Heavy-light *N*+1 clusters of two-dimensional fermions

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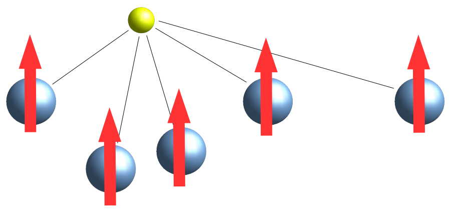
arXiv: 2310.11330

(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

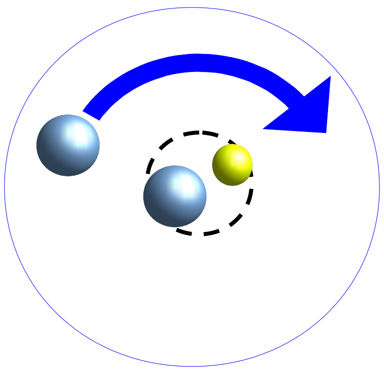
Attractive exchange potential of the light atom ~1/m

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

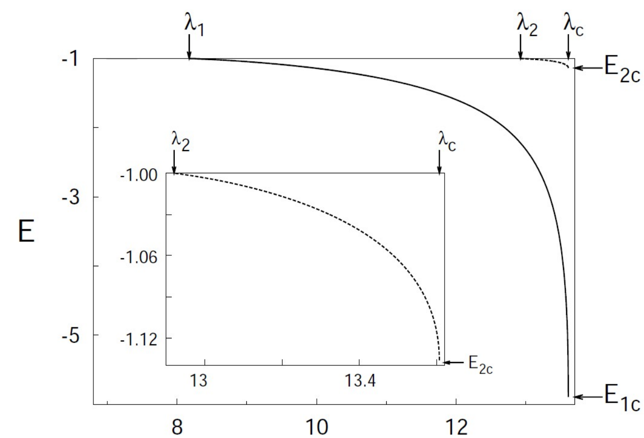
- space dimension D
- number of heavy atoms N
- mass ratio M/m
- dimer size a (can be used as the length unit)

3D 2+1-trimer

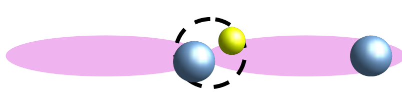
Emergence of a trimer state for M/m>8.2 [Kartavtsev & Malykh'2006]

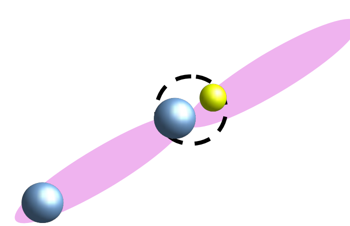


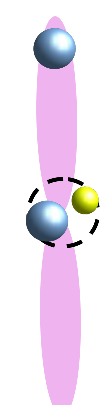
- *M/m*<8.2 p-wave atom-dimer scattering resonance
- *M/m*>8.2 (non-efimovian) trimer state with L=1



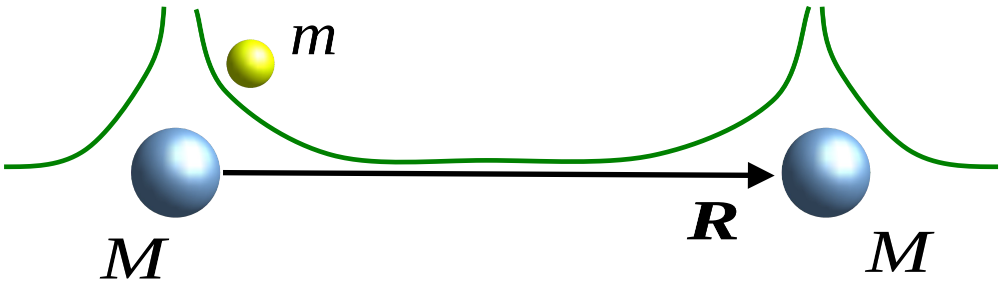
p_x, p_y, and p_z orbitals:

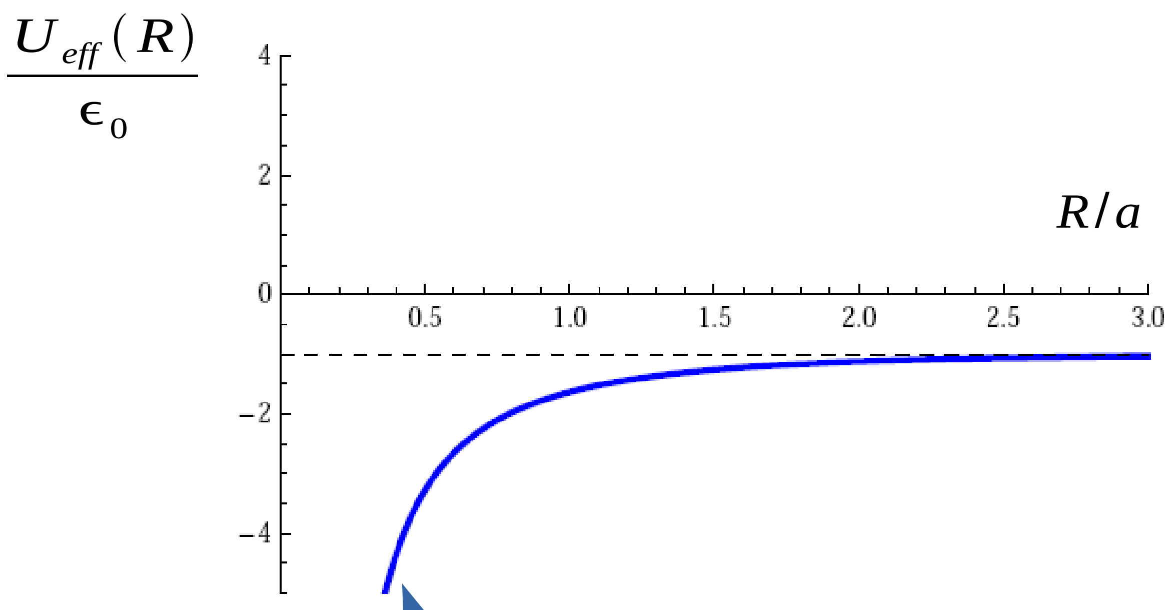






Born-Oppenheimer picture

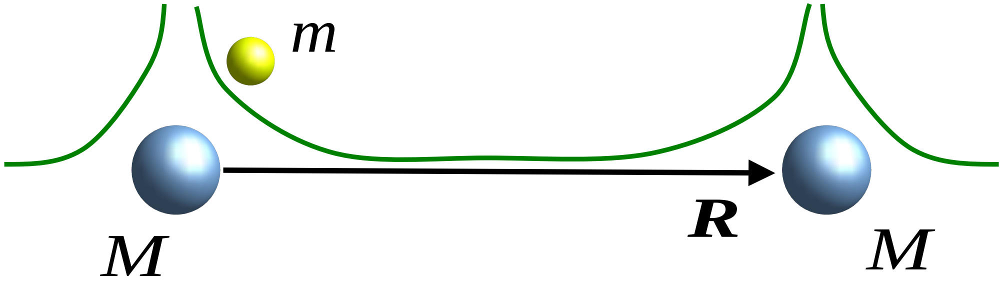




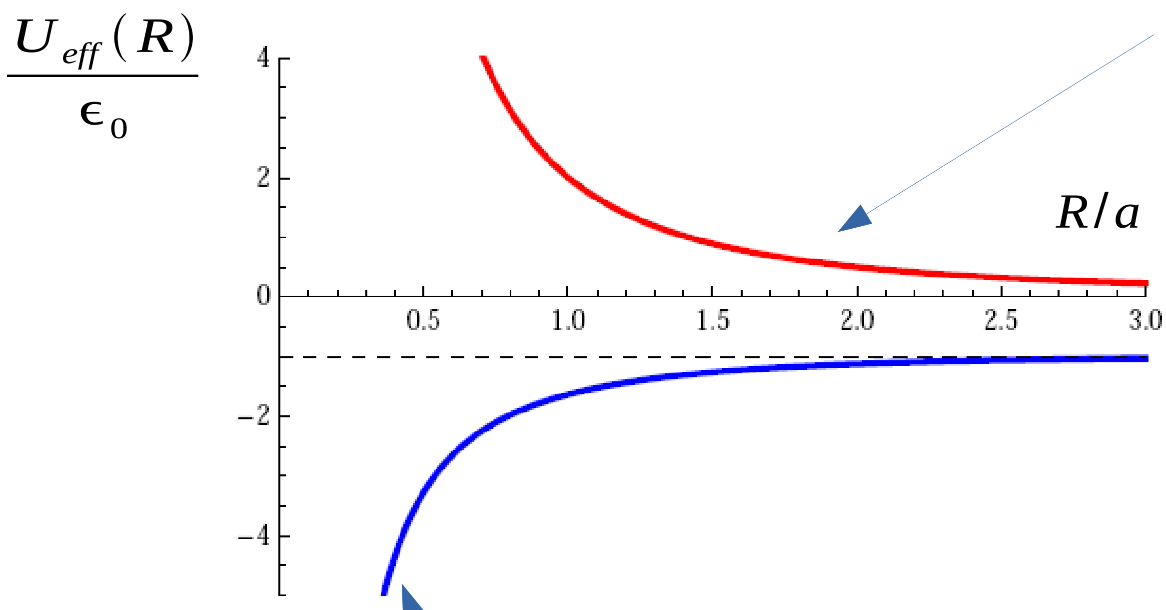
$$U_{eff}(R) \approx -\frac{\hbar^2}{2ma^2} = -|\epsilon_0|$$

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

Born-Oppenheimer picture



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



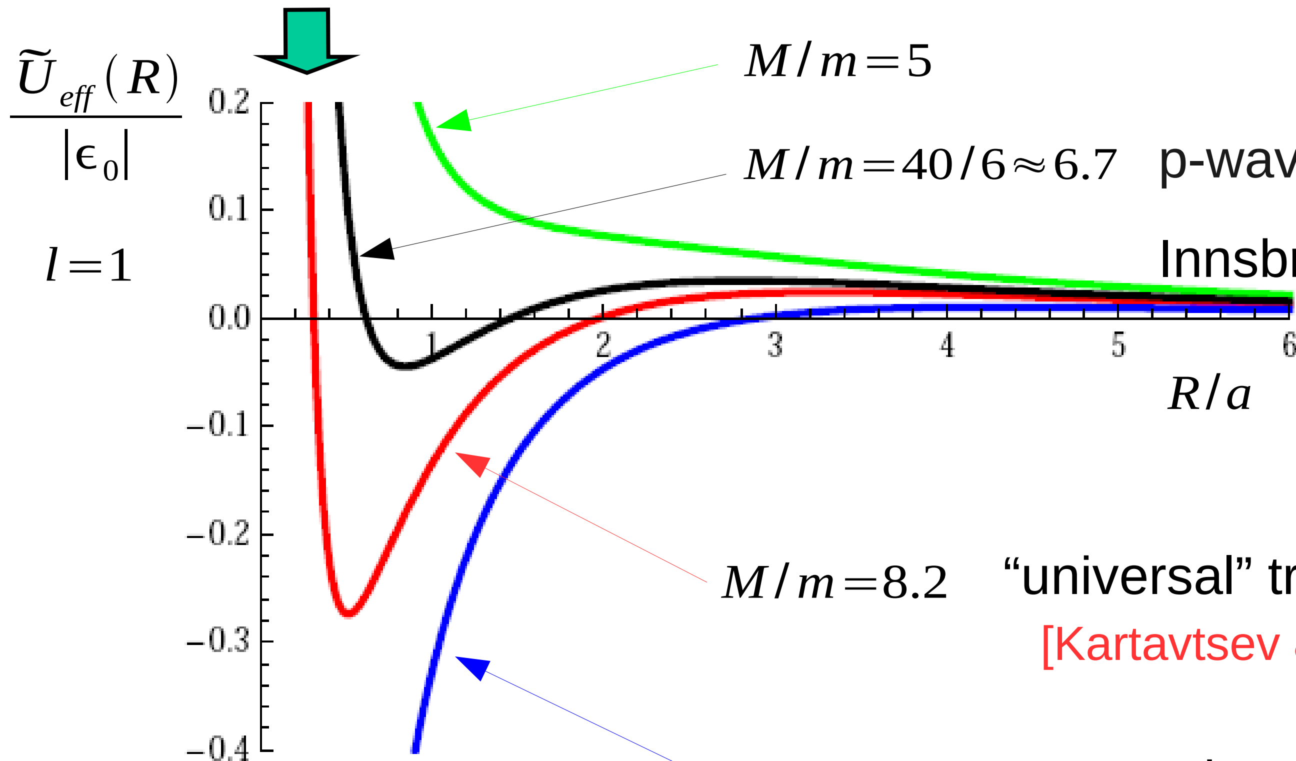
$$U_{eff}(R) \approx -\frac{\hbar^2}{2ma^2} = -|\epsilon_0|$$

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

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

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

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



$M/m=5$

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

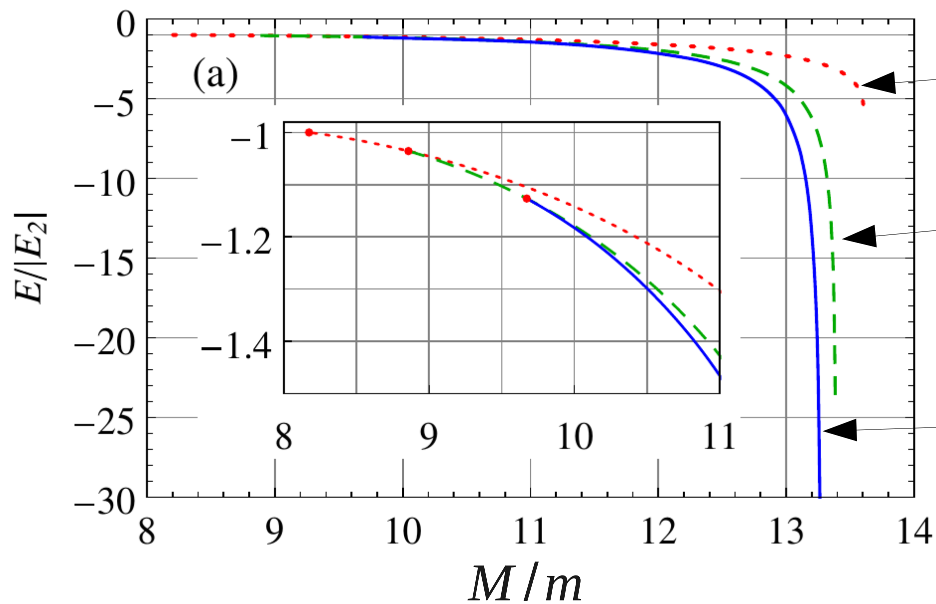
Innsbruck exp: [Jag et al'14]

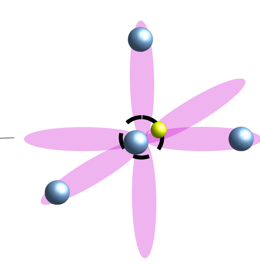
$M/m=8.2$ "universal" trimer state at threshold [Kartavtsev & Malykh'06]

$M/m>13.6$ 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

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

3D: $\tilde{U}_{eff}(R)=U_{eff}(R)+|\epsilon_0|+\frac{\hbar^2 l(l+1)}{MR^2}$ ⇒ $l=1\rightarrow(M/m)_c=8.2$

This is actually exact (not Born-Oppenheimer) number

different

2D: $\tilde{U}_{eff}(R)=U^{2D}_{eff}(R)+|\epsilon_0|+\frac{\hbar^2(l^2-1/4)}{MR^2}$ ⇒ Rough guess:

$$(M/m)^{2D}_c\approx\frac{l^2-1/4}{l(l+1)}(M/m)^{3D}_c=3.1$$

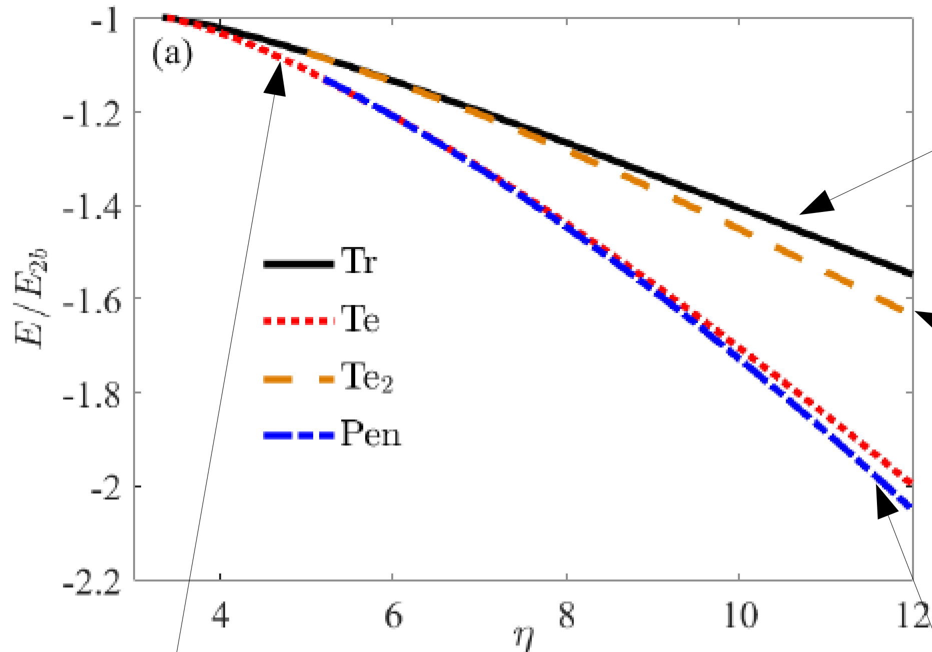
Exact ratio $(M/m)^{2D}_c=3.3$ [Pricoupenko & Pedri'10]

Centrifugal force weaker in 2D → p-wave resonance for smaller mass ratio!

… and in 1D $(M/m)^{1D}_c=1$ exactly!

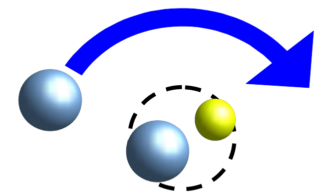
2D trimer, tetramer, pentamer...

[Liu & Peng & Cui'22]



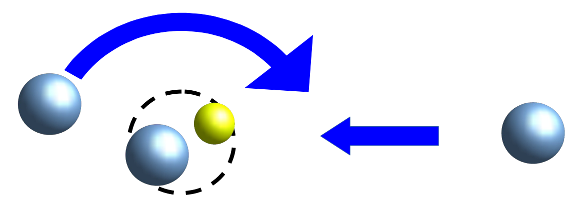
L=1 trimer $(M/m)_c = 3.33$

[Pricoupenko & Pedri'10]



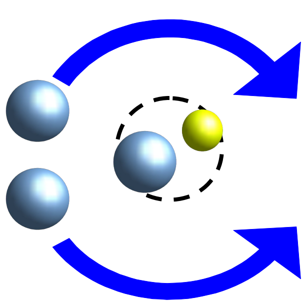
L=1 tetramer $(M/m)_c^{2D} = 5.0$

[Levinsen & Parish'13]



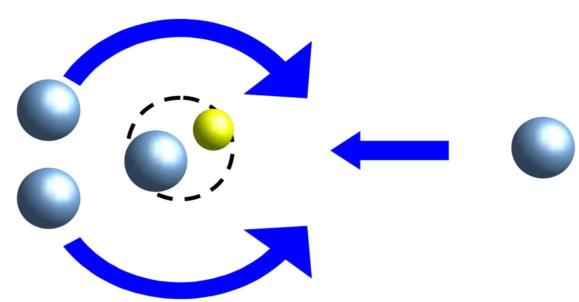
L=0 tetramer $(M/m)_c = 3.38$

[Liu & Peng & Cui'22]



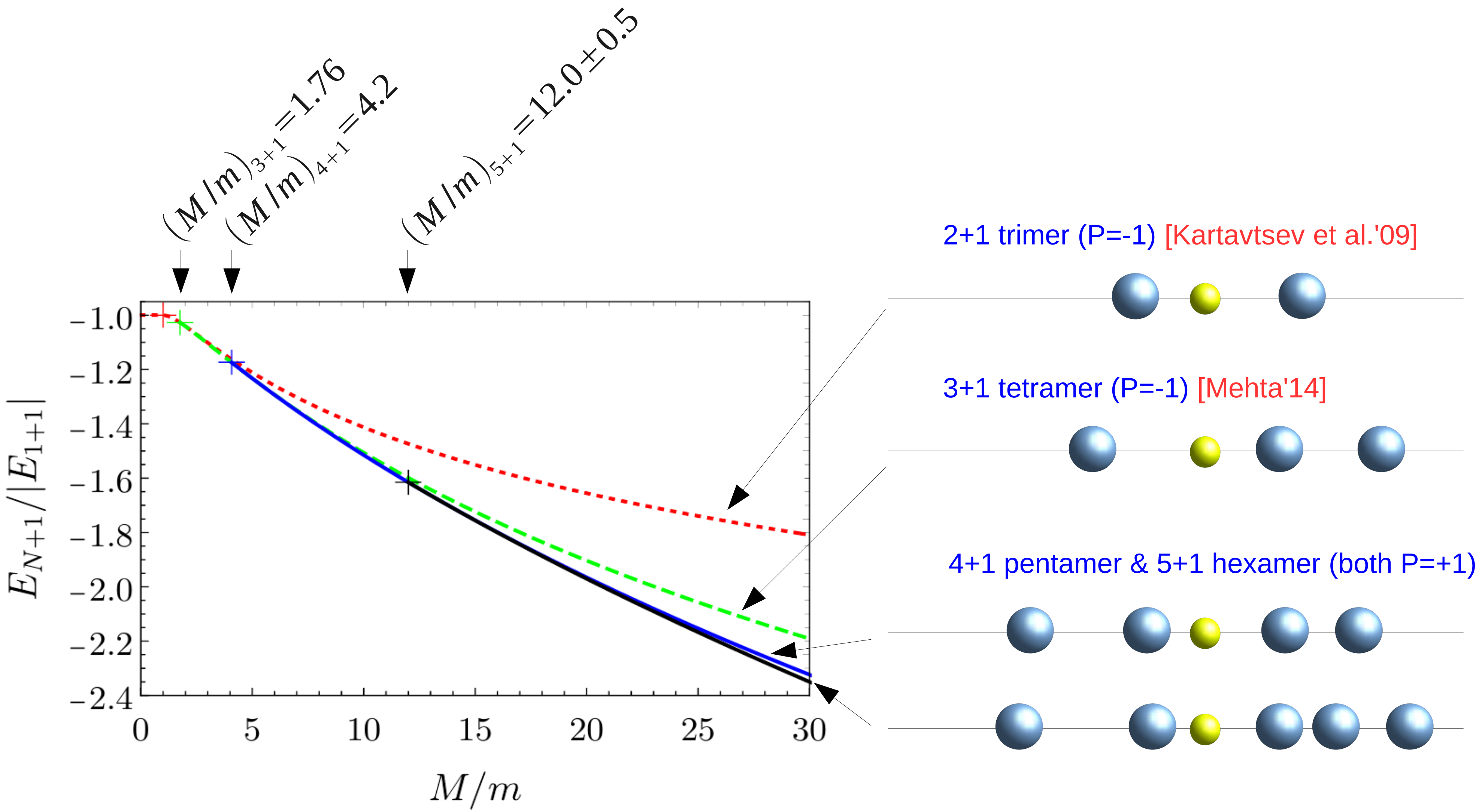
L=0 pentamer $(M/m)_c = 5.14$

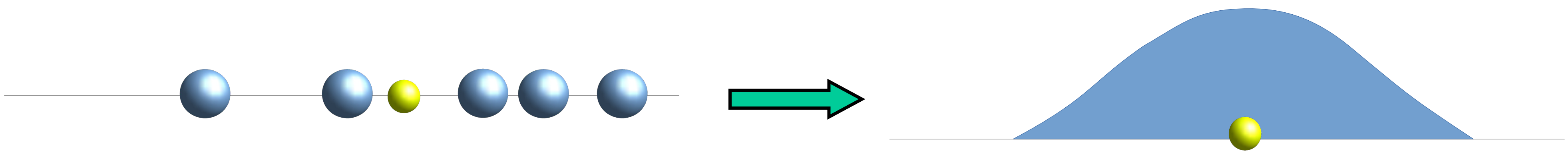
[Liu & Peng & Cui'22]



1D trimer, tetramer...(exact)

A. Tononi, J. Givois, DSP, Phys. Rev. A **106**, L011302 (2022)





$N \sim 1$ $\qquad$ $N \to \infty$

MF density functional (grand potential):

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

Mean field

Kinetic energy in the TF approximation

Lagrange multipliers

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

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

Rescaled grand potential:

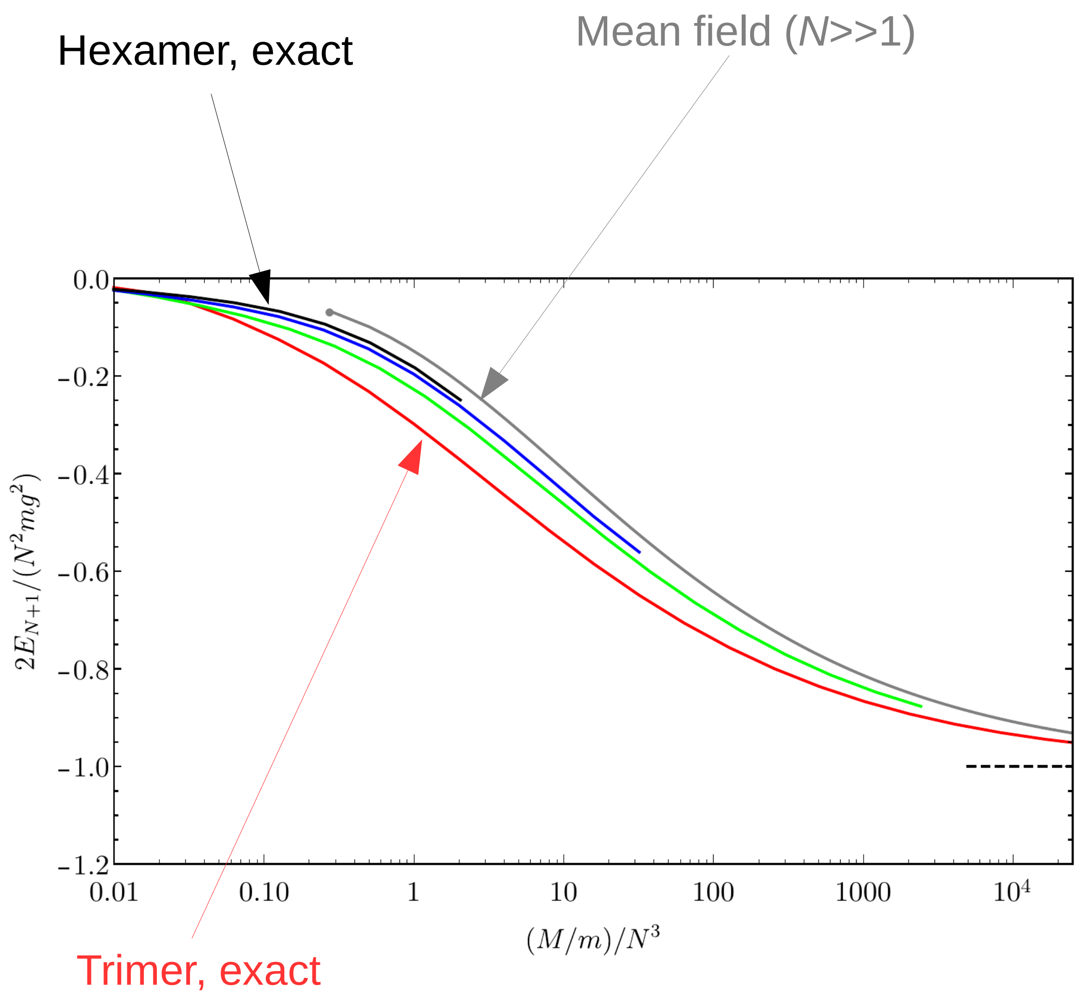
$$\frac{\Omega}{2mg^2N^2} = \int [|\tilde{\phi}'(u)|^2 - \tilde{n}(u)|\tilde{\phi}(u)|^2 + \alpha\tilde{n}^3(x) - \tilde{\epsilon}|\tilde{\phi}(u)|^2 - \tilde{\mu}\tilde{n}(u)]\, du$$

$$\int |\tilde{\phi}(u)|^2\, du = 1$$

$$\int \tilde{n}(u)\, du = 1$$

$$\alpha = \frac{\pi^2}{3}\frac{m}{M}N^3$$ = single control parameter!

Mean field VS exact



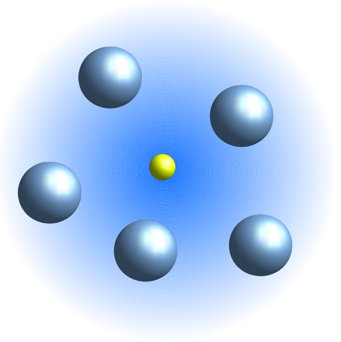
1D main conclusions:

- MF works fine, controlled by single parameter
- Thomas-Fermi → Hartree-Fock → hardly improves energy, but predicts structure of the wave function, parity...

More details: Tononi, Givois, DSP (2022) and Givois, Tononi, and DSP (2023)

2D N+1 clusters:

Mean field



Mean field + Thomas-Fermi assumptions

$$\hat{H} = \int \left(-\frac{\hat{\Psi}^\dagger_{\mathbf{r}} \nabla^2_{\mathbf{r}} \hat{\Psi}_{\mathbf{r}}}{2M} - \frac{\hat{\phi}^\dagger_{\mathbf{r}} \nabla^2_{\mathbf{r}} \hat{\phi}_{\mathbf{r}}}{2m} + g \hat{\Psi}^\dagger_{\mathbf{r}} \hat{\phi}^\dagger_{\mathbf{r}} \hat{\Psi}_{\mathbf{r}} \hat{\phi}_{\mathbf{r}} \right) d^2 r$$

$\phi(\mathbf{r})$ - light-atom wave function: $\int |\phi(\mathbf{r})|^2 d^2 r = 1$

$N n(\mathbf{r})$ - heavy-atom density: $\int n(\mathbf{r}) d^2 r = 1$

$$E = \frac{1}{2m} \int [|\nabla \phi(\mathbf{r})|^2 + \frac{\alpha}{2} n^2(\mathbf{r}) + \gamma n(\mathbf{r}) |\phi(\mathbf{r})|^2] d^2 r$$

$$\alpha = 4\pi \frac{m}{M} N^2$$

$$\gamma = 2mgN < 0$$

Thomas-Fermi assumption: density changes slowly on mean interparticle distance

Mean-field assumption:

$$\frac{mM}{M+m} |g| \ll 1$$

For $|\gamma| \sim 1$ and $\alpha \sim 1$ both TF and MF validity conditions are equivalent to: $N \gg 1$

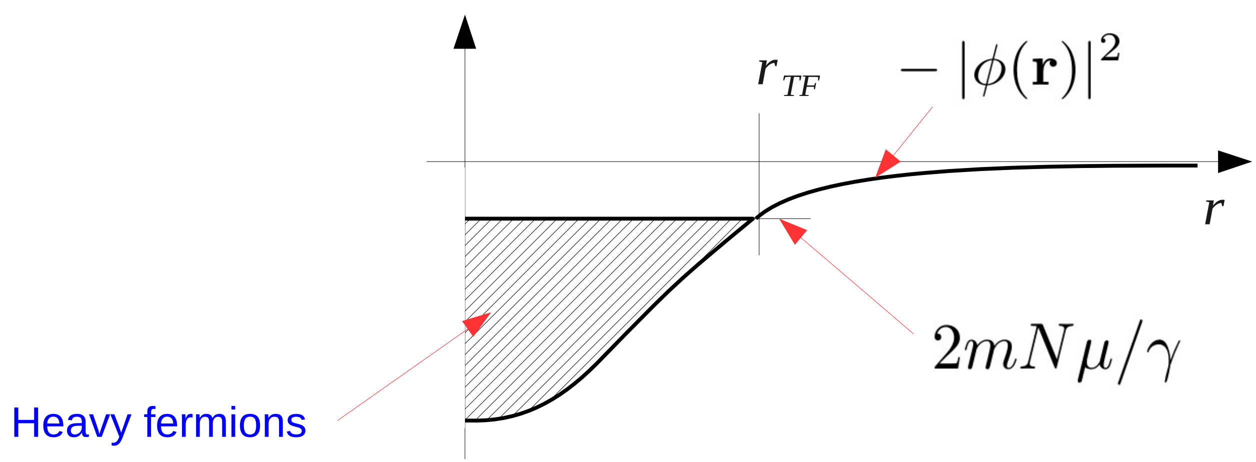
Mean field + Thomas-Fermi assumptions

$$E = \frac{1}{2m}\int [|\nabla\phi(\mathbf{r})|^2 + \frac{\alpha}{2} n^2(\mathbf{r}) + \gamma n(\mathbf{r})|\phi(\mathbf{r})|^2] d^2 r \qquad \alpha = 4\pi \frac{m}{M} N^2 \qquad \gamma = 2mgN < 0$$

$$\Omega = E - \int [\mu N n(\mathbf{r}) + \epsilon |\phi(\mathbf{r})|^2] d^2 r$$

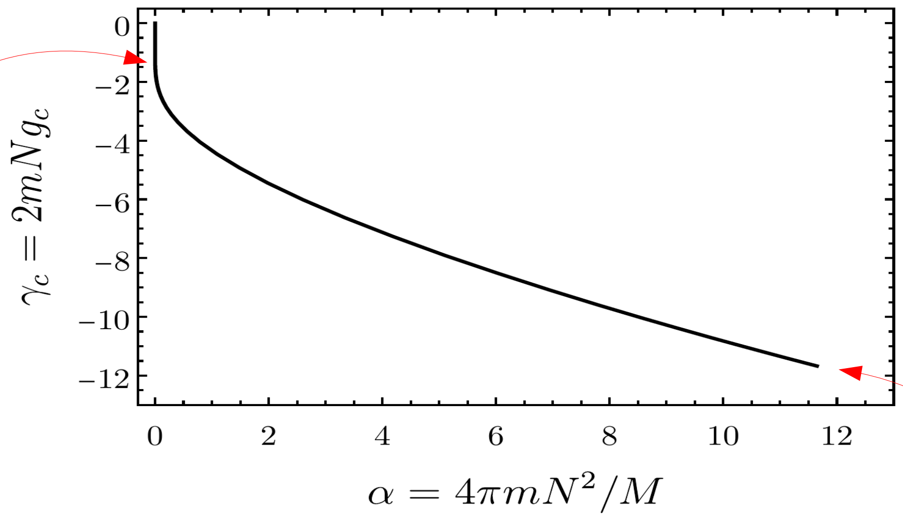
Minimization with respect to $\phi(\mathbf{r})$ → $-\nabla^2\phi(\mathbf{r}) + \gamma n(\mathbf{r})\phi(\mathbf{r}) = 2m\epsilon\phi(\mathbf{r})$

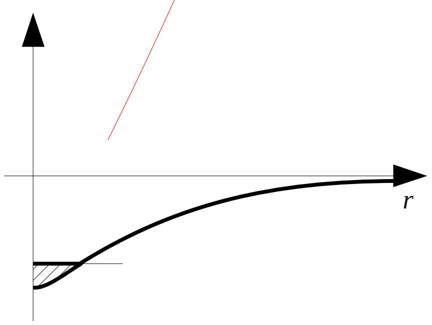
Minimization with respect to $n(\mathbf{r})$ → $n(\mathbf{r}) = -\frac{\gamma}{\alpha}\theta[|\phi(\mathbf{r})|^2 + 2mN\mu/\gamma]$

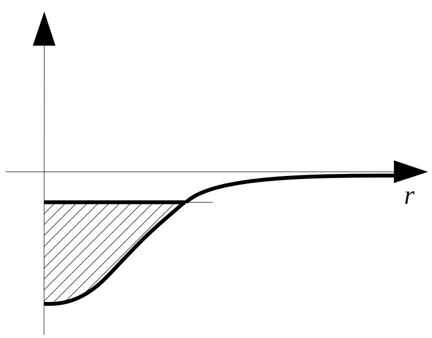


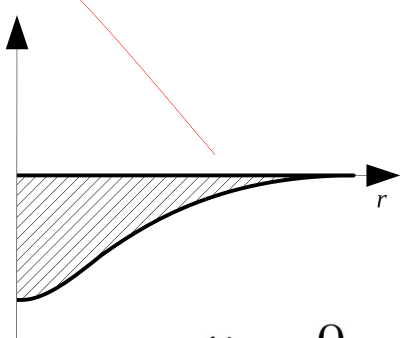
Mean field + Thomas-Fermi results

MF solution exists only for $\alpha < 2\pi C \approx 11.70$ i.e., $M/m > 1.074N^2$, and for a certain $\gamma = \gamma_c(\alpha)$









$\mu = 0$

Small α

$\gamma_c \approx 4\pi/\ln\alpha$

$$n(r) \approx \frac{4}{\alpha J_1(\sigma_1)\sigma_1} J_0\left(\sqrt{\frac{8\pi}{\alpha}}r\right)$$

$$-\nabla^2\phi(\mathbf{r}) + \gamma n(\mathbf{r})\phi(\mathbf{r}) = 2m\epsilon\phi(\mathbf{r})$$

$$n(\mathbf{r}) = -\frac{\gamma}{\alpha}\theta[|\phi(\mathbf{r})|^2 + 2mN\mu/\gamma]$$

$$\int |\phi(\mathbf{r})|^2 d^2r = 1 \qquad \int n(\mathbf{r}) d^2r = 1$$

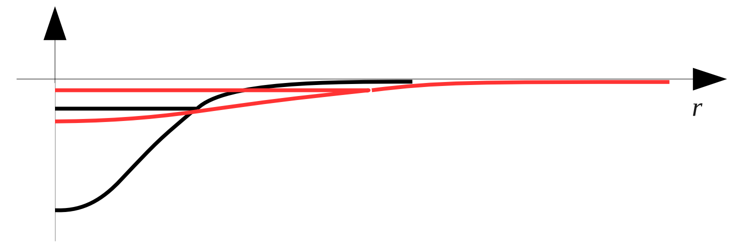
$$n(\mathbf{r}) = -\frac{\gamma}{\alpha}|\phi(\mathbf{r})|^2 \quad \alpha = -\gamma$$

$$-\nabla^2\phi + \gamma\phi^3 = 2m\epsilon\phi$$

Townes soliton [Chiao et al.'64, Bakkali-Hassani et al.'21, Chen&Hung'21]

Features/problems

- Scaling invariance



$$-\nabla^2\phi(\mathbf{r}) + \gamma n(\mathbf{r})\phi(\mathbf{r}) = 2m\epsilon\phi(\mathbf{r})$$

$$n(\mathbf{r}) = -\frac{\gamma}{\alpha}\theta[|\phi(\mathbf{r})|^2 + 2mN\mu/\gamma]$$

$$\int |\phi(\mathbf{r})|^2 d^2r = 1 \qquad \int n(\mathbf{r}) d^2r = 1$$

$\phi_0(r)$, $n_0(r)$, ϵ_0, μ_0 → $\phi_0(r/R)/R$, $n_0(r/R)/R^2$, $\epsilon = \epsilon_0/R^2$, $\mu = \mu_0/R^2$

If this set is a solution, the rescaled set is also a solution

- Vanishing energy E_0 → $E = E_0/R^2$ → $E = 0$

For bosonic Townes soliton see [Vlasov et al.'71, Pitaevskii'96, Bakkali-Hassani&Dalibard (Varenna Lectures'22)]

- What is $\gamma = 2mgN$? Is it an external parameter or not?

Solution for bosonic soliton [Hammer&Son'04]
g is the bare coupling constant, it gets renormalized

Solution = go beyond mean field

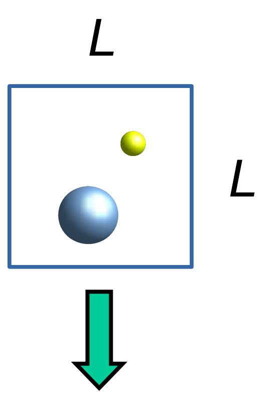
- Beyond-MF term is dominated by the diverging second-order Born integral

$$g = \frac{2\pi}{m_r \ln(2m_r|E_{1+1}|/\kappa^2)} \Longrightarrow g_r = g - \int_{1/\xi}^{\kappa} \frac{g^2}{k^2/(2m_r)} \frac{d^2k}{(2\pi)^2} = g - \frac{m_r g^2}{\pi} \ln(\kappa\xi)$$

κ - high-momentum cut-off, drops out from g_r (up to terms ~g^2)

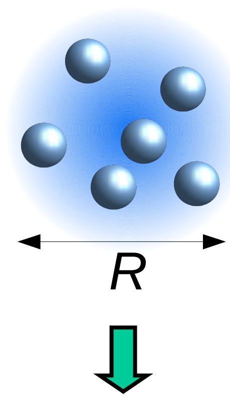
ξ - functional of $\phi(\mathbf{r})$ and $n(\mathbf{r})$, absorbs beyond-MF effects, ``typical length scale"

Two particles in a box



ξ ~L

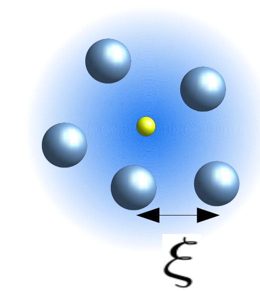
Townes soliton of attractive bosons



ξ ~R

[Hammer&Son'04]

***N*+1 fermionic cluster**



$$\xi = e^{1/2}/p_F$$

Local Fermi momentum of heavies

Minimization of BMF functional

$$E = \frac{1}{2m}\int [|\nabla\phi(\mathbf{r})|^2 + \frac{\alpha}{2}n^2(\mathbf{r}) + \gamma n(\mathbf{r})|\phi(\mathbf{r})|^2]d^2r \quad -\frac{1}{2m}\frac{\gamma^2}{2\pi N}\int n(\mathbf{r})|\phi(\mathbf{r})|^2 \ln\frac{e^{1/2}\kappa}{\sqrt{4\pi n(\mathbf{r})N}}d^2r$$

When $\gamma = \gamma_c(\alpha)$

$$\phi(r) = \phi_0(r/R)/R$$
$$n(r) = n_0(r/R)/R^2$$

Three MF terms separately are of order ~$1/R^2$, but their sum vanishes

The BMF term ~$(N^{-1}\ln N)/R^2$ << each MF term

The shape of the cluster unchanged, but there exists an optimal R

In the leading BMF order we thus have

$$E = \frac{1}{2mR^2}\int\left[(\gamma-\gamma_c)n_0(r)|\phi_0(r)|^2 - \frac{\gamma_c^2}{2\pi N}n_0(r)|\phi_0(r)|^2\ln\frac{e^{1/2}\kappa R}{\sqrt{4\pi n_0(r)N}}\right]d^2r$$

$$(\gamma-\gamma_c)/\gamma_c^2 \approx 1/\gamma_c - 1/\gamma$$
$$4\pi N/\gamma \approx \ln[4e^{-2\gamma_E}/(a\kappa)^2]$$

$$I_1 = \int n_0(r)\phi_0^2(r)d^2r$$
$$I_2 = \int n_0(r)\phi_0^2(r)\ln n_0(r)d^2r$$

$$R_{\min}^2 = \pi N a^2 e^{4\pi N/\gamma_c + I_2/I_1 + 2\gamma_E}$$

$$E_{N+1} = -\frac{I_1\gamma_c^2}{8\pi N m R_{\min}^2}$$

Need better mean field

$$E_{N+1} = -\frac{1}{2ma^2} e^{-4\pi N/\gamma_c - 2\ln N - I_2/I_1 - 2\gamma_E + \ln(I_1 \gamma_c^2) - 2\ln(2\pi) + o(N^0)}$$

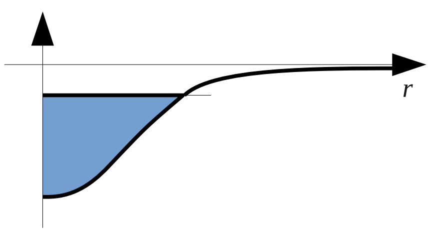
MF
cf. [Hammer&Son'04]

BMF
(aka, preexponential factor)

$$\gamma_c^{\mathrm{TF}}(\alpha = 4\pi N^2 m/M) \quad \Rightarrow \quad \gamma_c^{\mathrm{HF}}(M/m, N)$$

Thomas-Fermi MF functional

$$E = \frac{1}{2m}\int [|\nabla\phi(\mathbf{r})|^2 + \frac{\alpha}{2} n^2(\mathbf{r}) + \gamma n(\mathbf{r})|\phi(\mathbf{r})|^2] d^2r$$



$$-\nabla^2\phi(\mathbf{r}) + \gamma n(\mathbf{r})\phi(\mathbf{r}) = 2m\epsilon\phi(\mathbf{r})$$

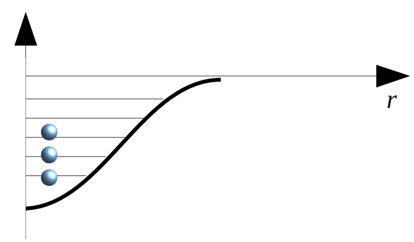
$$n(\mathbf{r}) = -\frac{\gamma}{\alpha}\theta[|\phi(\mathbf{r})|^2 + 2mN\mu/\gamma]$$

$$\int |\phi(\mathbf{r})|^2 d^2r = 1 \qquad \int n(\mathbf{r}) d^2r = 1$$

analytic results, but not precise on ~1/*N* level

Hartree-Fock MF functional

$$E = \frac{1}{2m}\int \left[|\nabla\phi(\mathbf{r})|^2 + \frac{m}{M}\sum_{i=1}^{N}|\nabla\Psi_i(\mathbf{r})|^2 + \gamma n(\mathbf{r})|\phi(\mathbf{r})|^2\right] d^2r$$



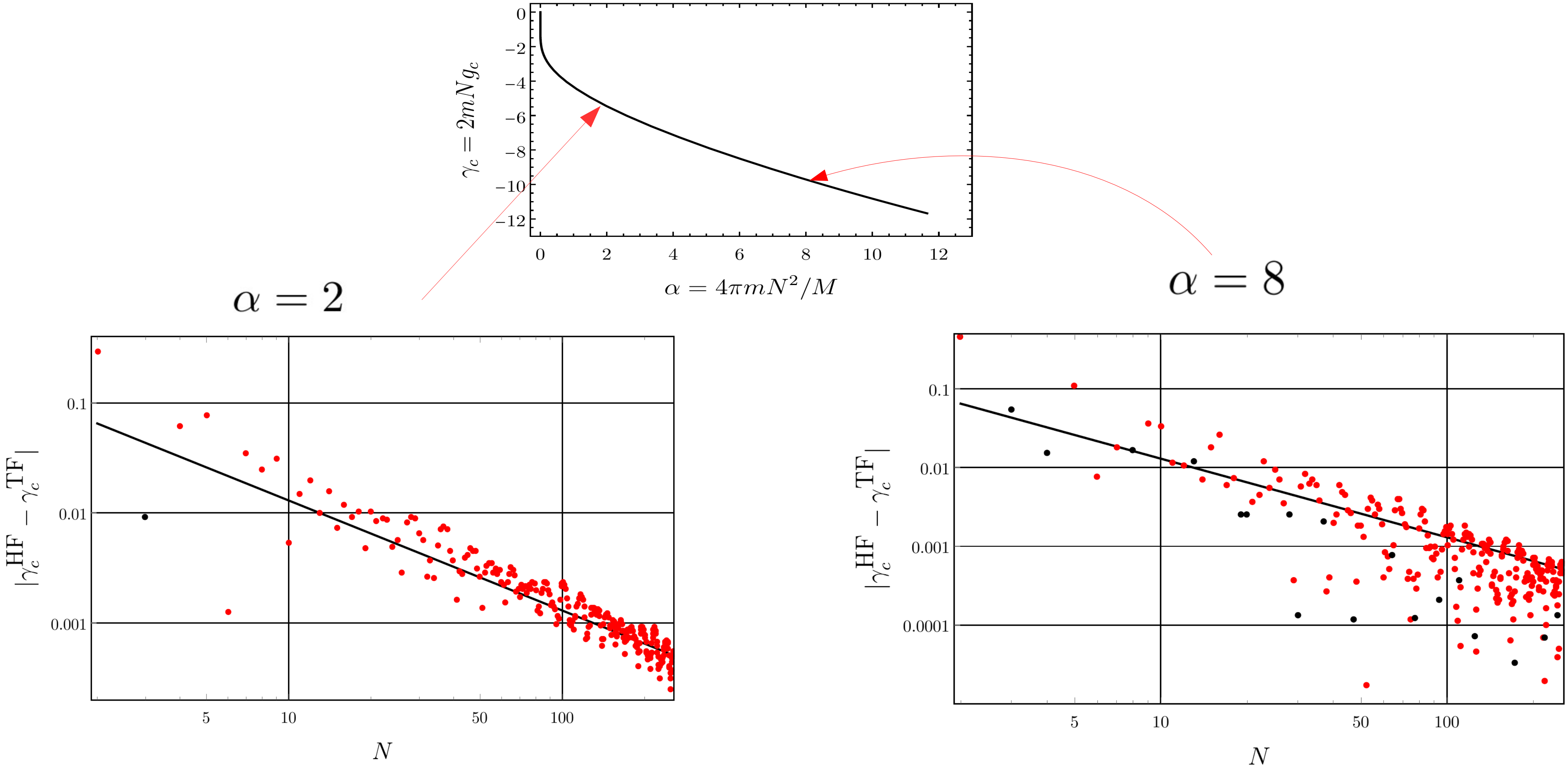
$$-\nabla^2\phi(\mathbf{r}) + \gamma n(\mathbf{r})\phi(\mathbf{r}) = 2m\epsilon\phi(\mathbf{r})$$

$$-\nabla^2\Psi_i + \frac{4\pi\gamma N}{\alpha}|\phi|^2\Psi_i = \omega_i\Psi_i$$

$$n(\mathbf{r}) = \sum_{i=1}^{N}|\Psi_i|^2/N$$

$$\int |\phi(\mathbf{r})|^2 d^2r = 1 \qquad \int n(\mathbf{r}) d^2r = 1$$

Hartree-Fock vs Thomas-Fermi



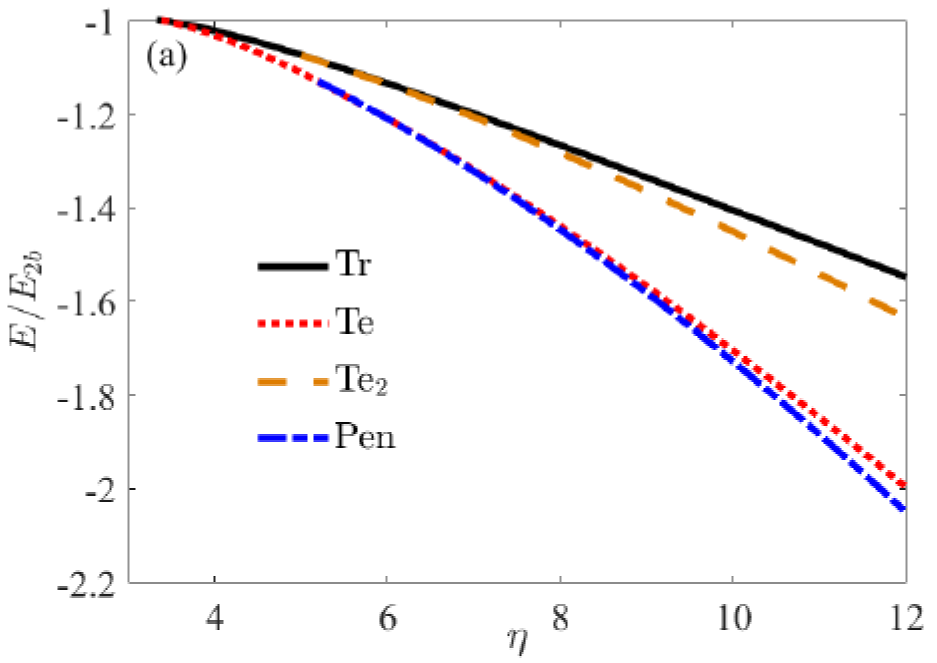
$$\gamma_c^{\mathrm{HF}} - \gamma_c^{\mathrm{TF}} \propto 1/N$$

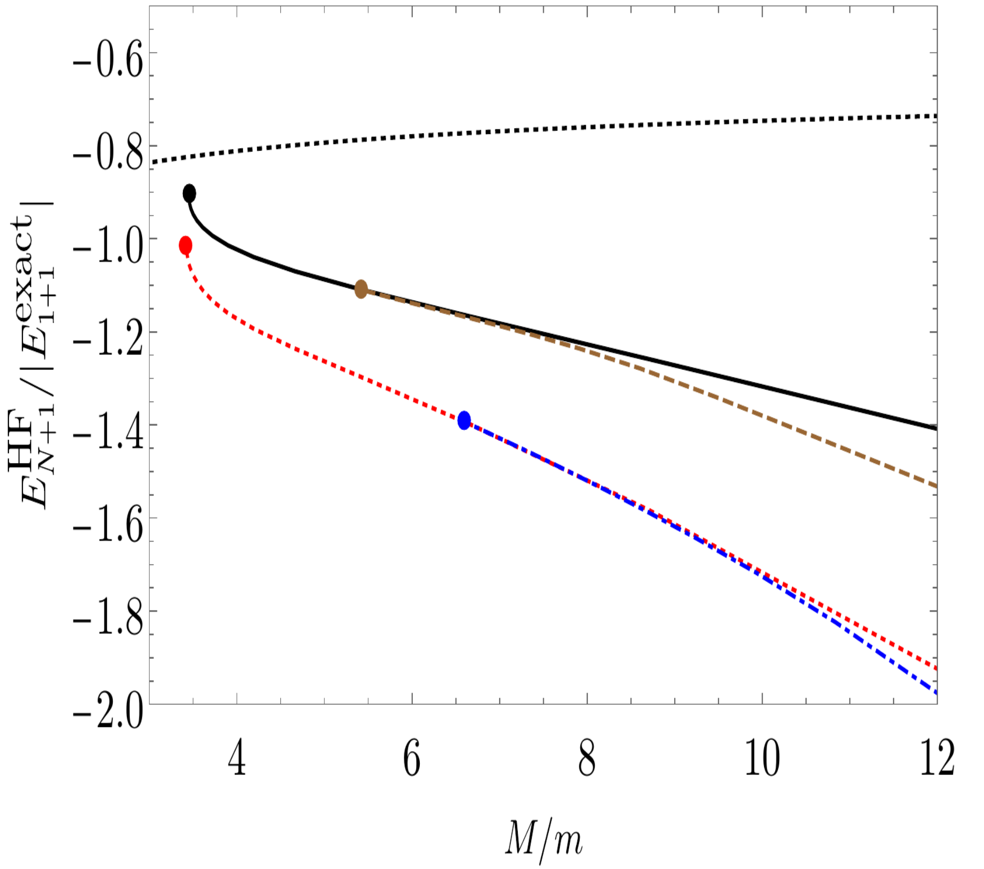
$$E_{N+1}^{\mathrm{TF}} = -\frac{1}{2ma^2} e^{-4\pi N/\gamma_c^{\mathrm{TF}} - 2\ln N + O(1)}$$

$$E_{N+1}^{\mathrm{HF}} = -\frac{1}{2ma^2} e^{-4\pi N/\gamma_c^{\mathrm{HF}} - 2\ln N - I_2/I_1 - 2\gamma_E + \ln(I_1\gamma_c^2) - 2\ln(2\pi) + o(N^0)}$$

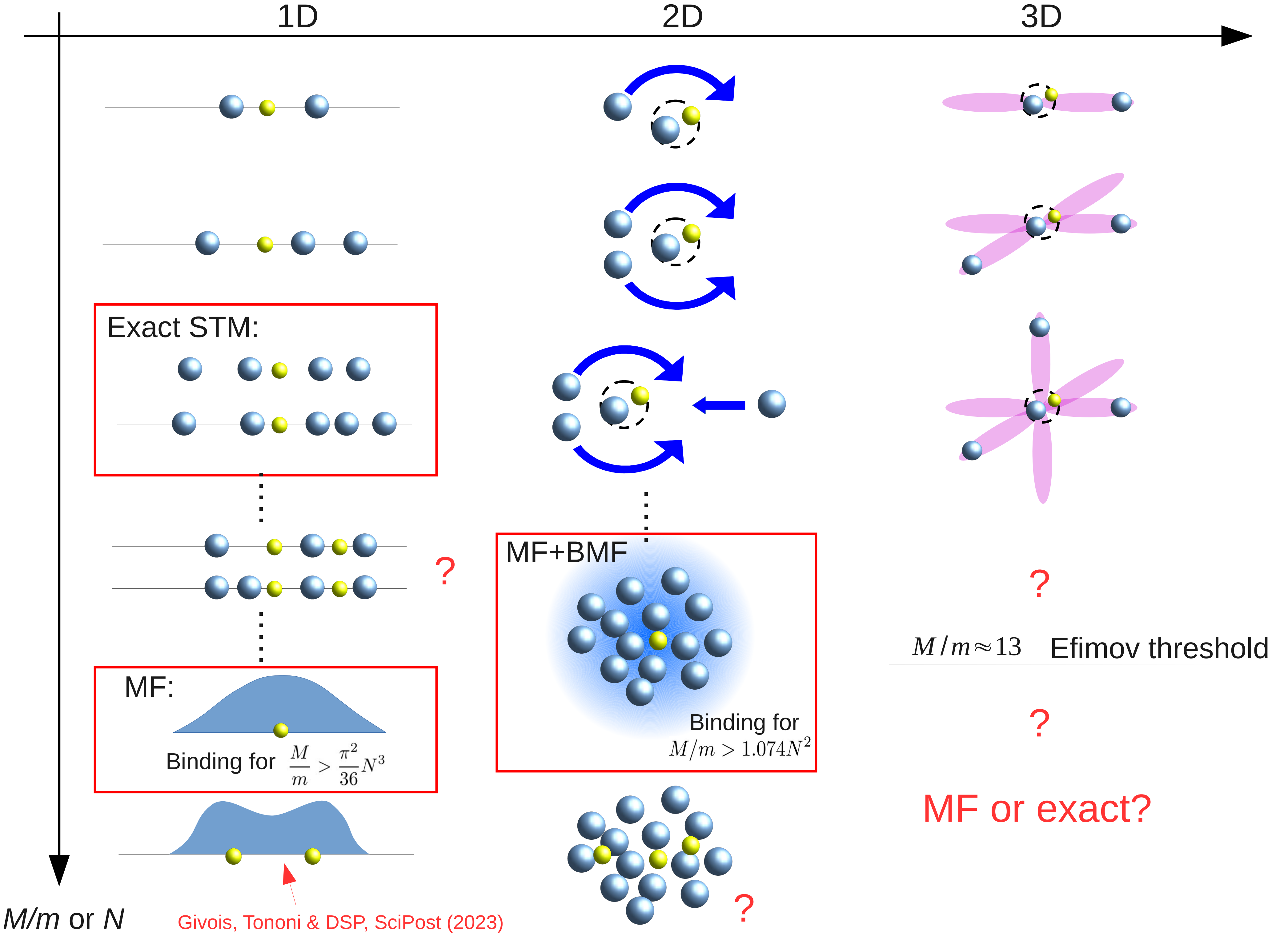
Exact vs Hartree-Fock

[Liu & Peng & Cui'22]





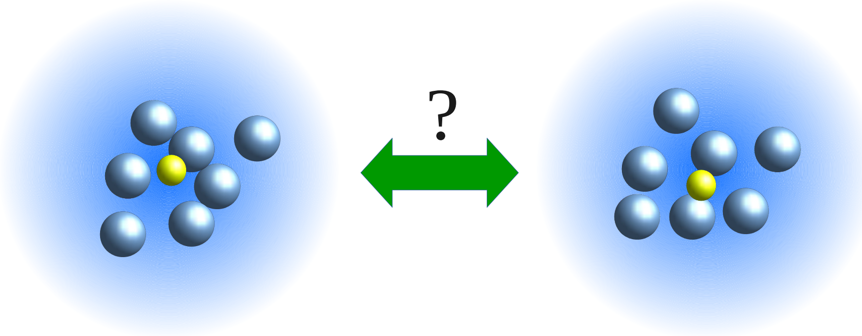
Summary and outlook



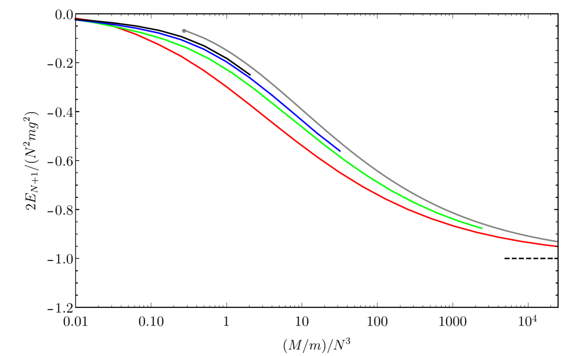
1D
2D
3D
Exact STM:
MF:
Binding for $\frac{M}{m} > \frac{\pi^2}{36} N^3$
?
MF+BMF
Binding for $M/m > 1.074N^2$
?
?
$M/m \approx 13$ Efimov threshold
?
MF or exact?
M/m or N
Givois, Tononi & DSP, SciPost (2023)

Outlook

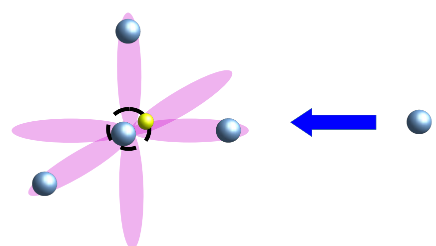
- Binding of two or more *N*+1 clusters



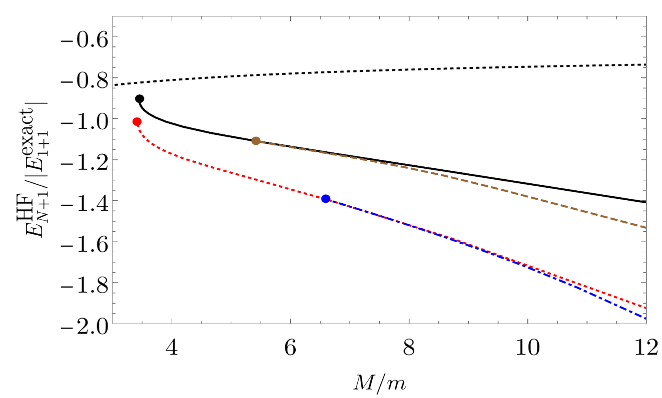
- Include BMF in the 1D case



- Hexamer in 3D?



- HF + fixed-node diffusion Monte Carlo



- ...

Thank you!