Energies of dilute Fermi gases

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Many-body quantum system with N particles in large box $\Lambda = [0, L]^3$ and Hamiltonian

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

- Kinetic energy: Laplacian $-\frac{\hbar^2}{2m}\Delta_{x_j} = -\Delta_{x_j}$. (Units with $\hbar = 2m = 1$.)
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I.e. energy in state $\psi_N \in L^2([0, L]^{3N})$ is

$$\langle \psi_N | H_N | \psi_N \rangle = \int \cdots \int_{[0,L]^{3N}} \left[\sum_{j=1}^{N} |\nabla_{x_j} \psi_N(x_1, \ldots, x_N)|^2 \right.$$
$$\left. + \sum_{1 \le j < k \le N} V(x_j - x_k) |\psi_N(x_1, \ldots, x_N)|^2 \right] \mathrm{d}x_1 \ldots \mathrm{d}x_N.$$

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We consider the **ground state energy**

$$E_N = \inf_{\psi_N : \|\psi_N\|_{L^2} = 1} \langle \psi_N | H_N | \psi_N \rangle ,$$

Appropriate wave functions ψ_N depend on particle statistics.

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- **Bosons**: Symmetric wave functions:

$$\psi_N(x_1, \ldots, x_j, \ldots, x_k, \ldots, x_N) = \psi_N(x_1, \ldots, x_k, \ldots, x_j, \ldots, x_N)$$

- **Spin-polarized / Spinless Fermi gas**: Anti-symmetric wave functions:

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  Can be realized experimentally using Feshbach resonances (for e.g. ^{6}Li, ^{40}K): "*p*-wave fermions"

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We consider ground state energy density in thermodynamic limit

$$e(\rho) = \lim_{\substack{L\to\infty \\ N/L^3\to\rho}} \inf_{\substack{\psi_N \text{ appropriate statistics} \\ \|\psi_N\|_{L^2}=1}} \frac{\langle \psi_N | H_N | \psi_N \rangle}{L^3},$$

Dilute regime $\longrightarrow$ Scattering lengths

Dilute limit: Interparticle spacing $\rho^{-1/3}$ large compared to lengthscale of interaction.

(Think, V has finite range R_0, then $\rho^{-1/3} \gg R_0$, i.e.; $\rho R_0^3 \ll 1$.)

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$\rightsquigarrow$ Study minimal energy of two particles in large box $\Lambda = [0, L]^3$ with

- no symmetry (bosons or fermions of different spin) $\rightsquigarrow$ s-wave: $E \simeq \frac{8\pi a_s}{L^3}$
- fermionic symmetry (fermions of same spin) $\rightsquigarrow$ p-wave: $E \simeq \frac{4\pi^2}{L^2} + \frac{16\pi^3 a_p^3}{L^5}$

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Definition

The s- and p-wave scattering lengths a_s and a_p are defined by

$$4\pi a_s = \inf\left\{\int_{\mathbb{R}^3}\left(|\nabla f|^2 + \frac{1}{2}Vf^2\right)\mathrm{d}x : f(x) \to 1 \text{ for } |x| \to \infty\right\},$$

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

$$8\pi a_s = \int_{\mathbb{R}^3} f_s V \approx \int_{\mathbb{R}^3} V, \quad 24\pi a_p^3 = \int_{\mathbb{R}^3} |x|^2 f_p V \approx \int_{\mathbb{R}^3} |x|^2 V \quad \text{for smooth and small } V.$$

Two particles in a (periodic) box

Non-interacting ground state: (Easy exercise)

$$\psi_0(x,y) = \begin{cases} \frac{1}{L^3} & \text{for different spins,} \\ \frac{2}{L^3}\cos\left(\frac{2\pi}{L}\frac{x^1+y^1}{2}\right)\sin\left(\frac{\pi}{L}(x^1-y^1)\right) & \text{for same spins,} \end{cases}$$

Interacting ground state is of form $\psi(x,y) = f(x-y)\psi_0(x,y)$ for some f. (By translation invariance)

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The interacting ground state is given by the non-interacting ground state multiplied by the scattering function $f_{s/p}$.

Asymptotic energy expansions

Theorem (Spin-$\frac{q-1}{2}$ Fermi gas (Lieb–Seiringer–Solovej 2005))

Let $V \geq 0$ be radial and of compact support (finite range). Then,

$$e(\rho) = \frac{3}{5}\left(\frac{6\pi^2}{q}\right)^{2/3}\rho^{5/3} + 4\pi a_s \rho^2 \left(1 - \frac{1}{q}\right)(1 + o(1)), \qquad a_s^3\rho \ll 1.$$

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- Kinetic energy of free gas.
- Interaction energy.
  - Energy of one pair of different spins is $8\pi a_s / L^3$. (Definition of a_s)
  - $\sum_{1 \leq \sigma < \tau \leq q} N_\sigma N_\tau$ many such pairs ($= N_\uparrow N_\downarrow$ in spin-$\frac{1}{2}$ case)
  - Balance of spins: $\rho_\sigma = \frac{\rho}{q}$. ($\rho_\uparrow = \rho_\downarrow = \frac{\rho}{2}$ for spin-$\frac{1}{2}$ case)

  $\rightsquigarrow$ Energy density $\sum_{1 \leq \sigma < \tau \leq q} 8\pi a_s \rho_\sigma \rho_\tau = \frac{q(q-1)}{2} 8\pi a_s (\frac{\rho}{q})^2 = 4\pi a_s \rho^2 (1 - \frac{1}{q})$.

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Theorem (Spinless Fermi gas (L.–Seiringer 2024))

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$$e(\rho) = \frac{3}{5}(6\pi^2)^{2/3}\rho^{5/3} + \frac{12\pi}{5}(6\pi)^{2/3} a_p^3 \rho^{8/3}(1 + o(1)), \qquad a_p^3\rho \ll 1.$$

1st order perturbation theory — Naive $a^3\rho^{8/3}$

- Take trial state ψ_F ground state of free gas: (easy calculation)

$$\lim_{\substack{N,L\to\infty \\ N/L^3=\rho}} \frac{\langle \psi_F | H_N | \psi_F \rangle}{L^3} = \frac{3}{5}(6\pi^2)^{2/3}\rho^{5/3} + \frac{1}{2}\int_{\mathbb{R}^3} \rho^{(2)}(x,0) V(x)\,\mathrm{d}x.$$

- Taylor expand $\rho^{(2)}(x,0) \simeq \frac{(6\pi^2)^{2/3}}{5}\rho^{8/3}|x|^2$ and use $\int_{\mathbb{R}^3} |x|^2 V(x)\,\mathrm{d}x \approx 24\pi a_p^3$

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Need to treat interactions more precisely

Recall from two-particle problem:

The interacting ground state is given by the non-interacting ground state multiplied by the scattering function $f_{s/p}$.

$\rightsquigarrow$ Use f_p to construct better trial state.

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$$\psi_N(x_1,\ldots,x_N) = \frac{1}{\sqrt{C_N}}\prod_{1\le i<j\le N} f_p(x_i - x_j)D_N(x_1,\ldots,x_N)$$

D_N Slater determinant (think free ground state ψ_F), C_N normalization constant.

Cluster expansion

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Compute energy (easy calculation)

$$\langle \psi_N | H_N | \psi_N \rangle = E_0 + \iint_{[0,L]^6} \rho^{(2)}_{\mathrm{Jas}}(x_1, x_2) \left(\left| \frac{\nabla f_p(x_1 - x_2)}{f_p(x_1 - x_2)} \right|^2 + \frac{1}{2} V(x_1 - x_2) \right) \mathrm{d}x_1 \, \mathrm{d}x_2$$

$$+ \text{3-body term}$$

E_0 kinetic energy of D_N, $\rho^{(2)}_{\mathrm{Jas}}$ the 2-particle density.

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Think $\rho^{(2)}_{\mathrm{Jas}}(x_1,x_2) \simeq f_p(x_1-x_2)^2 \rho^{(2)}(x_1,x_2)$. (Recall $12\pi a_p^3 = \int_{\mathbb{R}^3} (|\nabla f_p|^2 + \frac{1}{2} V f_p^2)|x|^2\,\mathrm{d}x$.)

Compute $\rho^{(2)}_{\mathrm{Jas}} \rightsquigarrow$ **Cluster expansion**: Way of calculating $\rho^{(n)}_{\mathrm{Jas}}$. (Formal calculations of Gaudin–Gillespie–Ripka 1971.) (Hard) combinatorics problem.