Binding of heavy fermions by a single light atom in one dimension

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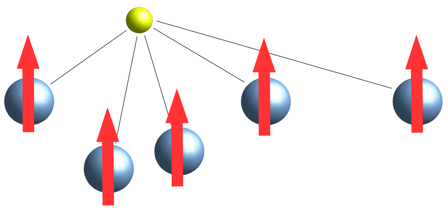
(N+1)-body problem

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



Kinetic energy of the heavy atoms ~1/*M*

competes with

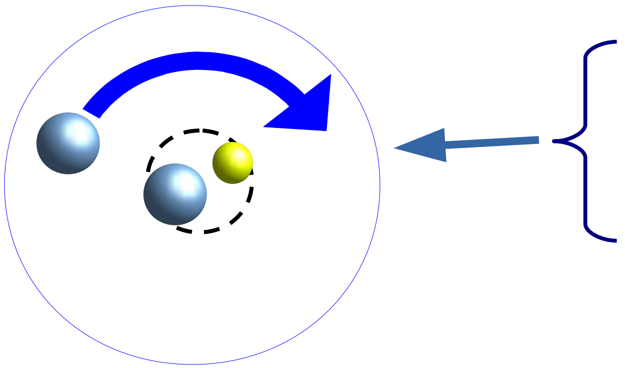
Attractive exchange potential of the light atom ~1/*m*

Parameters of the free-space zero-range N+1-body problem:

- space dimension *D*
- number of heavy atoms *N*
- mass ratio *M/m*
- dimer size *a* (can be used as the length unit)

3D 2+1-trimer

Emergence of a trimer state for M/m>8.2 [Kartavtsev & Malykh'2006]

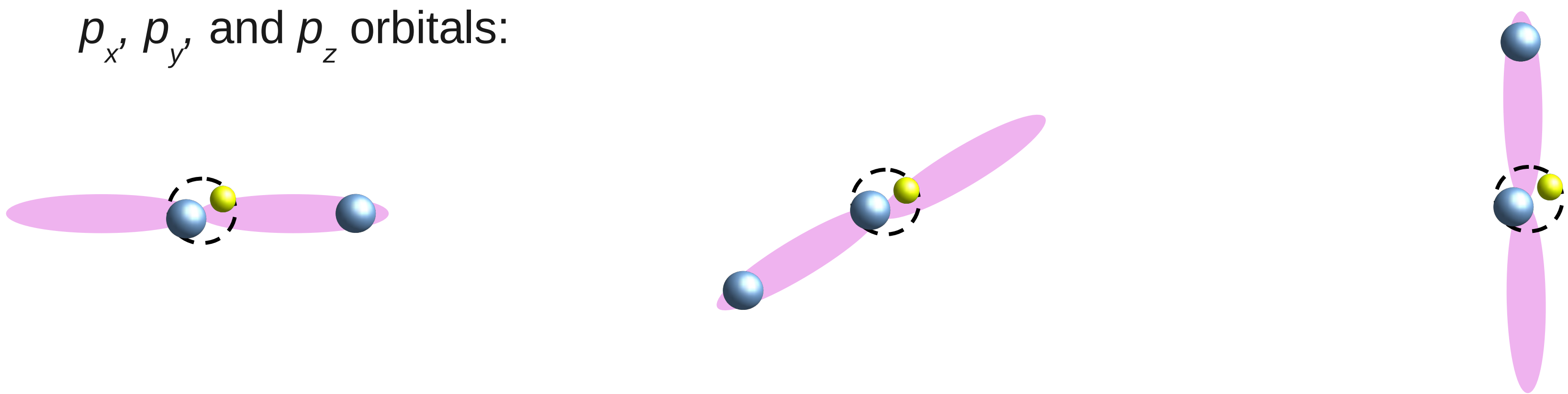


$M/m<8.2$ p-wave atom-dimer scattering resonance

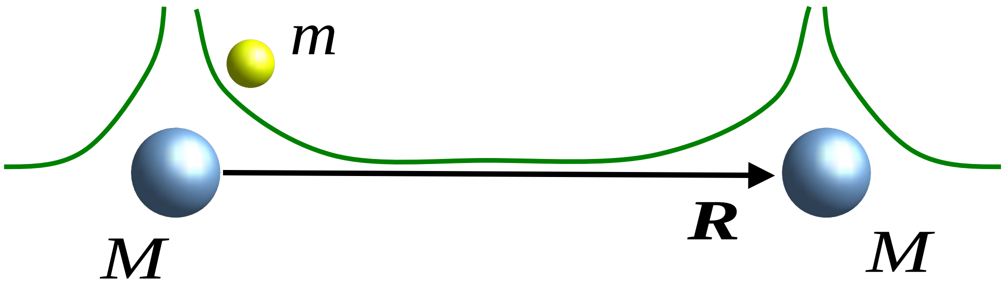
$M/m>8.2$ trimer state with L=1

Bound trimer state, NOT EFIMOV

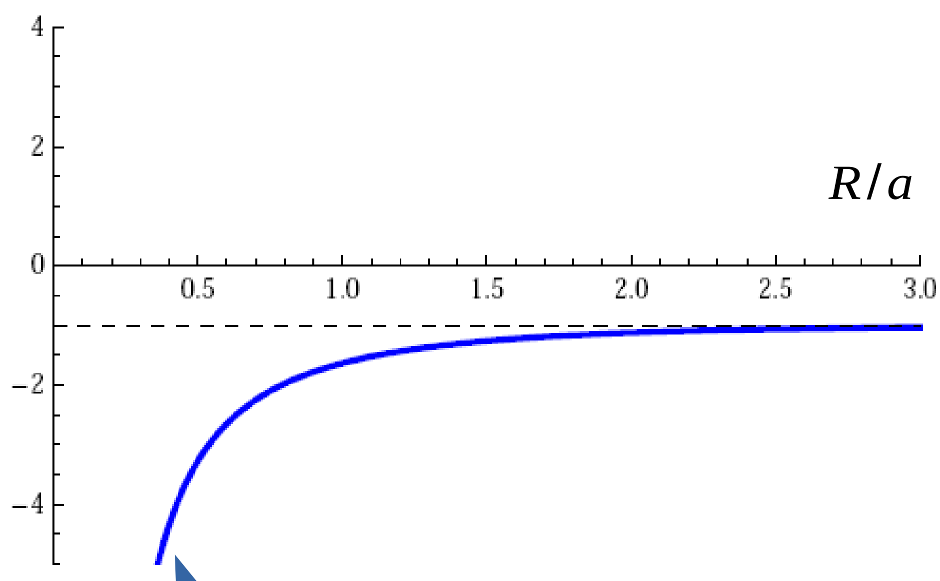
p_x, p_y, and p_z orbitals:



Born-Oppenheimer picture



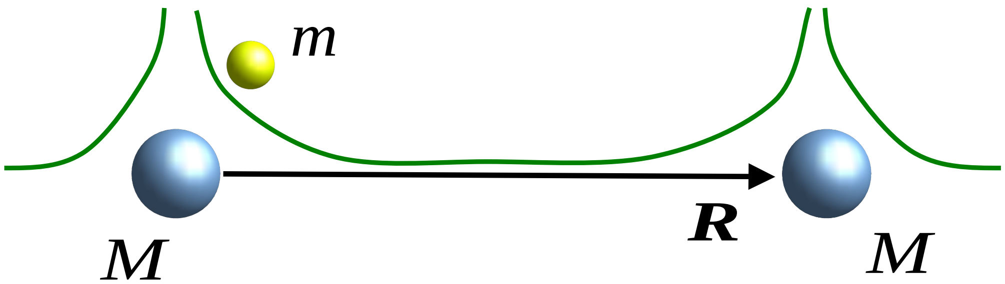
$$\frac{U_{eff}(R)}{\epsilon_0}$$

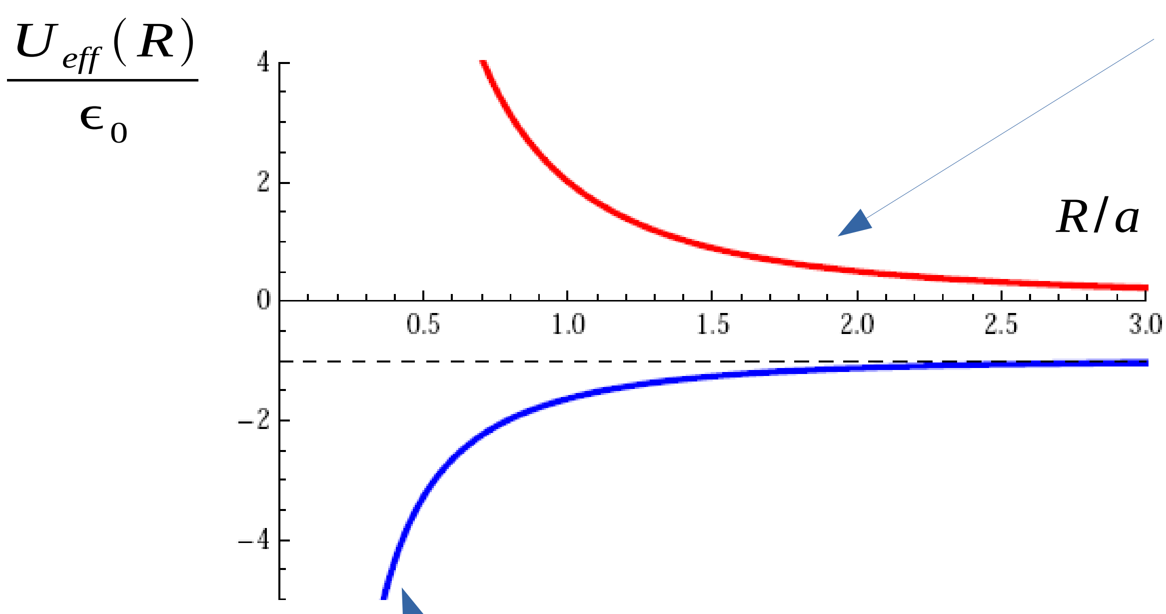


$$U_{eff}(R) \approx -\frac{\hbar^2}{2ma^2} = -|\epsilon_0|$$

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

Born-Oppenheimer picture





$$U_{centrifugal}(R) = \frac{\hbar^2 l(l+1)}{MR^2}$$

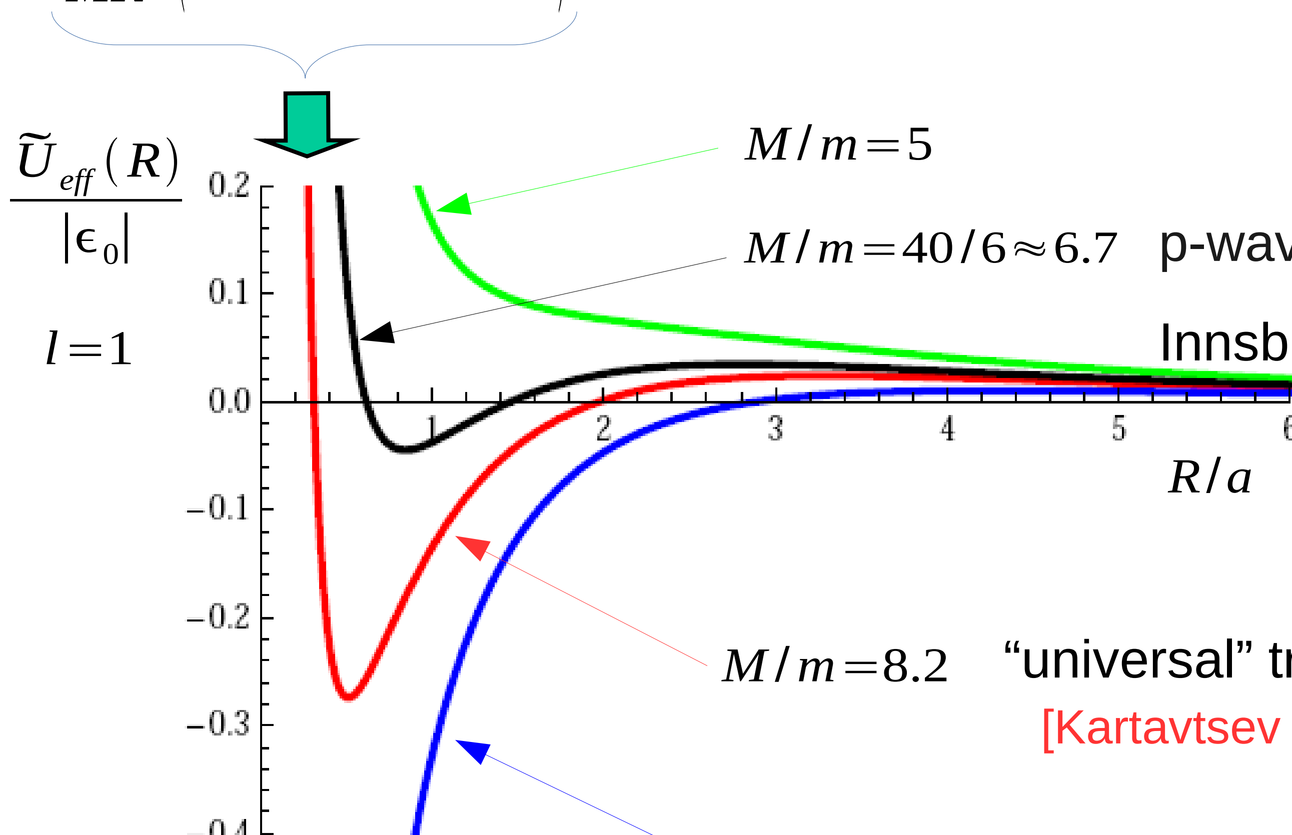
$$U_{eff}(R) \approx -\frac{\hbar^2}{2ma^2} = -|\epsilon_0|$$

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

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

$$\frac{\hbar^2}{MR^2}\left(l(l+1)-0.16\frac{M}{m}\right)$$

$$\tilde{U}_{eff}(R)=U_{eff}(R)+|\epsilon_0|+\frac{\hbar^2 l(l+1)}{MR^2}$$



$M/m=5$

$M/m=40/6\approx 6.7$ p-wave scattering resonance !

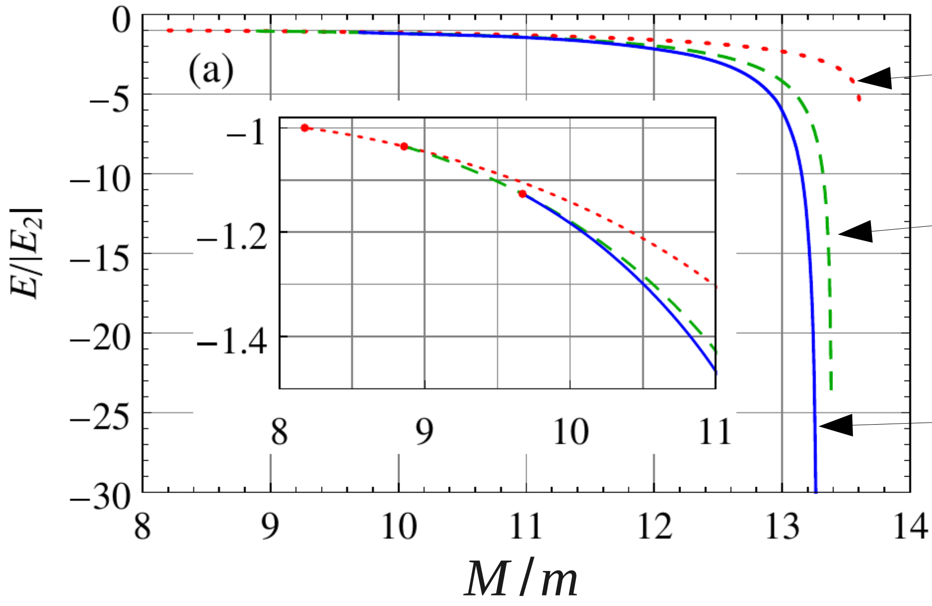
Innsbruck exp: [Jag et al'14]

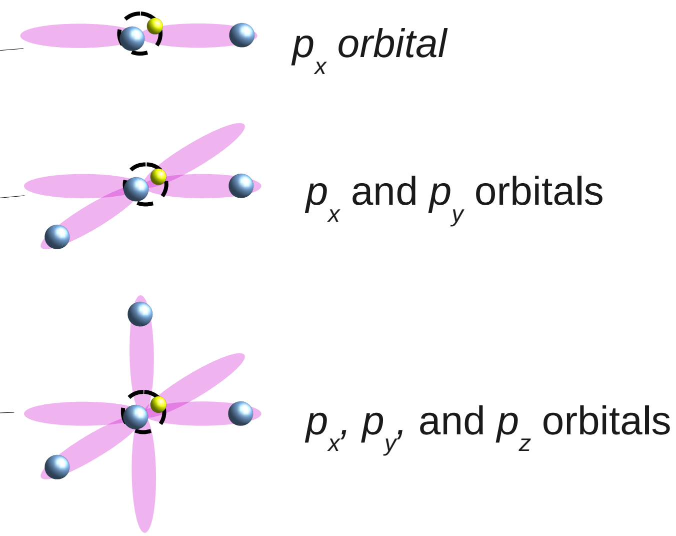
$M/m=8.2$ “universal” trimer state at threshold [Kartavtsev & Malykh'06]

$M/m>13.6$ many trimer (Efimov) states [Efimov'73]

3D trimer, tetramer, pentamer,...

	Symmetry L^{π}	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^+	8.862(1) Blume'12, Bazak&DSP'17	13.384 Castin,Mora&Pricoupenko'10
4+1 pentamer	0^-	9.672(6) Bazak&DSP'17	13.279(2) Bazak&DSP'17
N+1-mer	?	?	?

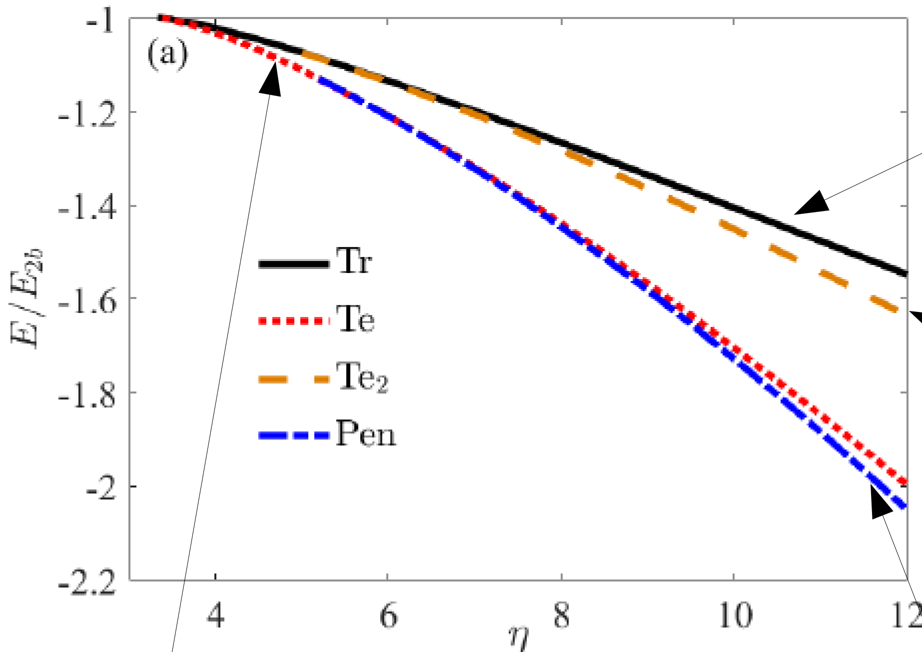




pentamer = closed *p*-shell

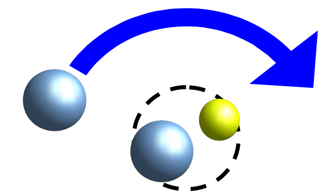
2D trimer, tetramer, pentamer...

[Liu & Peng & Cui'22]



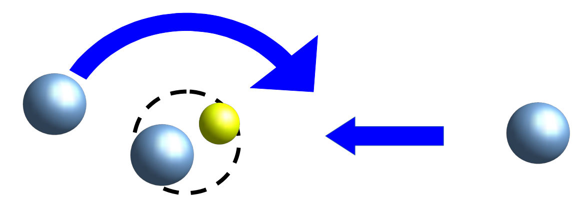
L=1 trimer $(M/m)_c = 3.33$

[Pricoupenko & Pedri'10]



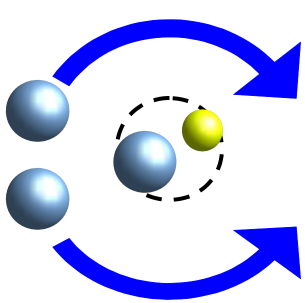
L=1 tetramer $(M/m)_c^{2D} = 5.0$

[Levinsen & Parish'13]



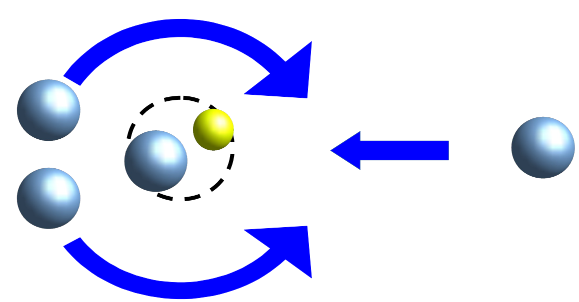
L=0 tetramer $(M/m)_c = 3.38$

[Liu & Peng & Cui'22]



L=0 pentamer $(M/m)_c = 5.14$

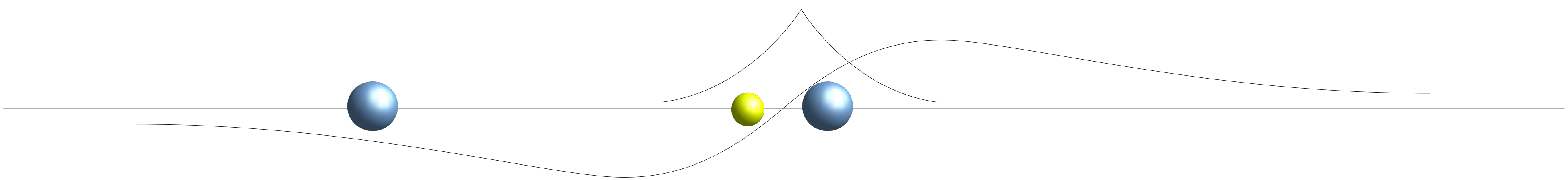
[Liu & Peng & Cui'22]



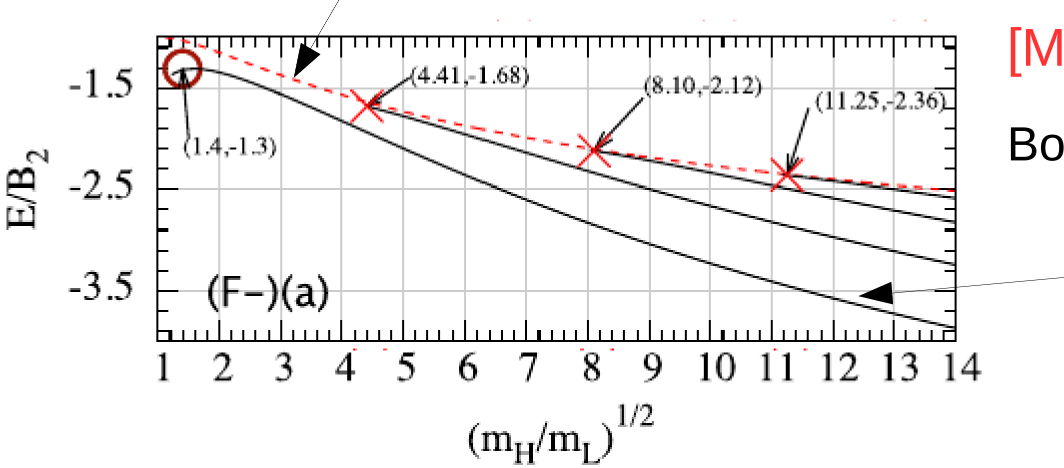
1D trimer, tetramer...

1D N+1 problem: no shell effects, no Efimov effect, “easy” calculations...

Ideal testbed for various few-body and many-body approaches!

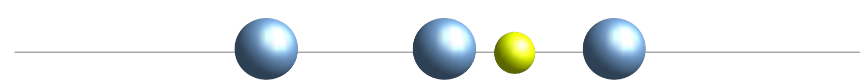


Odd-parity trimer for $M/m>1$ [Kartavtsev & Malykh & Sofianos'09]



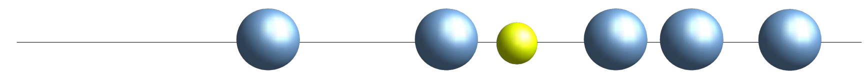
[Mehta'14]

Born-Oppenheimer treatment of the tetramer



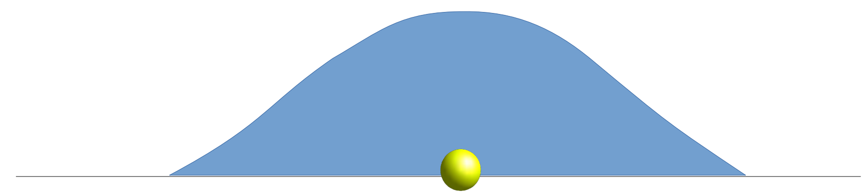
Outline

- Exact Skorniakov & Ter-Martirosian (STM) calculations for $N \leq 5$

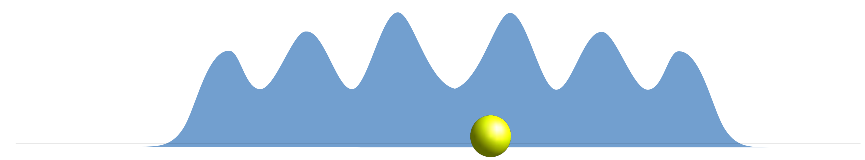


- Mean-field theory for $N \to \infty$

  - Thomas-Fermi for the heavies



  - Hartree-Fock for the heavies



- Applying MF for $N \leq 5$
  - trying to understand...
  - trying to improve...

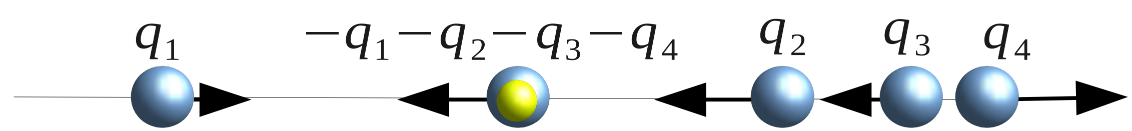
- Summary/Outlook

STM equation

$$\left[-\frac{1}{2m}\frac{\partial^2}{\partial x^2} - \sum_{i=1}^{N}\frac{1}{2M}\frac{\partial^2}{\partial x_i^2} + g\sum_{i=1}^{N}\delta(x_i - x) - E\right]\Psi(x_1,\ldots,x_{N-1},x_N,x) = 0$$

$$g = -1/(m_r a) < 0 \qquad E_{1+1} = -1/(2m_r a^2) \qquad m_r = Mm/(M+m)$$

$$\Psi(x_1,\ldots,x_{N-1},x_N,x=x_N) \xrightarrow{\text{Fourier}} F(q_1,\ldots,q_{N-1},q_N) \xrightarrow{q_N = -\sum_{i=1}^{N-1} q_i} F(q_1,\ldots,q_{N-1})$$



Skorniakov and Ter-Martirosian equation (STM) [L.Pricoupenko'11, A.Pricoupenko&DSP'19]:

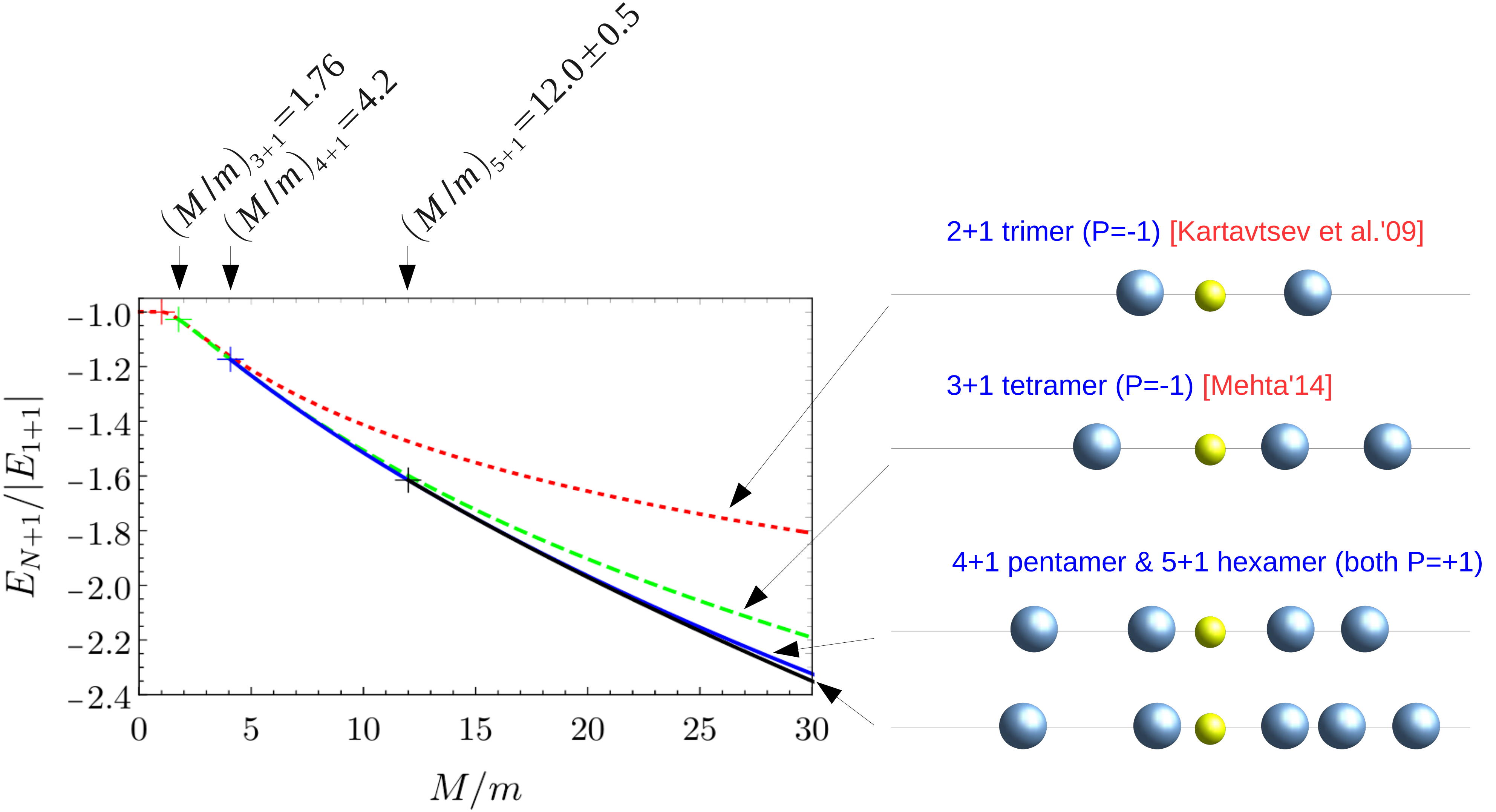
$$\left[\frac{a}{2} - \frac{1}{2\kappa(q_1,\ldots,q_{N-1})}\right]F(q_1,\ldots,q_{N-1}) = -\int\frac{dp}{2\pi}\frac{\sum_{j=1}^{N-1}F(q_1,\ldots,q_{j-1},p,q_{j+1},\ldots,q_{N-1})}{\kappa^2(q_1,\ldots,q_{N-1}) + (p + \frac{m_r}{m}\sum_{i=1}^{N-1}q_i)^2}$$

$$\kappa(q_1,\ldots q_{N-1}) = \sqrt{-2m_r E + \frac{m_r}{M+m}(\sum_{i=1}^{N-1}q_i)^2 + \frac{m_r}{M}\sum_{i=1}^{N-1}q_i^2}$$

STM:

- natural account of zero-range interactions
- removes one relative coordinate (1+1 dimer problem is analytic)
- ...

STM results



$(M/m)_{3+1}$=1.76
$(M/m)_{4+1}$=4.2
$(M/m)_{5+1}$=12.0±0.5
$E_{N+1}/|E_{1+1}|$
M/m
-1.0
-1.2
-1.4
-1.6
-1.8
-2.0
-2.2
-2.4
0
5
10
15
20
25
30
2+1 trimer (P=-1) [Kartavtsev et al.'09]
3+1 tetramer (P=-1) [Mehta'14]
4+1 pentamer & 5+1 hexamer (both P=+1)

Mean field #1 Thomas-Fermi

$$\Omega = \int [|\phi'(x)|^2/2m + gn(x)|\phi(x)|^2 + \pi^2 n^3(x)/6M - \epsilon|\phi(x)|^2 - \mu n(x)]\, dx$$

Mean field

Kinetic energy in the TF approximation

Lagrange multipliers

$$\int |\phi(x)|^2\, dx = 1$$

$$\int n(x)\, dx = N$$

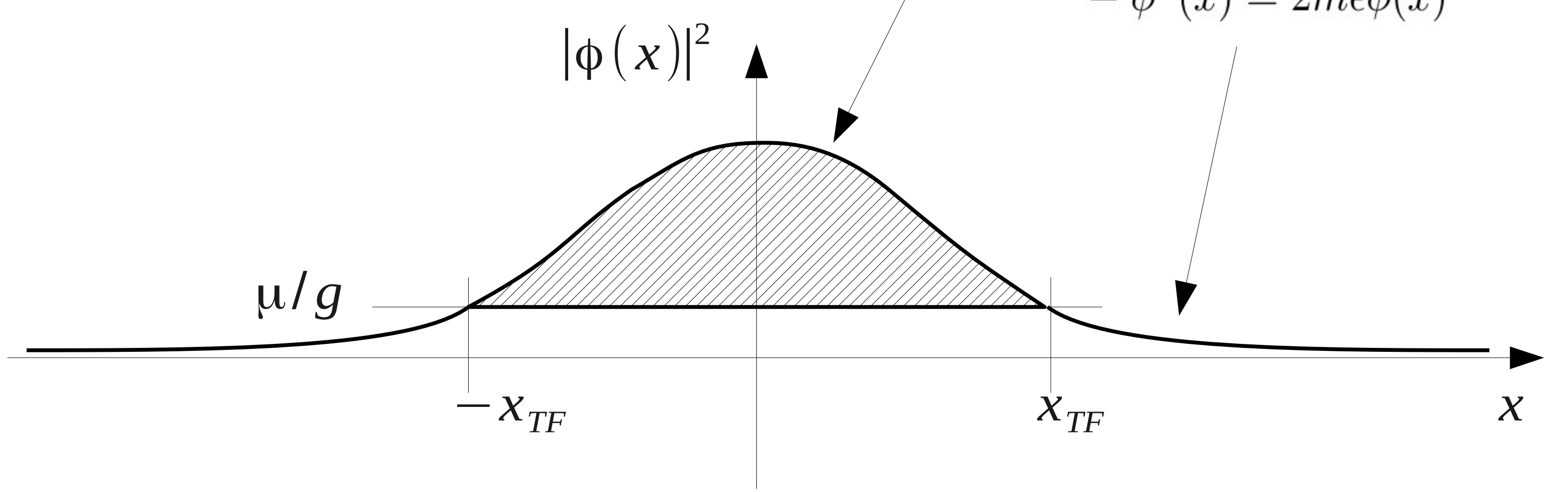
Minimization with respect to $n(x)$ →

$$n(x) = \begin{cases} \sqrt{-2Mg[|\phi(x)|^2 - \mu/g]}/\pi, & |\phi(x)|^2 > \mu/g \\ 0, & |\phi(x)|^2 \le \mu/g \end{cases}$$

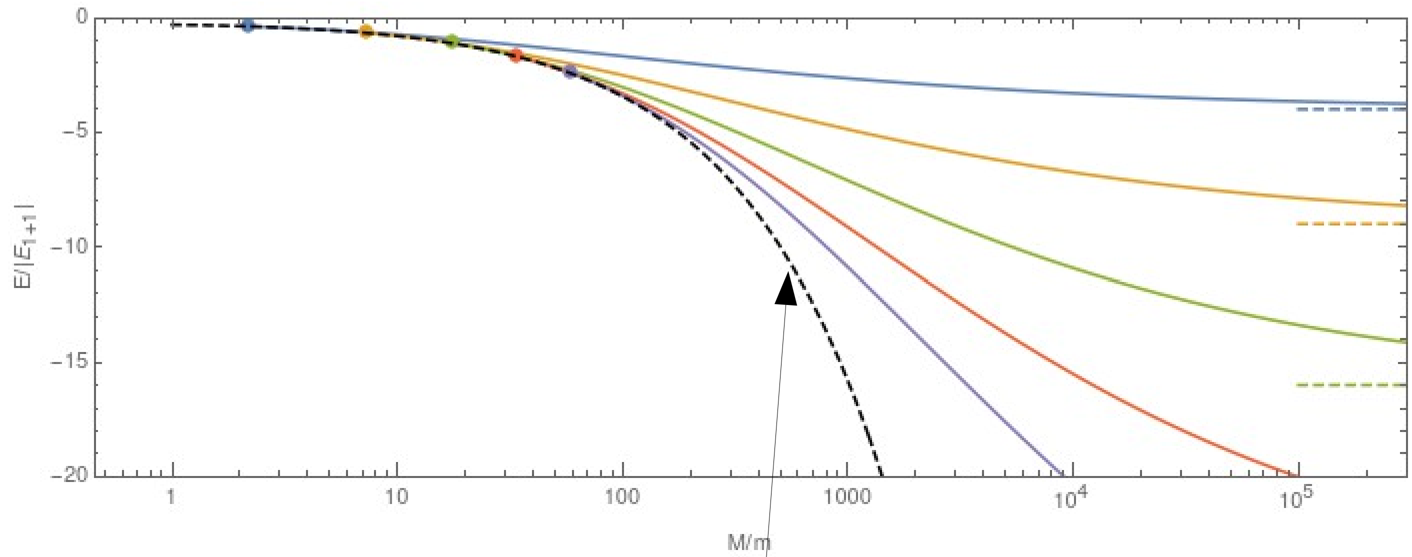
Minimization with respect to $\phi(x)$ →

$$-\phi''(x) - \frac{\sqrt{-8Mm^2g^3}}{\pi}\sqrt{|\phi(x)|^2 - \mu/g}\,\phi(x) = 2m\epsilon\phi(x)$$

$$-\phi''(x) = 2m\epsilon\phi(x)$$



Mean field #1 Thomas-Fermi



$E_{N+1}/|E_{1+1}| \approx -N^2$

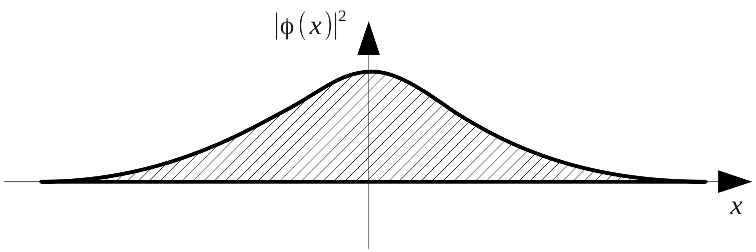
Light atom bound in the potential $N g \delta(x)$

N+1 cluster binds at

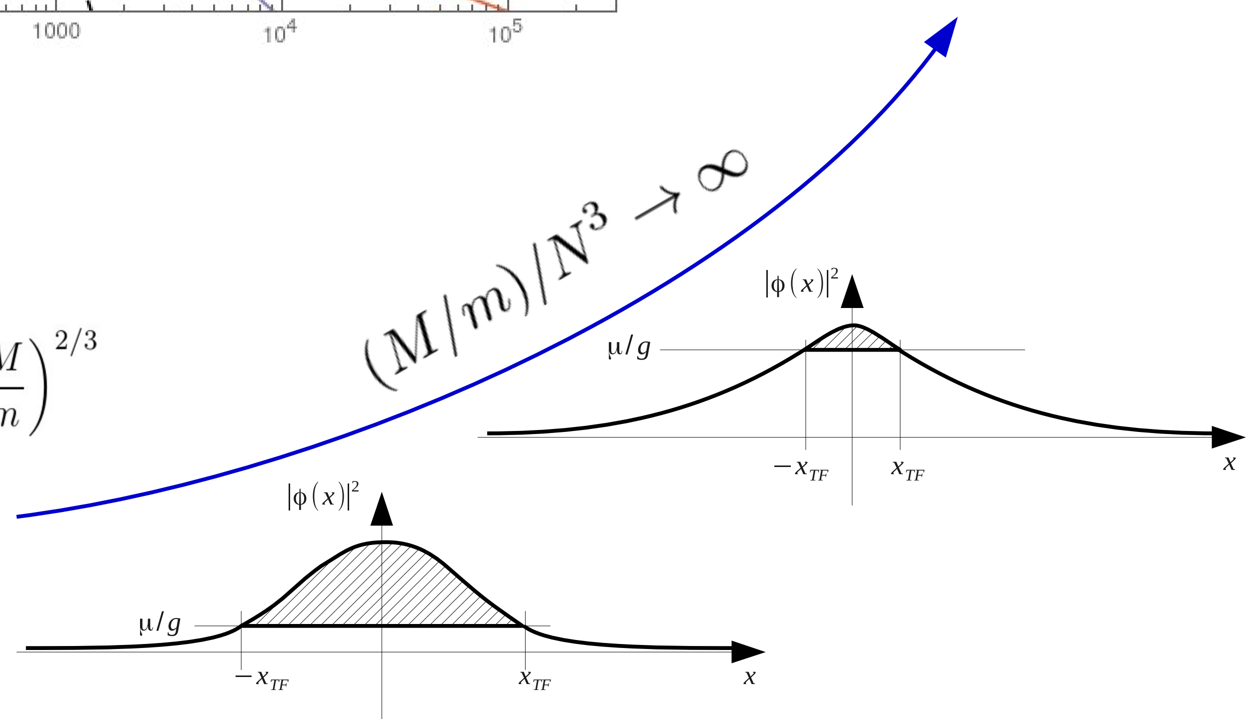
$$(M/m)/N^3 = \pi^2/36$$

$$E = \epsilon + \int \frac{\pi^2 n^3(x)}{6M}\, dx = -\frac{mg^2}{30} N^2 = -\frac{mg^2}{30}\left(\frac{36}{\pi^2}\frac{M}{m}\right)^{2/3}$$

$$\phi(x) = \frac{-3\pi\epsilon}{\sqrt{-8Mg^3}} \frac{1}{\cosh^2(\sqrt{-m\epsilon/2}x)}$$



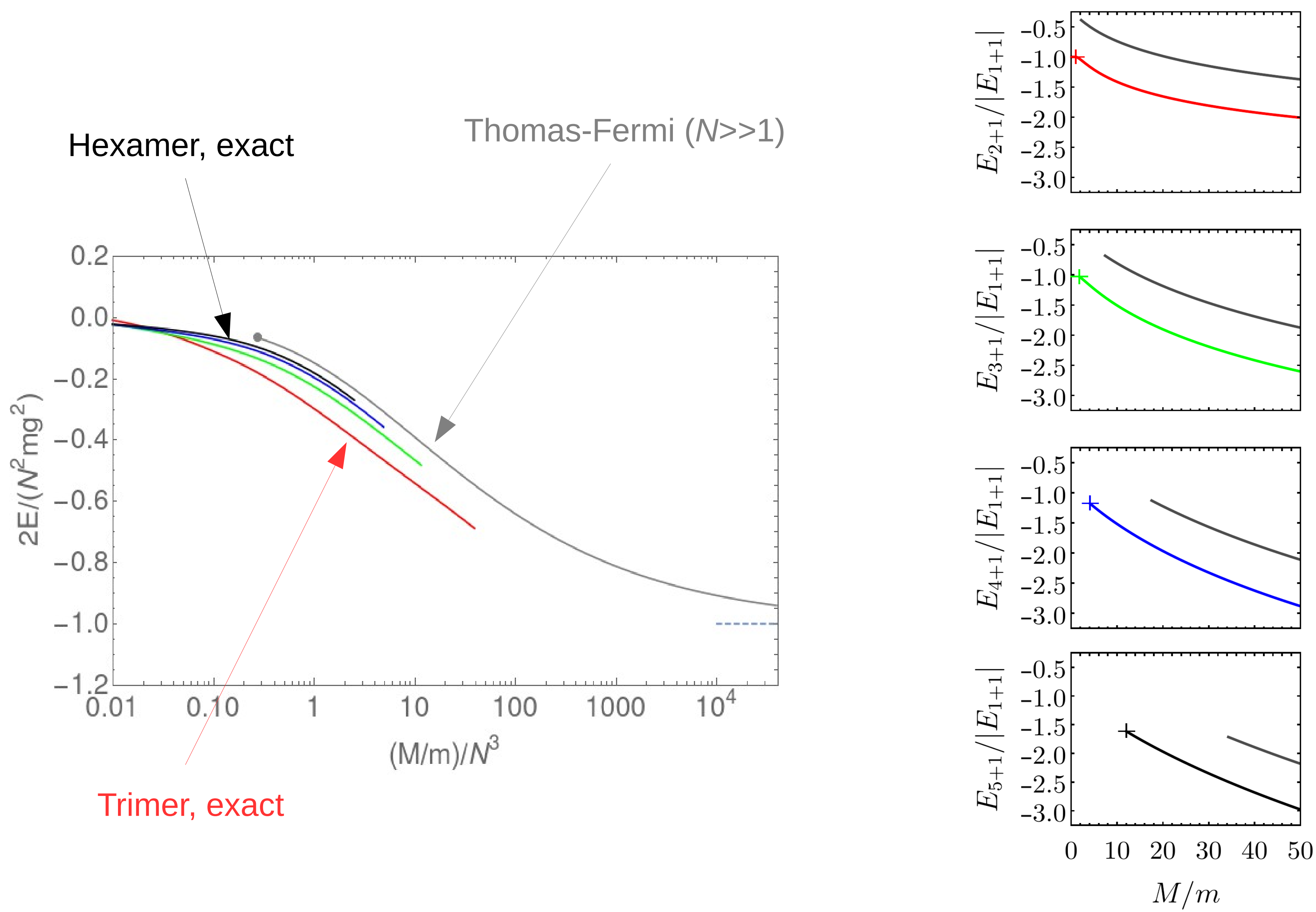
$\mu/g = 0 \qquad x_{TF} = \infty$



$(M/m)/N^3$ controls everything: $E_{N+1}/mg^2 = N^2 f[(M/m)/N^3]$

Typical lengthscales ~a/*N* → validity condition: *N*>>1

Thomas-Fermi VS exact



Who is (mostly) responsible for the discrepancy: the MF treatment of the interaction or the local TF approximation for the kinetic energy?

Mean field #2 Hartree-Fock

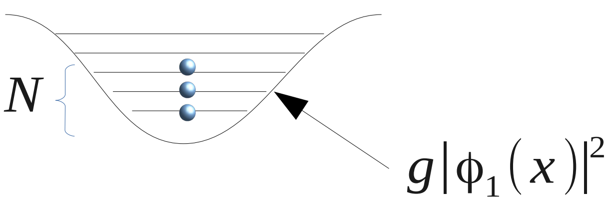
$$H = \int \left(-\frac{\hat{\Psi}_x^\dagger \partial_x^2 \hat{\Psi}_x}{2M} - \frac{\hat{\phi}_x^\dagger \partial_x^2 \hat{\phi}_x}{2m} + g \hat{\Psi}_x^\dagger \hat{\phi}_x^\dagger \hat{\Psi}_x \hat{\phi}_x \right) dx$$

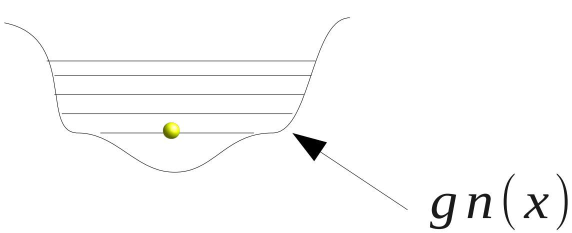
Variational ansatz

$$|v\rangle = \int dx \phi_1(x) \hat{\phi}_x^\dagger \int dx_1 ... dx_N \frac{\det[\Psi_\nu(x_\eta)]}{\sqrt{N!}} \prod_{\eta=1}^{N} \hat{\Psi}_{x_\eta}^\dagger |0\rangle$$

Minimization with respect to the orbitals →

$$-\partial_x^2 \phi_1(x)/2m + g n(x) \phi_1(x) = \epsilon_1 \phi_1(x),$$
$$-\partial_x^2 \Psi_\nu(x)/2M + g|\phi_1(x)|^2 \Psi_\nu(x) = E_\nu \Psi_\nu(x)$$
$$n(x) = \sum_{\nu=1}^{N} |\Psi_\nu(x)|^2$$



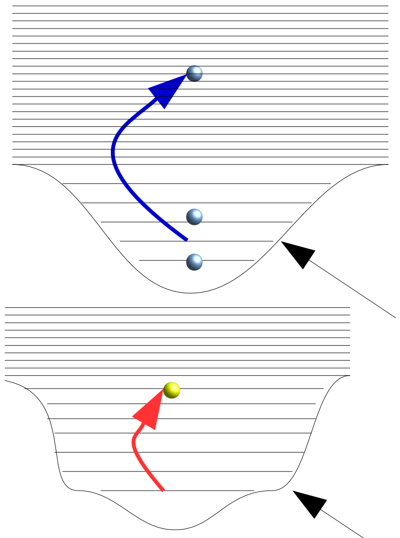


$$E_{N+1} = \langle v| H |v\rangle = \epsilon_1 + \sum_{\nu=1}^{N} E_\nu - g \int |\phi_1(x)|^2 n(x)\, dx$$

Very similar energies as in the mean-field Thomas-Fermi case!

TF is good enough?

"Improved" Hartree-Fock



$$-\partial_x^2\phi_1(x)/2m + gn(x)\phi_1(x) = \epsilon_1\phi_1(x),$$
$$-\partial_x^2\Psi_\nu(x)/2M + g|\phi_1(x)|^2\Psi_\nu(x) = E_\nu\Psi_\nu(x)$$

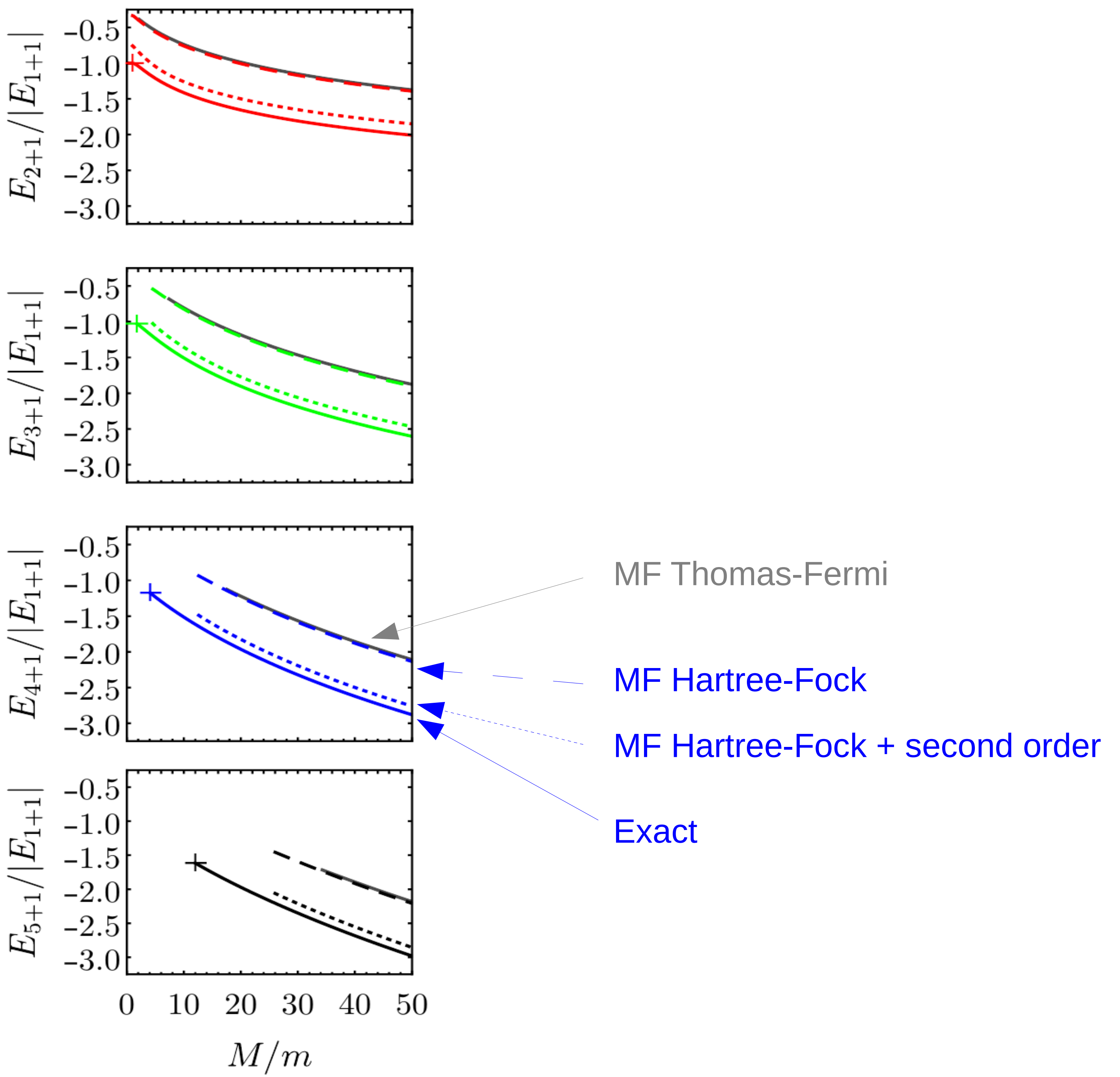
Orthonormal single-particle basis

Hamiltonian couples $|v\rangle$ with states $|v'\rangle$ where the light atom and one of the heavy atoms are excited

$$E_{N+1} = \langle v|\,H\,|v\rangle + \sum_{v'\neq v} \frac{|\,\langle v'|\,H\,|v\rangle\,|^2}{E_v^{(0)} - E_{v'}^{(0)}}$$

Computationally cheap, further corrections are more difficult

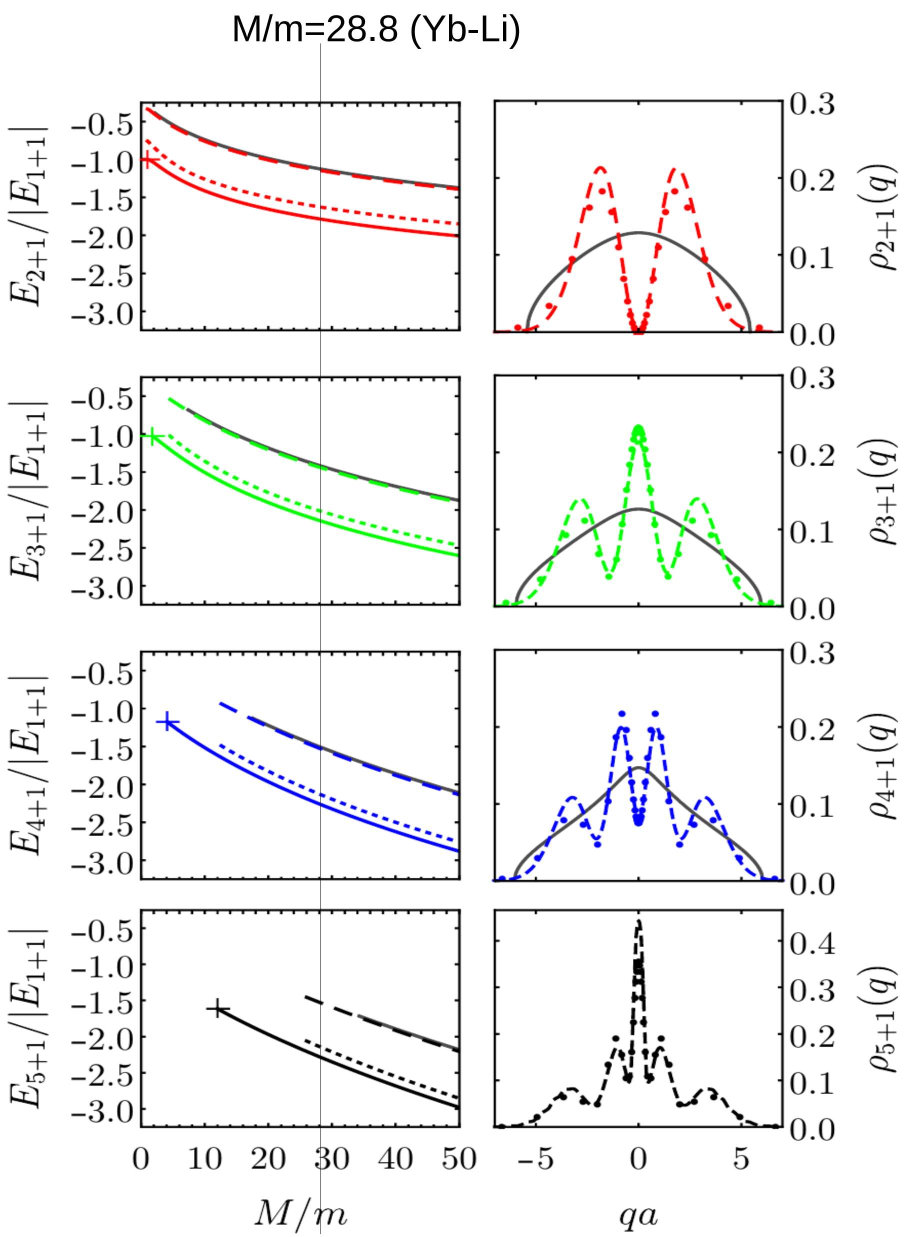
Results

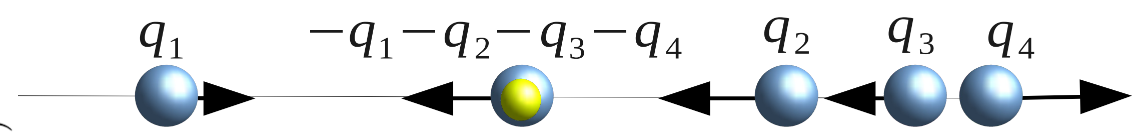


$E_{2+1}/|E_{1+1}|$
$E_{3+1}/|E_{1+1}|$
$E_{4+1}/|E_{1+1}|$
$E_{5+1}/|E_{1+1}|$
-0.5
-1.0
-1.5
-2.0
-2.5
-3.0
0
10
20
30
40
50
M/m
MF Thomas-Fermi
MF Hartree-Fock
MF Hartree-Fock + second order
Exact

Momentum correlations

$\Psi(x_1, ..., x_{N-1}, x_N, x = x_N)$ —Fourier→ $F(q_1, ..., q_{N-1}, q_N)$ —$q_N = -\sum_{i=1}^{N-1} q_i$→ $F(q_1, ..., q_{N-1})$





Exact (STM)

Hartree-Fock $|v\rangle$

$\Psi(x_1, ..., x_{N-1}, x_N, x)$

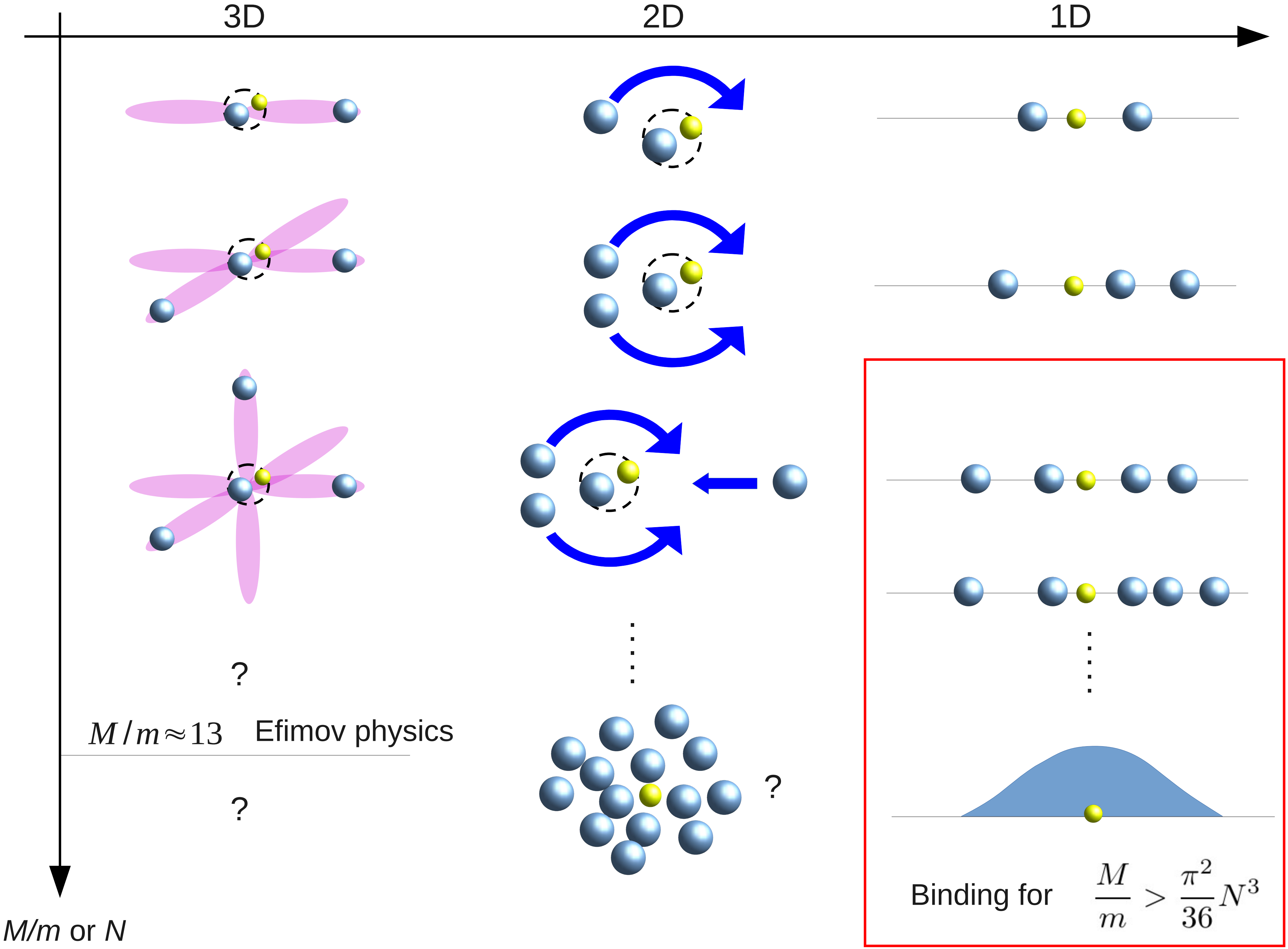
$F(q_1, ..., q_{N-1})$

Thomas-Fermi

$$\rho_{N+1}(q) = \int |F(q, q_2, ..., q_{N-1})|^2 \, dq_2 ... dq_{N-1}$$

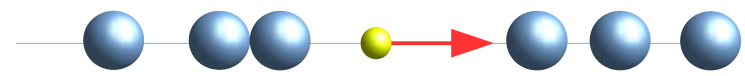
Momentum distribution of N-1 heavy fermions once the heavy-light pair is removed from the system (photoassociation)

Summary and outlook


3D
2D
1D
?
$M/m \approx 13$ Efimov physics
?
?
Binding for $\frac{M}{m} > \frac{\pi^2}{36} N^3$
M/m or N

Related (1D) research

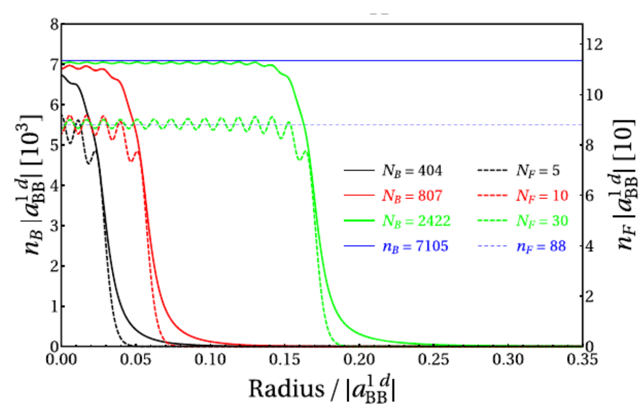
1D polaron or impurity (Fermi, Bose, solvable or not) [lots of literature]



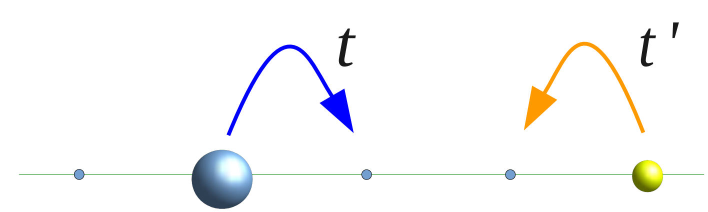
Self-bound Bose–Fermi liquids in lower dimensions

Debraj Rakshit[1,2], Tomasz Karpiuk[3], Paweł Zin[4], Mirosław Brewczyk[3], Maciej Lewenstein[2,5] and Mariusz Gajda[1]

Mean field, Hartree-Fock...



1D lattice mixtures with asymmetric tunnelling (many-body phases)
DMRG
[Burovski-Orso-Jolicoeur-Roux'09-11, Dalmonte-Roschilde et al.'12]



Thank you!