Ground state of the 2D attractive Fermi gas: from few to many body

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Motivation

Two-dimensional Fermi systems constitute a challenging puzzle in theoretical physics. Analytical solutions are scarce and mean field investigations are limited due to the strong influence of quantum and thermal fluctuations.

We apply a *fully ab-initio Quantum Monte Carlo* algorithm to extract multiple ground state properties for systems across a wide range or particle numbers. The approach is not limited to the homogeneous configuration in the ground state and was also applied to trapped systems [1] and systems at finite temperature [2] recently.

Path integral & hybrid Monte Carlo

To project a trial wavefunction $|\psi_T\rangle$ on the ground state, we discretize imaginary time and decouple the interaction with a *Hubbard-Stratonovich transformation*. We can subsequently collect all factors into a path integral and write for the partition function

$$\mathscr{Z} = \langle\psi_T|e^{-\beta\hat{H}}|\psi_T\rangle = \int \mathscr{D}\sigma \,\det U_\sigma^{(\uparrow)}\,\det U_\sigma^{(\downarrow)} \equiv \int \mathscr{D}\sigma\, e^{-S[\sigma]}.$$

The determinants in the integrand originate from using single-particle Slater determinants as trial wavefunctions. We compute the above integral with the *hybrid Monte Carlo (HMC)* algorithm that produces a Markov chain of σ configurations based on the Metropolis algorithm.

2D fermions: essential properties

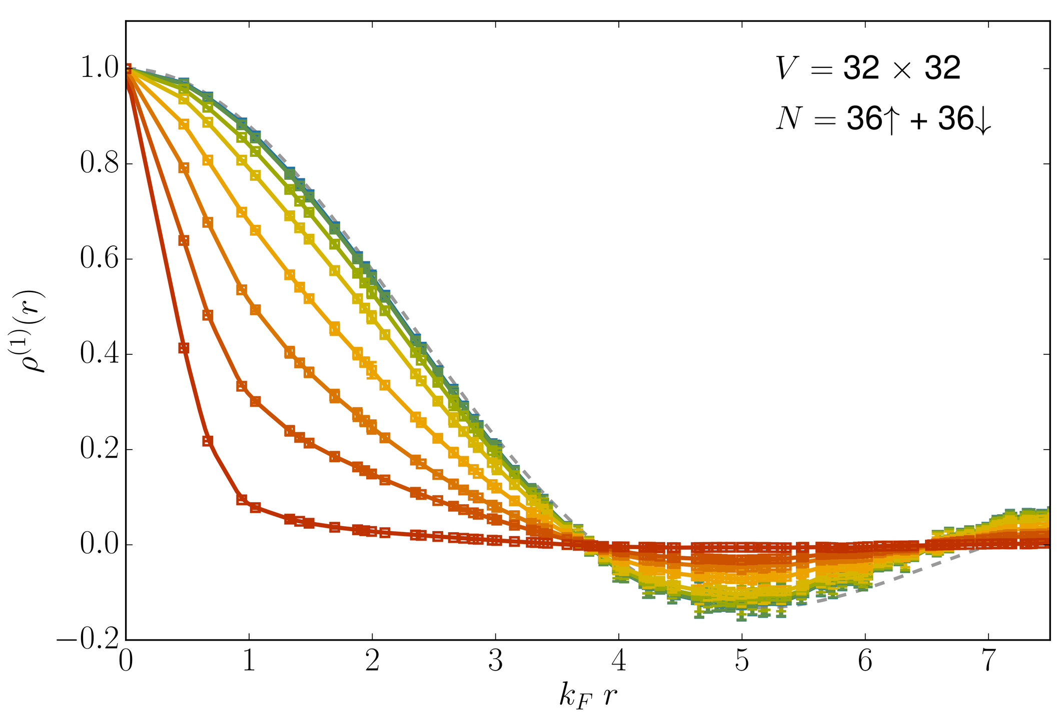
We study a two-component 2D Fermi gas with contact interaction [3], described by

$$\hat{H} = -\sum_{s=\uparrow,\downarrow}\sum_{\mathbf{x}} \hat{\psi}_s^\dagger(\mathbf{x})\frac{\hbar^2\nabla^2}{2m_s}\hat{\psi}_s(\mathbf{x}) + g\sum_{\mathbf{x}}\hat{n}_\uparrow(\mathbf{x})\,\hat{n}_\downarrow(\mathbf{x}).$$

With the convention $\hbar = m = c = 1$, the interaction parameter g becomes dimensionless. To fix the physics we renormalize the coupling with the binding energy ε_B and use $\eta \equiv \frac{1}{2}\ln\frac{\varepsilon_F}{\varepsilon_B} = \ln(k_F a_0)$.

a) One-body density matrix

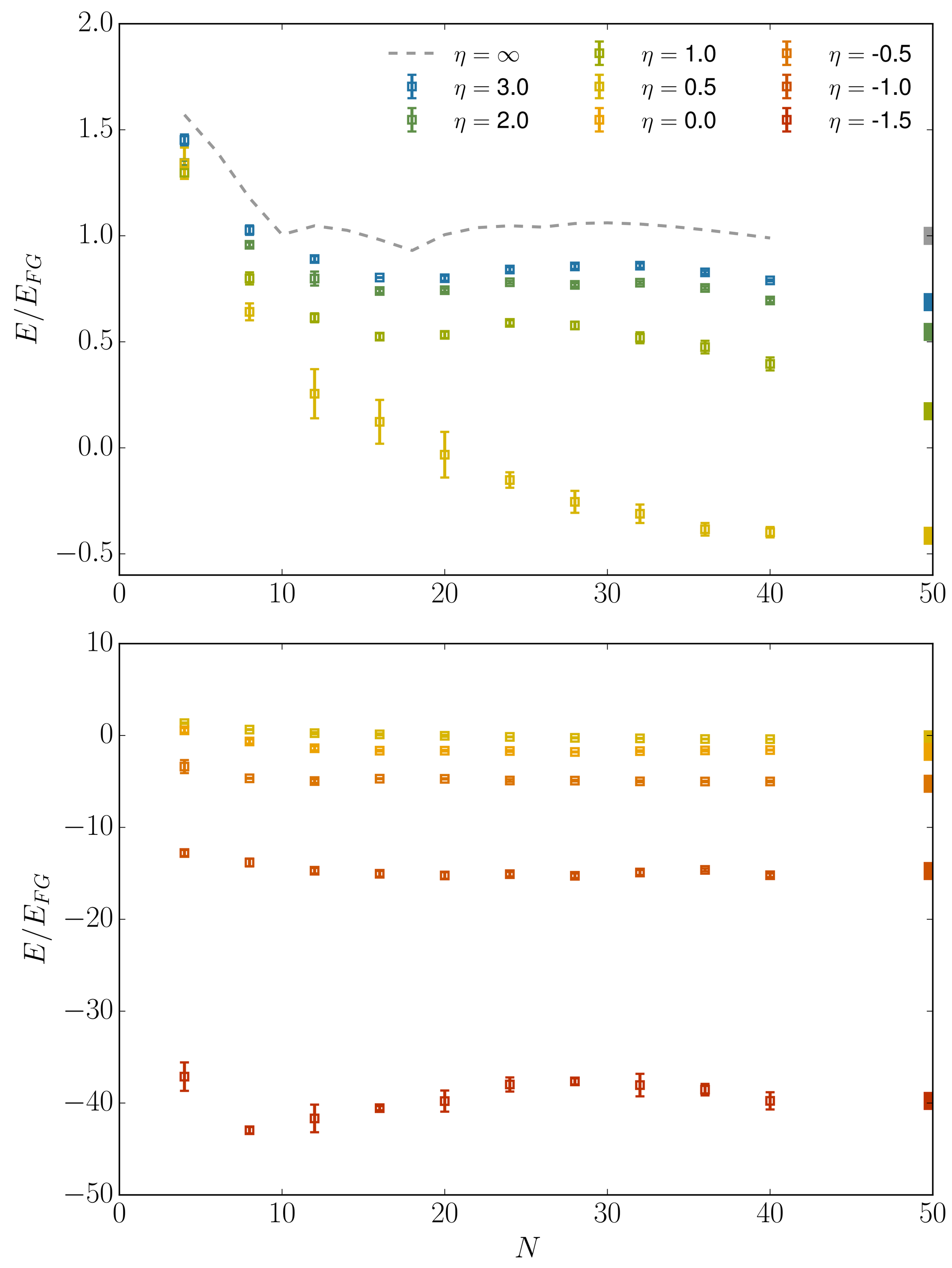
$$\rho_1^{(s)}(r) = \langle\hat{\psi}_{(s)}^\dagger(x+r)\,\hat{\psi}_{(s)}(x)\rangle$$



- $\rho_1 \sim e^{-r/a}$ at large coupling due to formation of dimers
- weakly coupled systems resemble the result of the non-interacting gas in the continuum (dashed gray line)

b) Ground-state energy

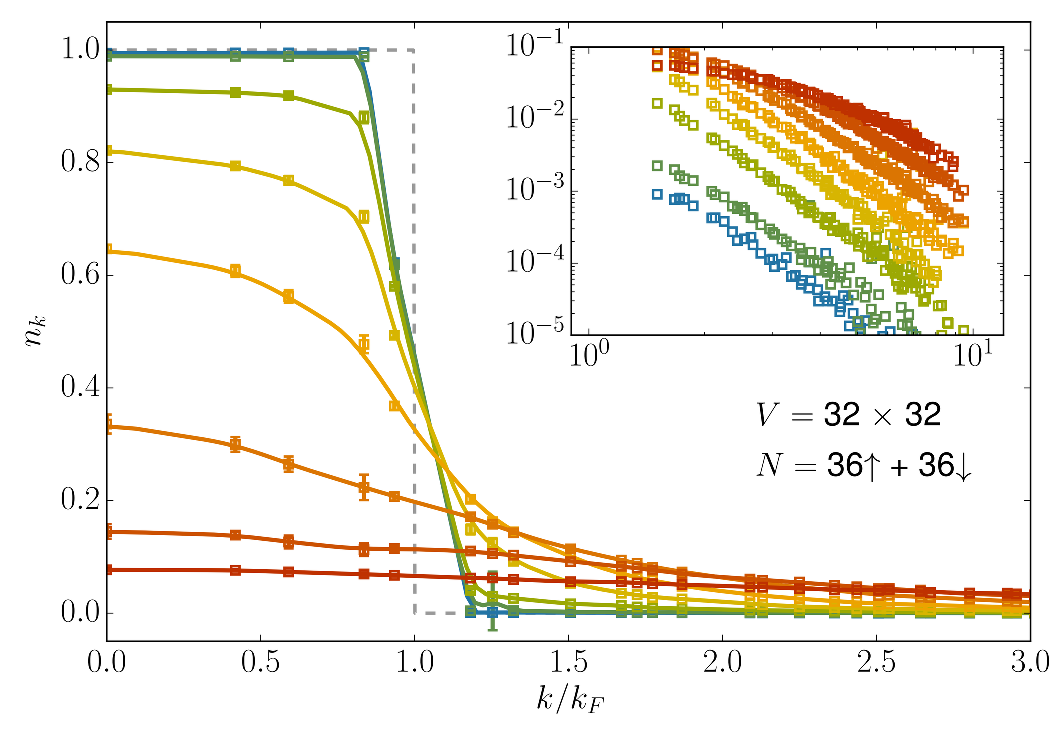
$$\langle E\rangle = -\frac{\partial \ln\mathscr{Z}}{\partial\beta} = -\frac{1}{\mathscr{Z}}\frac{\partial\mathscr{Z}}{\partial\beta}$$



- ground-state energy converges to the value in the thermodynamic limit (TL) as function of N (TL values obtained with FN-DMC [4])
- shell structure only visible for weakly coupled systems, washes out for stronger interaction
- strongly coupled regime (negative values of η) dominated by pair-binding energy

c) Momentum distribution & contact

$$\rho_1^{(s)}(x,x') = \sum_{k,k'}\phi_k^*(x)\,n_{k,k'}^{(s)}\,\phi_{k'}(x')$$



- Fermi surface washes out with increasing coupling indicating formation of composite bosons
- k^{-4} behavior at large momenta, onset shifted towards higher k with increased coupling

Imbalanced systems: complex Langevin

As one moves towards *mass- and spin-imbalanced Fermi systems*, the product of the determinants in the path integral is not guaranteed to be positive semidefinite and one encounters a *sign problem*. In this case the numerical effort of probabilistic approaches such as importance sampling scales exponentially with the system size.

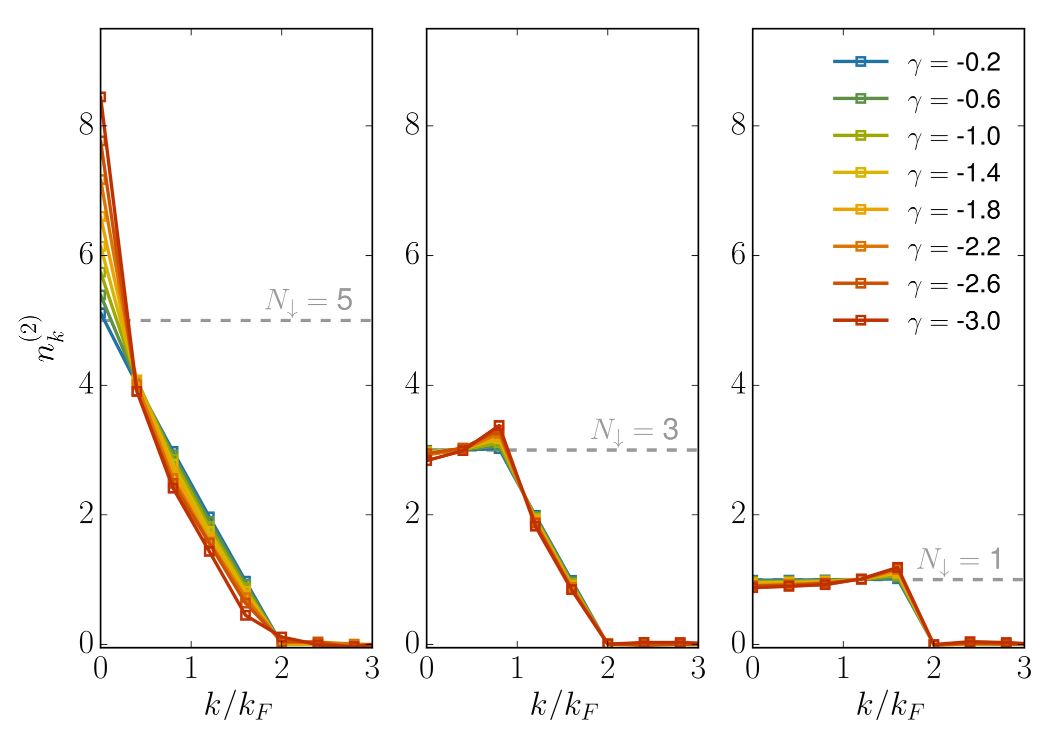
To avoid this issue one can exploit the idea of *stochastic quantization* [5], which states that the stationary distribution of a random process governed by the Langevin equation

$$\frac{\partial\sigma}{\partial t} = -\frac{\delta S[\sigma]}{\delta\sigma} + W$$

equals the distribution of a corresponding Euclidean path integral. Here, W comprises a Gaussian noise term which produces the random distribution of field configurations, or in other words, a random walk in configuration space.

This approach can be extended to complex auxiliary fields in a straightforward manner. The complexification allows to tackle systems governed by a complex action as demonstrated in case of relativistic theories [6]. It has been shown recently that an extension to non-relativistic systems is possible and perfect agreement of complex Langevin results with various other methods was observed for one dimensional mass-imbalanced Fermi systems [7].

a) First results for spin-polarized 1D fermions



b) Outlook

Motivated by these advances, we aim to apply the complex Langevin algorithm to 2D fermionic systems and study

- *FFLO pairing* in polarized 2D systems,
- effect of *mass imbalance in 2D systems* and
- thermodynamics of polarized 2D Fermi systems

in subsequent investigations.

References

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Support

HIC for FAIR Helmholtz International Center

HGS-HIRe for FAIR Helmholtz Graduate School for Hadron and Ion Research