Self-binding of a Fermi-Fermi atomic mixture with zero-range attraction in 1D

Andrea Tononi

Laboratoire Physique Théorique et Modèles Statistiques,
CNRS, Université Paris-Saclay

Orsay 07/09/2023

based on

[1] [AT, J. Givois, and D. S. Petrov, PRA **106**, L011302 (2022)]

[2] [J. Givois, AT and D. S. Petrov, SciPost Physics **14**, 091 (2023)]

Ultracold atomic gases

- Neutral atomic gases, either bosonic or fermionic
- Experiments with $N \sim 10^4$ atoms cooled at $T \sim 1\,\mu$K
- Bose-Einstein condensate or degenerate Fermi gas

- Typical density: $n \sim 10^{20}$ atoms/m^3
- Potential range: $b \sim a \sim 1\,$nm $\ll d = n^{-1/3} \sim 1\,\mu$m

  $\Rightarrow$ interatomic interactions can be well approximated as *zero-range* interactions with s-wave scattering length a.

Ultracold atomic gases in D=2 and D=1

Atomic gases are 3D systems.
Experimental techniques to study their physics (*effectively*) also in 1D and 2D geometries. How?

- Atoms are confined in space using external fields (e.g. magnetic potentials $U(\vec{r}) \sim -\vec{\mu} \cdot \vec{B}(\vec{r})$)
- Single point-like atom moving in the potential $U(\vec{r}) = \frac{m}{2}\omega_x^2 x^2 + \frac{m}{2}\omega_y^2 y^2 + \frac{m}{2}\omega_z^2 z^2$
- If the energy scales of the system $\langle k_B T \rangle$, $\langle gn \rangle \ll \hbar\omega_i$,

  $\Rightarrow$ the atoms are confined to the ground state of the harmonic oscillator along the direction i.

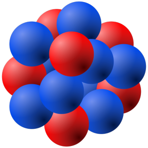
- Motion confined along *one* direction: 2D system
- Motion confined along *two* directions: 1D system

Physical system of this talk

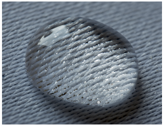
Fermionic atoms confined in a 1D geometry.

Two-component mixture of different fermions.

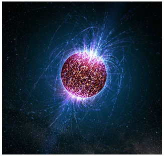
Mixtures of fermionic particles form self-bound states:



nuclei



liquids



neutron stars

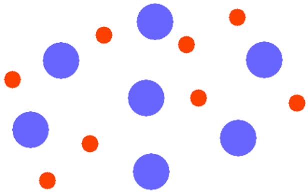
Can we describe fermionic binding with simple models?

Ultracold fermionic mixtures

N_h heavy fermions with mass M

$+$

N_l light fermions with mass m



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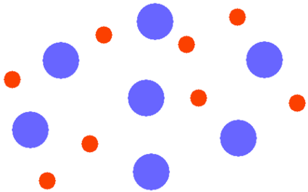

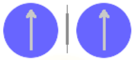

Noninteracting heavy

Noninteracting light

Heavy-light attraction

Ultracold fermionic mixtures

$$\hat{H} = \int \left(-\frac{\hat{\Psi}^\dagger_{\mathbf{r}} \nabla^2 \hat{\Psi}_{\mathbf{r}}}{2M} - \frac{\hat{\phi}^\dagger_{\mathbf{r}} \nabla^2 \hat{\phi}_{\mathbf{r}}}{2m} + g \hat{\Psi}^\dagger_{\mathbf{r}} \hat{\phi}^\dagger_{\mathbf{r}} \hat{\Psi}_{\mathbf{r}} \hat{\phi}_{\mathbf{r}} \right) d\mathbf{r}, \qquad g < 0$$

Ultracold fermionic mixtures

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Competition between:

- Kinetic energy of heavy fermions
- Kinetic energy of light fermions
- Heavy-light attraction

Ultracold fermionic mixtures

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Competition between:

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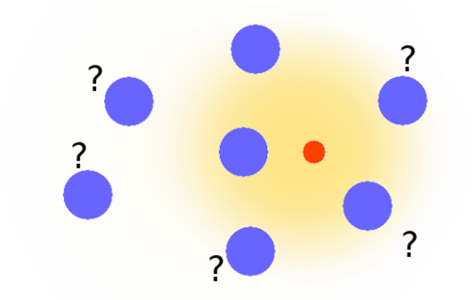
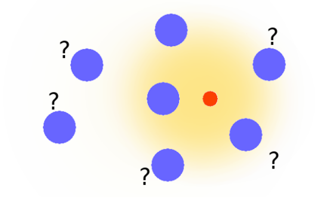
- Kinetic energy of light fermions
- Heavy-light attraction

Possibility to form **bound states** of heavy and light fermions:

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



The (N+1)-body problem:



Few simple parameters:

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

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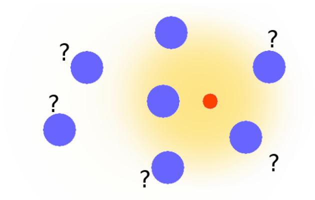


Few simple parameters:

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

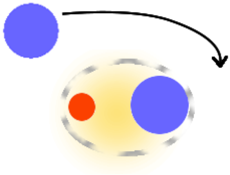
$N+1$ clusters form for sufficiently large M/m.

Studied in $D = 3, 2, 1$. Previous literature?

D=3: 2+1 (trimer)

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

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



[Kartavtsev, et al., J. Phys. B **40**, 1429 (2007)]

D=3: 2+1 (trimer) , 3+1 (tetramer), 4+1 (pentamer)

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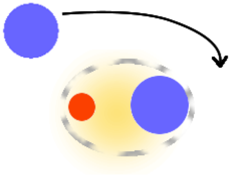
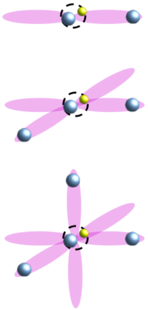


[Kartavtsev, et al., J. Phys. B **40**, 1429 (2007)]

Completing the p-wave shell:



Tetramer at $M/m > 8.86$
(p_x, p_y orbitals),

Pentamer at $M/m > 9.67$
(p_x, p_y, p_z orbitals)

[Bazak, Petrov, PRL **118**, 083002 (2017)]

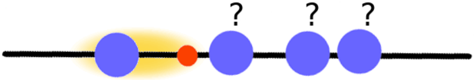
D=1

No shell effect, numerically treatable.

- 2+1 (trimer) at $M/m \geq 1$
  [Kartavtsev, et al. JETP **108**, 365 (2009)]
- 3+1 (tetramer) through Born-Oppenheimer theory
  [Mehta, PRA **89**, 052706 (2014)]

...and then?

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



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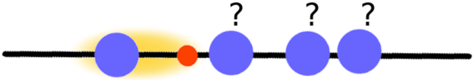
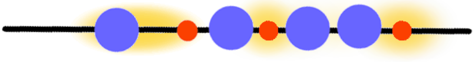


[1] [A. Tononi, J. Givois, and D. S. Petrov, PRA **106**, L011302 (2022)]

What is the ground state of the $N_h + N_l$ system?

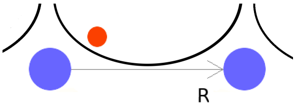


[2] [J. Givois, A. Tononi and D. S. Petrov, SciP. Phys. **14**, 091 (2023)]

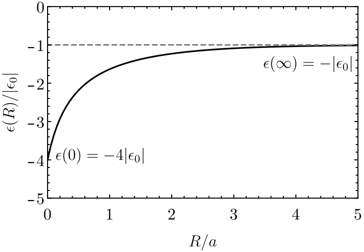
Outline

- Introduction and motivation
- [1] Bound states of $N + 1$ fermions in 1D
  - Born-Oppenheimer theory of the trimer
  - Exact $N + 1$ results for $N \leq 5$
  - Mean-field results for large N: Thomas-Fermi approximation
- [2] Self-bound mixtures of $N_h + N_l$ fermions
- Conclusions and perspectives

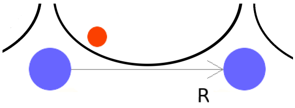
Born-Oppenheimer theory of the 1D trimer



1 light atom, in the field of
2 **fixed** heavy fermions



Born-Oppenheimer theory of the 1D trimer



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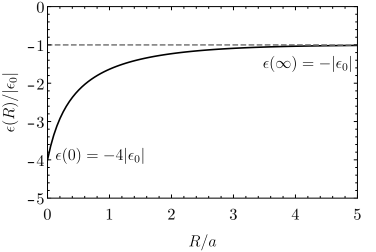
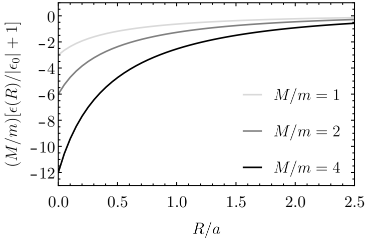


Heavy fermion with reduced mass $M/2$ in the effective potential:

$$\left[-\frac{\hbar^2}{M}\frac{\partial^2}{\partial R^2}+\epsilon_m(R)-E\right]\chi(R)=0$$

The depth of the potential well...

...is "tuned" by M/m:



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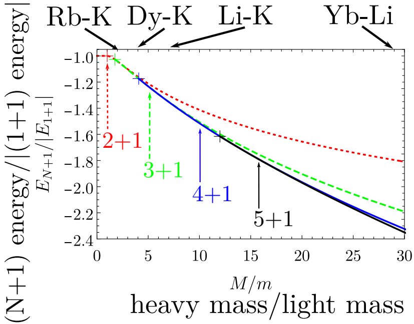
Our results



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

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

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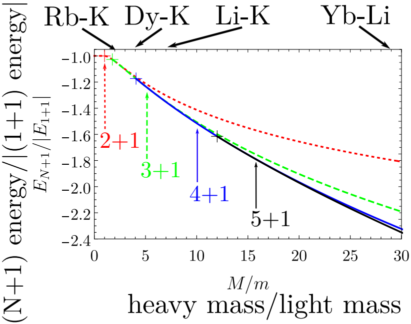

We identify the critical mass ratios:

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

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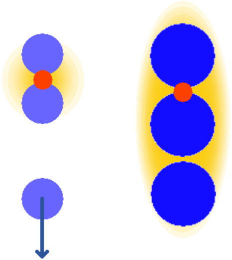

[A. Tononi, J. Givois, and D. S. Petrov, PRA **106**, L011302 (2022)]

The Skorniakov-Ter Martirosian equation

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

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

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

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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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Fourier transform: $F(q_1,...,q_{N-1},q_N)$

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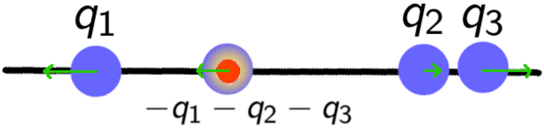
Fourier transform: $F(q_1,...,q_{N-1},q_N)$

In center of mass coordinates $q_N=-\sum_{i=1}^{N-1}q_i$ we have:
$F(q_1,...,q_{N-1})$



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)]

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

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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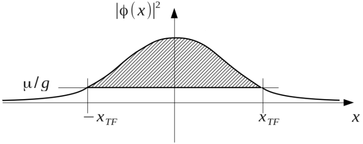
Minimize with n and with ϕ:

$$-\frac{\phi''(x)}{2m} + gn(x)\phi(x) = \epsilon\phi(x),$$

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

when $|\phi(x)|^2 > \mu/g$.



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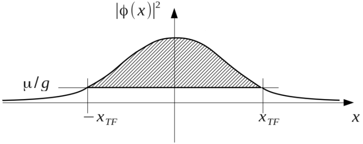
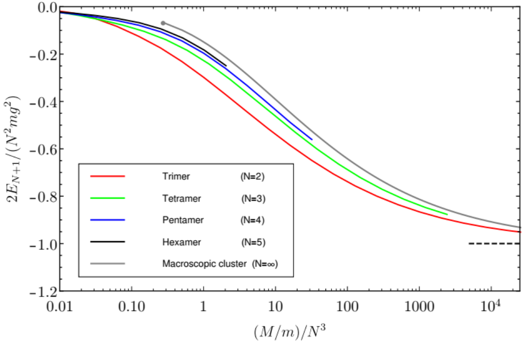


When $\mu = 0$, $\phi(x) \propto \cosh^{-2}(\sqrt{-m\epsilon/2}x)$, and **threshold for binding a new heavy atom**: $\left(\frac{M}{m}\right)_{N+1} = \frac{\pi^2}{36} N^3$

Thomas-Fermi approach

We extend the theory for $\mu \neq 0$, and calculate cluster energies.

Thomas-Fermi approach (grey curve), computationally cheap and works at large N:



What is the source of discrepancy with the small-N exact results: TF approximation or mean field? 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:

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

Hartree-Fock approach

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

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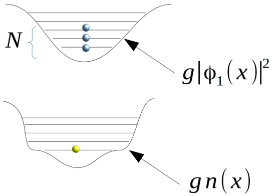
Minimizing $E_{N+1} - \epsilon_1 - \mu N$ with respect to the orbitals yields:

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

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

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



$N-1$ 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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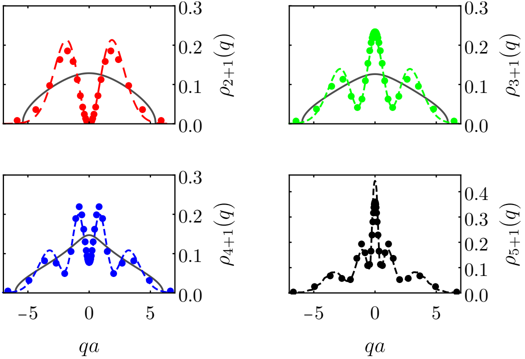
We find that Hartree-Fock reproduces very well these momentum correlations:



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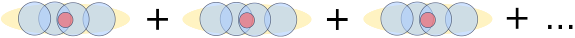
When clusters of type $N + 1$ can form, can they bind together?



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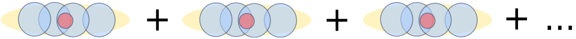
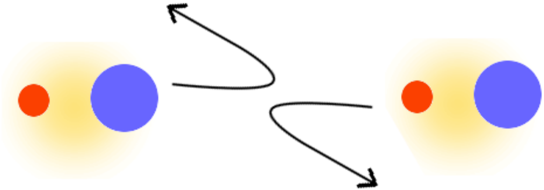


Nontrivial problem...



- BCS-BEC crossover (mass-balanced): the dimers repel each other
- BCS-BEC crossover (mass-imbalanced): the dimers repel or form trimers

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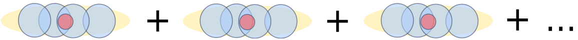

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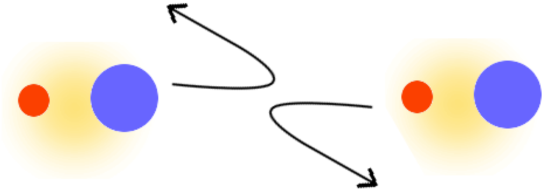

- ▷ BCS-BEC crossover (mass-balanced): the dimers repel each other
- ▷ BCS-BEC crossover (mass-imbalanced): the dimers repel or form trimers

Can the mass imbalance help?

Thomas-Fermi approach

Extending the previous approach to many light fermions:

$$\Omega = \int dx \big[\sum_{i=1}^{N_l} \left(\frac{|\partial_x \phi_i|^2}{2m} + gn|\phi_i|^2 \right) + \frac{\pi^2 n^3}{6M} - \sum_{i=1}^{N_l} \epsilon_i |\phi_i|^2 - \mu n \big],$$

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Rescaling with the length scale $\lambda = 1/(2m|g|N)$ gives:

$$\frac{\Omega}{2mg^2N^2} = \int du \Big[\sum_{i=1}^{N_l} \left(|\partial_u \tilde{\phi}_i|^2 - \tilde{n}|\tilde{\phi}_i|^2 \right) + \alpha \tilde{n}^3 - \sum_{i=1}^{N_l} \tilde{\epsilon}_i |\tilde{\phi}_i|^2 - \tilde{\mu}\tilde{n} \Big],$$

which depends only on:
N_l and $\alpha = (\pi^2/3)N^3 m/M$, with $N = N_h/N_l$.

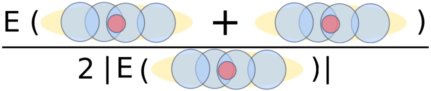
Minimize the functional and solve the equations of motion.

$\Rightarrow$ energy, and the heavy and light atoms densities $\forall \alpha$

Binding of several $N+1$ clusters

Binding energy per (N+1)-cluster.

For instance, $N_h = 8$, $N_l = 2$:



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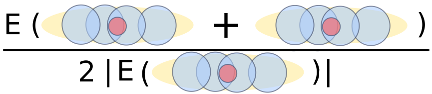
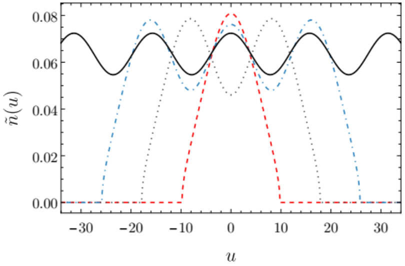
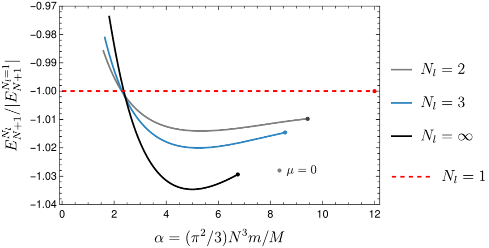




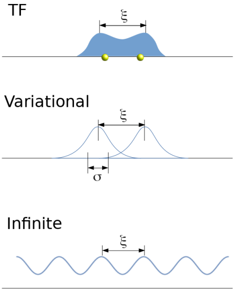
density profiles

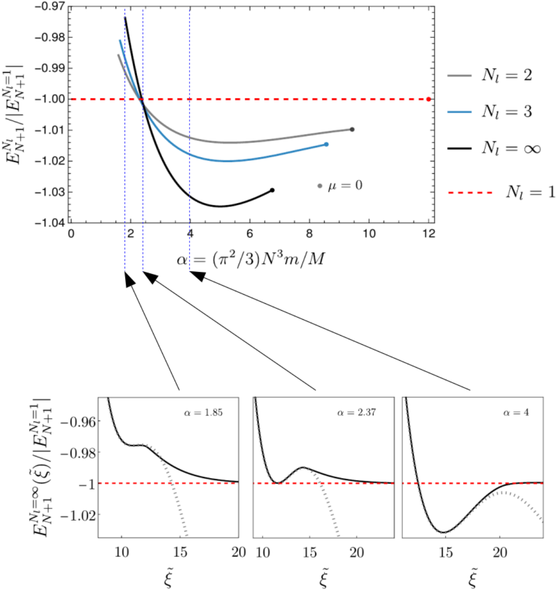


binding energy per (N+1)-cluster

Interaction between the $N+1$ clusters

$E(\xi)$, various cases:





Repulsive interaction at $\xi \gg 0$

(Meta)stable minimum at $\xi \sim 1$.

Outline

- ▷ Introduction and motivation
- ▷ [1] Bound states of $N + 1$ fermions in 1D
  - ▷ Born-Oppenheimer theory of the trimer
  - ▷ Exact $N + 1$ results for $N \leq 5$
  - ▷ Mean-field results for large N: Thomas-Fermi approximation
- ▷ [2] Self-bound mixtures of $N_h + N_l$ fermions
- ▷ 2D preliminary results
- ▷ Conclusions and perspectives

2D preliminary results

Mean-field TF approximation in 2D:

$$\Omega = \int d^2 r \Big[\sum_{i=1}^{N_I} \left(\frac{|\nabla \phi_i|^2}{2m} + gn|\phi_i|^2 \right) + \frac{\pi n^2}{M} - \sum_{i=1}^{N_I} \epsilon_i |\phi_i|^2 - \mu n \Big],$$

Method: iterative solution.

Preliminary:

- We find a solution of the binding problem for $N_I = 1$. More atoms can be bound for larger mass ratio.

  (given a bound state wavefunction $\phi(\rho)$, also $\lambda\,\phi(\lambda\rho)$ is a solution)

- Not clear if two $N+1$ clusters bind

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Binding of N heavy fermions by a light atom:
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Conclusions

Binding of N heavy fermions by a light atom:
for larger mass ratio more atoms can be bound.

- Exact results up to $N = 5$
- **TF theory**: analytical and works for large N
- **HF theory**: reproduces well energy and correlations at small and large N

Fermionic mixture in 1D:
self-binding in a specific region of parameters.

Perspectives

- Self binding in 2D?

- What is the minimum N to observe the self-bound state?

  ...open question!

Thank you for your attention!

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