Finite-range effects in dilute quantum gases

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Motivation

- Formation of liquid drops of Bose-Bose mixtures and dipolar atoms leads to denser systems than usual quantum gases
- Even if these drops are ultradilute they can show departure of universality in terms of the s-wave scattering length
- Terms beyond the Lee-Huang-Yang in the perturbative series for bosons are not known, but probably depend on the effective range, p-wave scattering length, ...
- We have used a combination of quantum Monte Carlo (QMC) methods and Density Functional Theory (DFT) to estimate first corrections to the universal terms
- Measurable effects observed in experiments with liquid droplets and in the Fermi polaron in two dimensions

Outline

- Quantum Monte Carlo methods
- Formation of drops in Bose-Bose mixtures. Limitations of the LHY correction
- A new functional for Bose-Bose-liquids
- Formation of dipolar drops. Improvements on the current theory: QMC-based functional
- Finite-range effects in the 2D Fermi polaron
- Summary

Diffusion Monte Carlo (DMC)

Starting point: Schrödinger equation for N particles in imaginary time

$$-\frac{\partial \Psi(\boldsymbol{R},t)}{\partial t} = (H - E)\Psi(\boldsymbol{R},t)$$

$$\text{WALKER} \longrightarrow \boldsymbol{R} = (\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N)$$

Expanding $\Psi(\boldsymbol{R},t)$,

$$\Psi(\boldsymbol{R},t) = \sum_n c_n \, \exp[-(E_n - E)t] \, \Phi_n(\boldsymbol{R})$$

with

$$H \, \Phi_n(\boldsymbol{R}) = E_n \, \Phi_n(\boldsymbol{R})$$

When $t \to \infty \Longrightarrow \Phi_0(\boldsymbol{R})$: GROUND STATE

PIGS

The path integral ground state method (PIGS) is a $T = 0$ version of PIMC method.

At any imaginary time τ,

$$\Psi(\mathbf{R}, \tau) = e^{-\tau H} \Psi_T(\mathbf{R}) = \sum_{n=0}^{\infty} c_n e^{-\tau E_n} \Psi_n(\mathbf{R})$$

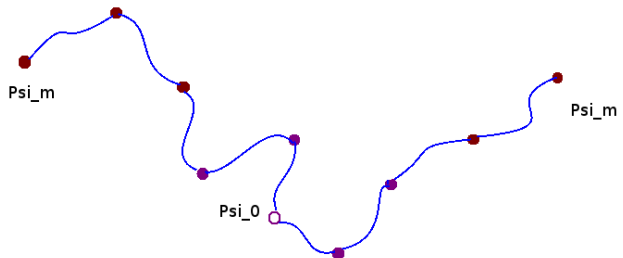
When $\tau \to \infty$ only the ground-state survives,

$$\Psi_0(\mathbf{R}) = \lim_{\tau \to \infty} \Psi(\mathbf{R}, \tau) = \lim_{\tau \to \infty} \int d\mathbf{R}' G(\mathbf{R}, \mathbf{R}', \tau) \Psi_T(\mathbf{R}')$$

PIGS is based on the convolution property of the Green's function

$$\Psi(\mathbf{R}_M) = \int \prod_{j=0}^{M-1} d\mathbf{R}_j G(\mathbf{R}_{j+1}, \mathbf{R}_j, \epsilon) \Psi_T(\mathbf{R}_0)$$

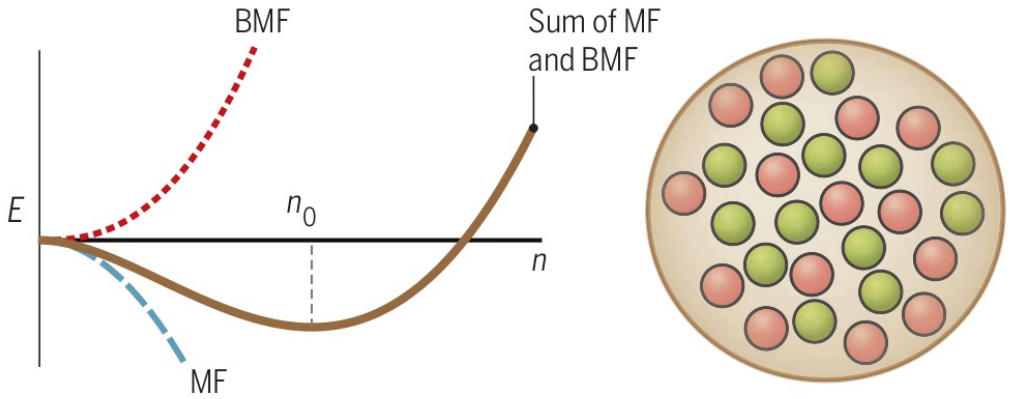
with $\epsilon = \tau / M$



Drops in Bose mixtures

Using mean-field (MF) theory plus LHY correction Petrov predicts the existence of very dilute liquid drops when $g_{12}^2 \simeq g_{11} g_{22}$ (Phys. Rev. Lett. **115**, 155302, (2015)).

Drops are stabilized by competition between the attractive MF term $\sim n^2$ and the repulsive LHY term $\sim n^{5/2}$.



Similar predictions in 1D and 2D geometries (D. S. Petrov, G. E. Astrakharchik, Phys. Rev. Lett. **117**, 100401 (2016))

Drops in Bose mixtures

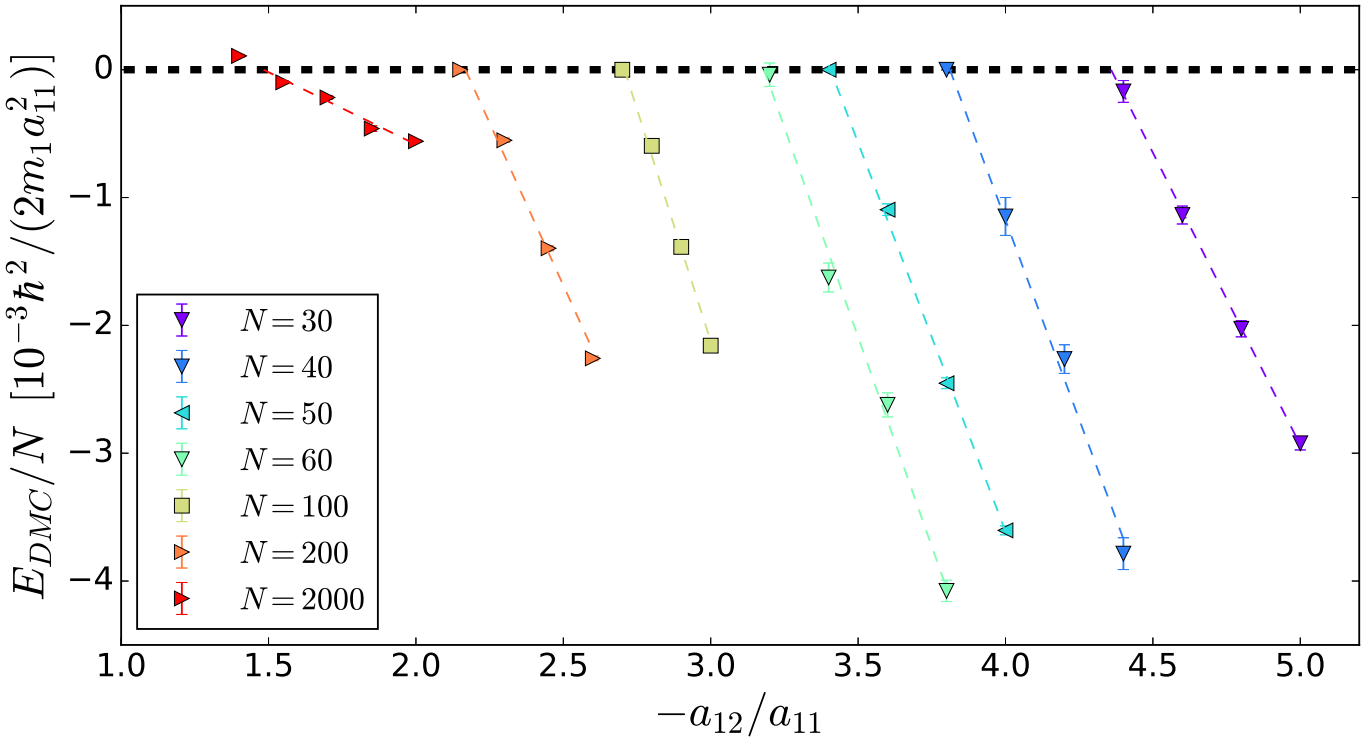
- Following Petrov proposal and experimental results from ICFO we carried out a DMC study on formation of self-bound (liquid) drops
- The Hamiltonian

$$H = -\frac{\hbar^2}{2}\sum_{i=1}^{N}\frac{\boldsymbol{\nabla}_i^2}{m_i} + \sum_{i,j}^{N_\alpha,N_\beta} V^{(\alpha,\beta)}(r_{ij})$$

- Repulsive interaction (HS) between equal species and attractive (SW) between different ones
- Trial-wave functions: Jastrow model with two-body factors from solutions of the two-body problem
- To reduce number of variables, we take $m_\alpha = m_\beta \equiv m$ and $a_{\alpha\alpha} = a_{\beta\beta}$. $a_{\alpha\beta} < 0$, no dimer bound state

Drops in Bose mixtures

By changing the depth of attractive potential, increasing a_{12}, the system evolves from a gas $E > 0$ to a self-bound liquid drop $E < 0$



V. Cikojević, K. Dželalija, P. Stipanović, L. Vranješ Markić, J. B., PRB **97**, 140502(R) (2018)

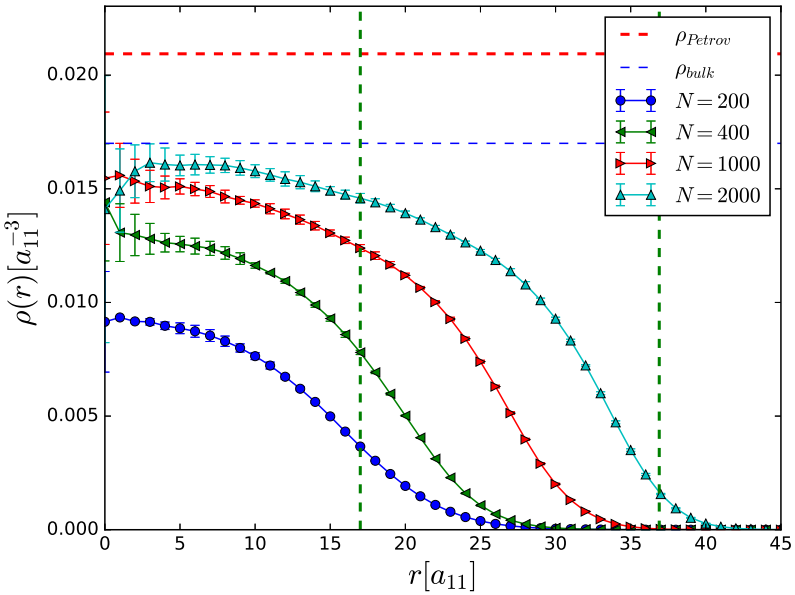
Drops in Bose mixtures

Density profiles show the characteristic liquid behavior

Notice the very low density in the center ($\rho_0 \simeq 10^{17}$ cm^{-3}). Five orders of magnitude lower than for ^{4}He.

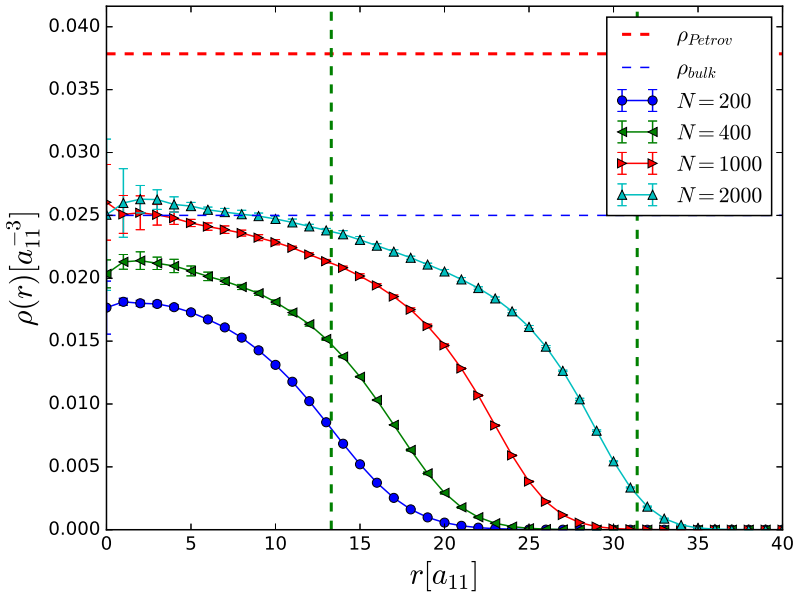
$a_{12} = -3.09 a_{11}$

$\rho_0/\rho_0^{\rm LHY} = 0.81$



$a_{12} = -3.81 a_{11}$

$\rho_0/\rho_0^{\rm LHY} = 0.66$

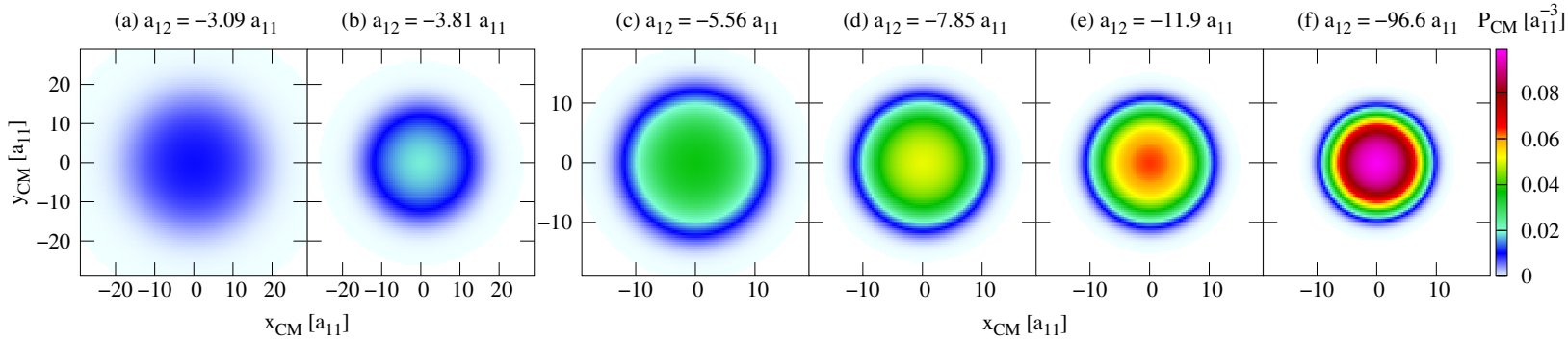


Drops in Bose mixtures

Our results also show the evolution of the drop going to larger attraction.

Even by increasing a_{12} an order of magnitude we do not see collapse.

Central density increases and size reduces, but not in an exponential way.

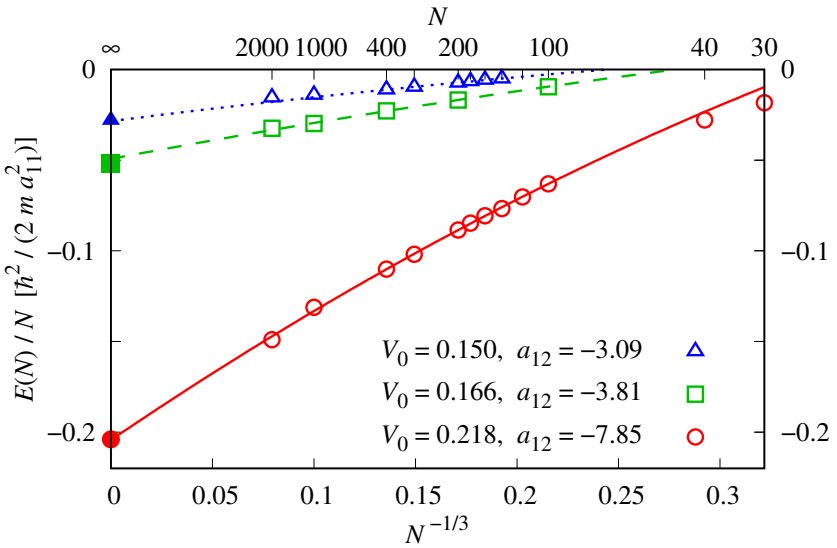


Drops in Bose mixtures

The energy of the drop can be fitted to a liquid-drop model:
$E(N)/N = E_v + xE_s + x^2E_c$, with $x \equiv N^{-1/3}$

E_v is the energy per particle of bulk phase, E_s is a surface term and E_c a curvature contribution

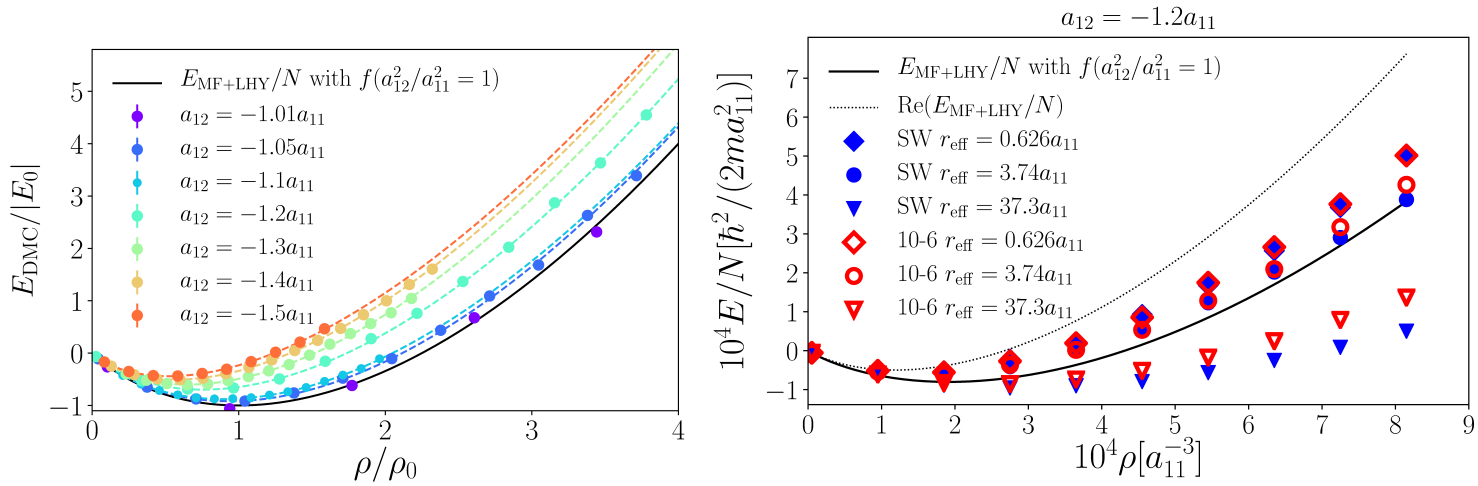
The surface tension of the liquid can be obtained as $t = E_s/(4\pi r_0^2)$ with $4\pi r_0^3 \rho_0/3 = 1$



Bose-Bose droplets

- Critical atom numbers in experiments are much larger than the capabilities of DMC
- To make the connection with experiments we rely on a DFT+LDA approach
- The idea is similar to the one used extensively in liquid Helium
- The new function is built by using the DMC equation of state of the bulk liquid

Bose-Bose droplets



Left: Energy of the bulk liquid for different scattering lengths, compared with MF+LHY theory. *Right:* Universality in terms of the s-wave scattering length and effective range.

QMC-based new functional

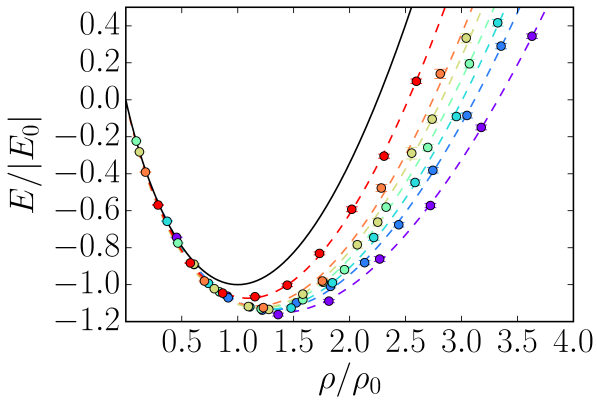
$$\mathcal{E}=\frac{\hbar^2}{2m}N|\nabla\phi|^2+\frac{25\pi^2\hbar^2|a_{11}+a_{12}|^3}{49152ma_{11}^5}\left[-3\frac{N^2|\phi|^4}{\rho_0}+\beta\frac{(N|\phi|^2)^{\gamma+1}}{\rho_0^\gamma}\right]$$

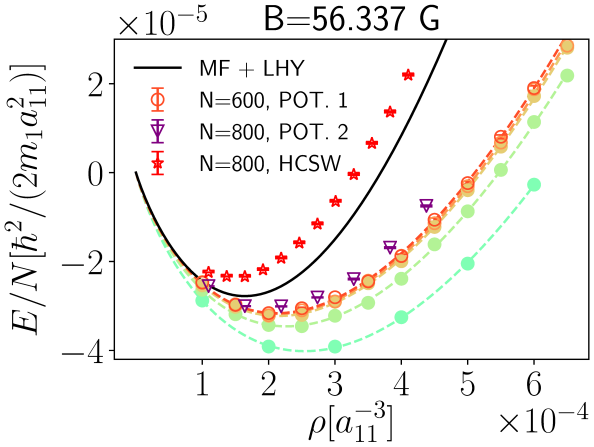
MF+LHY values: $\beta=2,\ \gamma=1.5$

V. Cikojević *et al.*, Phys. Rev. A **99**, 023618 (2019)

Bose-Bose droplets

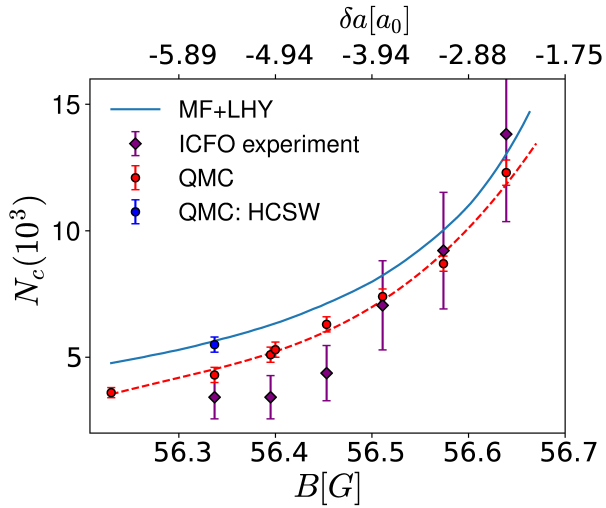
Application to the experiment of Cabrera *et al.* (Science 359, 301 (2018))
composed by a mixture of two hyperfine levels of ^{39}K

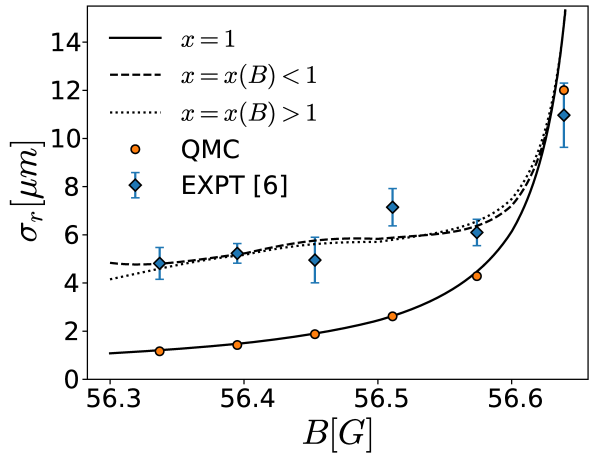




QMC results for the bulk liquid phase (V. Cikojević *et al.*, NJP **22**, 053045 (2020))

Comparison with experiment





Dipolar droplets

$\Longrightarrow$ Hamiltonian of the system

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \frac{C_{dd}}{4\pi}\sum_{i<j}\frac{1-3\cos^2\theta_{i,j}}{r_{i,j}^3} + V_{HC} + V_{trap}\ ,$$

with V_{HC} a short-range repulsive interaction.

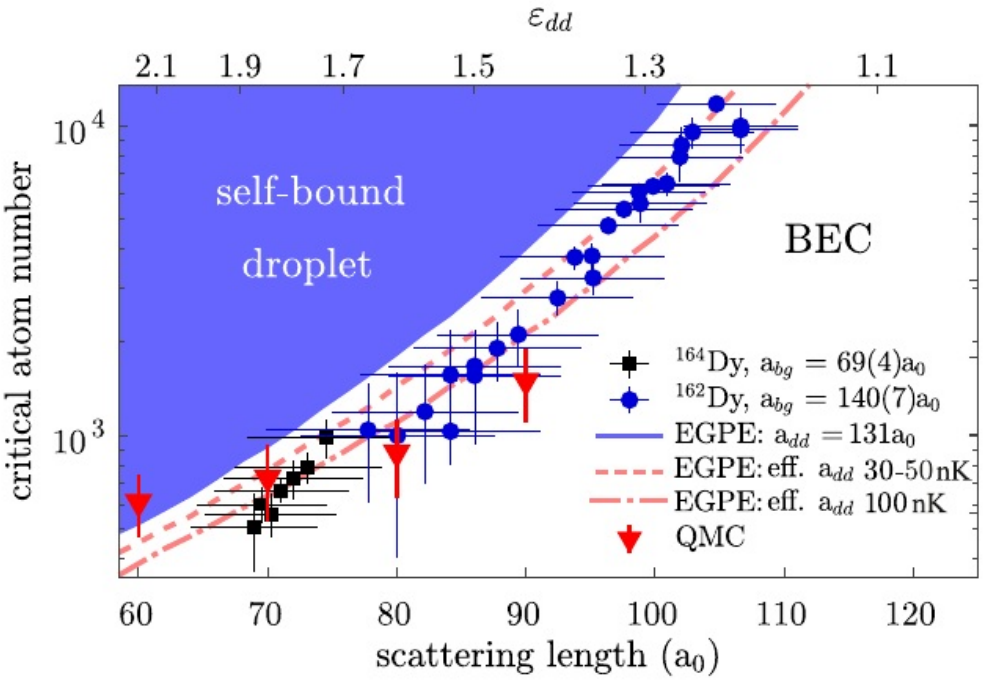
$\Longrightarrow$ Notice the anisotropic character of the dipolar interaction and the combination between repulsive and attractive pairs.

$\Longrightarrow$ The short-range potential part is able to stabilize the system and controls the phase of the system: gas, liquid, ...

$\Longrightarrow$ We use PIGS ($T = 0$) to determine the critical atom number for formation of self-bound systems (drops).

Dipolar droplets

The inclusion of the LHY term seems not to be accurate enough to describe relevant properties of dipolar droplets such as the critical atom number

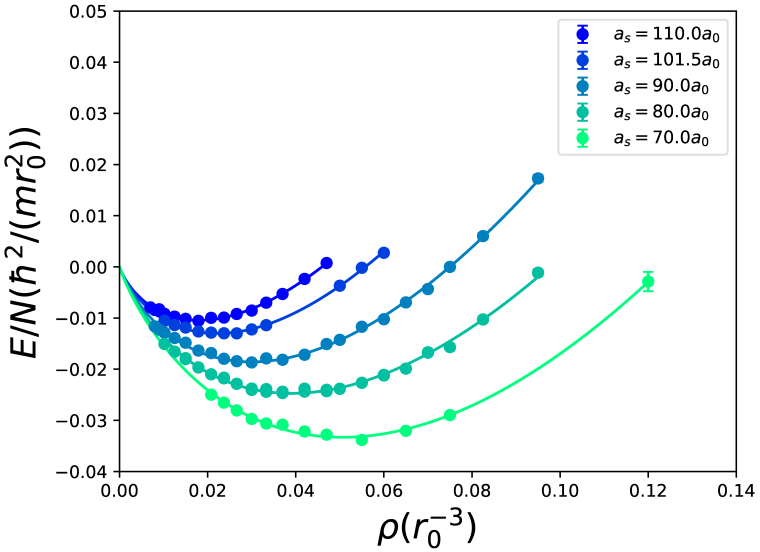


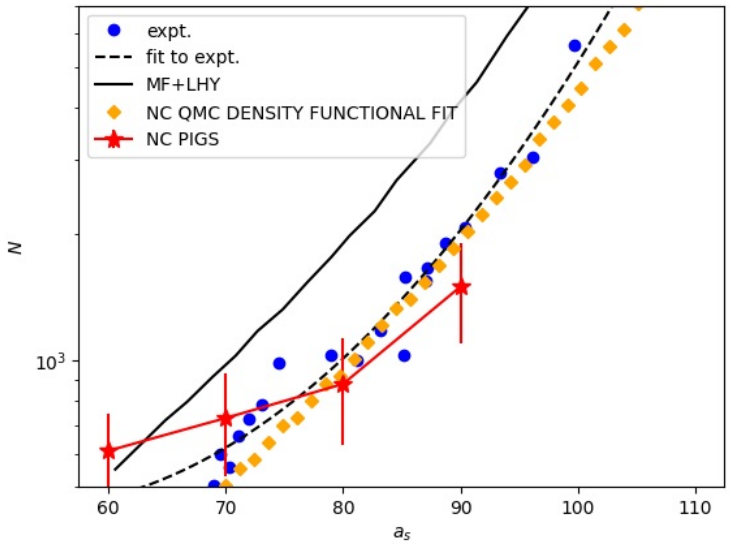
$$\epsilon_{dd} = a_{dd}/a_s, a_{dd} = \mu_0 \mu^2 m/(12\pi\hbar^2)$$

F. Böttcher *et al.*, Phys. Rev. Res. **1**, 033088 (2019)

Dipolar droplets

We are working in a QMC-DFT approach to include efficiently the finite-range effects of the dipolar interaction





Left: DMC results for the equation of state of the bulk liquid; *right:* Our predictions for the critical atom number N_c introducing in the functional the DMC equation of state (work is in progress)

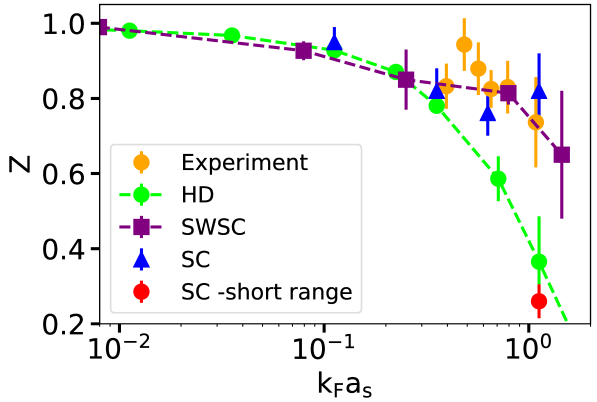
Fermi polaron in 2D

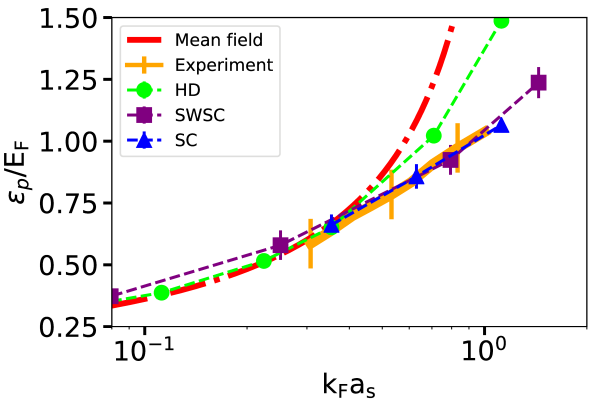
- We studied the repulsive Fermi polaron in a two-component, two-dimensional system of fermionic atoms inspired by the results of a recent experiment with ^{173}Yb atoms [N. Darkwah Oppong *et al.*, Phys. Rev. Lett. **122**, 193604 (2019)]
- We use the diffusion Monte Carlo method to report properties such as the polaron energy and the quasi-particle residue that have been measured in that experiment
- We show that the effective range, together with the scattering length, is needed in order to reproduce the experimental results.
- The Hamiltonian of the system is

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla_{\downarrow}^2 - \frac{\hbar^2}{2m}\sum_{i=1}^{N_\uparrow}\nabla_i^2 + \sum_{j=1}^{N_\uparrow} V^{\rm int}(r_{\downarrow j})$$

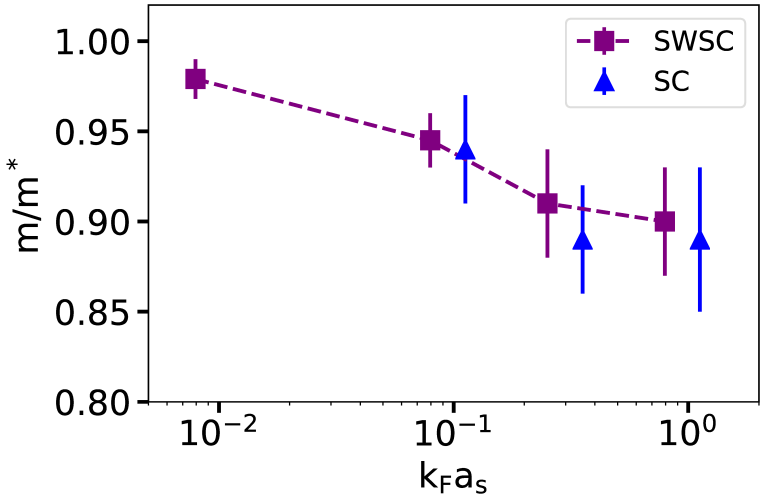
Fermi polaron in 2D

Comparison with experiment (R. Bombín *et al.*, PRA **103**, L041302 (2021)). *Left*, quasi-particle residue; *right*, polaron energy)





Effective mass of the polaron



Summary

- Several experiments in the field of dilute quantum gases point to the necessity of including many-body effects in the theory
- We use QMC methods to go beyond perturbative approximations
- With the QMC data for bulk we build new functionals that seem to produce better results
- The knowledge of the effective range of the atomic interactions helps to improve the results and generate an approximate universal equation of state in terms of two scattering parameters

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THANKS FOR YOUR ATTENTION!