Exact numerical results on the pairing gap, spectral functions, and dynamical response in the two-dimensional Fermi gas

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Using an exact numerical method, we estimate from first principles the pairing gap, the spectral function and response functions for a two-dimensional cold Fermi gas in the BEC-BCS crossover at zero temperature.
Outline

• The cold gas Hamiltonian
• The Auxiliary-Field Quantum Monte Carlo Method
• The calculation of dynamical correlation functions
• The estimation of the pairing gap
• Predictions for the spectral function and response functions: visualization of the BEC-BCS crossover
• Conclusions and perspectives
The cold gas hamiltonian

$\frac{1}{2}$-spin fermions with attractive zero-range interaction

$$\hat{H} = \sum_{\sigma} \int dx \hat{\psi}_\sigma^\dagger (x) \left( -\frac{\hbar^2}{2m} \nabla^2 \right) \hat{\psi}_\sigma (x) - g \int dx \hat{\psi}_\uparrow^\dagger (x) \hat{\psi}_\downarrow^\dagger (x) \hat{\psi}_\downarrow (x) \hat{\psi}_\uparrow (x)$$

• Strongly correlated quantum many body system in the crossover regime
• Relevant model in condensed matter physics, nuclear physics and nuclear astrophysics
• It can be controlled experimentally with unprecedented accuracy
Why two dimensions?

• It is supposed to be a relevant model for high-temperature superconductors
• It could be interesting for pasta phases in neutron stars
• Quantum fluctuations in two-dimensions are expected to be stronger than in three-dimensions
• The BEC-BCS crossover has been less explored in two-dimensions
The lattice hamiltonian

\[ \hat{H} = \sum_{k, \sigma} \varepsilon(k) \hat{c}^\dagger_{k, \sigma} \hat{c}_{k, \sigma} + U \sum_{\mathbf{R}} \hat{n}_{\mathbf{R}, \uparrow} \hat{n}_{\mathbf{R}, \downarrow} \quad \varepsilon(k) = t \ |k|^2 \]

On-site attractive interaction \( U \) tuned to obtain the physical scattering length of the problem in the continuum.

N particles on a lattice with \( M = L \times L \) sites.

Bulk properties obtained via extrapolation to the continuum and thermodynamic limit.
\[ \hat{H} = \sum_{\mathbf{k}, \sigma} \varepsilon(\mathbf{k}) \hat{c}^\dagger_{\mathbf{k}, \sigma} \hat{c}_{\mathbf{k}, \sigma} + U \sum_{\mathbf{R}} \hat{n}_{\mathbf{R}, \uparrow} \hat{n}_{\mathbf{R}, \downarrow} \quad \varepsilon(\mathbf{k}) = t \ |\mathbf{k}|^2 \]

\( \mathbf{k} \in [-\pi, \pi] \times [-\pi, \pi] \) \quad \text{Brillouin zone}

\( \text{Square lattice with } M = L \times L \text{ sites, hosting } N \text{ particles} \)

- The parameters are given by:

\[ t = \frac{\hbar^2}{2m\Delta^2} \quad \text{Hopping} \]

\[ \text{Lattice parameter} \]

\[ U \frac{t}{t} = -\frac{4\pi}{\ln(k_F a) - \ln(C \ n)} \quad n = \frac{N}{L^2}, \quad k_F = \frac{\sqrt{2\pi n}}{\Delta} \]

- Dilute limit: \( n \ll 1 \)
- Continuum limit: \( L \to +\infty \)
- Thermodynamic limit: \( N \to +\infty \)
- Keeping fixed the interaction parameter: \( \ln(k_F a) \)
The Auxiliary-Field Quantum Monte Carlo Method

• Wave-function based projector Quantum Monte Carlo methodology.

\[ |\Psi_0\rangle \propto \lim_{\beta \to +\infty} \exp(-\beta \hat{H}) |\phi_T\rangle \]

• In the simplest case, the trial wave function is chosen to be a Slater determinant with N particles

\[ |\phi_T\rangle = \hat{c}_{u_1}^\dagger \cdots \hat{c}_{u_N}^\dagger |0\rangle \]
• The imaginary time propagator is decomposed in small time propagators

$$\exp \left( -\beta \hat{H} \right) = \left( \exp \left( -\delta \tau \hat{H} \right) \right)^M$$

• The Hubbard-Stratonovich transformation is then used to approximate

$$\exp \left( -\delta \tau \hat{H} \right) \simeq \int dx \ p(x) \ \hat{B}(x)$$
$\hat{B}(x)$ is a single particle propagator: it maps Slater determinants into Slater determinants

$$\exp \left( -\delta \tau \hat{H} \right) | \phi \rangle$$

$$| \phi \rangle = \hat{c}^\dagger_{u_1} \cdots \hat{c}^\dagger_{u_N} | 0 \rangle$$

$$| \phi' \rangle = \hat{c}^\dagger_{\hat{B}(x) u_1} \cdots \hat{c}^\dagger_{\hat{B}(x) u_N} | 0 \rangle$$
In general a complex quantity, in some situations can be real and non-negative, so it can be sampled...
• Explicit Hubbard-Stratonovich transformation (charge decomposition):

\[ e^{-\delta \tau U \hat{n}_{R,\uparrow} \hat{n}_{R,\downarrow}} = e^{-\delta \tau U (\hat{n}_{R,\uparrow} + \hat{n}_{R,\downarrow} - 1)/2} \sum_{\mathbf{X}(\mathbf{R})=\pm 1} \frac{1}{2} e^{\gamma \mathbf{X}(\mathbf{R})} (\hat{n}_{R,\uparrow} + \hat{n}_{R,\downarrow} - 1) \]
\[ \cosh \gamma = e^{\delta \tau |U|/2} \]

• The is no fermion sign problem:

\[ \frac{\langle \Psi_0 | \hat{\mathcal{O}} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = \sum_{\mathbf{X}} \mathcal{W}(\mathbf{X}) \mathcal{O}(\mathbf{X}) \]
\[ \langle \phi_{L} | = \langle \phi_{T} | \prod_{l=M+1}^{2M} \hat{B}(\mathbf{x}_l) | \phi_{R} \rangle = \prod_{l=1}^{M} \hat{B}(\mathbf{x}_l) | \phi_{T} \rangle \]

\[ \mathcal{W}(\mathbf{X}) \propto \prod_{l=1}^{M} p(\mathbf{x}_l) \langle \phi_{L} | \phi_{R} \rangle \]
\[ \mathcal{W}(\mathbf{X}) \geq 0 \quad \text{No sign problem!} \]
\[ \text{in the spin-balanced case} \]
Manifold of $N$ particles
Slater Determinants

\[ \hat{O} \]

\[ \langle \phi_L | \psi_R \rangle \]

\[ \langle \phi_T | \psi_T \rangle \]

\[ \left( \begin{array}{ccc} u_1(R_1) & \ldots & u_N(R_1) \\ u_1(R_2) & \ldots & u_N(R_2) \\ u_1(R_3) & \ldots & u_N(R_3) \\ \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots \\ u_1(R_{L\times L}) & \ldots & u_N(R_{L\times L}) \end{array} \right) \otimes \left( \begin{array}{ccc} u_{N+1}(R_1) & \ldots & u_N(R_1) \\ u_{N+1}(R_2) & \ldots & u_N(R_2) \\ u_{N+1}(R_3) & \ldots & u_N(R_3) \\ \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots \\ u_{N+1}(R_{L\times L}) & \ldots & u_N(R_{L\times L}) \end{array} \right) \]

Dilute system: $N \ll L \times L$

Manifold of $N$ particles Slater Determinants

stored as a matrix
• With this method we can compute any expectation value on the ground state of the physical system.
The calculation of dynamical correlation functions

\[ \frac{\langle \Psi_0 | \hat{O} e^{-\tau \hat{H}} \hat{O}^\dagger | \Psi_0 \rangle}{\langle \Psi_0 | e^{-\tau \hat{H}} | \Psi_0 \rangle} \]

Manifold of N particles Slater Determinants
• Standard approaches rely on commutators:

\[
\frac{\langle \Psi_0 | \hat{O} e^{-\tau \hat{H}} \hat{O}^\dagger | \Psi_0 \rangle}{\langle \Psi_0 | e^{-\tau \hat{H}} | \Psi_0 \rangle}
\]

\[
\int dx \ p(x) \hat{B}(x) \hat{O}^\dagger | \phi_R \rangle \quad \overset{?}{\rightarrow} \quad \int dx \ p(x) \hat{O}^\dagger \hat{B}(x) | \phi_R \rangle
\]

• This in general requires at least (Number of sites)^3 operations.
• Not effi
• We intr
Dynamical Green functions

\[ \frac{\langle \Psi_0 | \hat{O} e^{-\tau \hat{H}} \hat{O}^\dagger | \Psi_0 \rangle}{\langle \Psi_0 | e^{-\tau \hat{H}} | \Psi_0 \rangle} \]

\[ \hat{O} = \hat{c}_R, \uparrow \]

- We simply add a column to the matrices
- The dependence of the complexity on the number of lattice sites does not change with respect to static computations

\[ \langle \phi_L | \hat{O} \hat{O}^\dagger | \phi_R \rangle \]

\[ \langle \phi_T | \]

Manifold of N particles Slater Determinants

N+1 particles Slater Determinants
Dynamical structure factors

\[
\frac{\langle \Psi_0 | \hat{O} e^{-\tau \hat{H}} \hat{O}^\dagger | \Psi_0 \rangle}{\langle \Psi_0 | e^{-\tau \hat{H}} | \Psi_0 \rangle} = \hat{n}_{\mathbf{R}, \uparrow} = \hat{c}_{\mathbf{R}, \uparrow}^\dagger \hat{c}_{\mathbf{R}, \uparrow}
\]

- One Slater determinant is transformed into a linear combination of two determinants.
- The dependence of the complexity on the number of lattice sites does not change with respect to static computations.

\[
\hat{n}_{\mathbf{R}, \uparrow} = \frac{e^{\hat{n}_{\mathbf{R}, \uparrow}} - 1}{e - 1}
\]
• The method allows us to provide unbiased estimations of correlation functions in imaginary time

• Dynamical Green functions

\[ G^p(\mathbf{k}, \tau) = \langle \hat{c}_k e^{-\tau(\hat{H} - \mu \hat{N})} \hat{c}_k^{\dagger} \rangle \quad G^h(\mathbf{k}, \tau) = \langle \hat{c}_k^{\dagger} e^{-\tau(\hat{H} - \mu \hat{N})} \hat{c}_k \rangle \]

• Spin density and density correlation functions

\[ F^{S,D}(\mathbf{k}, \tau) = \langle (\hat{n}_k, \uparrow \pm \hat{n}_k, \downarrow) e^{-\tau \hat{H}} (\hat{n}_{-k, \uparrow \pm \hat{n}_{-k, \downarrow}}) \rangle \]

• With a very favourable complexity as a function of the lattice size
What can we learn from these correlation functions?

• Dynamical Green functions

• Pairing gap $\Delta$

$$E_{0}^{N+1} - E_{0}^{N} = \mu + \Delta$$

$$E_{0}^{N-1} - E_{0}^{N} = -\mu + \Delta$$

• Spectral function

$$A(k, \omega) = \Im \left( \frac{1}{\omega - \hat{H} + i0^{+}} \langle \hat{c}_{k}^\dagger \rangle + \langle \hat{c}_{k} \rangle \right)$$
• Spin density and density structure factors:

• Spin and density structure factors

\[ S^{D,S}(\mathbf{k}, \omega) = \frac{1}{2\pi N} \int_0^{+\infty} dt \, e^{i\omega t} \langle \hat{n}^{D,S}_\mathbf{k}(t) \hat{n}^{D,S}_{-\mathbf{k}}(0) \rangle \]
Why do we need dynamical correlations to compute the pairing gap?

- A static computation requires three independent simulations, with N, N+1 and N-1 particles.
- For the spin unbalanced cases, fermion sign problem is present.
- The complexity does not change if we compute the dynamical correlations.
The estimation of the pairing gap

\[ E_0^{N+1} - E_0^N = \mu + \Delta \]
\[ E_0^{N-1} - E_0^N = -\mu + \Delta \]

\[ G^p(\mathbf{k}, \tau) = \langle \hat{c}_k e^{-\tau(\hat{H} - \mu \hat{N})} \hat{c}_k^\dagger \rangle \]
\[ G^h(\mathbf{k}, \tau) = \langle \hat{c}_k^\dagger e^{-\tau(\hat{H} - \mu \hat{N})} \hat{c}_k \rangle \]

• Quasi particles dispersion relations:

• Particles
  \[ \omega^+(\mathbf{k}) = - \lim_{\tau \to +\infty} \frac{\log (G^p(\mathbf{k}, \tau))}{\tau} \]

• Holes
  \[ \omega^-(\mathbf{k}) = - \lim_{\tau \to +\infty} \frac{\log (G^h(\mathbf{k}, \tau))}{\tau} \]
\[
\log \left( k_F a \right) = 1.5
\]
\[
N = 50
\]
\[
L = 41 \times 41
\]
\[
\frac{k}{k_F} = 1
\]

Estimation of uncertainty includes QMC error bar, uncertainty on fitting parameters and interval in imaginary time.
$\log(k_F a) = 1.5$

$N = 50$

$L = 41 \times 41$

$\frac{k}{k_F} = 1$

Estimation of uncertainty includes QMC error bar, uncertainty on fitting parameters and interval in imaginary time
- Momentum dependent quasi-particles energies: BEC regime

\[ \ln(k_F a) = 0 \]

We compute the correlations functions for \( N = 18, 26, 42, 50 \) particles on lattices with 25x25, 35x35, 39x39 and 41x41 sites.
• Momentum dependent quasi-particles energies: BCS regime

\[ \ln(k_F a) = 1 \]

We compute the correlations functions for \( N = 18, 26, 42, 50 \) particles on lattices with 25x25, 35x35, 39x39 and 41x41 sites.
• Pairing gap is the minimum (maximum) of the particles (holes) dispersion
• Results for the pairing gap in the BEC-BCS crossover

\[ \frac{\left( \Delta + \varepsilon_b/2 \right)}{\varepsilon_F} \]

- this work
- Galea et al. (2016)
- Bertaina and Giorgini (2011)
- mean field
A similar calculation for repulsive Hubbard model at half-filling

Charge gap as a function of the interaction parameter

Small U: Slater insulator

Large U: Mott insulator with charge gap close to the one-dimensional exact result from Bethe ansatz
Predictions for the spectral function and response functions: visualization of the BEC-BCS crossover

$$A(k, \omega) = \Im \left( \frac{1}{\omega + \hat{H} + i0^+} \hat{c}_k \right) + \left( \frac{1}{\omega - \hat{H} + i0^+} \hat{c}_k \right)$$

• This function can be directly measured in ARPES experiments
• It provides a map of the single-particle states accessible for the many body system
We use the state-of-art Genetic Inversion via Falsification of theories method to estimate the spectral function.

\[ G^p(k, \tau) = \langle \hat{c}_k e^{-\tau(\hat{H} - \mu \hat{N})} \hat{c}_k^\dagger \rangle \]

\[ G^h(k, \tau) = \langle \hat{c}_k^\dagger e^{-\tau(\hat{H} - \mu \hat{N})} \hat{c}_k \rangle \]

\[ A(k, \omega) = \Im \left( \frac{1}{\omega + \hat{H} + i0^+} \langle \hat{c}_k \rangle + \langle \hat{c}_k^\dagger \frac{1}{\omega - \hat{H} + i0^+} \hat{c}_k^\dagger \rangle \right) \]
Statistical and computational intelligence approach to analytic continuation in Quantum Monte Carlo

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\[ \frac{\omega}{\epsilon_F} \]

(a) \( \ln(k_F a) = 0 \)
(b) \( \ln(k_F a) = 0.5 \)
(c) \( \ln(k_F a) = 1 \)
(d) \( \ln(k_F a) = 1.5 \)

BEC
BCS
Response functions and visualization of the BEC-BCS crossover: atoms or molecules?

\[ S^{D,S}(k, \omega) = \frac{1}{2\pi N} \int_{0}^{+\infty} dt \, e^{i\omega t} \langle \hat{n}^{D,S}_k(t) \hat{n}^{D,S}_{-k}(0) \rangle \]

- This function can be directly measured in two-photons Bragg scattering experiments, or, in condensed matter physics, in neutron scattering experiments.
- It provides a map of the collective excitations of the system.
\[
\left\langle \left( \hat{n}_{\mathbf{k},\uparrow} \pm \hat{n}_{\mathbf{k},\downarrow} \right) e^{-\tau \hat{H}} \left( \hat{n}_{-\mathbf{k},\uparrow} \pm \hat{n}_{-\mathbf{k},\downarrow} \right) \right\rangle
\]

Density and spin density imaginary time correlation functions

Analytic continuation problem

\[ S^{D,S}(\mathbf{k}, \omega) \] (spin) density structure factors

Can be measured experimentally using two-photons Bragg spectroscopy
• The high momentum behavior contains information about the recoil of single atoms or molecules, depending on the regime
(a) $\ln(k_Fa) = 0$
(b) $\ln(k_Fa) = 0.5$
(c) $\ln(k_Fa) = 1$
(d) $\ln(k_Fa) = 1.5$
Conclusions and perspectives

• Using an exact method, we computed dynamical correlations in imaginary time for the Fermi gas with zero range attractive interactions
• We provided an unbiased estimation of the pairing gap through the BEC-BCS crossover
• Performing analytic continuation, we provided predictions for the spectral function and the dynamical structure factors, which allow us to visualize the crossover
• We plan to extend the calculations to cold atoms in optical lattices, systems with spin-orbit coupling ...
Thank you for the attention