Ground state energy of the dilute spin-polarized Fermi gas

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Introduction

Fermi gas in box $\Lambda = [0, L]^3$. Hamiltonian

$$H_N = \sum_{i=1}^{N} -\Delta_{x_i} + \sum_{1\le j<k\le N} V(x_j - x_k).$$

Interaction V is

- Repulsive: $V \ge 0$,
- Radial and compactly supported,
- Possibly with a 'hard core': $V(x) = +\infty$ for $|x| \le R_0$.

Spin-polarized (=**spinless**) fermions: Antisymmetric wave functions

$$\psi_N \in L^2_a(\Lambda^N; \mathbb{C}) = \bigwedge^N L^2(\Lambda; \mathbb{C}).$$

Ground state energy per particle

$$\frac{e(\rho)}{\rho} = \lim_{\substack{N,L\to\infty \\ N/L^3=\rho}} \frac{E_N}{N}, \qquad E_N = \inf_{\psi_N \in L^2_a(\Lambda^N;\mathbb{C})} \frac{\langle \psi_N | H_N | \psi_N \rangle}{\langle \psi_N | \psi_N \rangle}.$$

Dilute limit: Particle density ρ small compared to **p-wave scattering length** of V.

Scattering length

Definition. *The **p-wave scattering length** a is given by*

$$12\pi a^3 = \inf\left\{ \int_{\mathbb{R}^3} |x|^2 \left(|\nabla f(x)|^2 + \frac{1}{2} V(x) |f(x)|^2 \right) \mathrm{d}x : f(x) \to 1 \text{ as } |x| \to \infty \right\}.$$

*Minimizing f is the **p-wave scattering function**.*

Definition. *The **p-wave effective range** r_{eff} is given by*

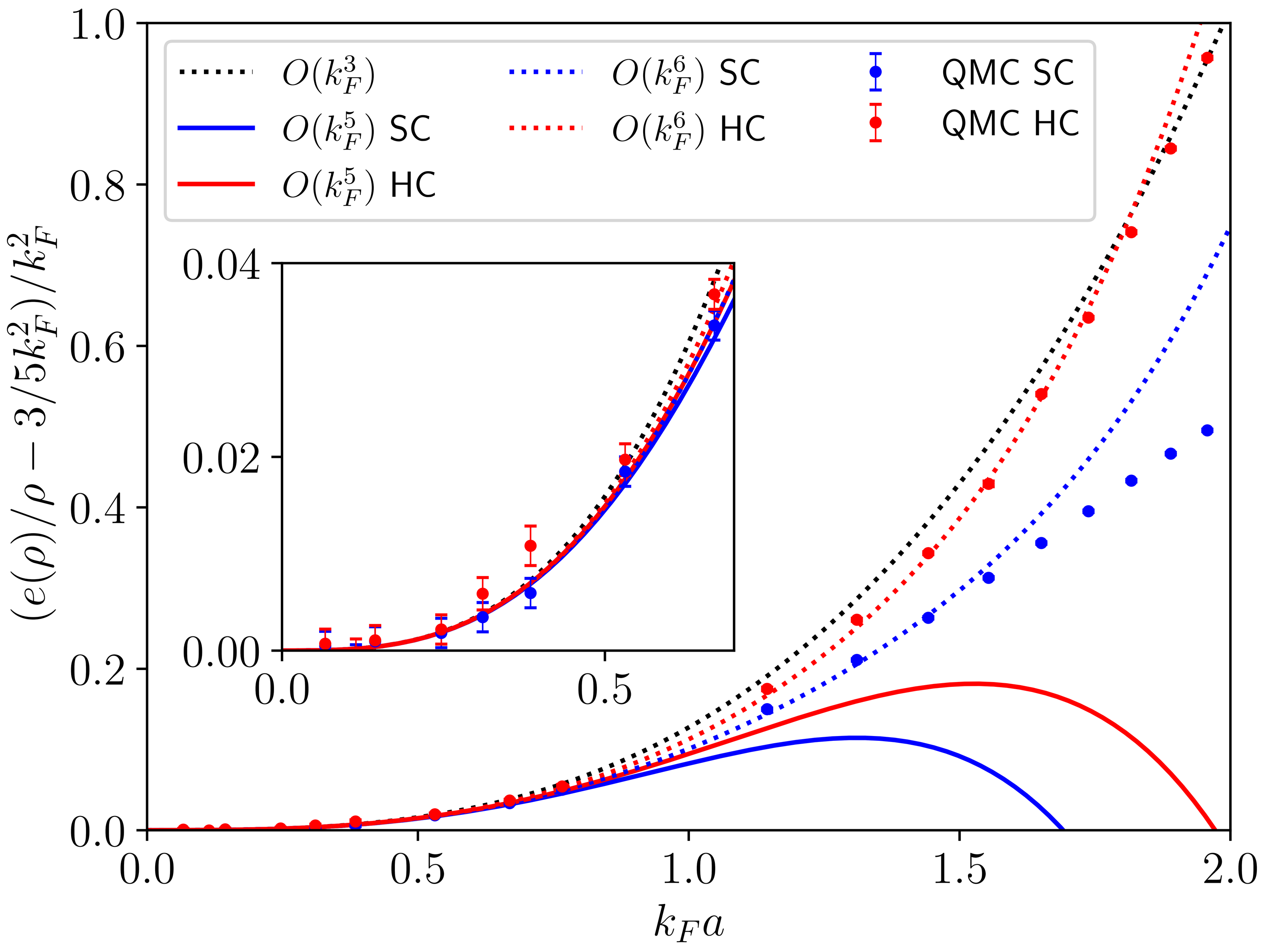
$$r_{\mathrm{eff}}^{-1} = \frac{1}{10\pi a^6} \int_{\mathbb{R}^3} |x|^4 \left(|\nabla f(x)|^2 + \frac{1}{2} V(x) |f(x)|^2 \right) \mathrm{d}x,$$

where f is the p-wave scattering function.

Conjecture

Physics prediction: (Fermi momentum $k_F = (6\pi^2)^{1/3}\rho^{1/3}$)

$$\frac{e(\rho)}{\rho} = k_F^2 \left[\frac{3}{5} + \frac{2}{5\pi} a^3 k_F^3 - \frac{1}{35\pi} a^6 r_{\mathrm{eff}}^{-1} k_F^5 + \frac{2066 - 312\log 2}{10395\pi^2} a^6 k_F^6 + \dots \right].$$



QMC are Quantum Monte Carlo computations from (Bertaina, Tarallo and Pilati, Phys Rev A (2023)).
SC and HC are 'soft' and 'hard core' interactions.

Main theorems

Theorem. *Let $V \ge 0$ be radial and compactly supported. Then, for small ak_F, (with Fermi momentum $k_F = (6\pi^2)^{1/3}\rho^{1/3}$)*

$$\frac{e(\rho)}{\rho} \le k_F^2 \left[\frac{3}{5} + \frac{2}{5\pi} a^3 k_F^3 - \frac{1}{35\pi} a^6 r_{\mathrm{eff}}^{-1} k_F^5 + O\left((ak_F)^{5+1/7} |\log ak_F|^6 \right) \right].$$

Theorem. *Let $V \in L^1$ be non-negative, radial and compactly supported. Then, for small ak_F,*

$$\frac{e(\rho)}{\rho} \ge k_F^2 \left[\frac{3}{5} + \frac{2}{5\pi} a^3 k_F^3 + O((ak_F)^{3+3/10} |\log ak_F|) \right].$$

Naive heuristics

1st order perturbation theory

Ground state of free system ($V \equiv 0$): Slater determinant of momenta in Fermi ball $B_F = \{|k| \le k_F\} \cap \frac{2\pi}{L}\mathbb{Z}^3$

$$\psi_F(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \det[f_k(x_j)]_{\substack{k\in B_F, \\ 1\le j\le N}}, \qquad f_k(x) = L^{-3/2} e^{ikx}.$$

Interacting energy of free state

$$\frac{1}{N} \langle \psi_F | H_N | \psi_F \rangle = \frac{3}{5} k_F^2 + \frac{1}{2} \rho^{-1} \int V(x) \rho_F^{(2)}(x, 0)\, \mathrm{d}x.$$

Taylor expand $\rho_F^{(2)}$ and use 1st term in Born series for scattering length:

$$\rho_F^{(2)}(x, 0) \approx \frac{1}{5} k_F^2 \rho^2 |x|^2, \qquad 24\pi a^3 \approx \int |x|^2 V(x)\, \mathrm{d}x.$$

Conclude

$$\frac{1}{N} \langle \psi_F | H_N | \psi_F \rangle \approx k_F^2 \left[\frac{3}{5} + \frac{2}{5\pi} a^3 k_F^3 \right].$$

Implementing correlations

Upper bound

Trial state of **Jastrow** type:

$$\psi_{\mathrm{Jas}}(x_1, \dots, x_N) = \frac{1}{\sqrt{C_N}} \prod_{1\le j<k\le N} f(x_j - x_k) \psi_F(x_1, \dots, x_N).$$

Compute $\langle \psi_{\mathrm{Jas}} | H_N | \psi_{\mathrm{Jas}} \rangle$ using **Fermionic cluster expansion**.

Lower bound

Define unitary e^B with

$$B = \sum_{1\le i<j\le N} P_i \otimes P_j [1 - f(x_i - x_j)] Q_i \otimes Q_j - \text{h.c.}.$$

$P = \chi(-\Delta \le k_F^2)$ and $Q = \mathbb{1} - P$ projections onto small and large momenta. As operators:

$$e^{-B} H_N e^B = N k_F^2 \left[\frac{3}{5} + \frac{2}{5\pi} a^3 k_F^3 \right] + H_N^{\mathrm{eff}} + \mathcal{E}.$$

With $H_N^{\mathrm{eff}} \ge 0$ as operators and $\mathcal{E}$ small error.

References

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A. B. Lauritsen and R. Seiringer. "Ground state energy of the dilute spin-polarized Fermi gas: Lower bound". arXiv:2402.17558 [math-ph]. 2024

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