Ground state energy and pressure of a dilute spin-polarized Fermi gas*

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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 $-\Delta_{x_j}$
- Interaction energy: Pairwise interaction $v \ge 0$, radial and of compact support.

For ground state energy:

- Spin-$\frac{1}{2}$ Fermi gas: Realize H_n on $L^2_a(\Lambda^n; \mathbb{C}^2) = \bigwedge^n L^2(\Lambda; \mathbb{C}^2)$ or $L^2_a(\Lambda^{n_\uparrow}) \otimes L^2_a(\Lambda^{n_\downarrow})$ if fixed number of spin $\uparrow$ and $\downarrow$
- Spin-polarized Fermi gas: Realize H_n on $L^2_a(\Lambda^n) = \bigwedge^n L^2(\Lambda)$

For the pressure: Realize on Fock spaces

$$\mathcal{F} = \bigoplus_{n=0}^{\infty} \bigwedge^n L^2(\Lambda; \mathbb{C}^2) \quad = \bigoplus_{n=0}^{\infty} L^2_a(\Lambda^n; \mathbb{C}^2) \quad \text{spin-1/2 fermions}$$

$$\mathcal{F} = \bigoplus_{n=0}^{\infty} \bigwedge^n L^2(\Lambda) \quad = \bigoplus_{n=0}^{\infty} L^2_a(\Lambda^n) \quad \text{spin-polarized fermions}$$

Interested in ground state energy in the thermodynamic limit

$$e(\rho) = \lim_{\substack{L\to\infty \\ N/|\Lambda|\to\rho}} \inf_{\psi\in L^2_a(\Lambda^N)} \frac{\langle\psi|H_N|\psi\rangle / \langle\psi|\psi\rangle}{|\Lambda|},$$

$$e(\rho_\uparrow,\rho_\downarrow) = \lim_{\substack{L\to\infty \\ N_\sigma/|\Lambda|\to\rho_\sigma}} \inf_{\psi\in L^2_a(\Lambda^{N_\uparrow})\otimes L^2_a(\Lambda^{N_\downarrow})} \frac{\langle\psi|H_N|\psi\rangle / \langle\psi|\psi\rangle}{|\Lambda|}$$

or pressure in the thermodynamic limit

$$\psi(\beta,\mu) = \lim_{L\to\infty} \frac{1}{\beta|\Lambda|} \log \mathrm{Tr}_{\mathcal{F}}\left[e^{-\beta(\mathcal{H}-\mu\mathcal{N})}\right] = \lim_{L\to\infty} \sup_{\Gamma} P_\Lambda[\Gamma]$$

at temperature $T = 1/\beta > 0$ and chemical potential μ.

- $\mathcal{H} = \bigoplus_{n=0}^\infty H_n$ is the Hamiltonian on Fock space.
- $\mathcal{N} = \bigoplus_{n=0}^\infty n$ is the number operator.
- $P_\Lambda[\Gamma]$ is the pressure functional of the state Γ. A state Γ is an operator on $\mathcal{F}$ with $0 \le \Gamma \le 1$ and $\mathrm{Tr}_{\mathcal{F}}\,\Gamma = 1$.

$$L^3 P_\Lambda[\Gamma] = \mathrm{Tr}_{\mathcal{F}}[\mathcal{H}\Gamma] - \frac{1}{\beta}S(\Gamma) = \mathrm{Tr}_{\mathcal{F}}[\mathcal{H}\Gamma] + \frac{1}{\beta}\mathrm{Tr}_{\mathcal{F}}\left[\Gamma\log\Gamma\right].$$

Scattering lengths

Dilute limit: ρ small compared to scattering length of v, i.e. $a^3\rho \ll 1$.

$\rightsquigarrow$ Expect only pairwise interactions (to leading order)

$\rightsquigarrow$ Study minimal energy of two particles in a box with

- no symmetry (fermions of different spin) $\rightsquigarrow$ s-wave,
- fermionic symmetry (fermions of same spin) $\rightsquigarrow$ p-wave.

Definition

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

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

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

$$8\pi a_s \simeq \int v, \qquad 24\pi a_p^3 \simeq \int |x|^2 v \qquad \text{for smooth and small } v.$$

Bosons

Realize $H_N = \sum_{j=1}^N -\Delta_{x_j} + \sum_{1\le i<j\le N} v(x_i - x_j)$ on $L_s^2(\Lambda^N) = L^2(\Lambda)^{\otimes_{\mathrm{sym}} N}$.

Theorem (Dyson 1957; Lieb–Yngvason 1998 (+ many others))

For appropriate v we have

$$e_{\mathrm{Bose}}(\rho) = 4\pi a_s \rho^2 \left[1 + \frac{128}{15\sqrt{\pi}}(a_s^3\rho)^{1/2} + o((a_s^3\rho)^{1/2})\right], \qquad a_s^3\rho \ll 1.$$

- Energy of one pair of particles is $8\pi a_s/L^3$. (Short calculation)
- There are $N(N-1)/2 \simeq N^2/2$ many pairs.

$\rightsquigarrow$ Energy density $4\pi a_s\rho^2$.

Goal for fermions: Find "analogue of $4\pi a_s\rho^2$" for both zero and positive temperature.

Spin-1/2 Fermi gas

Theorem (Lieb–Seiringer–Solovej 2005)

Let $v \geq 0$ be radial and of compact support. Then for $a_s^3\rho \ll 1$

$$e(\rho_\uparrow, \rho_\downarrow) = \frac{3}{5}(6\pi^2)^{2/3}\left(\rho_\uparrow^{5/3} + \rho_\downarrow^{5/3}\right) + 8\pi a_s \rho_\uparrow \rho_\downarrow + a_s \rho^2 \delta(a_s^3\rho),$$

with $\rho = \rho_\uparrow + \rho_\downarrow$ and $-C(a_s^3\rho)^{1/39} \leq \delta(a_s^3\rho) \leq C(a_s^3\rho)^{2/27}$.

Theorem (Seiringer 2006)

Let $v \geq 0$ be radial and of compact support. Then for small $a_s^3\rho$ uniformly in $T = 1/\beta \lesssim \rho^{2/3}$

$$\psi(\beta, \mu) = \psi_0(\beta, \mu) - 2\pi a_s \rho^2 [1 + o(1)].$$

- Kinetic energy/pressure of free gas.
- Interaction energy. Similar to $4\pi a_s \rho^2$ for the Bose gas:
  - Energy of one pair of spin-↑ and spin-↓ is $8\pi a_s / L^3$. (Short calculation)
  - $N_\uparrow N_\downarrow$ many such pairs $\rightsquigarrow$ Energy density $8\pi a_s \rho_\uparrow \rho_\downarrow$.
- $T_F \sim \rho^{2/3}$ is the **Fermi temperature**. For higher temperatures expect thermal effects stronger than quantum and so gas should behave like classical gas.

Next order

$$e(\rho_\uparrow, \rho_\downarrow) = \frac{3}{5}(6\pi^2)^{2/3}\left(\rho_\uparrow^{5/3} + \rho_\downarrow^{5/3}\right) + 8\pi a_s \rho_\uparrow \rho_\downarrow + a_s \rho^2 \delta(a_s^3 \rho).$$

Expect the **Huang-Yang term** for $\rho_\uparrow = \rho_\downarrow = \rho/2$

$$\delta(a_s^3\rho) = c_{\mathrm{HY}} a_s \rho^{1/3} + o(a_s \rho^{1/3}), \qquad c_{\mathrm{HY}} = \frac{4(11 - 2\log 2)}{35\pi^2}\left(\frac{3}{4\pi}\right)^{4/3}$$

$\rightsquigarrow$ "Optimal" error is $\delta(a_s^3\rho) = O((a_s^3\rho)^{1/3})$.

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Expect the **Huang-Yang term** for $\rho_\uparrow = \rho_\downarrow = \rho/2$

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$\rightsquigarrow$ "Optimal" error is $\delta(a_s^3\rho) = O((a_s^3\rho)^{1/3})$.

Bounds on the error: (Assume always $v \geq 0$ radial and compactly supported.)

$-(a_s^3\rho)^{1/39} \lesssim \delta(a_s^3\rho) \lesssim (a_s^3\rho)^{2/27}$	(Lieb–Seiringer–Solovej 2005)
$-(a_s^3\rho)^{1/9} \lesssim \delta(a_s^3\rho) \lesssim (a_s^3\rho)^{2/9}$	v smooth (Falconi–Giacomelli–Hainzl–Porta 2021)
$-(a_s^3\rho)^{1/5} \lesssim \delta(a_s^3\rho) \lesssim (a_s^3\rho)^{1/3}$	v smooth (Giacomelli 2022)
$\delta(a_s^3\rho) \lesssim_\varepsilon (a_s^3\rho)^{1/3-\varepsilon}$ for any $\varepsilon > 0$	(L. 2023)

Spin-polarized Fermi gas

Theorem (L.–Seiringer 2023)

Let $v \geq 0$ be radial and of compact support. Then for $a_p^3\rho \ll 1$

$$e(\rho) \leq \frac{3}{5}(6\pi^2)^{2/3}\rho^{5/3} + \frac{12\pi}{5}(6\pi)^{2/3}a_p^3\rho^{8/3}\left[1 - \frac{1}{14}(6\pi^2)^{2/3}a_p^3 R_{\text{eff}}^{-1}\rho^{2/3}(1+o(1))\right].$$

$$R_{\text{eff}}^{-1} = \frac{1}{10\pi a_p^6}\int_{\mathbb{R}^3}|x|^4\left(|\nabla f_p(x)|^2 + \frac{1}{2}v(x)|f_p(x)|^2\right)\mathrm{d}x \qquad \text{the effective range.}$$

Expected from physics literature with $=$ (Efimov–Amus'ya 1965; Efimov 1966; Ding–Zhang 2019)

Theorem (L.–Seiringer 2023)

Let $v \geq 0$ be radial and of compact support. Then for $a_p^3\rho \ll 1$ uniformly in $T = 1/\beta \lesssim \rho^{2/3}$

$$\psi(\beta,\mu) \geq \psi_0(\beta,\mu) - 12\pi c_{\beta,\mu}a_p^3\rho^{8/3}[1+o(1)].$$

$T_F \sim \rho^{2/3}$ is the **Fermi temperature**. For higher temperatures expect thermal effects stronger than quantum and so gas should behave like classical gas.

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

Zero temperature:

- Take trial state ψ_{free} ground state of free gas:

$$\lim_{N,|\Lambda|\to\infty} \frac{\langle \psi_{\text{free}}|H_N|\psi_{\text{free}}\rangle}{|\Lambda|} = \frac{3}{5}(6\pi^2)^{2/3}\rho^{5/3} + \frac{1}{2}\int \rho^{(2)}(x,0)v(x)\,\mathrm{d}x.$$

- Taylor $\rho^{(2)}(x,0) \simeq \frac{(6\pi^2)^{2/3}}{5}\rho^{8/3}|x|^2$ and use $\int |x|^2 v(x)\,\mathrm{d}x \simeq 24\pi a_p^3$
- $\rightsquigarrow$ Energy density $\frac{3}{5}(6\pi^2)^{2/3}\rho^{5/3} + \frac{12\pi}{5}(6\pi^2)^{2/3}a_p^3\rho^{8/3}$.

Positive temperature:

- Compute pressure functional of free state:

$$\lim_{L\to\infty} P_\Lambda[\Gamma_{\text{free}}] = \psi_0(\beta,\mu) - \frac{1}{2}\int \rho^{(2)}(x,0)v(x)\,\mathrm{d}x.$$

- Taylor expand $\rho^{(2)}(x,0) \simeq c_{\beta,\mu}|x|^2\rho^{8/3}$ and use $\int |x|^2 v(x) \simeq 24\pi a_p^3$.
- $\rightsquigarrow$ Pressure contribution $-12\pi c_{\beta,\mu}a_p^3\rho^{8/3}$.

Need to include interactions in trial state $\rightsquigarrow$ include the scattering functions f_p in trial state.

Cluster expansion (spin-polarized case at zero temperature)

We consider Jastrow-type trial state

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

f_p now scaled and cut-off version of scattering function, D_N Slater determinant, C_N normalization constant.

Compute energy

$$\langle \psi_N | H_N | \psi_N \rangle = E_0 + \iint \rho^{(2)}_{\mathrm{Jas}}(x_1, x_2) \left(\left| \frac{\nabla f(x_1 - x_2)}{f(x_1 - x_2)} \right|^2 + \frac{1}{2} v(x_1 - x_2) \right) \mathrm{d}x_1 \, \mathrm{d}x_2$$

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

E_0 kinetic energy of Slater determinant, $\rho^{(2)}_{\mathrm{Jas}}$ the 2-particle density. Think $\rho^{(2)}_{\mathrm{Jas}}(x_1, x_2) \simeq f(x_1 - x_2)^2 \rho^{(2)}(x_1, x_2)$.

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

Sketch of calculation of normalization constant C_N:

$$C_N = \int \cdots \int \prod_{i<j} f_{ij}^2 |D_N|^2 = \int \cdots \int \prod_{e \in \text{Complete graph}} (1 + g_e) \det[\gamma_{ij}]_{i,j \le N}$$

$$= \int \cdots \int \left[1 + \sum_{p=2}^{N} \binom{N}{p} \sum_{G \in \mathcal{G}_p} \prod_{e \in G} g_e \right] \det[\gamma_{ij}]_{i,j \le N}$$

$$= N! \left[1 + \sum_{p=2}^{N} \frac{1}{p!} \int \cdots \int \sum_{G \in \mathcal{G}_p} \prod_{e \in G} g_e \det[\gamma_{ij}]_{i,j \le p} \right]$$

$$= N! \left[1 + \sum_{p=2}^{\infty} \frac{1}{p!} \int \cdots \int \sum_{G \in \mathcal{G}_p} \prod_{e \in G} g_e \sum_{\pi \in \mathcal{S}_p} (-1)^{\pi} \prod_{j=1}^{p} \gamma_{j\pi(j)} \right].$$

- $g(x) = f(x)^2 - 1$, and for $e = (i,j)$ denote $g_e = g_{ij} = g(x_i - x_j) = f(x_i - x_j)^2 - 1$.
- $\gamma_{ij} = \gamma^{(1)}(x_i; x_j) = \frac{1}{L^3} \sum_{k \in M_F} e^{ik(x_i - x_j)}$ the one-particle density matrix of ψ_N. Here M_F is some set of momenta (think $M_F \simeq B_F$ the Fermi ball).
- $|D_N|^2 = \det[\gamma^{(1)}(x_i; x_j)]_{1 \le i,j \le N}$, the square of the Slater determinant.
- $\mathcal{G}_p$: Set of all graphs on p vertices with all vertices degree ≥ 1.

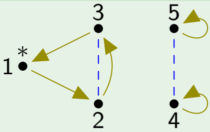
Definition (Diagrams)

- $\mathcal{G}_p^q$: Set of all graphs on q "external" and p "internal" vertices with all internal vertices degree ≥ 1.
- A **diagram** (π, G) (on (q, p) vertices) is a pair of
  - a permutation $\pi \in \mathcal{S}_{q+p}$ (viewed as a directed graph)
  - a graph $G \in \mathcal{G}_p^q$.
- $\mathcal{D}_p^q$: Set of all diagrams (on (q, p) vertices).
- Value of $(\pi, G) \in \mathcal{D}_p^q$ is

$$\Gamma^q_{\pi,G}(x_1, \ldots, x_q) := (-1)^\pi \int \cdots \int \prod_{e \in G} g_e \prod_{j=1}^{p} \gamma_{j\pi(j)} \, \mathrm{d}x_{q+1} \ldots \mathrm{d}x_{q+p}.$$

- A diagram (π, G) is **linked** if $\pi \cup G$ is connected.
- $\mathcal{L}_p^q$: Set of all linked diagrams (on (q, p) vertices).
- $\tilde{\mathcal{L}}_p^q$: Set of all diagrams (on (q, p) vertices) with each linked component having ≥ 1 external vertex.

Example



$$= \iiiint g_{23} g_{45} \gamma_{12} \gamma_{23} \gamma_{31} \gamma_{44} \gamma_{55} \, \mathrm{d}x_2 \, \mathrm{d}x_3 \, \mathrm{d}x_4 \, \mathrm{d}x_5$$

Decomposing into linked components gives ("standard" cluster expansion)

$$\frac{C_N}{N!} = 1 + \sum_{p=2}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{D}_p} \Gamma_{\pi,G} = \exp\left[\sum_{p=2}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p} \Gamma_{\pi,G}\right].$$

Similarly

$$\rho_{\text{Jas}}^{(q)} = \left[\prod_{1\le i<j\le q} f_{ij}^2\right] \sum_{p=0}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\tilde{\mathcal{L}}_p^q} \Gamma_{\pi,G}^q = \left[\prod_{1\le i<j\le q} f_{ij}^2\right] \left[\rho^{(q)} + \sum_{p=1}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\tilde{\mathcal{L}}_p^q} \Gamma_{\pi,G}^q\right].$$

Valid for both zero and positive temperature – only different $\gamma^{(1)}$'s

Absolute convergence:

$$\sum_{p=2}^{\infty} \frac{1}{p!} \left| \sum_{(\pi,G)\in\tilde{\mathcal{L}}_p^q} \Gamma_{\pi,G}^q \right| < \infty.$$

(Non-trivial) combinatorics: reduces to

$$\rho \int |g(x)|\,\mathrm{d}x \int |\gamma^{(1)}(x;0)|\,\mathrm{d}x = \rho \times a_p^3 \left|\log a_p^3 \rho\right| \times \int_{[0,L]^3} |\gamma^{(1)}(x)|\,\mathrm{d}x < c_q.$$

Absolute convergence at zero temperature

Absolute convergence

$\gamma^{(1)}(x) = \frac{1}{L^3}\sum_{k\in M_F} e^{ikx}$. Thus absolute convergence if

$$a_p^3\rho \left|\log a_p^3\rho\right| \times \frac{1}{L^3}\int_{[0,L]^3} \left|\sum_{k\in M_F} e^{ikx}\right| \mathrm{d}x < c.$$

Introduce Fermi polyhedron:

For Fermi ball B_F and Fermi polyhedron P_F (Kolomoitsev–Lomako 2018):

$$\frac{1}{L^3}\int_{[0,L]^3} \left|\sum_{k\in B_F} e^{ikx}\right| \mathrm{d}x \sim N^{1/3}, \qquad \frac{1}{L^3}\int_{[0,L]^3} \left|\sum_{k\in P_F} e^{ikx}\right| \mathrm{d}x \lesssim s(\log N)^3.$$

s is number of corners of P_F – some parameter to choose.

- Finite size error from kinetic energy $\sim N^{-1/3}\rho^{5/3}$.
- Leading energy density from interaction $\sim a_p^3\rho^{8/3}$.

$\rightsquigarrow$ Need $N^{-1/3}\rho^{5/3} \ll a_p^3\rho^{8/3}$, i.e. $N^{1/3}a_p^3\rho \gg 1$.

$\rightsquigarrow$ **Can't use Fermi ball.**

Absolute convergence at positive temperature

Absolute convergence

$$\gamma^{(1)}(x) = \frac{1}{L^3} \sum_{k \in \frac{2\pi}{L}\mathbb{Z}^3} \frac{1}{1 + e^{\beta|k|^2 - \beta\mu}} e^{ikx}, \qquad \int_\Lambda |\gamma^{(1)}(x)| \, \mathrm{d}x \le C\rho\beta^{3/2}.$$

Thus absolute convergence if

$$a_p^3\rho \left| \log a_p^3\rho \right| \beta^{3/2}\rho < c.$$

Uniform in volume

Satisfied for not too small temperatures:

$$T = \frac{1}{\beta} > C\rho^{2/3}(a_p^3\rho|\log a_p^3\rho|)^{2/3} \sim T_F(a_p^3\rho|\log a_p^3\rho|)^{2/3}.$$

For smaller temperatures compare to zero-temperature problem to prove theorem.

Thanks for your attention!

A. B. Lauritsen. "Almost optimal upper bound for the ground state energy of a dilute Fermi gas via cluster expansion". arXiv:2301.08005 [math-ph]. 2023.

A. B. Lauritsen and R. Seiringer. "Ground state energy of the dilute spin-polarized Fermi gas: Upper bound via cluster expansion". arXiv:2301.04894 [math-ph]. 2023.

A. B. Lauritsen and R. Seiringer. "Pressure of a dilute spin-polarized Fermi gas: Lower bound". arXiv:2307.01113 [math-ph]. 2023.