Binding of heavy fermions by a single light atom in 1D

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Trento

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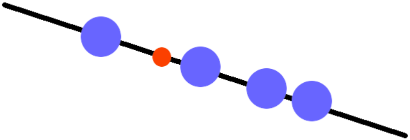
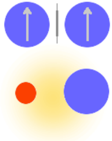
based on
[A. Tononi, J. Givois, and D. S. Petrov, arXiv:2205.01018, accepted in PRA as a Letter]

The system

$$\hat{H} = \int \left(-\frac{\hat{\Psi}_x^\dagger \partial_x^2 \hat{\Psi}_x}{2M} - \frac{\hat{\phi}_x^\dagger \partial_x^2 \hat{\phi}_x}{2m} + g \hat{\Psi}_x^\dagger \hat{\phi}_x^\dagger \hat{\Psi}_x \hat{\phi}_x \right) dx, \qquad g < 0$$



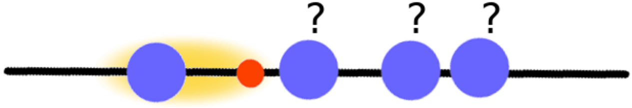
N heavy fermions of mass M
1 light atom of mass m



Noninteracting heavy

heavy-light attraction

How many heavy fermions can be bound by a single light atom in 1D?



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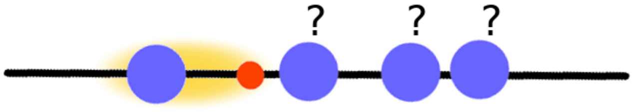
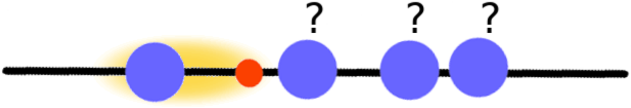


Competition between:

- Kinetic energy of heavy atoms $\sim 1/M$
- (Effective) attractive heavy-heavy potential, mediated by the exchange of the light atom $\sim 1/m$

The (N+1)-body problem



A well posed problem (clear question), with few simple parameters

- spatial dimension $D = 1$,
- scattering length a
- mass ratio M/m,
- number of heavy atoms N

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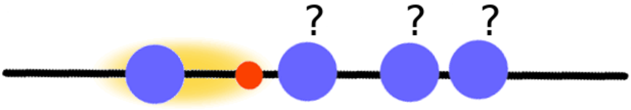

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- spatial dimension $D = 1$,
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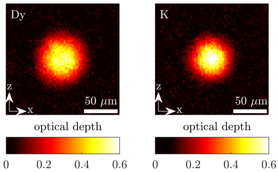
relevant for experiments with mass and density-imbalanced fermionic mixtures

^{173}Yb–^{6}Li, ^{53}Cr–^{6}Li, ^{40}K–^{6}Li, ^{161}Dy–^{40}K

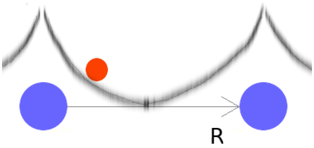


[Ravensbergen et al, PRA **98**, 063624 (2018)]

Outline

- Introduction and motivation
- Born-Oppenheimer theory of the 3D trimer
- Bound states of $N+1$ fermions in 1D
- Derivation of the results
  - Exact results for $N \leq 5$
  - Mean field: Thomas-Fermi approximation
  - Mean field: Hartree-Fock
- Conclusions and perspectives

2+1 (trimer) in the 3D Born-Oppenheimer picture



Light atom in the field of fixed heavy fermions
(distance $R = |\vec{R}_2 - \vec{R}_1|$)

$$-\frac{\hbar^2 \nabla^2_{\vec{r}}}{2m}\,\phi_R(\vec{r}) = \epsilon(R)\,\phi_R(\vec{r}), \qquad \phi_R(\vec{r} \to \vec{R}_i/2) \propto \frac{1}{|\vec{r} - \vec{R}_i/2|} - \frac{1}{a}$$

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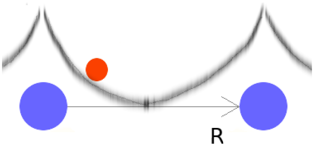

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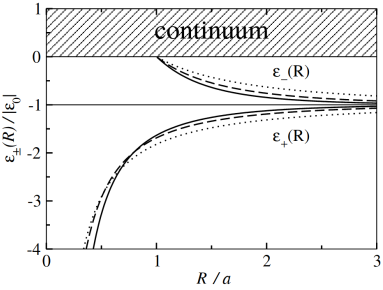
Small R:

$$\epsilon_{+,m}(R) \sim -\frac{\hbar^2}{mR^2}$$

Large R:

$\epsilon_{+,m}(R) \sim \epsilon_0$, dimer energy



[D. S. Petrov, arXiv:1206.5752]

2+1 (trimer) in the 3D Born-Oppenheimer picture

Schrödinger equation for heavy atom with reduced mass $M/2$ in the effective potential:

$$\left[-\frac{\hbar^2}{M}\frac{\partial^2}{\partial R^2}+U_{eff}(R)-E\right]\chi(R)=0,\quad U_{eff}(R)=\frac{\hbar^2 l(l+1)}{MR^2}+\epsilon_{+,m}(R)+|\epsilon_0|$$

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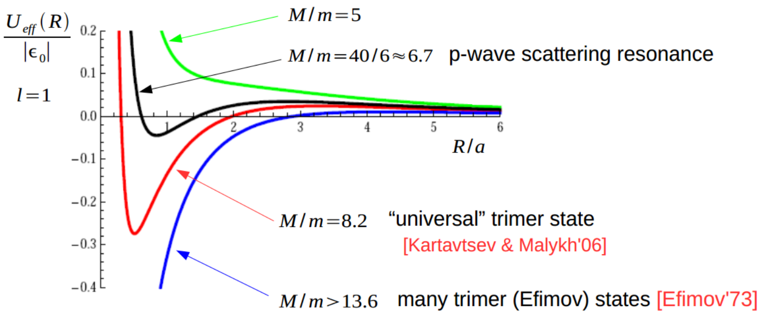
The light-mediated effective heavy-heavy potential is "tuned" by M/m:



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Binding in 1D

As in 3D, there is a **competition** between heavy kinetic energy and light-mediated heavy-heavy attraction.

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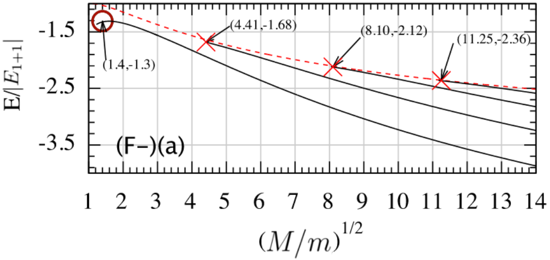
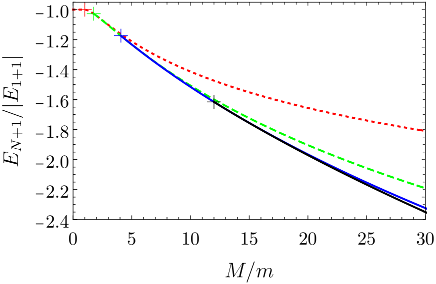
State of the art in 1D:

- Trimer (2+1 atoms) at $M/m \geq 1$ (red dashed curve)
  [Kartavtsev, et al. JETP **108**, 365 (2009)]
- Tetramer (3+1 atoms) through Born-Oppenheimer treatment (lowest black curve)
  [Mehta, PRA **89**, 052706 (2014)]



Our results



We provide the **exact solution of the quantum mechanical problem** up to $N = 5$.

($N = 2, 3, 4, 5$ here)

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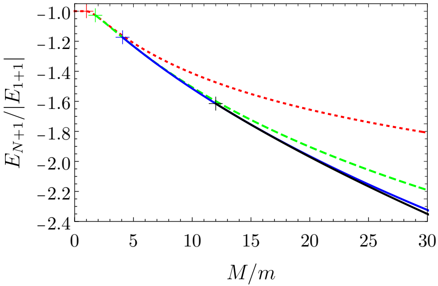

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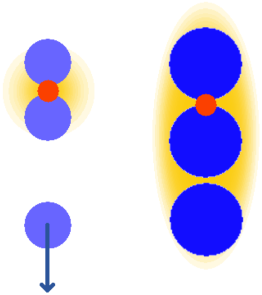
We identify the critical mass ratios:

$$(M/m)_{2+1} = 1,$$
$$(M/m)_{3+1} = 1.76,$$
$$(M/m)_{4+1} = 4.2,$$
$$(M/m)_{5+1} = 12.0 \pm 0.5$$



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Exact results: the Skorniakov-Ter Martirosian equation

Schrödinger equation for a system of N heavy plus 1 light fermions:

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

where $E<0$, and $g=-1/(m_r a)<0$, $m_r=mM/(m+M)$.

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where $E < 0$, and $g = -1/(m_r a) < 0$, $m_r = mM/(m + M)$.

Wave function of $(N-1)$ fermions plus a dimer:

$$\psi(x_1, ..., x_{N-1}, x_N, x_{N+1} = x_N)$$

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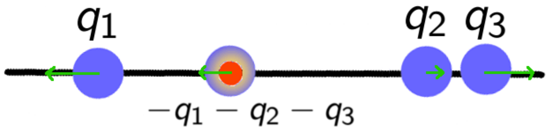
In center of mass coordinates $q_N=-\sum_{i=1}^{N}q_i$ we have:

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



Exact results: the Skorniakov-Ter Martirosian equation

$F(q_1, ..., q_{N-1})$ satisfies the STM equation

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

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

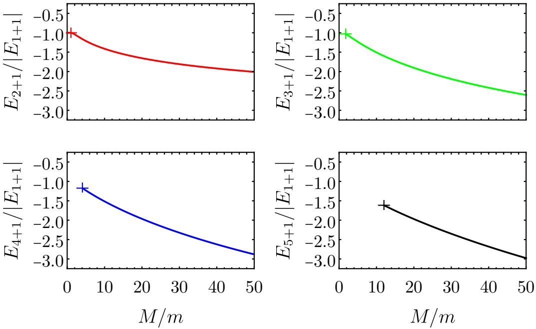
[Skorniakov, Ter-Martirosian, JETP **4**, 648 (1957)]

[Pricoupenko, Petrov, PRA **100**, 042707 (2019)]

Integro-differential equation that includes naturally zero-range interactions, and removes the dimer coordinates.

Exact results: the Skorniakov-Ter Martirosian equation

The exact solution of the STM equation gives the energies (continuous lines) of the $N+1$ clusters:



We also find that the trimer and tetramer have $P=-1$, while pentamer and hexamer have $P=+1$

Two questions

- Large N limit?
- Are there computationally-cheap methods that work also at small N?

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Thomas-Fermi approach

Large N limit: mean-field theory based on the Thomas-Fermi approximation for the heavy fermions

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

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minimizing Ω wrt ϕ and n: $-\phi_1''(x) + 2mgn(x)\phi_1(x) = 2m\epsilon\phi_1(x)$,

$n(x) = \sqrt{-2Mg(|\phi(x)|^2 - \mu/g)/\pi^2}$, when $|\phi(x)|^2 > \mu/g$.

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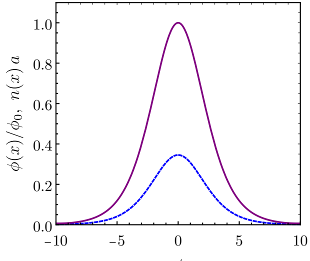
When $\mu = 0$ (threshold for binding a new heavy atom), analytical:

Threshold: $\left(\frac{M}{m}\right)_{N+1} = \frac{\pi^2}{36} N^3$

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

$$n(x) = \sqrt{-2Mg/\pi^2}\,|\phi(x)|$$



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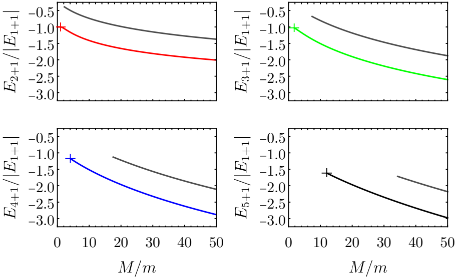
Thomas-Fermi approach (grey curves), analytical, computationally cheap, works at large N:



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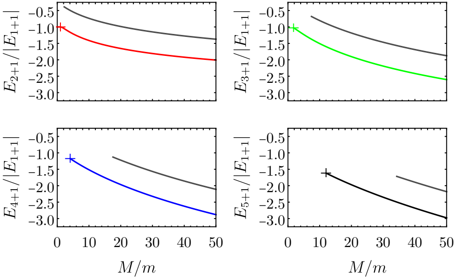

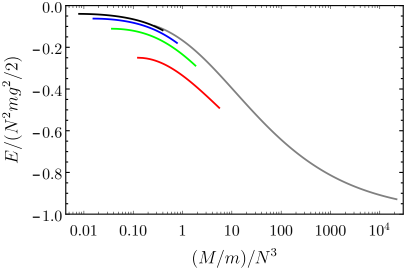

What is the main source of discrepancy with the small-N exact results? TF, mean field?

Hartree-Fock approach

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

Energy $E_{N+1} = \langle v | \hat{H} | v \rangle$, with the variational ansatz:

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

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

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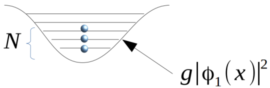
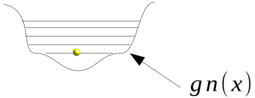
Minimizing $E_{N+1} - \epsilon_1 - \mu N$ with respect to the orbitals yields:

$$-\frac{\partial_x^2 \phi_1}{2m} + gn\, \phi_1 = \epsilon_1 \phi_1,$$

$$-\frac{\partial_x^2 \Psi_\nu}{2M} + g\, |\phi_1|^2 \Psi_\nu = E_\nu \Psi_\nu,$$

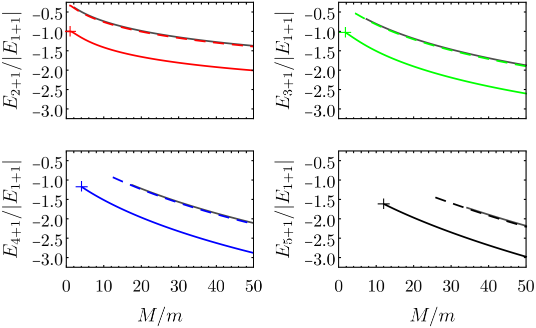
$$n = \sum_{\nu=1}^N |\Psi_\nu|^2$$





Hartree-Fock approach

$\rightarrow$ No improvement wrt TF energies (dashed lines)...



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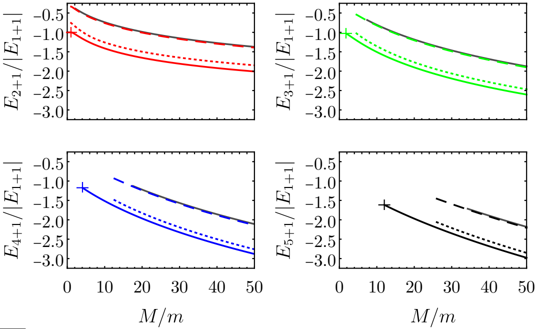

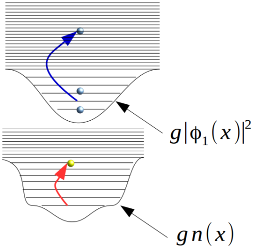

...the second-order correction (dotted lines)

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

gives good and **computationally cheap** agreement

$N-1$ atoms momentum distribution

All methods give access to the following quantity:

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

that can be used to compare their effectiveness at small N.

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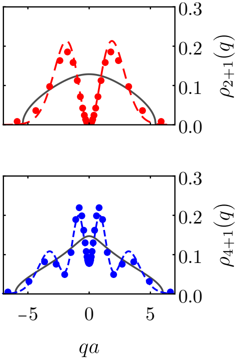
We find that Hartree-Fock reproduces very well these momentum correlations:



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Conclusions and perspectives

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(very different from 3D, where there are no $N+1$ states for $M/m \gtrsim 13$, meaning no 6+1 clusters!)

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- **HF theory**: reproduces well energy and correlations at small and large N

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Possible generalization to other setups:

- higher dimensions
- more particles

Thank you for your attention!

References:

— A. Tononi, J. Givois, and D. S. Petrov, arXiv:2205.01018, accepted in PRA as a Letter

— A. Pricoupenko, and D. S. Petrov, PRA **100**, 042707 (2019)