

Self-bound fermionic mixtures in 1D

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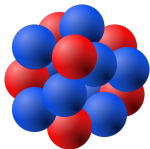
Barcelona

18/01–02/02 /2023

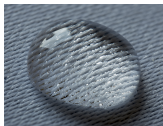
based on

- [1] [A. Tononi, J. Givois, and D. S. Petrov, PRA **106**, L011302 (2022)]
 - [2] [J. Givois, A. Tononi and D. S. Petrov, arXiv:2207.04742]
-

Mixtures of fermionic particles form self-bound states:



nuclei



liquids



neutron stars

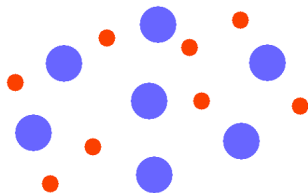
Can we describe fermionic binding with simple models?

Ultracold fermionic mixtures

N_h heavy fermions with mass M

+

N_l light fermions with mass m

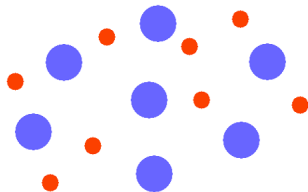


Ultracold fermionic mixtures

N_h heavy fermions with mass M

+

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Noninteracting heavy

Noninteracting light

Heavy-light attraction

Ultracold fermionic mixtures

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

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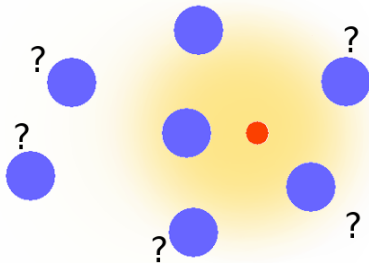
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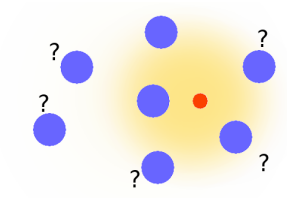
Possibility to form **bound states**
of **heavy** and **light** fermions:



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



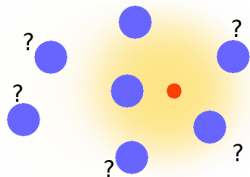
The $(N+1)$ -body problem:



Few simple parameters:

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

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

Studied in $D = 3, 2, 1$.

D=3: 2+1 (trimer)

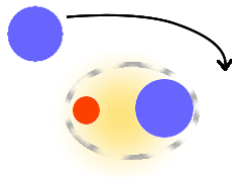
$$M/m < 8.2:$$

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)

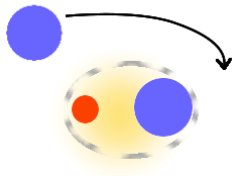
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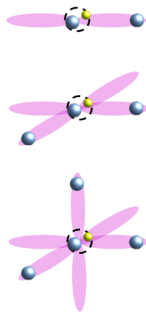
Completing the p-wave shell:

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)]

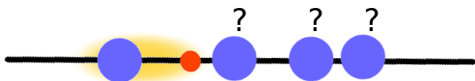
D=1

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)]

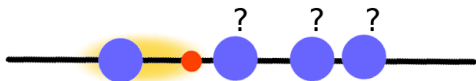
...and then?

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



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

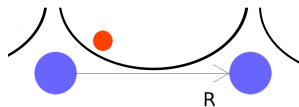


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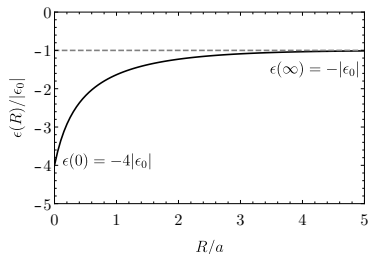
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- ▷ Introduction and motivation
- ▷ [1] Bound states of $N + 1$ fermions in 1D
 - ▷ Born-Oppenheimer theory of the trimer
 - ▷ Exact $N + 1$ results for $N \leq 5$
 - ▷ Mean-field results for large N : Thomas-Fermi approximation
- ▷ [2] Self-bound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

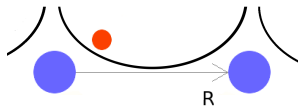
Born-Oppenheimer theory of the 1D trimer



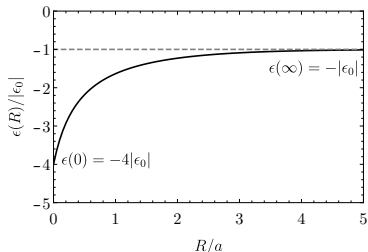
- 1 **light** atom, in the field of
- 2 **fixed heavy** fermions



Born-Oppenheimer theory of the 1D trimer



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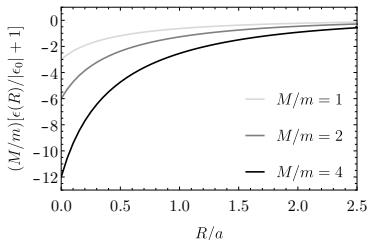


Heavy fermion with reduced mass $M/2$ in the effective potential:

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

The depth of the potential well...

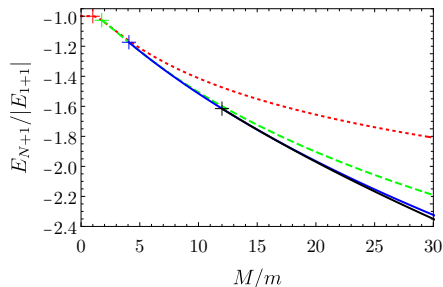
...is “tuned” by M/m :



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Our results

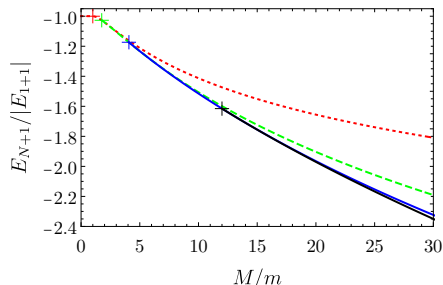


We provide the **exact**
solution of the quantum
mechanical problem up
to $N = 5$.

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

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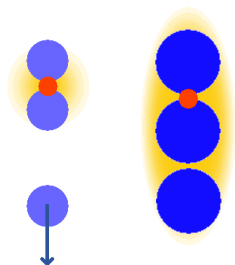
We identify the critical mass ratios:

$$(M/m)_{2+1} = 1,$$

$$(M/m)_{3+1} = 1.76,$$

$$(M/m)_{4+1} = 4.2,$$

$$(M/m)_{5+1} = 12.0 \pm 0.5$$



[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:

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

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:

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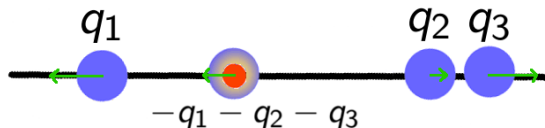
Wave function of $(N - 1)$ fermions plus a dimer:

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

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

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

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



The Skorniakov-Ter Martirosian equation

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

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

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

[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.

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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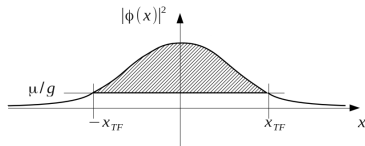
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Minimize with n and with ϕ :

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

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

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



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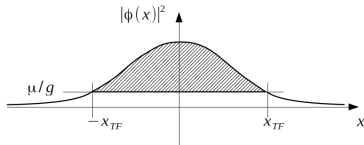
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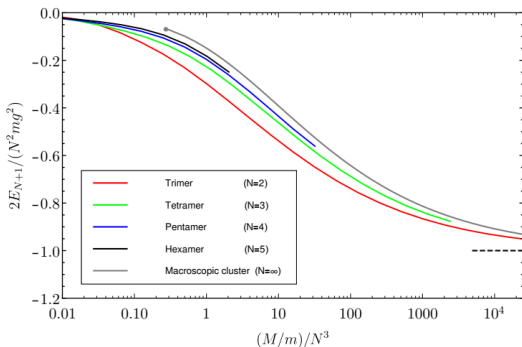


When $\mu = 0$, $\phi(x) \propto \cosh^{-2}(\sqrt{-m\epsilon/2}x)$, and **threshold for binding a new heavy atom:** $\left(\frac{M}{m}\right)_{N+1} = \frac{\pi^2}{36} N^3$

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

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

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

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

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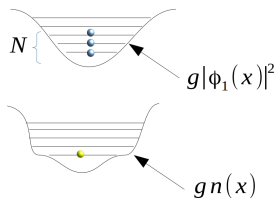
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Minimizing $E_{N+1} - \epsilon_1 - \mu N$ with respect to the orbitals yields:

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

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

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



$N - 1$ atoms momentum distribution

All methods give access to the following quantity:

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

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

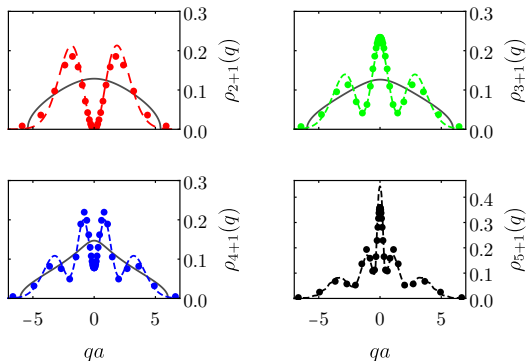
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We find that Hartree-Fock reproduces very well these momentum correlations:





“And now for something completely different.”

Monty Python

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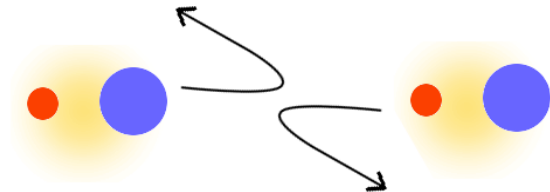
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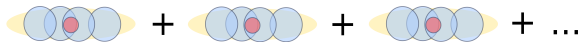


Nontrivial
problem...



- ▷ 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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- ▶ 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:

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

Thomas-Fermi approach

Extending the previous approach to many light fermions:

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

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

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

which depends only on:

$$N_l \text{ and } \alpha = (\pi^2/3)N^3m/M, \text{ with } N = N_h/N_l.$$

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

$$\frac{E(\text{diagram 1}) + E(\text{diagram 2})}{2 |E(\text{diagram 3})|}$$

The diagram shows three clusters of four overlapping circles each, with a red circle in the center. The top part of the equation shows two such clusters separated by a plus sign. The bottom part shows one such cluster enclosed in absolute value bars. The entire expression is divided by 2.

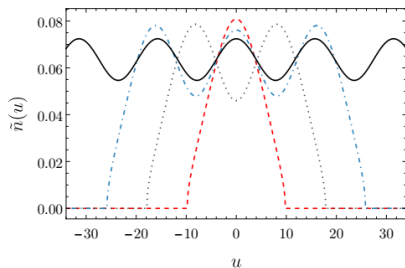
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Binding energy per
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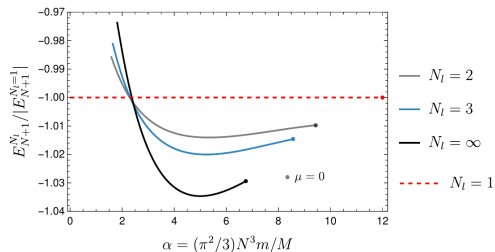
For instance, $N_h = 8$, $N_l = 2$:

$$E \left(\text{two } (N+1)\text{-clusters} \right) + \dots$$

$$\frac{E \left(\text{two } (N+1)\text{-clusters} \right) + \dots}{2 |E \left(\text{one } (N+1)\text{-cluster} \right)|}$$



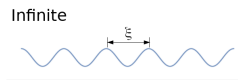
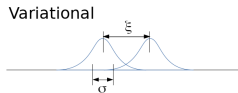
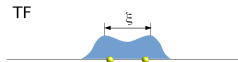
density profiles



binding energy per ($N+1$)-cluster

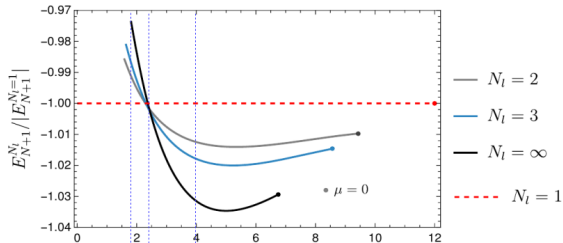
Interaction between the $N + 1$ clusters

$E(\xi)$, various cases:

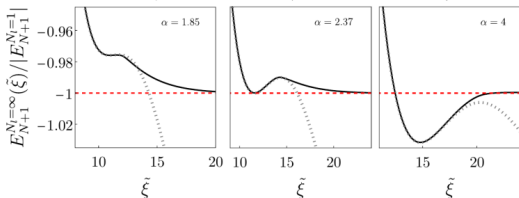


Repulsive
interaction at $\xi \gg 0$

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



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



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

Conclusions

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

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Binding of N heavy fermions by a light atom:
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Fermionic mixture in 1D:
self-binding in a specific region of parameters.

Perspectives

- Generalization to higher dimensions
- What is the minimum N to observe the self-bound state?
...I came to Barcelona to find it out! :)

Thank you for your attention!

References:

- A. Tononi, J. Givois, and D. S. Petrov, PRA **106**, L011302 (2022)
- J. Givois, A. Tononi and D. S. Petrov, arXiv:2207.04742
- A. Pricoupenko, and D. S. Petrov, PRA **100**, 042707 (2019)

$D = 3$ [Kartavtsev, et al., J. Phys. B **40**, 1429 (2007)], [Bazak, Petrov, PRL **118**, 083002 (2017)]

$D = 2$ [Pricoupenko, et al., PRA **82**, 033625 (2010)], [Blume, PRL **109**, 230404 (2012)], [Levinsen, et al., PRL **110**, 055304 (2013)], [Liu, et al. PRL **129**, 073401 (2022)]

$D = 1$ [Kartavtsev, et al. JETP **108**, 365 (2009)], [Mehta, PRA **89**, 052706 (2014)]