text{He}$  atoms form much deeper bound molecule than two  ${}^4\text{He}$  atoms

# Neutron-deuteron scattering

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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:

$$R_e \approx 10^{-13} \text{ cm}, \quad a \approx 4.5 \cdot 10^{-13} \text{ cm}$$

Ultracold atoms:

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

**Three Body Problem for Short Range Forces. I.  
Scattering of Low Energy Neutrons by Deuterons**

G. V. SKORNIAKOV AND K. A. TER-MARTIROSIAN

(Submitted to JETP editor July 23, 1955)

J. Exptl. Theoret. Phys. (U.S.S.R.) 31, 775-790 (November, 1956)

$$(\alpha - \gamma_k) \chi(\mathbf{k}) \quad (12)$$

$$+ 8\pi \int \frac{d\mathbf{k}'}{(2\pi)^3} \frac{\chi(\mathbf{k}')}{k^2 + k'^2 + \mathbf{k}\cdot\mathbf{k}' - (ME/\hbar^2) - i\tau} = 0.$$

The solution of this equation determines the wave function of the system, in accord with Eq. (11). For states with a definite quantity of momentum, Eq. (12) reduces to an equation for a function which depends on one independent variable, which can be solved numerically.

The idea for this consideration of the three body problem was supplied by L. D. Landau.

# Borromean binding

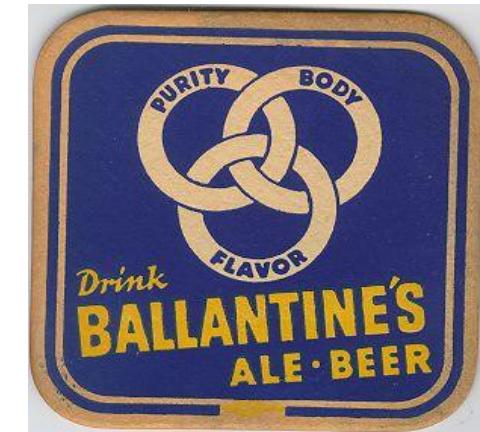
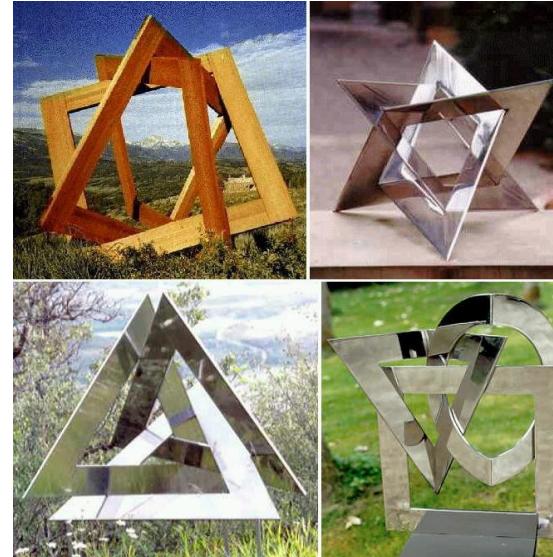
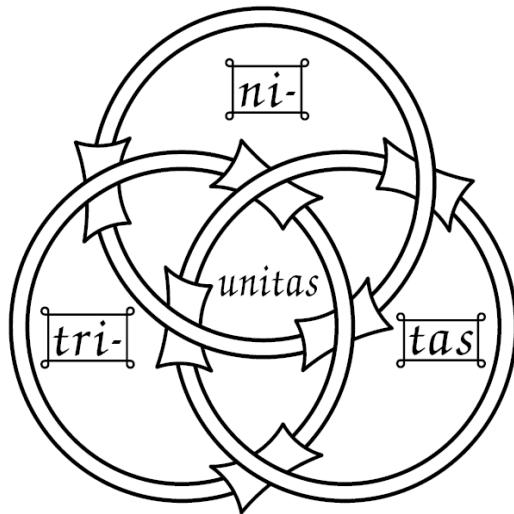


Borromean rings – symbol of strength in unity.  
Remove one ring and the other two fall apart

The symbol is used in a number of other applications

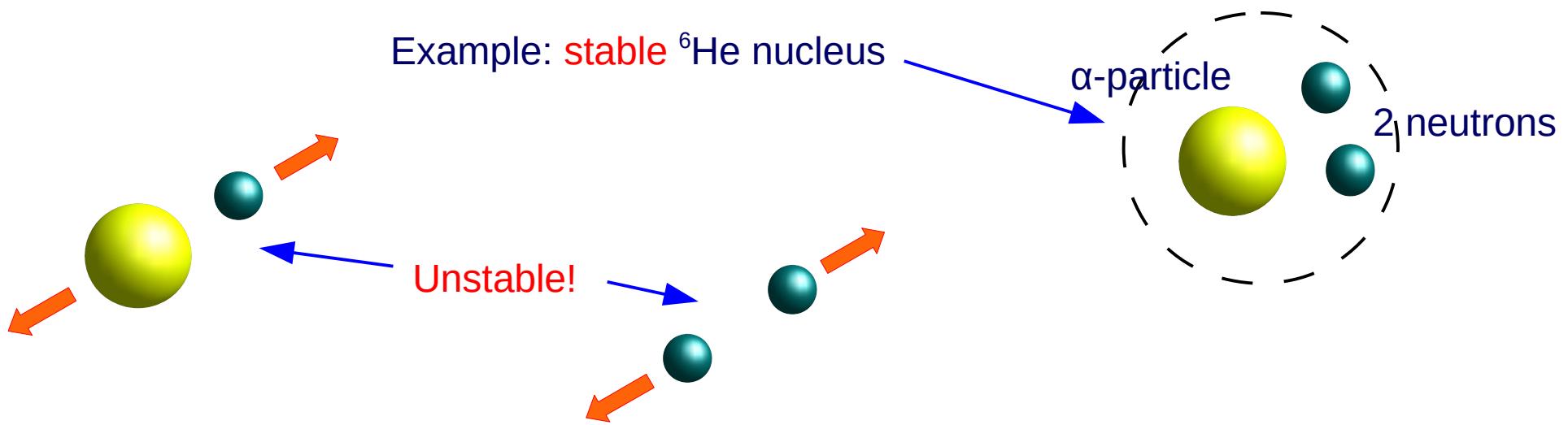
Borromean sculptures (John Robinson)

Christian Trinity

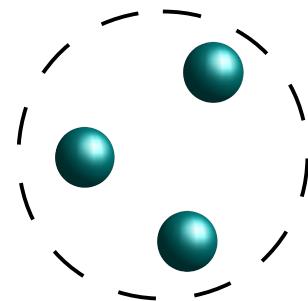


# Borromean binding

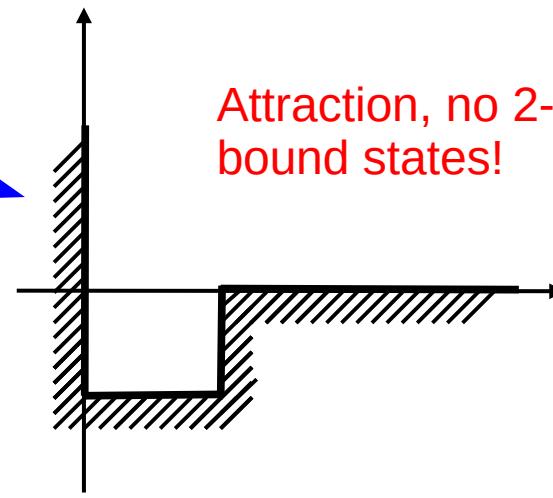
... in nuclear physics to represent halo nuclei



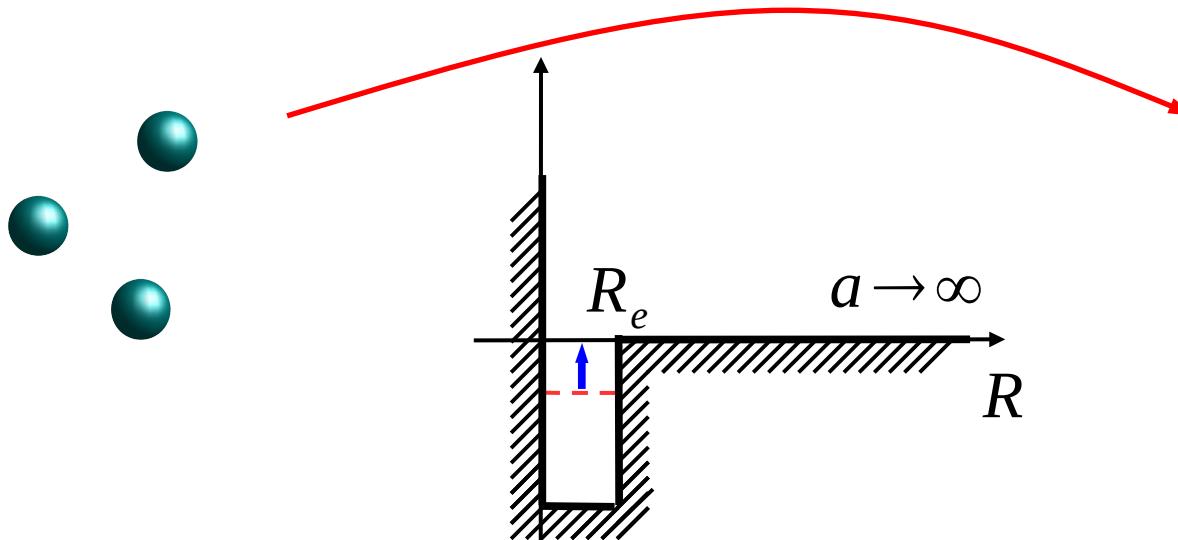
Not a big surprise. Three bosons  
attracting each other via this potential  
could form a trimer state



Attraction, no 2-body  
bound states!



# Efimov effect



Efimov (1970) found that the number of trimer states

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

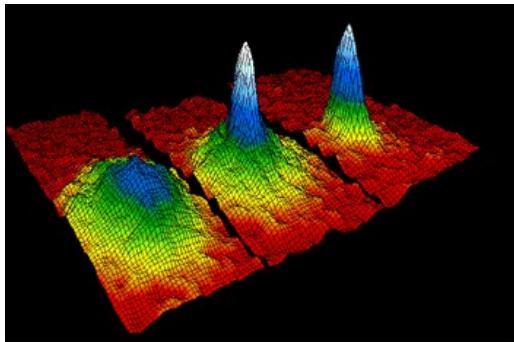
with the accumulation point at  $E=0$

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

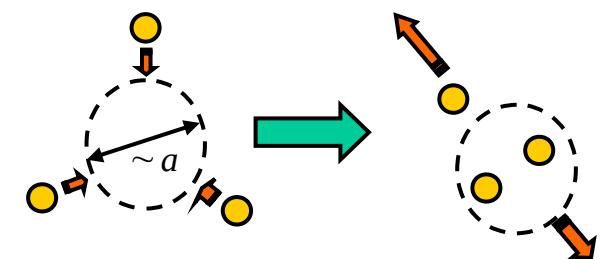
Theoretical papers:

Fedichev, Reynolds, and Shlyapnikov (1996)

Nielsen and Macek (1999)

Esry, Greene, and Burke (1999)

Bedaque, Braaten, and Hammer (2000)



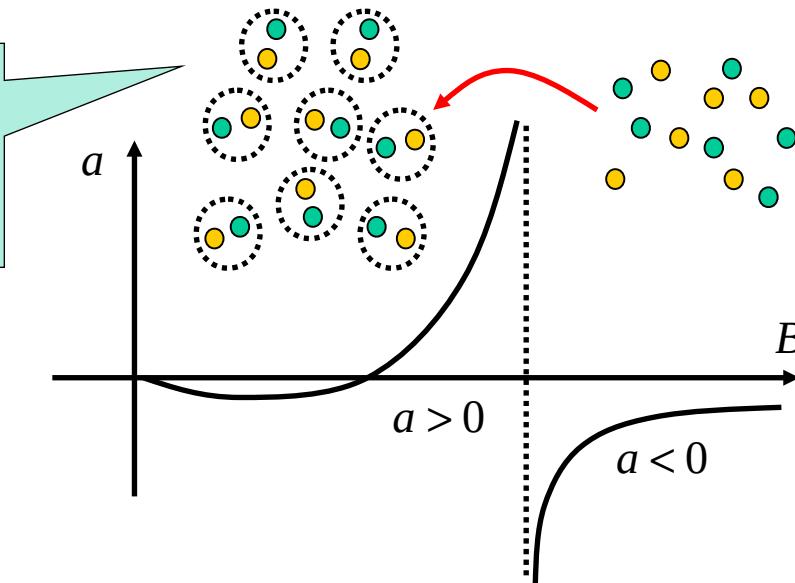
$$\alpha_{rec} \sim \hbar a^4 / m$$

MIT (1999) BEC + Feshbach resonance  $\rightarrow$  Strong losses

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

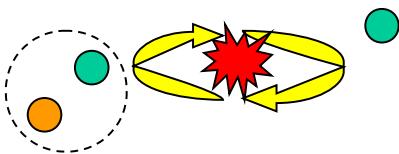
# 2003: BCS-BEC crossover, molecules

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



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

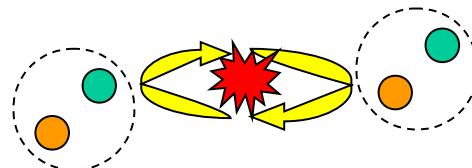
Few-body problem in this case is **non-efimovian**



$$a_{ad} = 1.2 a$$

Skorniakov,

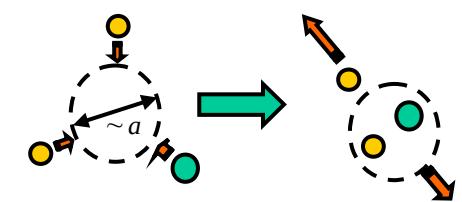
Ter-Martirosian (1957)



$$a_{dd} = 0.6 a$$

DSP, Salomon,

Shlyapnikov (2003)



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

DSP (2003)

# Modern history

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## Efimovian theme:

- Homonuclear bosons (Innsbruck, Florence, Rice, Ramat Gan, Paris)
- Heteronuclear mixtures (Florence, JILA, Heidelberg, Chicago...)
- Three-component Li (Heidelberg, PennState)
- Effective-range effects; wide and narrow resonances
- Van der Waals universality of the three-body parameters

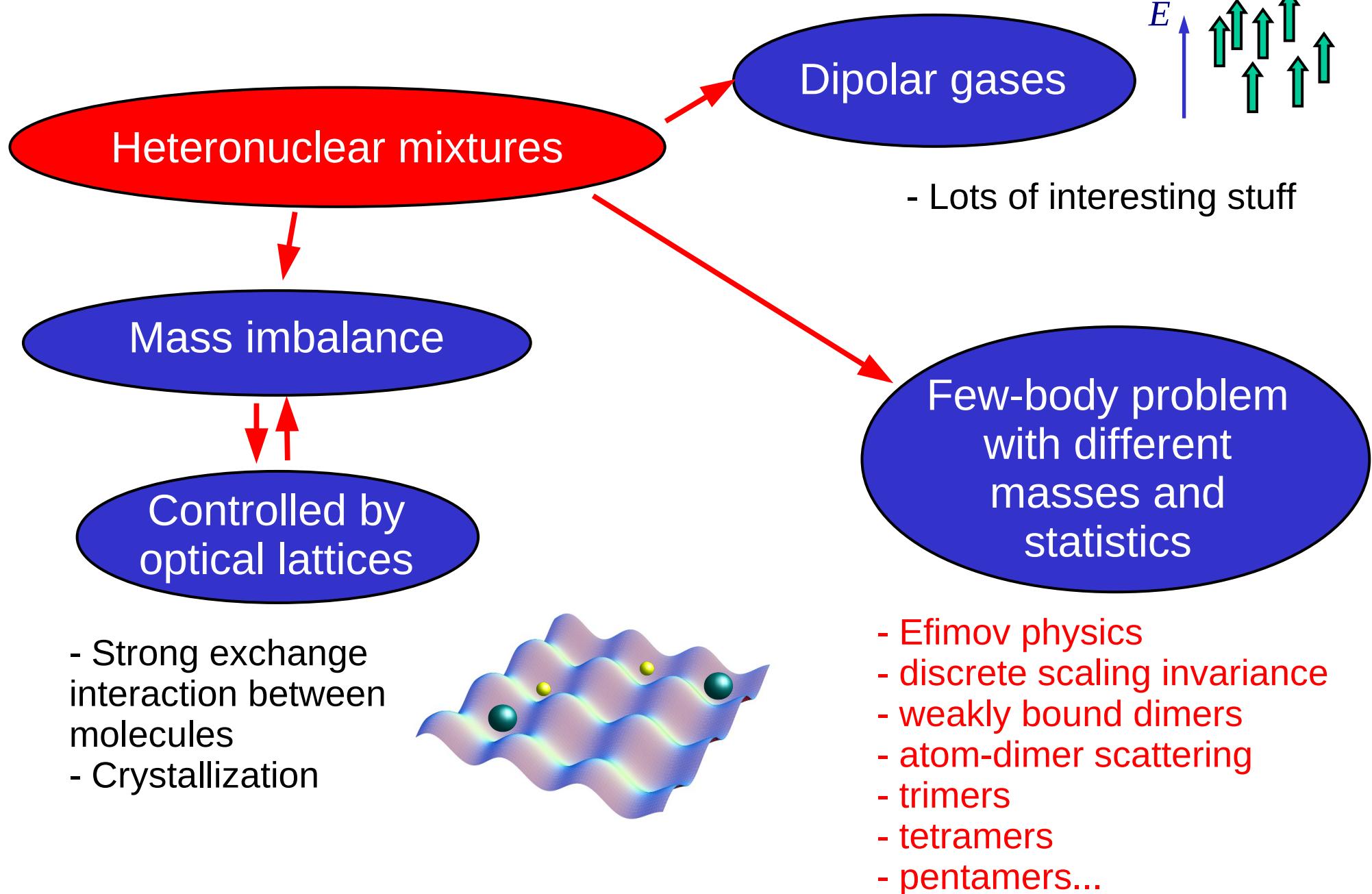
## Non-eftimovian theme:

- Fermi-Fermi Li-K mixture (Innsbruck, Singapour), Li-Cr (Florence), K-Dy (Innsbruck)...

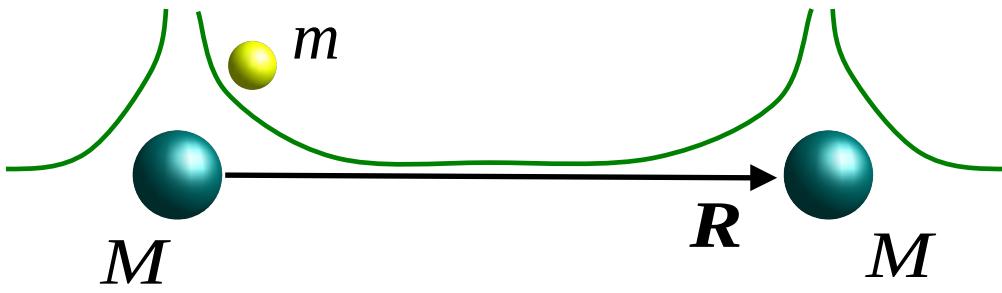
## Theory (mostly):

- Mixed-dimensional
- Rabi- and spin-orbit-coupled mixtures

Heavy-heavy-light problem



# 3-body problem. Born-Oppenheimer approximation



Effective interaction between heavy atoms is provided by exchange of the fast light particle.  
**Born-Oppenheimer approximation.**  
Fonseca, Redish, Shanley (1979)

Light atom wavefunction:

$$\Psi(\mathbf{r}) = \frac{\exp(-\kappa|\mathbf{r} - \mathbf{R}/2|)}{|\mathbf{r} - \mathbf{R}/2|} + \frac{\exp(-\kappa|\mathbf{r} + \mathbf{R}/2|)}{|\mathbf{r} + \mathbf{R}/2|}$$

Bethe-Peierls boundary condition gives:

$$\frac{1}{a} - \kappa + \frac{\exp(-\kappa R)}{R} = 0$$

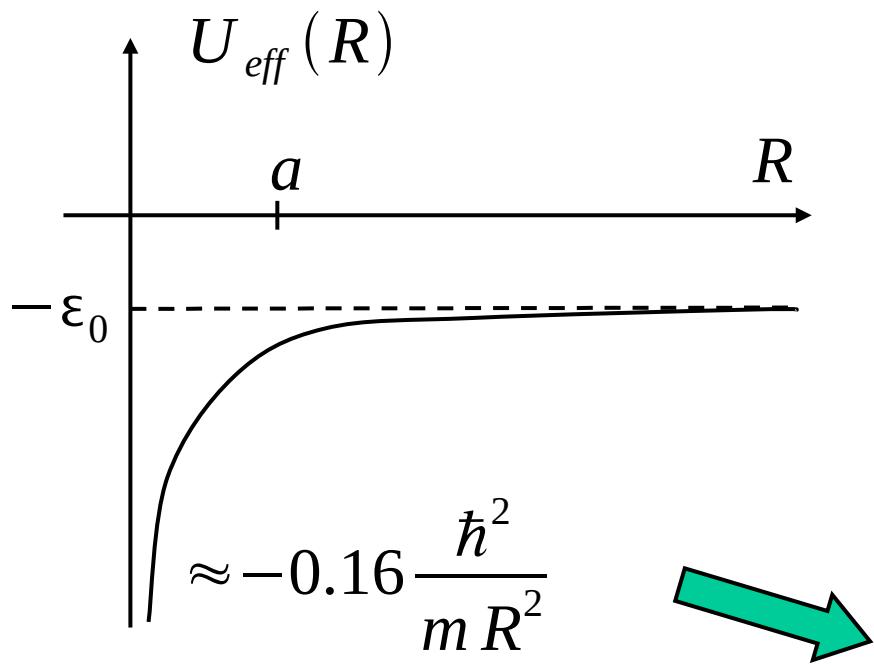
$$R \ll a \quad \rightarrow \quad \kappa \approx \frac{0.567}{R}$$

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

$$R \gg a \quad \rightarrow \quad \kappa \approx \frac{1}{a}$$

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

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



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

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

Heavy fermions  $\rightarrow l=1,3,5\dots$

Heavy bosons  $\rightarrow l=0,2,4\dots$

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

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

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

# Efimov effect. Discrete scaling symmetry

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

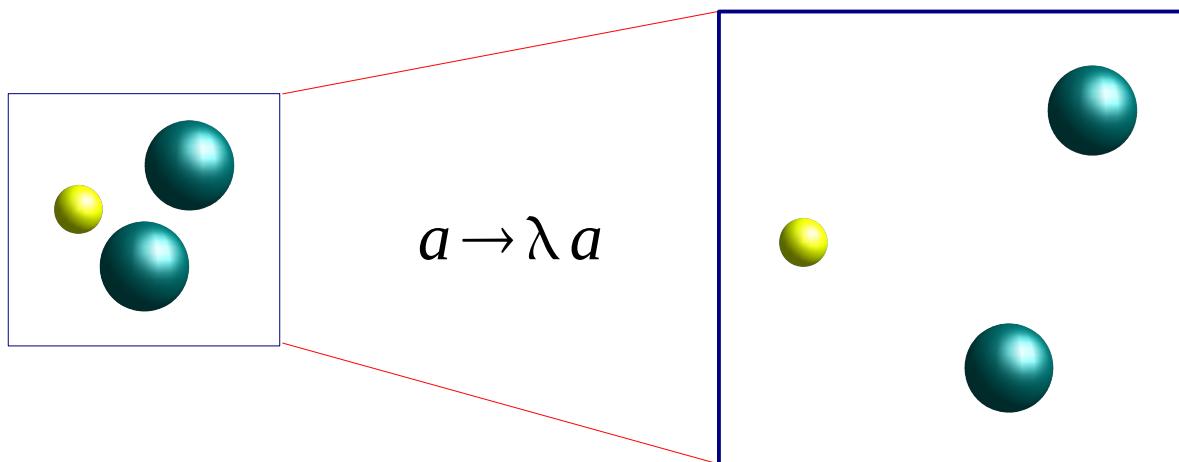
$$\chi(R) \propto R^\nu \quad \nu_{\pm} = 1/2 \pm \sqrt{\beta + 1/4}$$

$$\beta = \left( l(l+1) - 0.16 \frac{M}{m} \right) < -1/4 \rightarrow \nu_{\pm} = 1/2 \pm i s_0 \rightarrow \chi(R) \propto \sqrt{R} \sin(s_0 \log R / r_0)$$

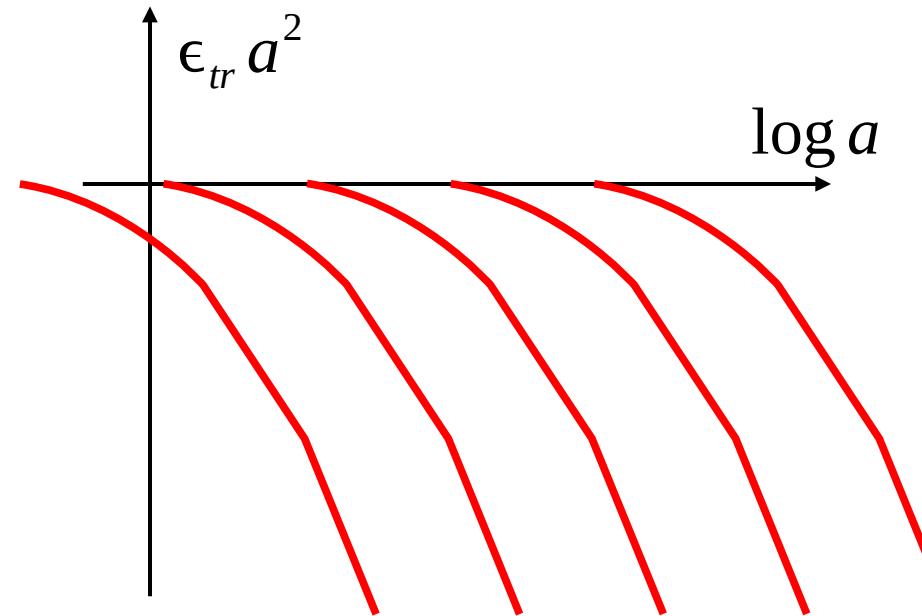
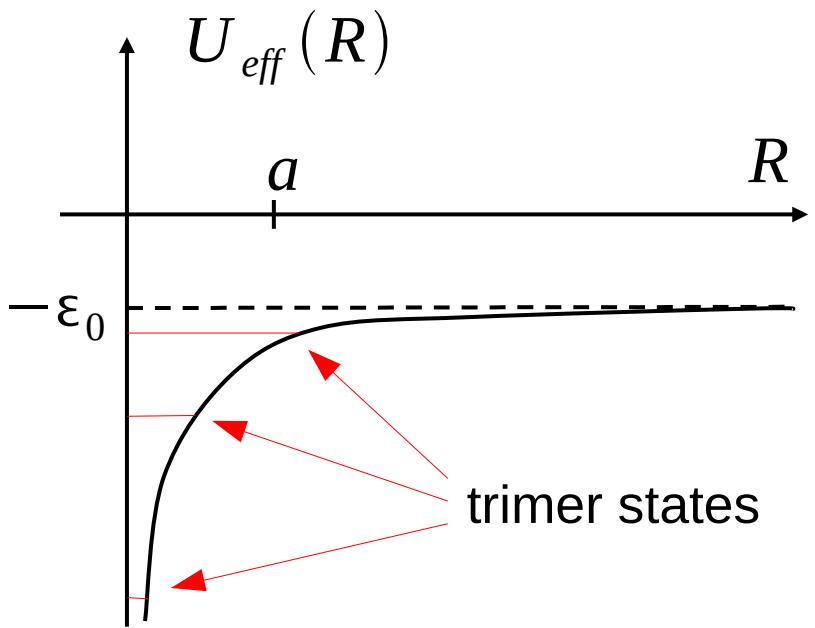
“Fall of a particle to the center in  $R^{-2}$  potential”. Infinite number of zeros of the wavefunction. Infinite number of trimer states. **Efimov effect**

Discrete scaling symmetry.  
Multiplicative factor  $\lambda = \exp(\pi/s_0)$

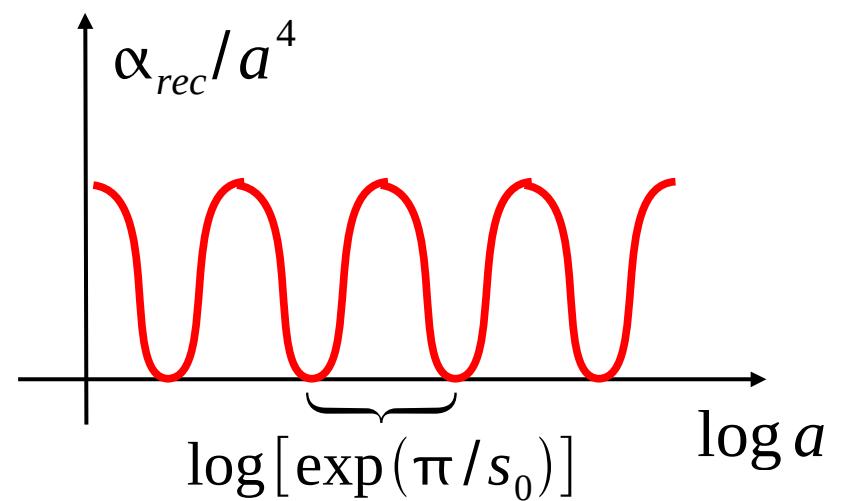
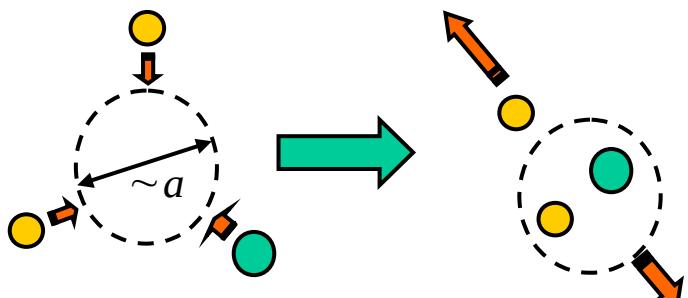
$$\chi(\lambda R) \propto \chi(R)$$



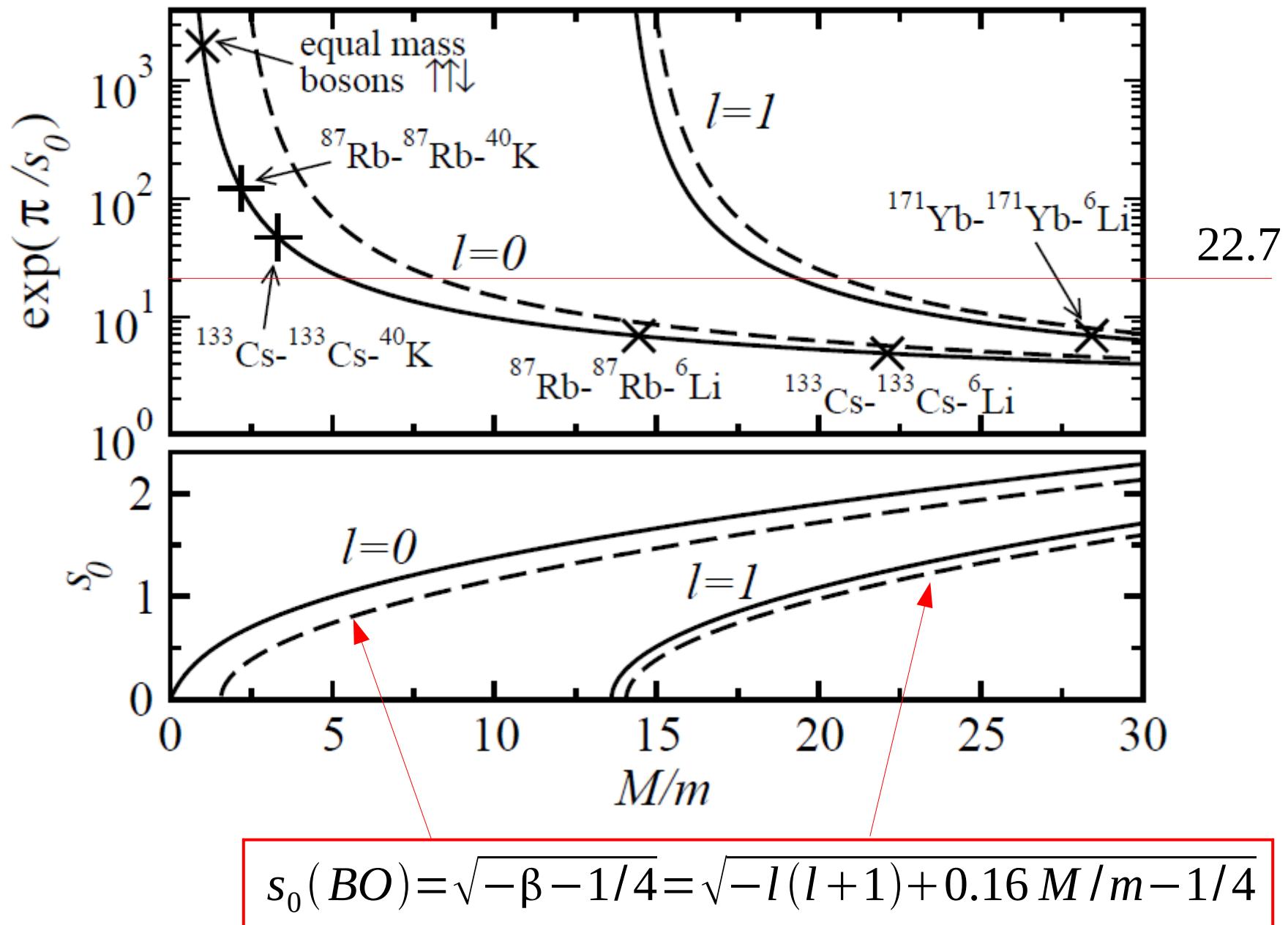
# Manifestation of discrete scaling symmetry



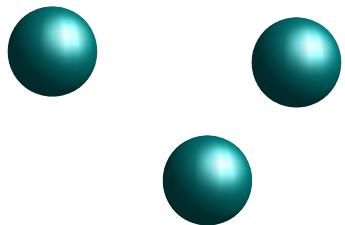
3-body recombination



# Values of $s_0$ and the scaling parameter $\lambda = \exp(\pi/s_0)$



# Observation of discrete scaling symmetry

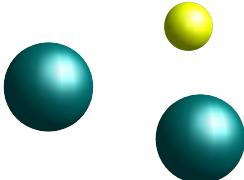


Cs-Cs-Cs, K-K-K, Li-Li-Li

Innsbruck, Florence, Heidelberg,  
PennState, Rice, Ramat Gan

Two Efimov features observed in  
Innsbruck (Huang et al (2014))

$$\lambda \approx 23$$



Rb-Rb-K

Florence, JILA

$$\lambda \approx 120$$

Rb-Rb-Li and Yb-Yb-Li

Cs-Cs-Li

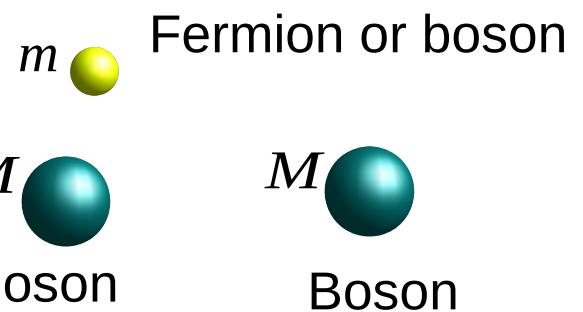
(Heidelberg, Chicago)

~3 Efimov features  
observed in 2014

$$\lambda \approx 7$$

$$\lambda \approx 5$$





## Recombination loss rates in a cold mixture:

Helfrich, Hammer, Petrov (2010)

Rate constant for three-body recombination to a weakly bound molecular level

$$\alpha_s = C(M/m) \frac{\sin^2[s_0 \log(a/a_{0*})] + \sinh^2 \eta_*}{\sinh^2(\pi s_0 + \eta_*) + \cos^2[s_0 \log(a/a_{0*})]} \frac{\hbar a^4}{m}$$

... and to deeply bound states

$$\alpha_d(a > 0) = C(M/m) \frac{\coth(\pi s_0) \sinh(\eta_*) \cosh(\eta_*)}{\sinh^2(\pi s_0 + \eta_*) + \cos^2[s_0 \log(a/a_{0*})]} \frac{\hbar a^4}{m}$$

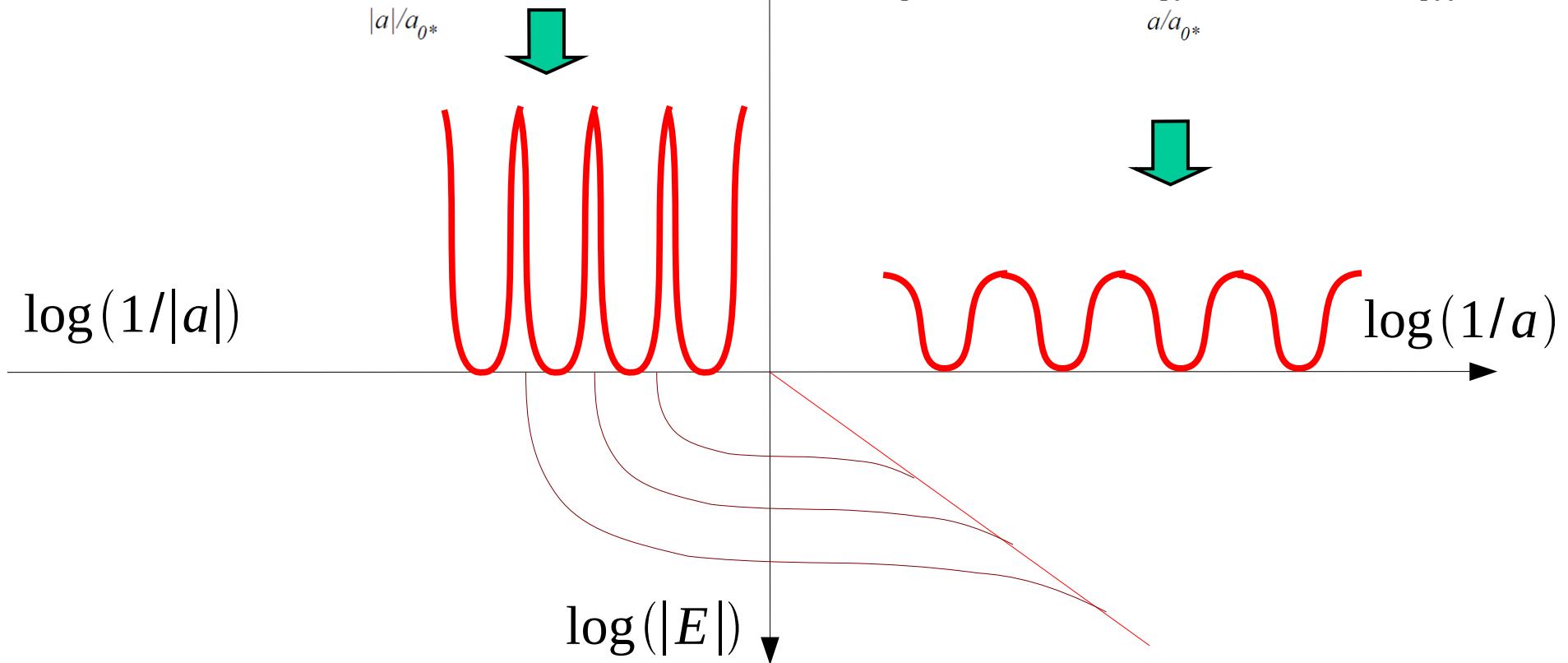
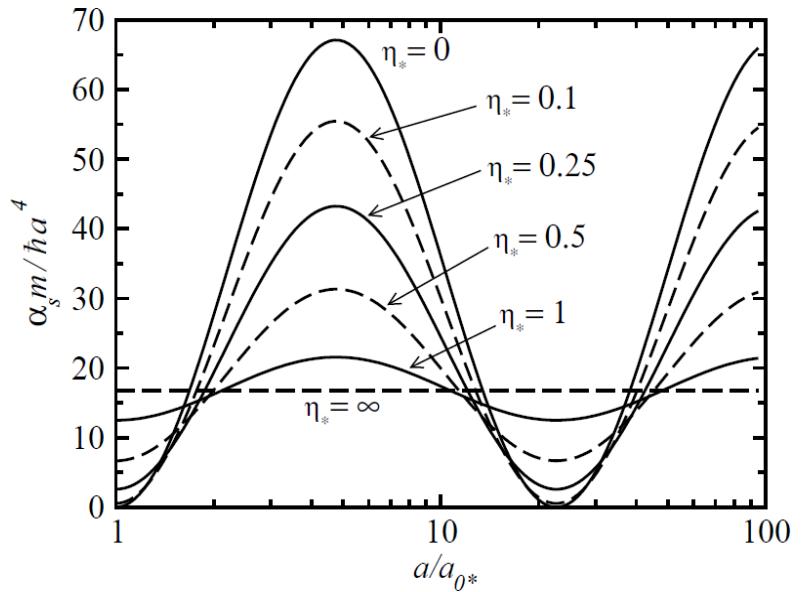
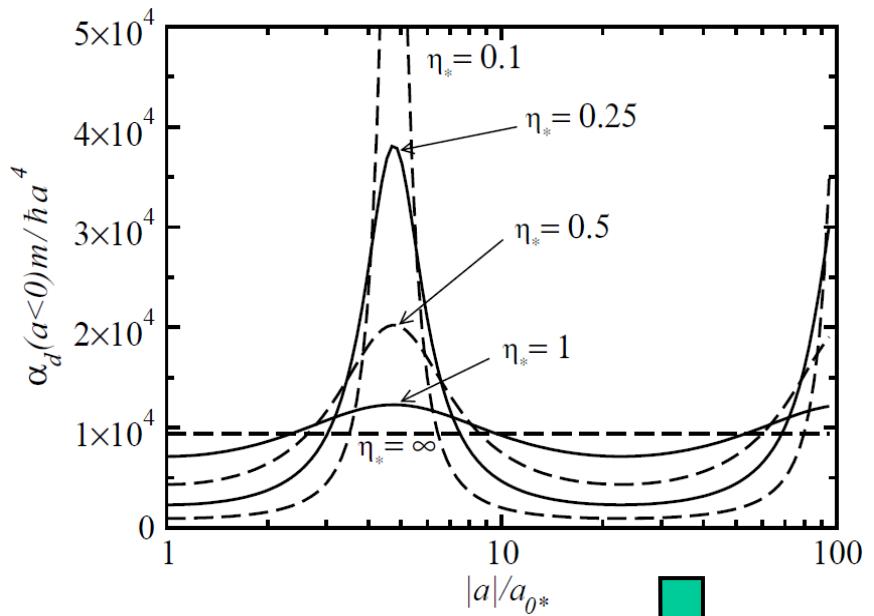
$$\alpha_d(a < 0) = C(M/m) \frac{\coth(\pi s_0) \sinh(\eta_*) \cosh(\eta_*)}{\sinh^2 \eta_* + \cos^2[s_0 \log(|a|/a_{0*})]} \frac{\hbar a^4}{m}$$

where

$$C(M/m) = 64 \left[ \left( \frac{M+m}{M} \right)^2 \arcsin \left( \frac{M}{M+m} \right) - \frac{\sqrt{m(2M+m)}}{M} \right]$$

$\eta_*$  - elasticity parameter  
 $a_{0*}$  - the value of  $a$  where  $\alpha_s(a)$  reaches its minimum

Recombination maxima symmetric with respect to the resonance center!



# Skorniakov and Ter-Martirosian zero-range approach

# 2D scattering by a curve

$$(-\nabla_{\rho}^2 - E) \psi(\rho) = 0$$

Homogeneous Helmholtz equation with boundary condition

$$[\partial \psi / \partial \mathbf{n}] = g(x) \psi$$



Introduce an auxiliary function  $f(x)$  (source or distribution of charges) defined on the boundary



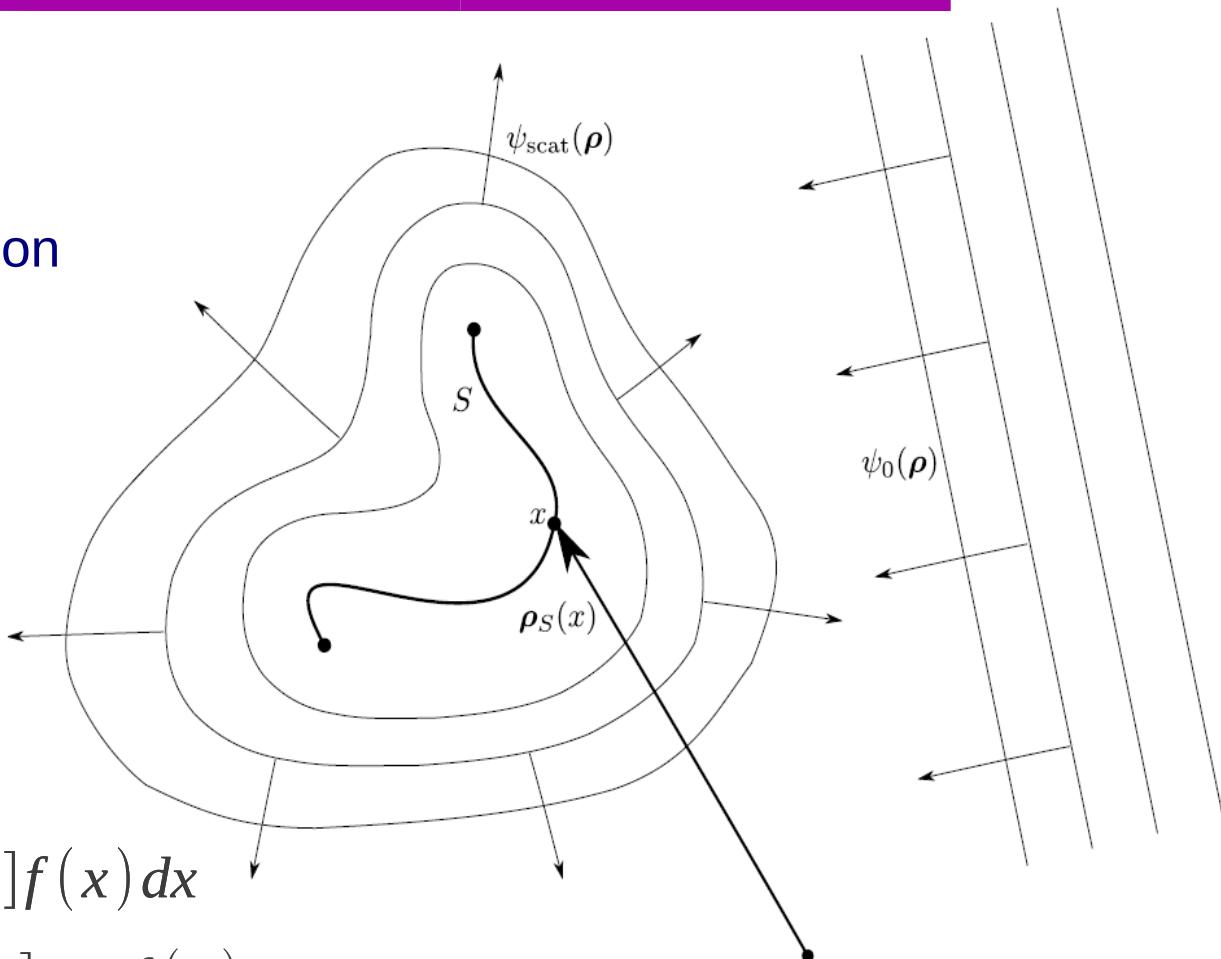
$$\psi(\rho) = \psi_0(\rho) + \int_S G_E[\rho - \rho_s(x)] f(x) dx$$

Gauss-Ostrogradsky:  $[\partial \psi / \partial \mathbf{n}] = -f(x)$

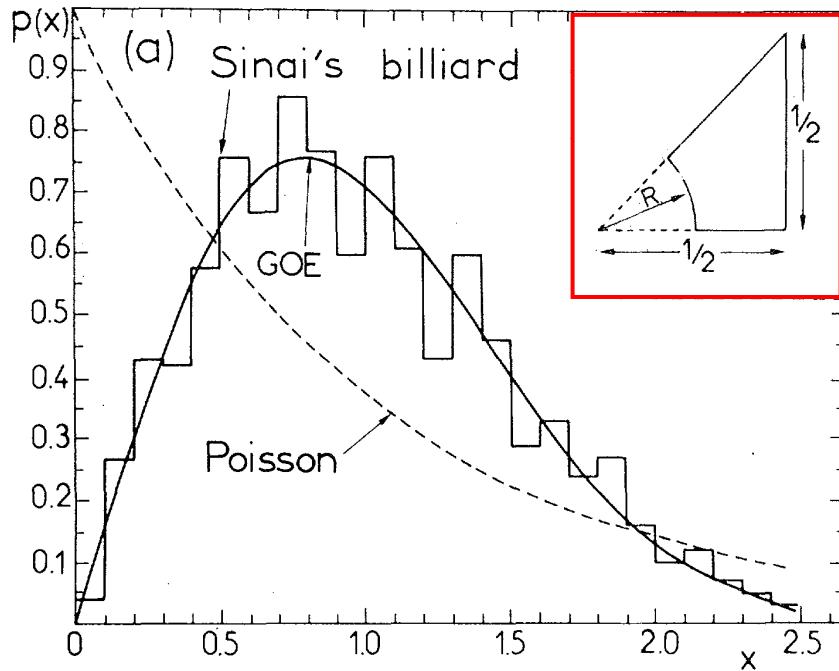


$$\int_S G_E[\rho_s(x) - \rho_s(x')] f(x') dx' + f(x)/g(x) = -\psi_0[\rho(x)]$$

Fredholm int. eq.



# Example: quantum billiard



Calculation of ~1000 energy levels  
of Sinai billiard

Bohigas, Giannoni, Schmit (1984)

They call the method Korringa-  
Kohn-Rostoker and cite Berry...

$$-\nabla_{\rho}^2 \psi(\rho) = E \psi(\rho) \quad \text{Helmholtz vs Fredholm ;)}$$

- huge 2D configurational space

+ sparse matrix

- difficult to implement boundary  
conditions

+ more general; works with any potential

$$\int_S K_E(x, x') f(x') dx' = \lambda f(x)$$

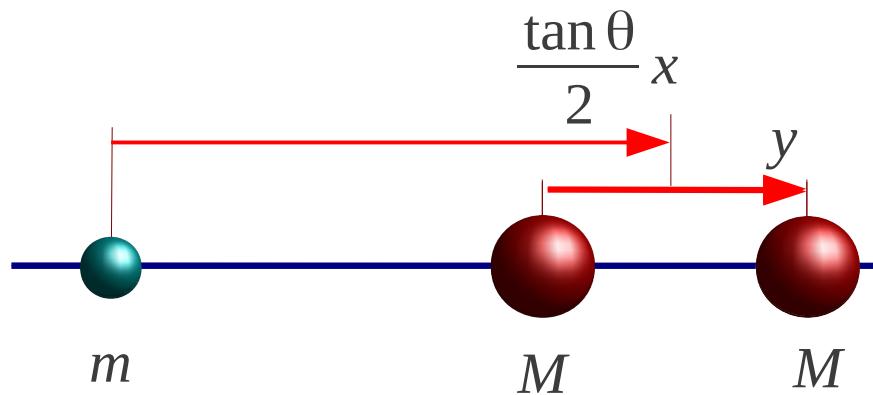
+ 1D configurational space

- full matrix

+ boundary conditions are taken  
into account naturally

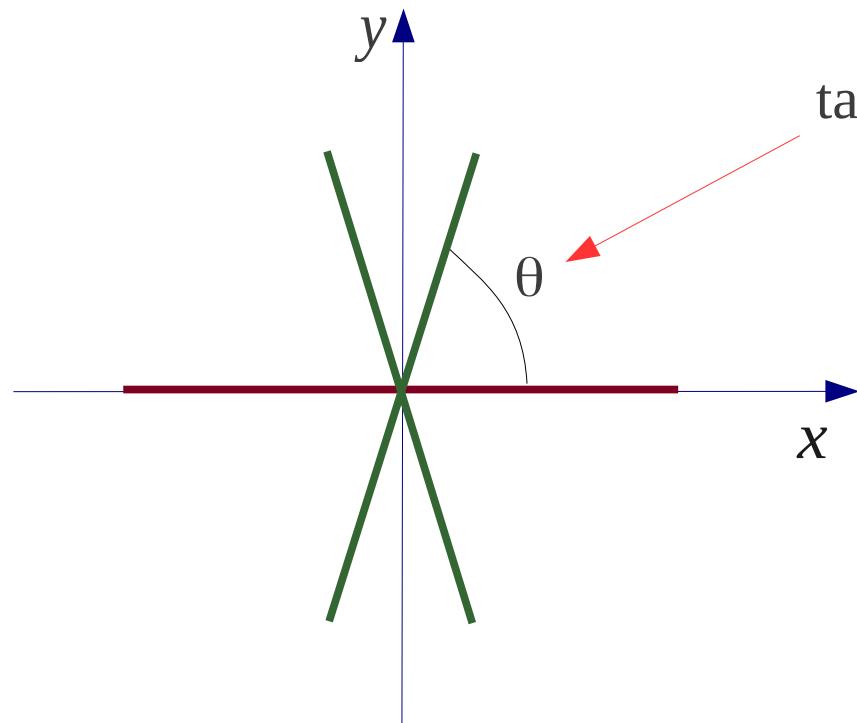
- only billiard

# 1D three-body = 2D one-body

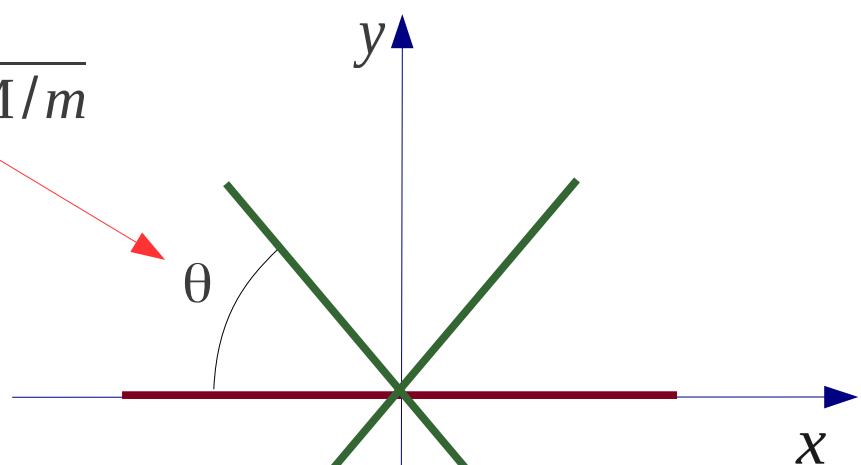


$$(-\partial^2/\partial x^2 - \partial^2/\partial y^2 - ME)\psi(\rho) = 0$$

$$[\partial \psi / \partial n] = -2\psi/a$$

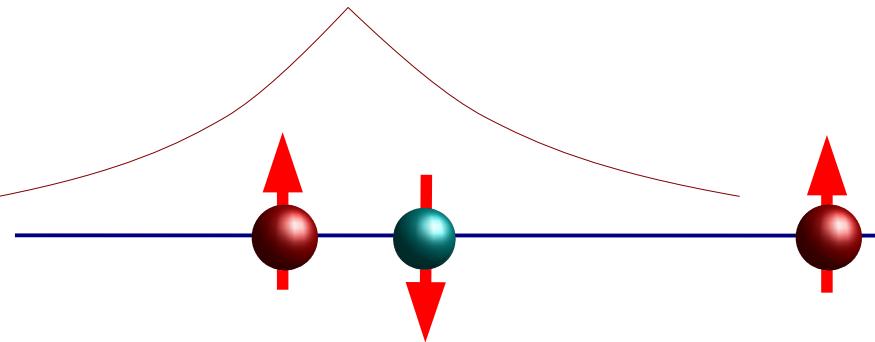


$$\tan \theta = \sqrt{1+2M/m}$$



Some simple applications

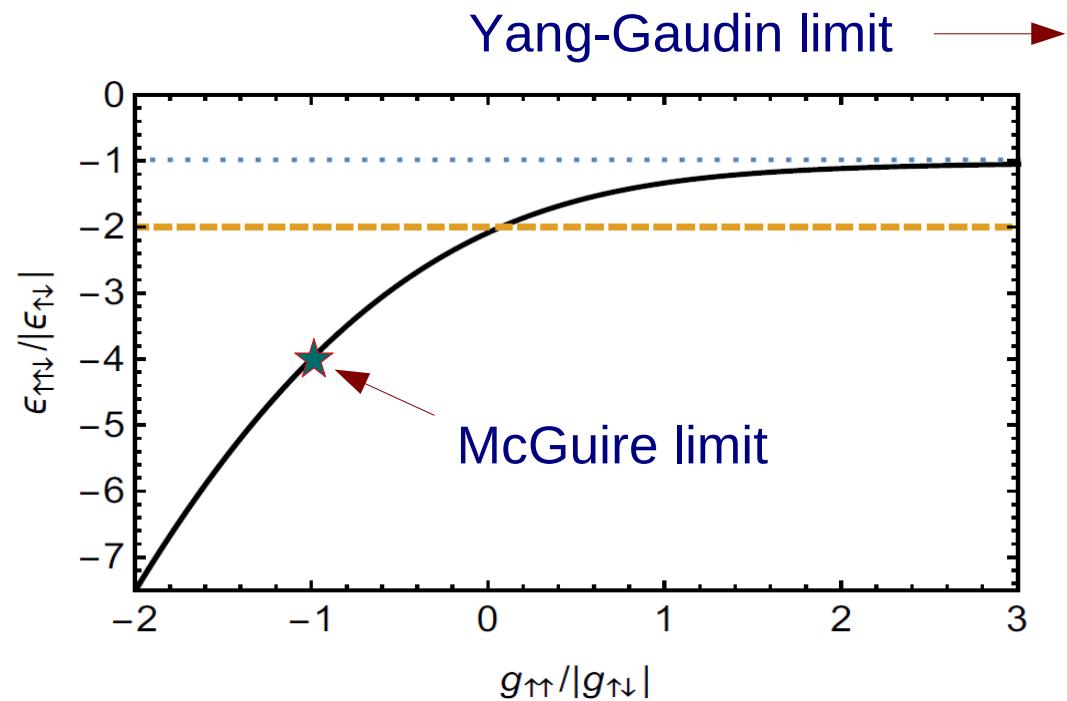
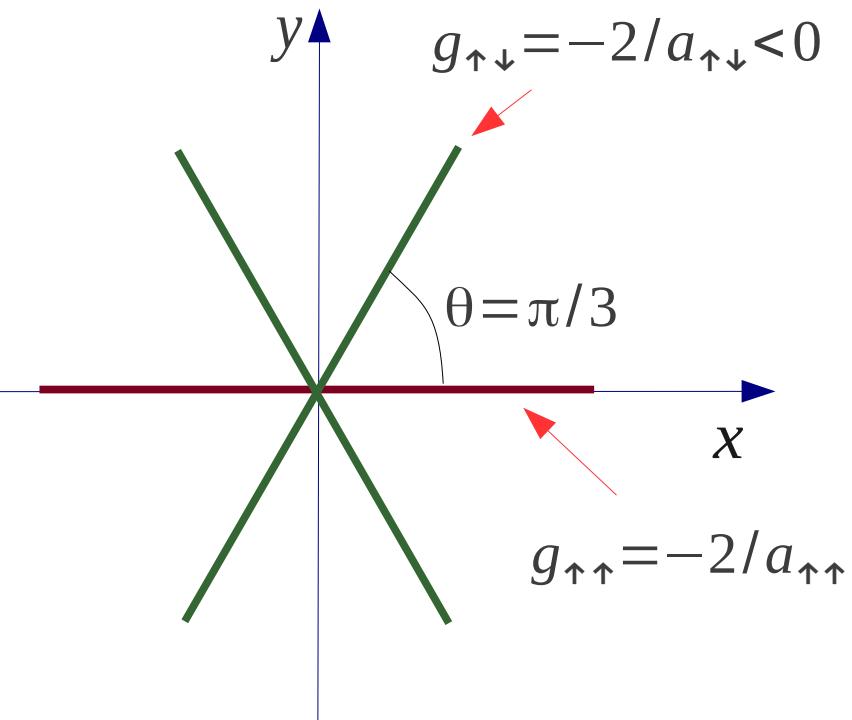
# Trimer in a Bose-Bose mixture



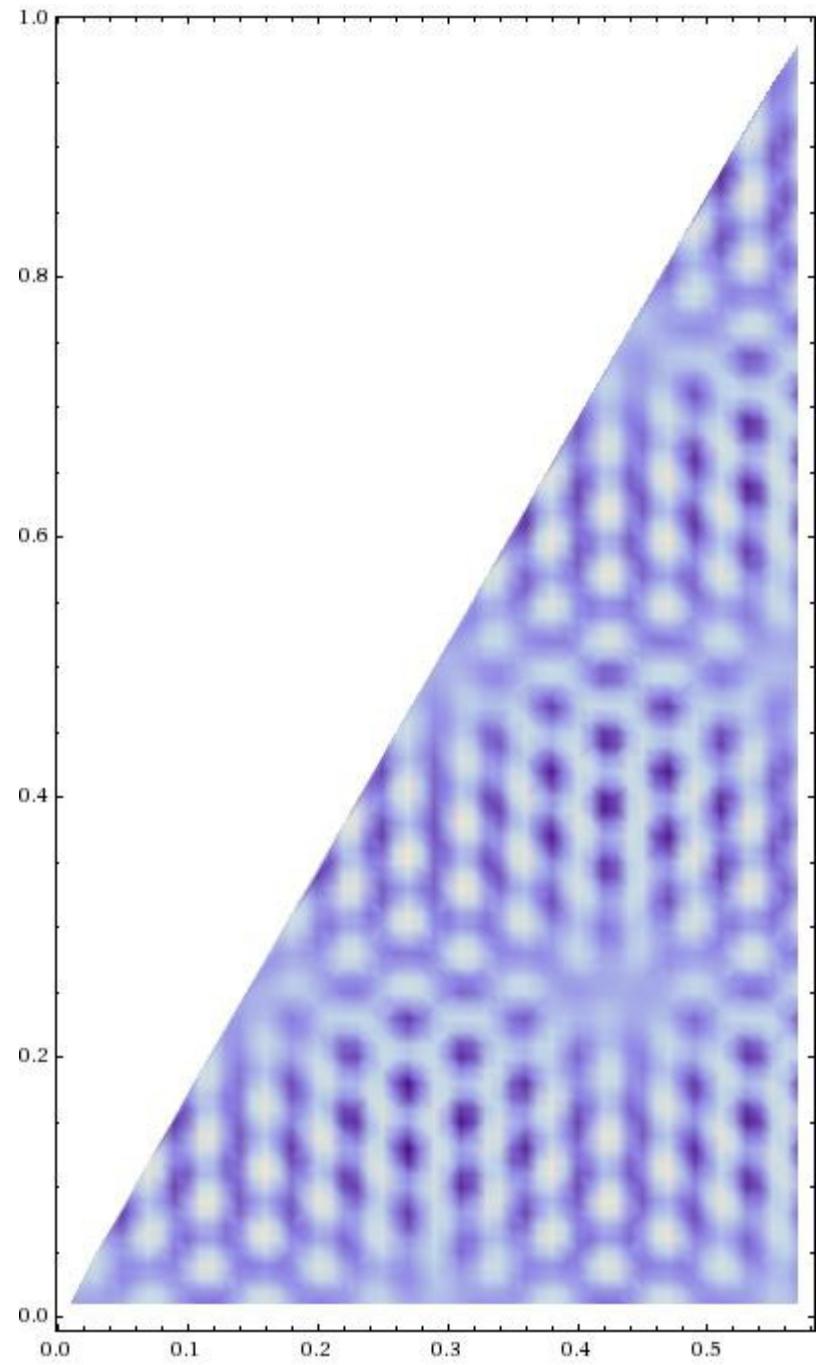
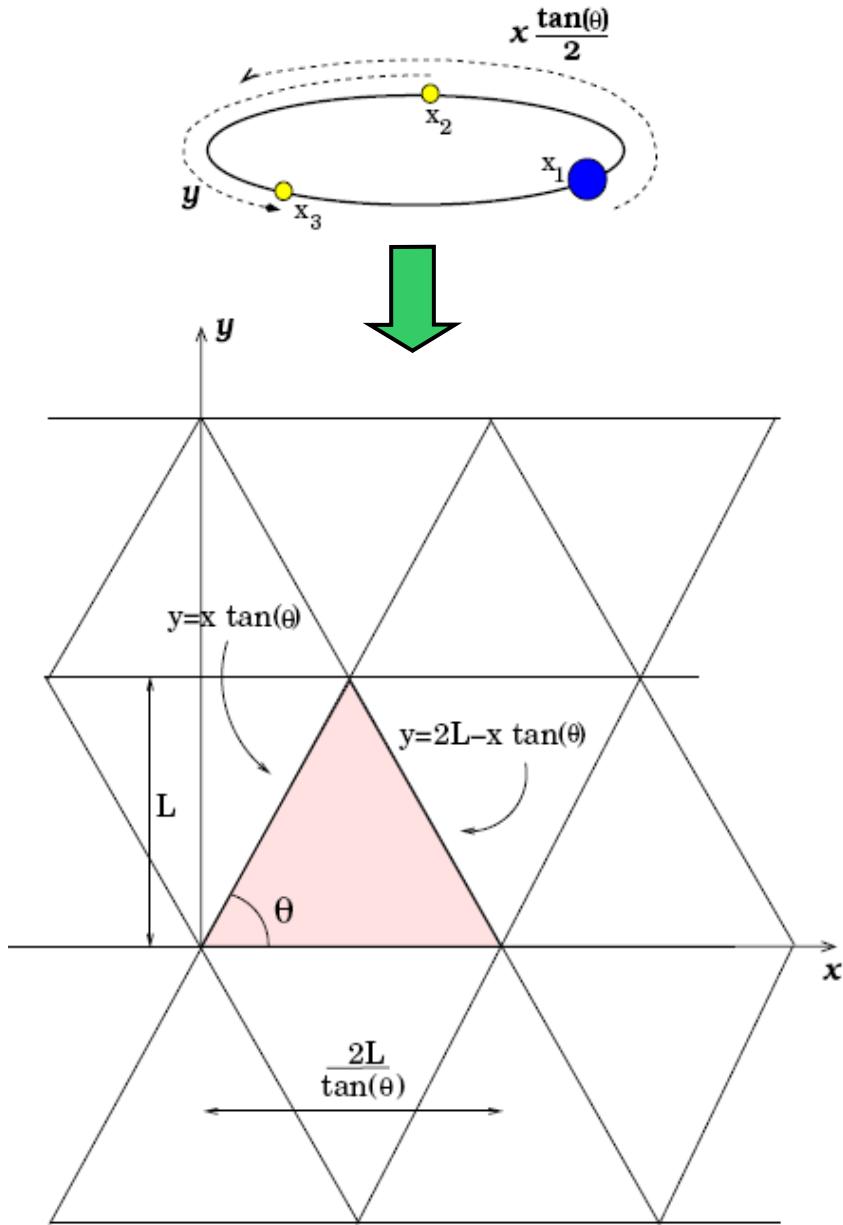
STM equation(s) in momentum space ( $f = gF$ )

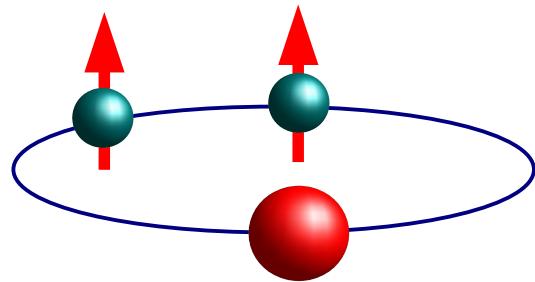
$$\left(1 + \frac{g_{\uparrow\uparrow}}{\sqrt{3p^2 - 4E}}\right) F_{\uparrow\uparrow}(p) = \int \frac{2g_{\uparrow\downarrow}F_{\uparrow\downarrow}(q)}{E - p^2 - pq - q^2} \frac{dq}{2\pi},$$

$$\left(1 + \frac{g_{\uparrow\downarrow}}{\sqrt{3p^2 - 4E}}\right) F_{\uparrow\downarrow}(p) = \int \frac{g_{\uparrow\downarrow}F_{\uparrow\downarrow}(q) + g_{\uparrow\uparrow}F_{\uparrow\uparrow}(q)}{E - p^2 - pq - q^2} \frac{dq}{2\pi}$$



# Equal-mass up-up-down fermions (Yang-Gaudin model)



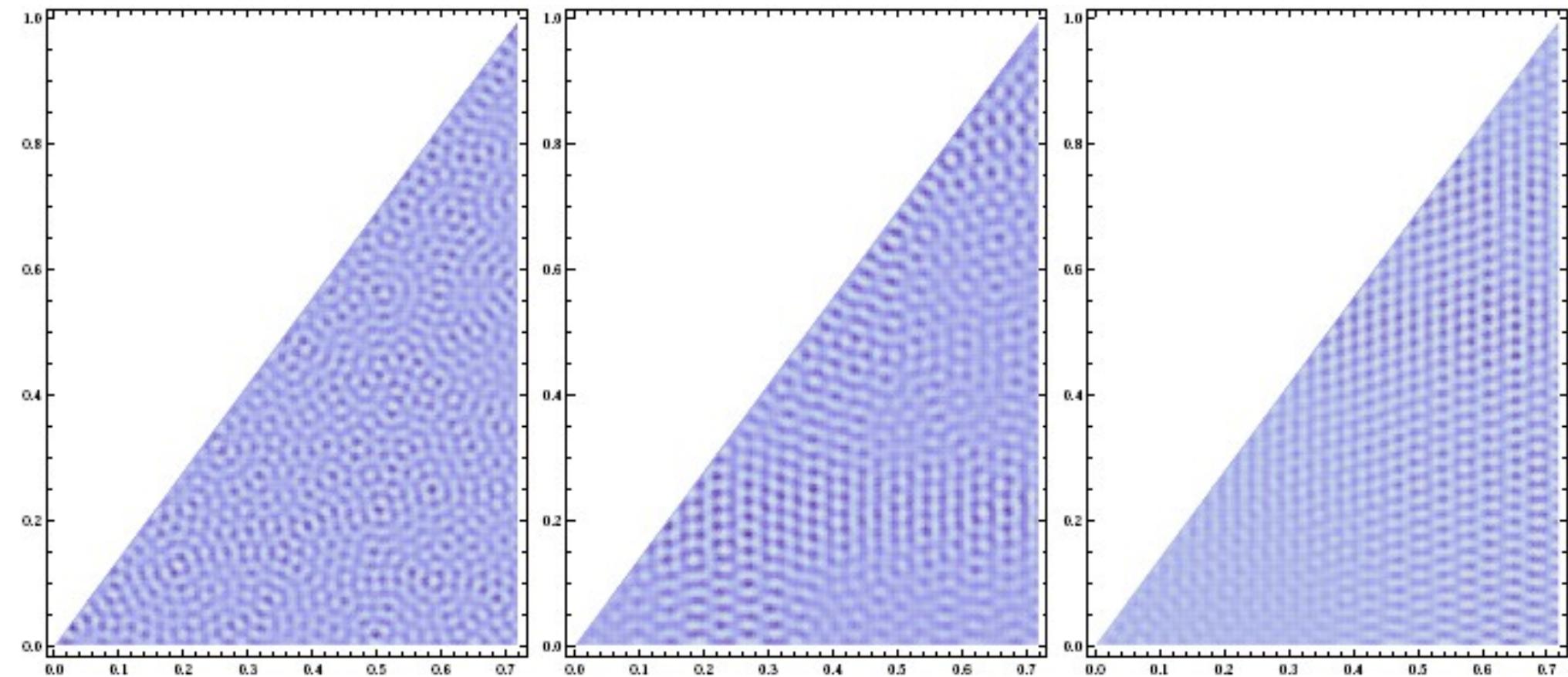


Rb-K-K Bose-Fermi-Fermi, non integrable  
M. Colome-Tatche and DSP (2011)

State number 1835

1296

1676



# Comparison with Born-Oppenheimer

$$(-\partial^2/\partial x^2 - \partial^2/\partial y^2 - ME)\psi(\rho) = 0$$

$$[\partial \psi / \partial n] = -2 \psi / a$$

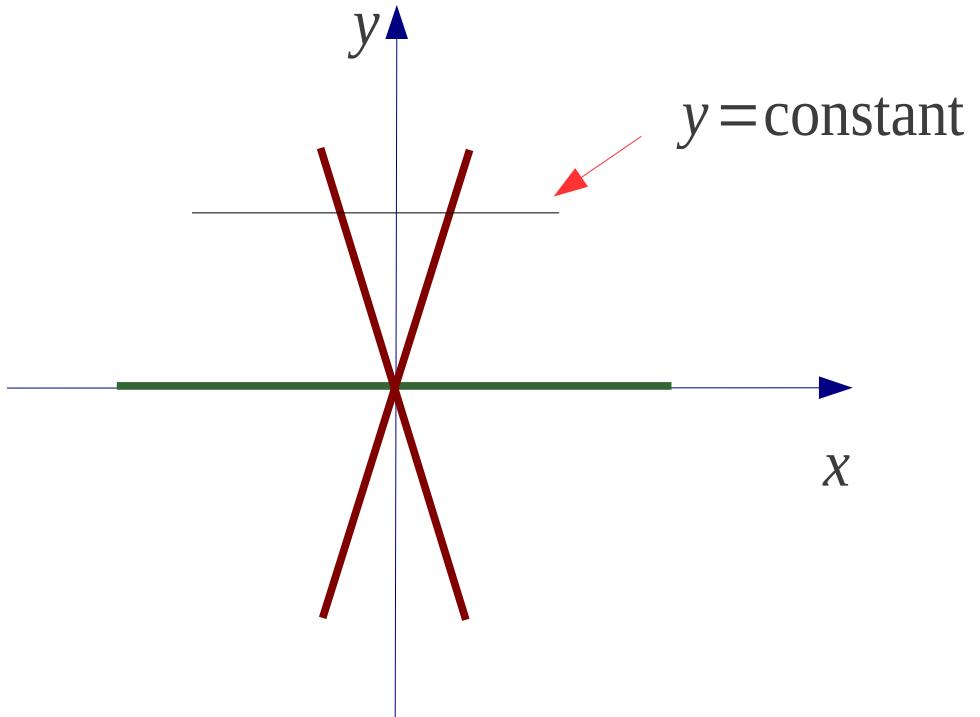


$$-\partial^2 \psi_y(x) / \partial x^2 = \lambda(y) \psi_y(x)$$

$$[\partial \psi_y / \partial x] = -2 \psi_y / a$$



$$[-\partial^2/\partial y^2 + \lambda(y)]\chi(y) = ME\chi(y)$$



# Comparison with hyperspherical approach

$$(-\partial^2/\partial x^2 - \partial^2/\partial y^2 - ME)\psi(\rho) = 0$$

$$[\partial \psi / \partial \mathbf{n}] = -2\psi/a$$

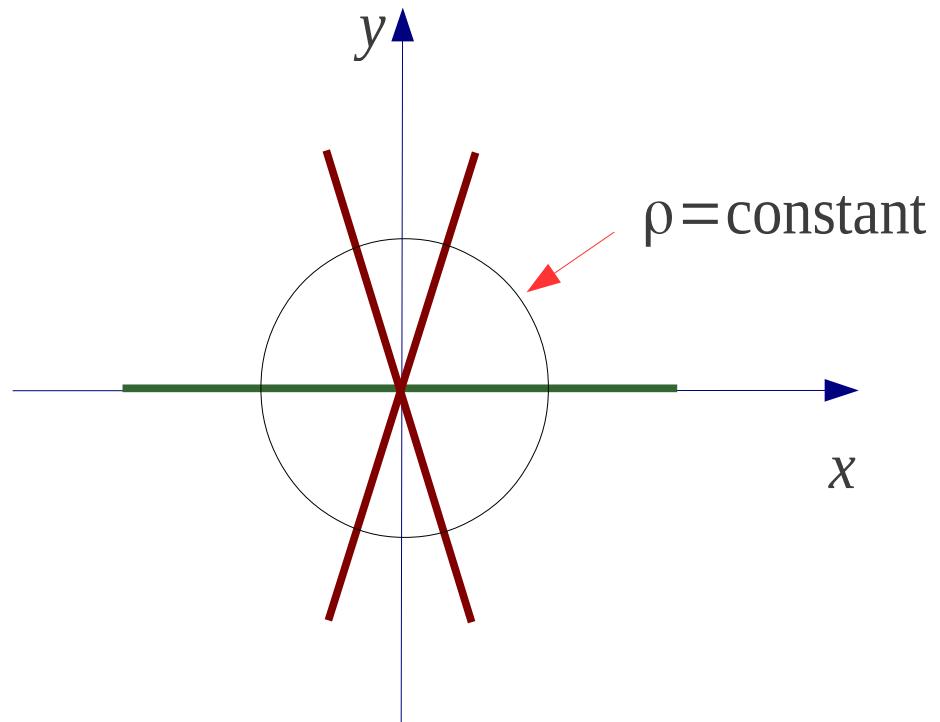


$$-\partial^2 \psi_{v,\rho}(\varphi)/\partial \varphi^2 = \lambda_v(\rho) \psi_{v,\rho}(\varphi)$$

$$\psi(\rho) = \sum_v \chi_v(\rho) \psi_{v,\rho}(\varphi)$$



$$\left[ -\nabla_\rho^2 + \frac{\lambda_v(\rho)}{\rho^2} - ME \right] \chi_v(\rho) + \sum_u \hat{K}_{vu} \chi_u(\rho) = 0$$



$$(\alpha - \gamma_k) \chi(\mathbf{k}) \quad (12)$$

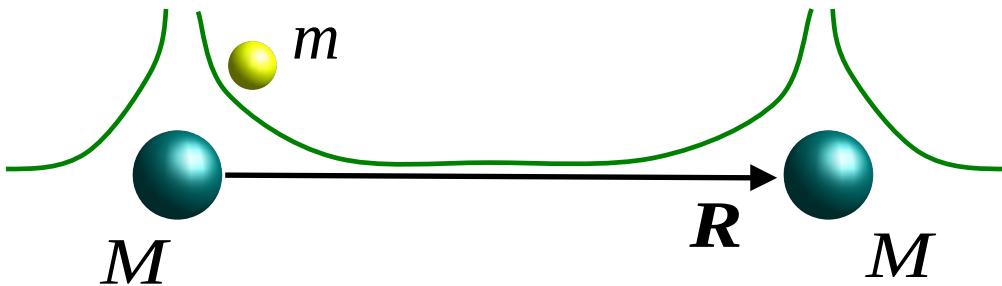
$$+ 8\pi \int \frac{d\mathbf{k}'}{(2\pi)^3} \frac{\chi(\mathbf{k}')}{k^2 + k'^2 + \mathbf{k}\cdot\mathbf{k}' - (ME/\hbar^2) - i\tau} = 0.$$

The solution of this equation determines the wave function of the system, in accord with Eq. (11). For states with a definite quantity of momentum, Eq. (12) reduces to an equation for a function which depends on one independent variable, which can be solved numerically.

The idea for this consideration of the three body problem was supplied by L. D. Landau.

# Heteronuclear Fermi-Fermi mixture in the non-efimovian regime

# 3-body problem. Born-Oppenheimer approximation



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

Light atom wavefunction:

$$\Psi(\mathbf{r}) = \frac{\exp(-\kappa|\mathbf{r} - \mathbf{R}/2|)}{|\mathbf{r} - \mathbf{R}/2|} + \frac{\exp(-\kappa|\mathbf{r} + \mathbf{R}/2|)}{|\mathbf{r} + \mathbf{R}/2|}$$

Bethe-Peierls boundary condition gives:

$$\frac{1}{a} - \kappa + \frac{\exp(-\kappa R)}{R} = 0$$

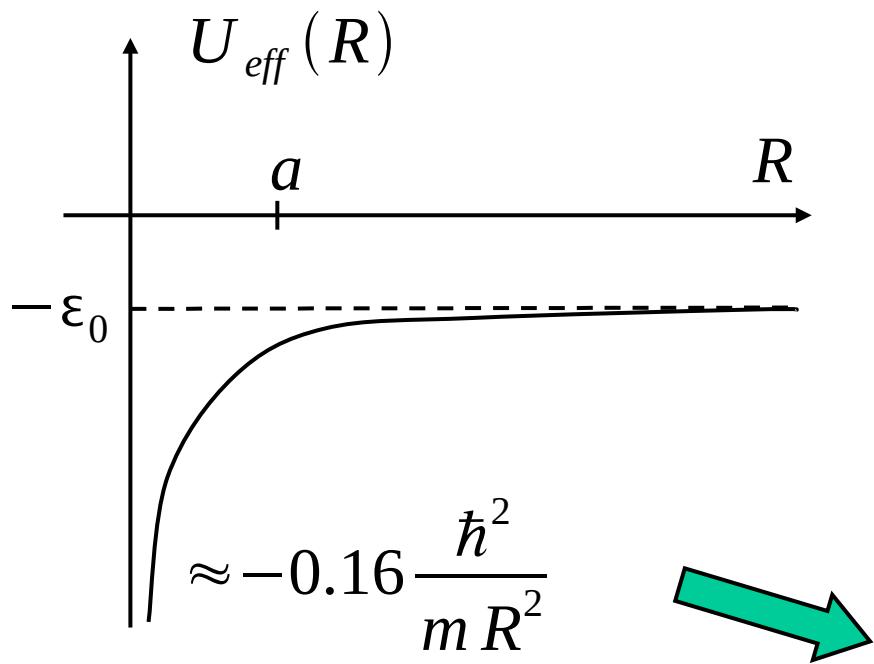
$$R \ll a \rightarrow \kappa \approx \frac{0.567}{R}$$

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

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

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

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



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

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

Heavy fermions  $\rightarrow l=1,3,5\dots$

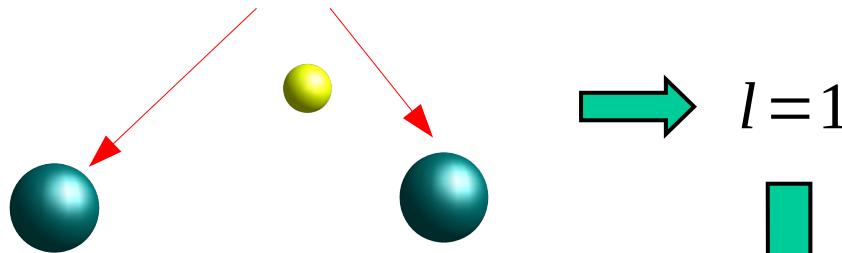
Heavy bosons  $\rightarrow l=0,2,4\dots$

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

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

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

# Identical fermions



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

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

$$\chi(R) \propto \sqrt{R} \sin(\sqrt{-1/4 - \beta} \log R/r_3)$$



“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**

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

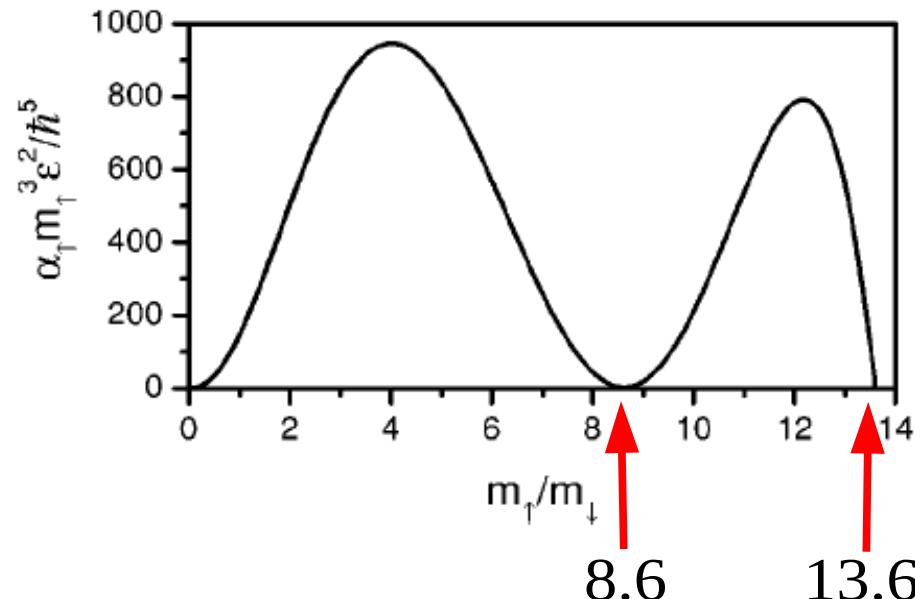
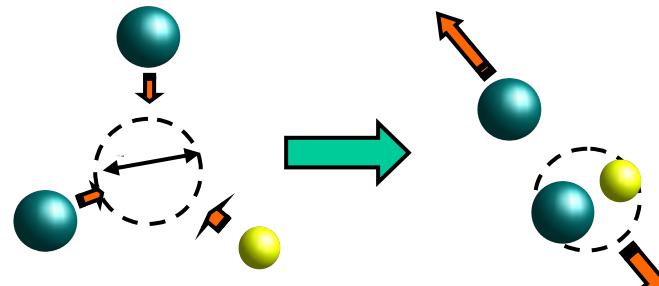
$$\chi(R) \propto R^{1/2 + \sqrt{\beta + 1/4}}$$



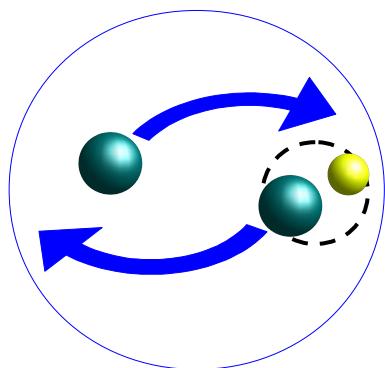
“Universal” regime in the sense that one needs no three-body parameter. **Fermi statistics wins over the induced attraction**

# Heavy-heavy-light problem, magic mass ratios

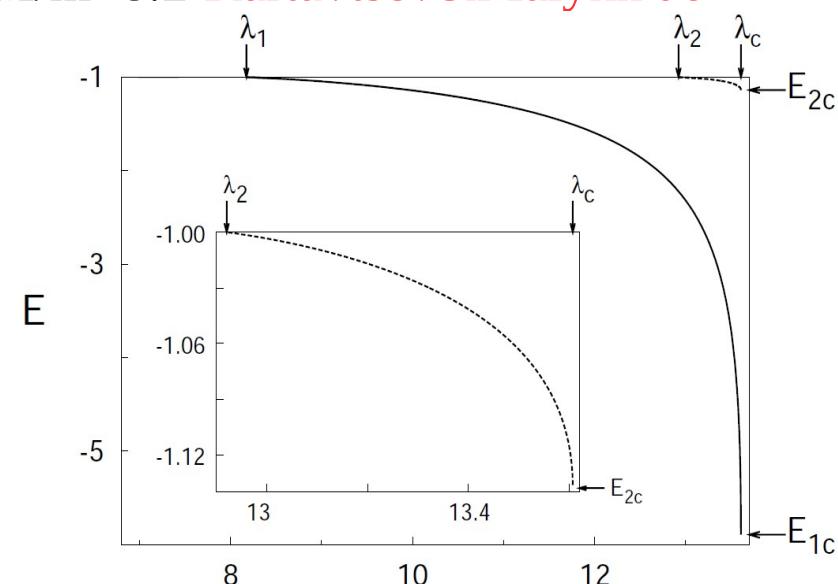
3-body recombination to a weakly bound level **DSP'03**



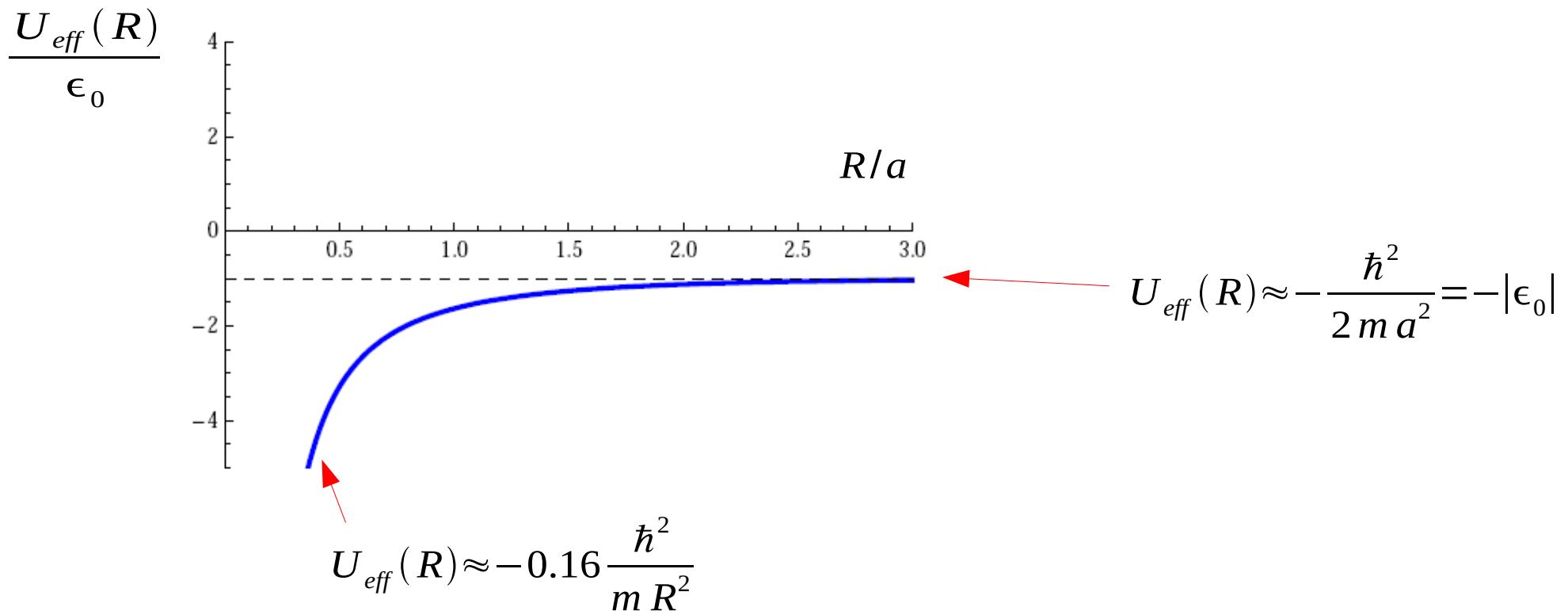
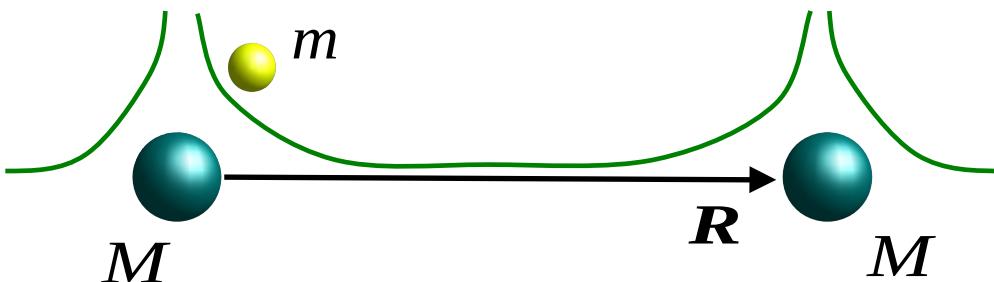
Emergence of a non-Efimovian trimer state for  $M/m > 8.2$  **Kartavtsev&Malykh'06**



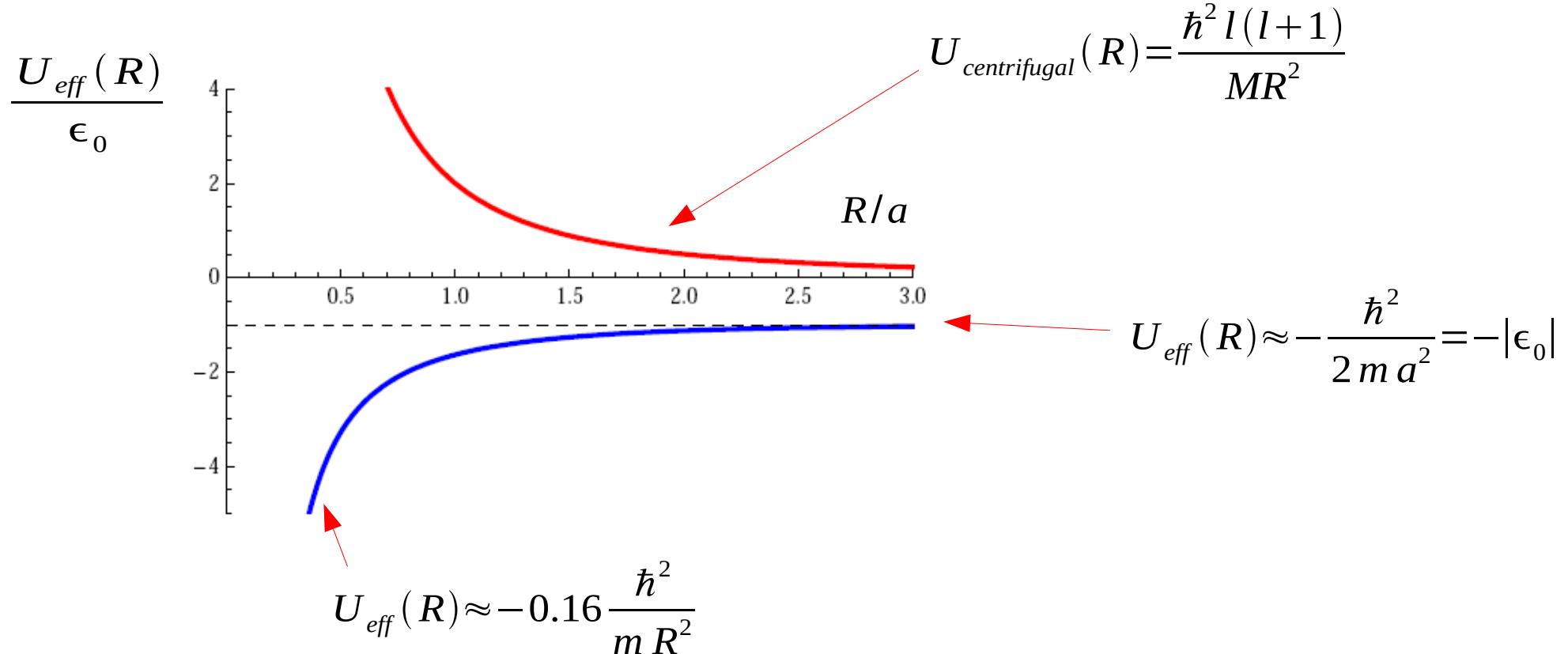
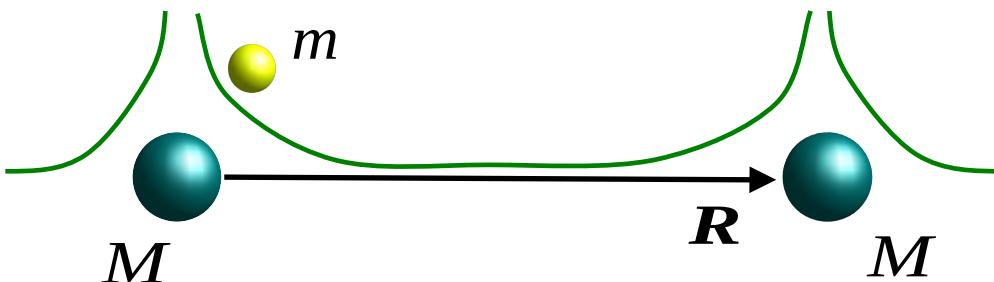
$M/m < 8.2$  *p*-wave atom-dimer scattering resonance  
 $M/m > 8.2$  trimer state with  $l=1$



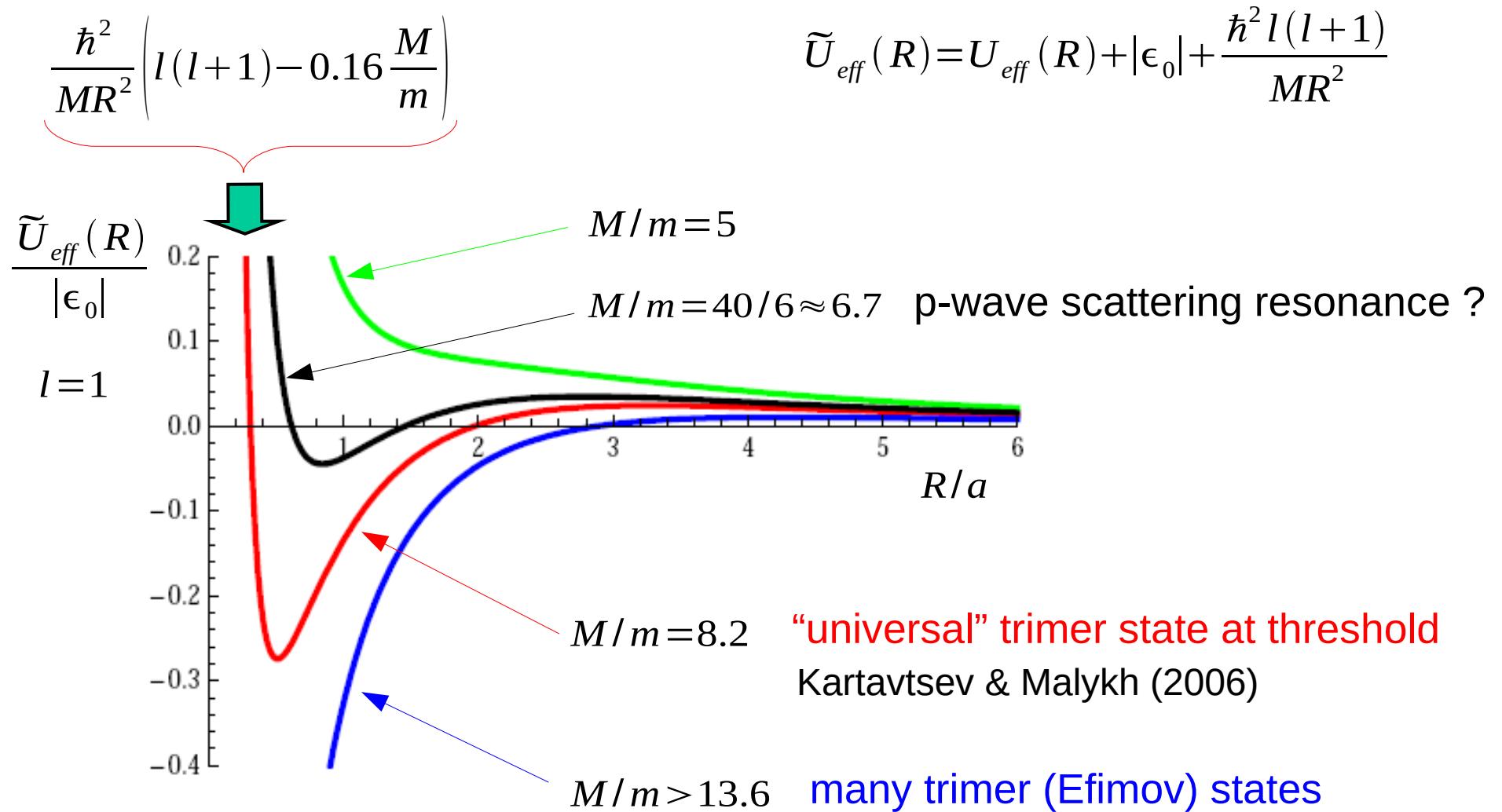
# Born-Oppenheimer approximation



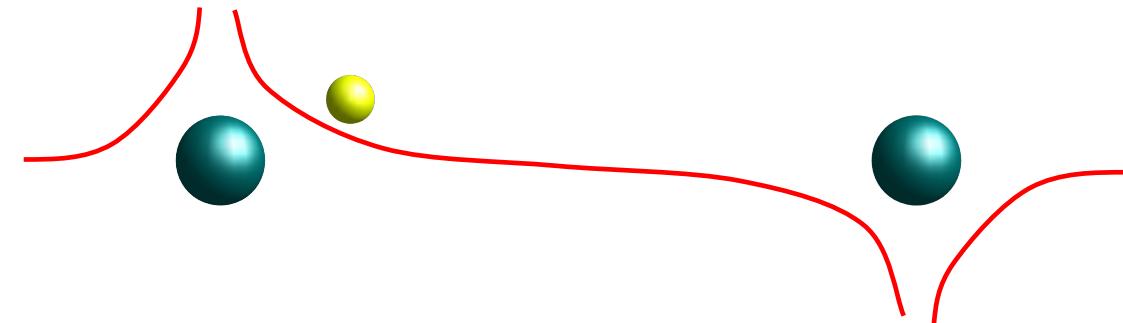
# Born-Oppenheimer approximation



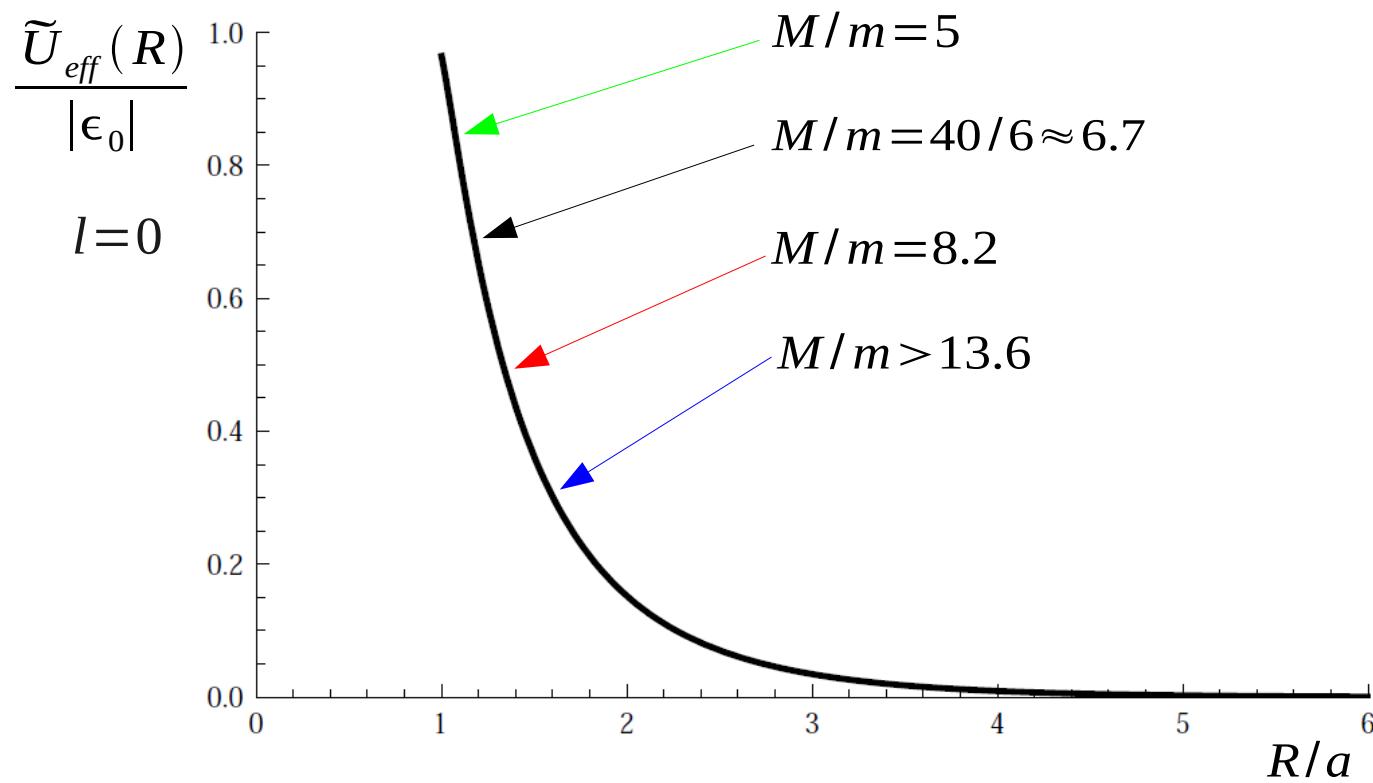
$$\left[ -\frac{\hbar^2}{M} \frac{\partial^2}{\partial R^2} + \tilde{U}_{eff}(R) \right] \chi(R) = E \chi(R)$$

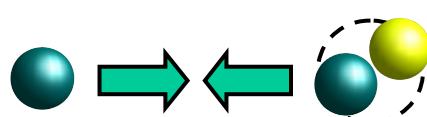


# S-wave atom-dimer repulsion

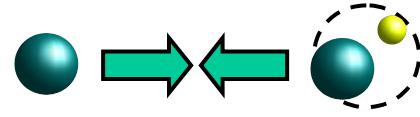
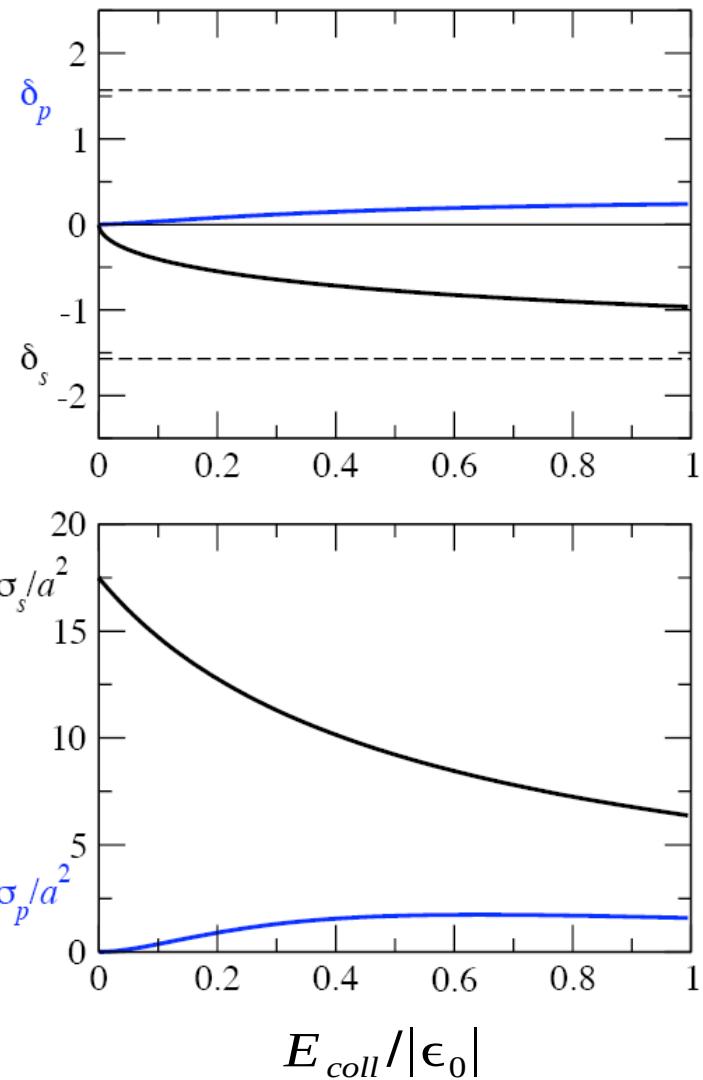


Light fermion in the  
antisymmetric “ungerade” state

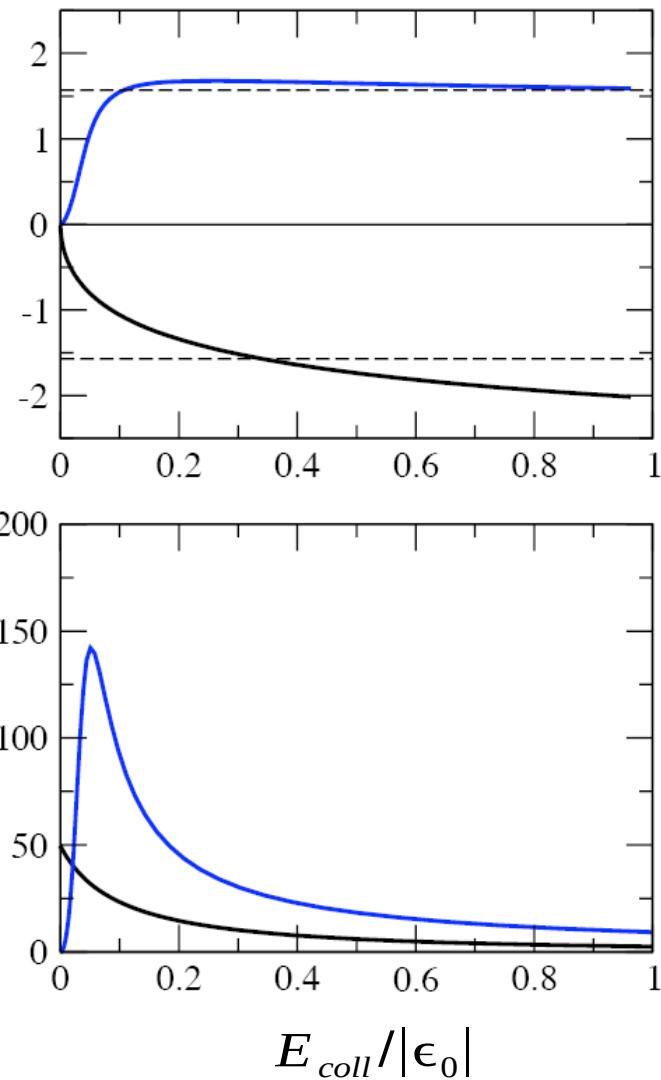




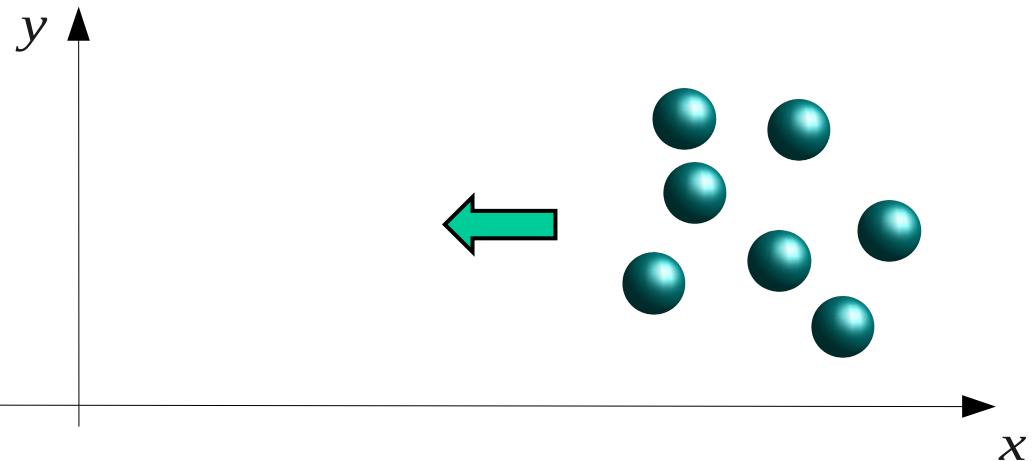
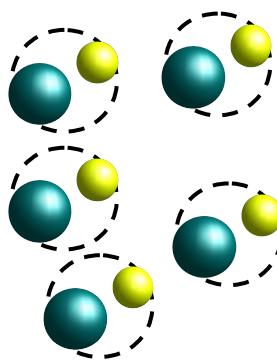
Equal mass



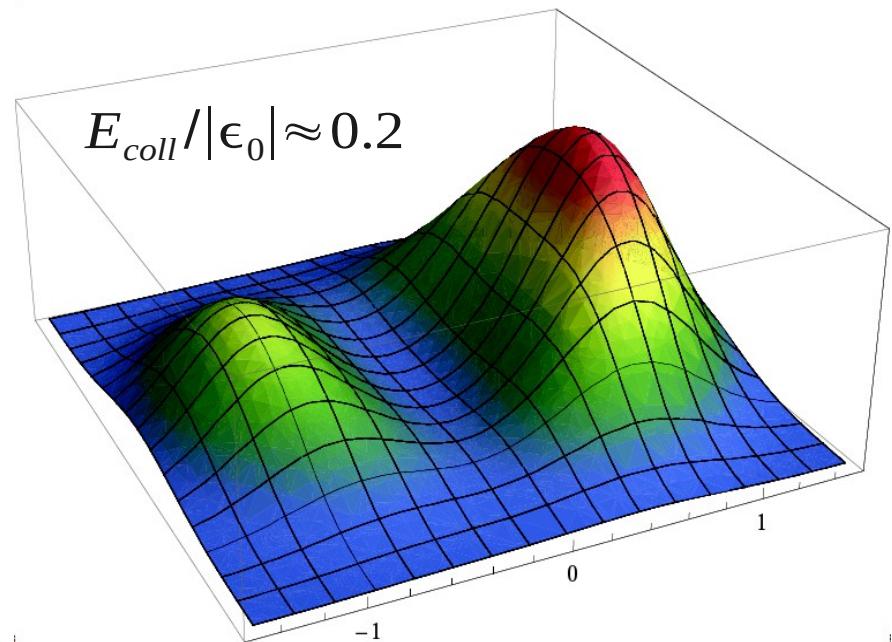
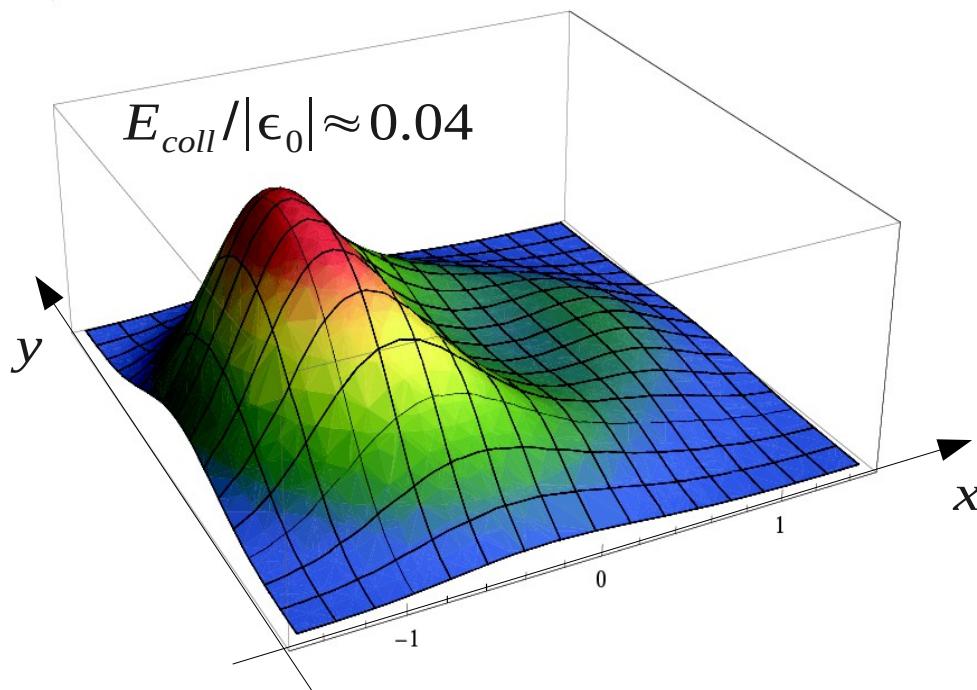
$^{40}\text{K}$ -( $^{40}\text{K}$ , $^{6}\text{Li}$ )



# Collision of atomic and molecular thermal clouds

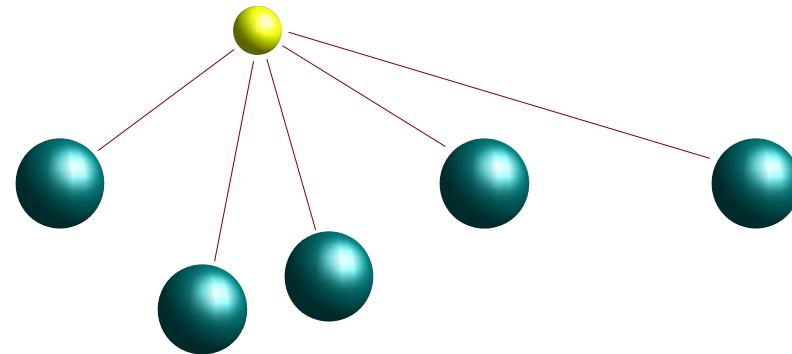


molecular column density



# (N+1)-body problem

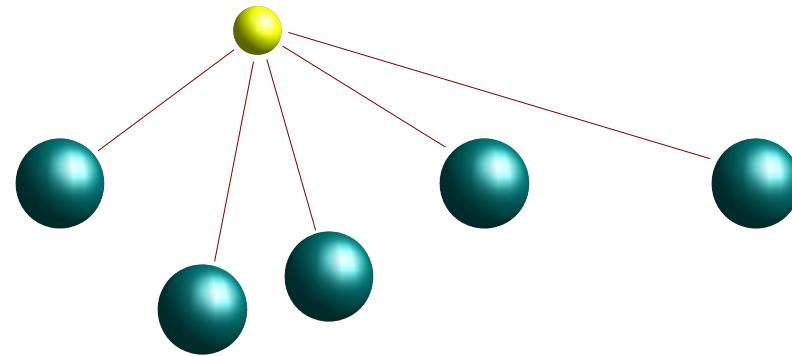
How many heavy fermions can be bound by a single light atom?



	Symmetry $L^\pi$	appear at $M/m >$	Efimovian for $M/m >$
2+1 trimer	 $1^-$	8.173 Kartavtsev&Malykh'06	13.607 Efimov'73
3+1 tetramer	 $1^+$	~9.5 Blume'12	13.384 Castin,Mora&Pricoupenko'10
4+1 pentamer	 ?	?	?
:	?	?	?
N+1-mer	 ?	?	?

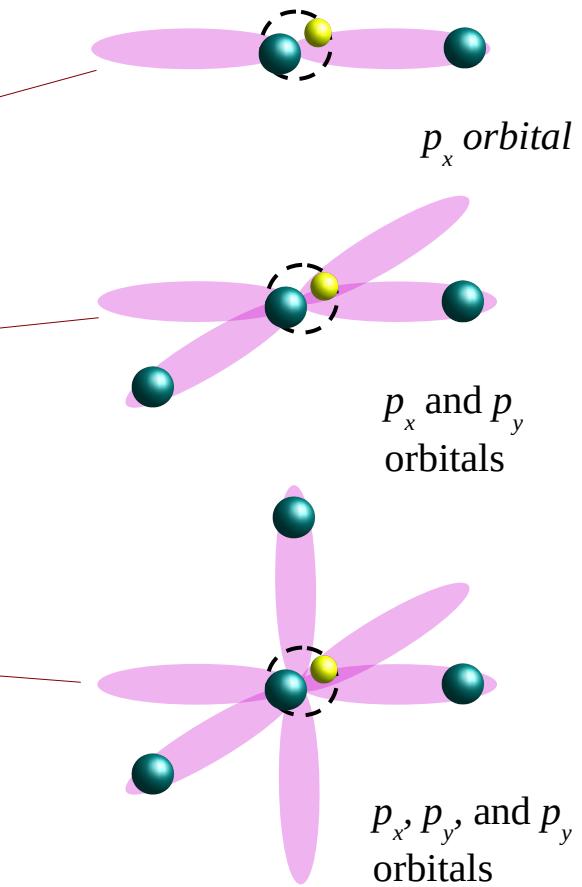
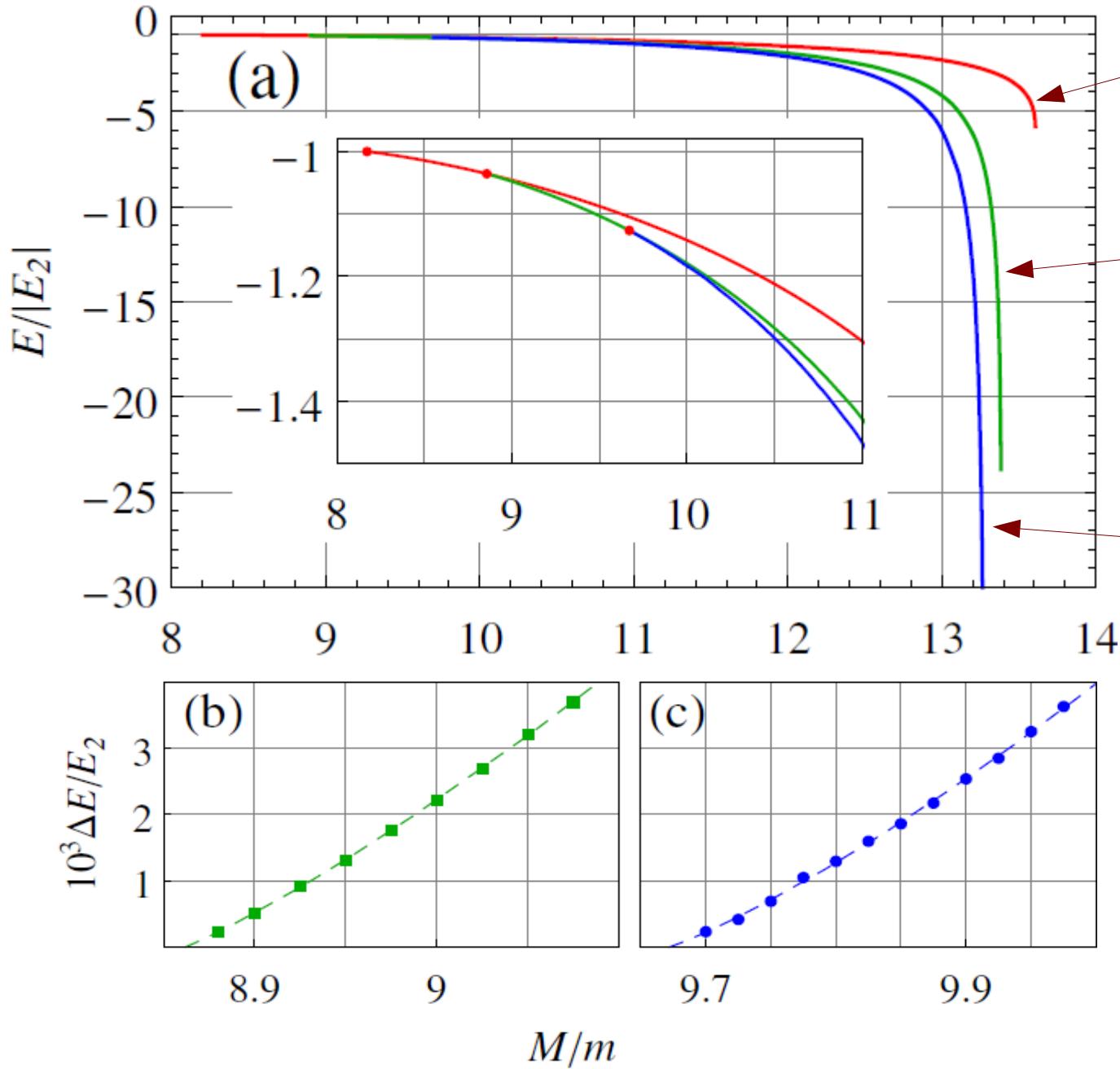
# (N+1)-body problem

How many heavy fermions can be bound by a single light atom?



B. Bazak and DSP (2017)

	Symmetry $L^\pi$	appear at $M/m >$	Efimovian for $M/m >$
2+1 trimer	 $1^-$	8.173 Kartavtsev&Malykh'06	13.607 Efimov'73
3+1 tetramer	 $1^+$	$\sim 9.5 \rightarrow 8.862(1)$ Blume'12	13.384 Castin,Mora&Pricoupenko'10
4+1 pentamer	 $0^-$	9.672(6)	13.279(2)
:	?	?	?
N+1-mer	 ?	?	?



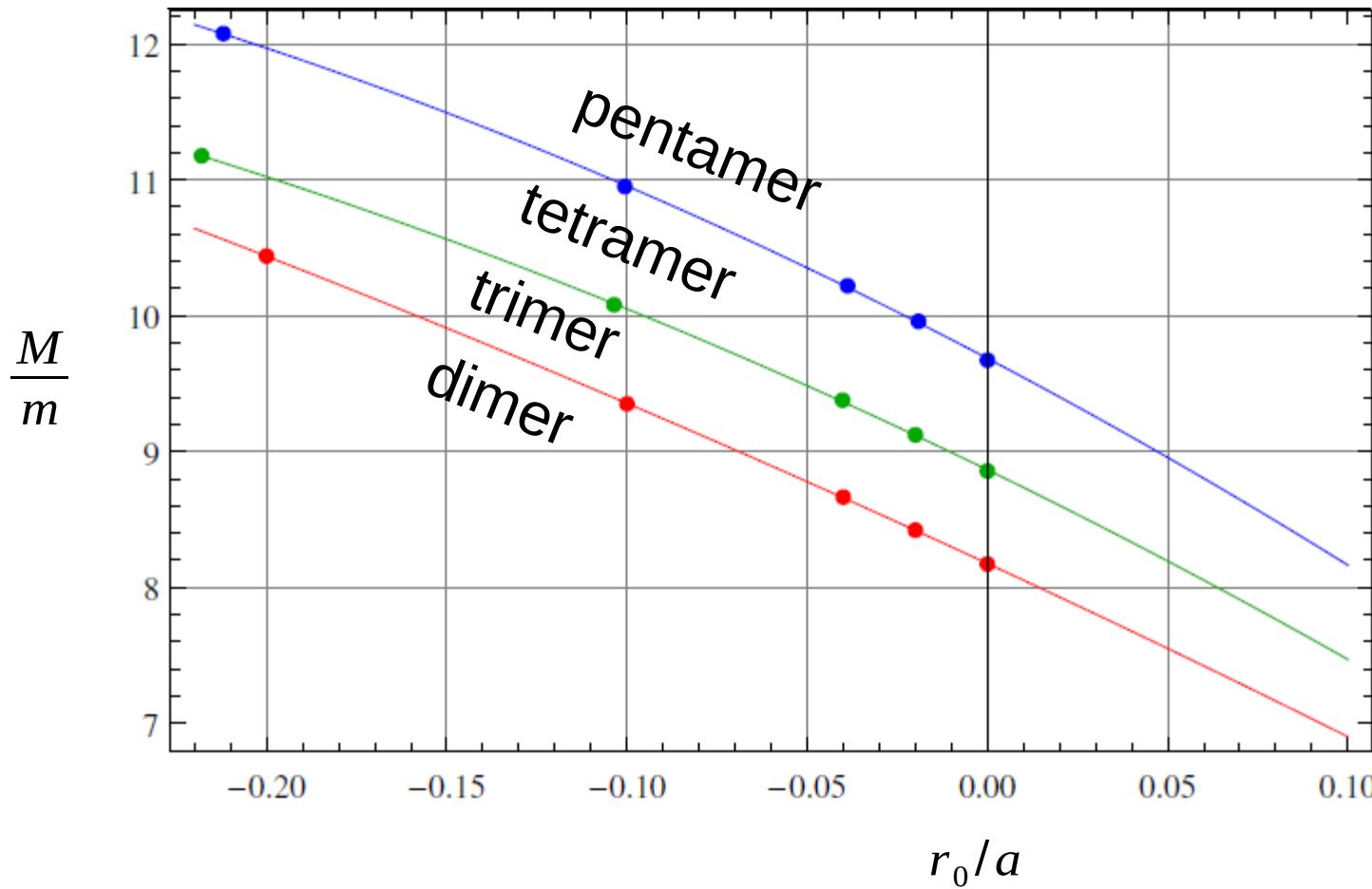
pentamer = closed  $p$ -shell

CONJECTURE:

No hexamer!  
(requires justification)

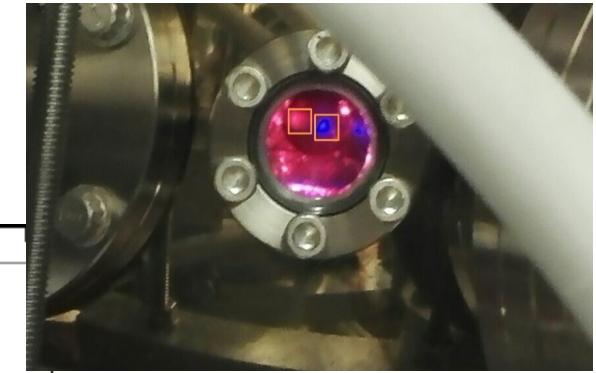
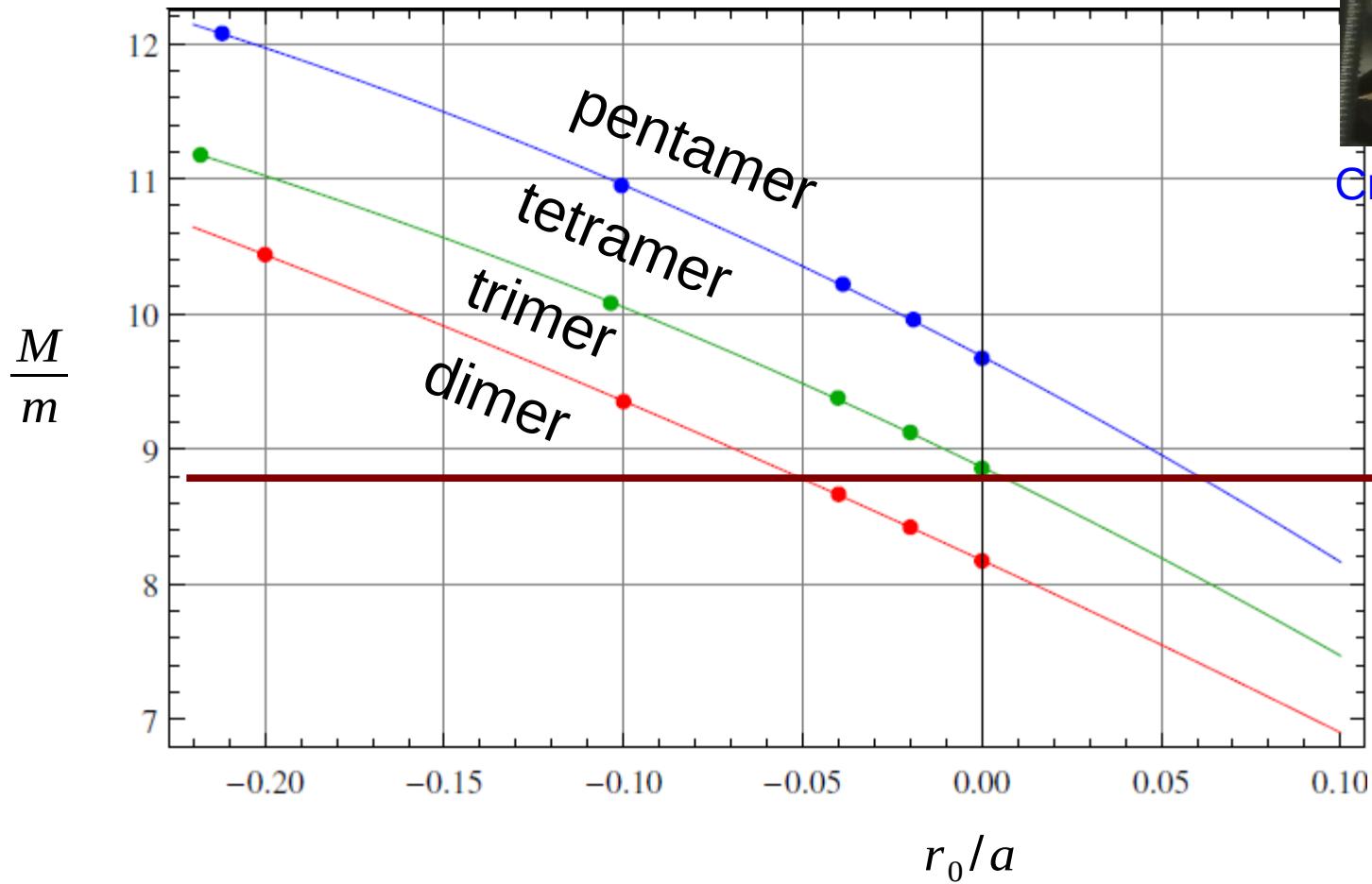
# Effective-range effects

$$\frac{1}{a} \longrightarrow \frac{1}{a} - \frac{r_0}{2} k^2$$



# Effective-range effects

$$\frac{1}{a} \longrightarrow \frac{1}{a} - \frac{r_0}{2} k^2$$



Cr-Li double MOT, Florence

$^{53}\text{Cr}-{}^6\text{Li}$

# Summary

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- History and basics of the zero-range few-body physics
- Efimovian and non-eftimovian regimes of three-body systems with zero-range interactions
- Approach of Skorniakov and Ter-Martirosian and its comparison with the Born-Oppenheimer and hyperspherical methods
- Universal trimers, tetramers, and pentamers in mass-imbalanced fermionic mixtures



