A kinetic Dirac interpolation theorem for homogeneous quasi-free fermions

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May 13, 2026

Abstract

How much exchange energy can a homogeneous fermion gas concede beyond the Dirac value, and what controls the deviation? We answer this question completely within the gauge-invariant quasi-free class. The bound we obtain interpolates between the Dirac constant $C_D(q)$, attained at the unpolarized Fermi ball, and the fully spin-polarized constant $C_D(1)$, attained in the large-kinetic-excess regime. The interpolation parameter is the homogeneous kinetic ratio $R = \tau/(K_D(q)\rho^{5/3}) \geq 1$, which the Pauli principle forces above unity. The proof rests on two classical inputs: the Riesz rearrangement inequality, which bounds the exchange integral by the value at indicator-of-ball occupations, and the bathtub principle, which converts the kinetic budget into a spin-polarization constraint. A short Lyapunov-style interpolation between ℓ^1 and $\ell^{5/3}$ then yields the explicit $\sqrt{R}$ law and the small-excess slope at $R = 1$. The result isolates what the quasi-free framework alone can establish about the Lieb–Oxford problem.

1 Introduction

How does the exchange energy of a homogeneous fermion gas depend on its kinetic budget? The classical Dirac formula $e_x = -C_D(q)\rho^{4/3}$ describes the unpolarized Fermi sea, but the same density supports a continuum of homogeneous quasi-free states with strictly larger kinetic energy. The natural question is whether, and how, the Dirac constant can degrade across that family. The Lieb–Oxford program identifies $C_D(q)$ as the right benchmark constant for unpolarized matter; outside the quasi-free class, getting a sharp universal lower bound is a longstanding open problem.

This note answers the homogeneous quasi-free version of the question in closed form. We work with gauge-invariant quasi-free states in the thermodynamic limit, parametrized by occupation functions $0 \leq n_\sigma(k) \leq 1$. The Pauli principle forces the homogeneous kinetic ratio

$$R = \frac{\tau}{K_D(q)\rho^{5/3}}$$

to be at least one, with equality only at the unpolarized Fermi ball. Theorem 2.1 states that for the entire quasi-free class

$$e_x(n) \geq -C_D(q)\min\{\sqrt{R},\, q^{1/3}\}\,\rho^{4/3},$$

which reduces to the Dirac bound $-C_D(q)\rho^{4/3}$ at $R = 1$ and saturates at the fully spin-polarized value $-C_D(1)\rho^{4/3}$ for $R \geq q^{2/3}$. The mechanism is transparent: kinetic excess can only widen the exchange constant by spin polarization, and the Pauli phase-space constraint converts a

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kinetic budget into a permitted level of polarization. The two-page proof combines the Riesz rearrangement inequality with the bathtub principle and an ℓ^p interpolation step.

The takeaway for the Lieb–Oxford problem is structural. The bound here is tight within the quasi-free framework; any further descent toward the Lieb–Oxford constant C_{LO} must therefore originate in genuine two-particle correlation, not in one-particle phase-space rearrangement.

Plan of the paper. Section 2 sets up notation and states the main theorem. Section 3 proves the one-spin exchange bound via Riesz rearrangement. Section 4 establishes the kinetic moment constraint via the bathtub principle. Section 5 assembles these ingredients into the proof of the main theorem and records the small-excess expansion.

2 Statement

Fix spin degeneracy q. A homogeneous gauge-invariant quasi-free fermion state in the thermodynamic limit is described by occupation functions

$$0 \le n_\sigma(k) \le 1, \qquad \sigma = 1, \dots, q, \qquad k \in \mathbb{R}^3.$$

Its spin densities and kinetic-energy densities are

$$\rho_\sigma = (2\pi)^{-3} \int_{\mathbb{R}^3} n_\sigma(k)\, \mathrm{d}k, \qquad \tau_\sigma = (2\pi)^{-3} \int_{\mathbb{R}^3} |k|^2 n_\sigma(k)\, \mathrm{d}k.$$

Set

$$\rho = \sum_{\sigma=1}^{q} \rho_\sigma, \qquad \tau = \sum_{\sigma=1}^{q} \tau_\sigma.$$

Let

$$K_D(q) = \frac{3}{5}(6\pi^2)^{2/3} q^{-2/3}, \qquad C_D(q) = \frac{3}{4}\left(\frac{6}{\pi}\right)^{1/3} q^{-1/3}.$$

Define the homogeneous kinetic ratio

$$R = \frac{\tau}{K_D(q)\rho^{5/3}}.$$

By the Pauli principle $R \ge 1$.

The exchange energy density of the quasi-free state is

$$e_x(n) = -\frac{1}{2}\sum_{\sigma=1}^{q}(2\pi)^{-6} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{4\pi}{|k-\ell|^2} n_\sigma(k) n_\sigma(\ell)\, \mathrm{d}k\, \mathrm{d}\ell.$$

Theorem 2.1 (Quasi-free kinetic Dirac interpolation)**.** *For every homogeneous quasi-free fermion state,*

$$e_x(n) \ge -C_D(q)\, \min\{\sqrt{R}, q^{1/3}\}\, \rho^{4/3}.$$

In particular, when $R \downarrow 1$,

$$e_x(n) \ge -C_D(q)\rho^{4/3} - \frac{1}{2}C_D(q)(R-1)\rho^{4/3} + O((R-1)^2)\rho^{4/3}.$$

Thus the lower bound has the Dirac constant as its small-excess kinetic limit.

Remark 2.2. The statement is positive, not a no-go result. Across the homogeneous quasi-free class, the Dirac constant follows from two ingredients alone: the Pauli phase-space constraint and the kinetic ratio. The large-R saturation value $C_D(1)$ is the fully spin-polarized exchange constant; it does not descend to the Lieb–Oxford constant C_{LO}, because quasi-free states carry no correlation energy beyond exchange.

3 Exchange rearrangement

Lemma 3.1 (One-spin exchange maximization)**.** *Let* $0 \le n(k) \le 1$ *and*

$$\rho_n = (2\pi)^{-3} \int n(k)\, \mathrm{d}k.$$

Then

$$\frac{1}{2}(2\pi)^{-6} \iint \frac{4\pi}{|k-\ell|^2} n(k) n(\ell)\, \mathrm{d}k\, \mathrm{d}\ell \le C_D(1)\rho_n^{4/3}.$$

Equality holds for the indicator of a ball, up to translation.

Proof. The kernel $|k-\ell|^{-2}$ is radially decreasing. By the Riesz rearrangement inequality, the left side is maximized, among all functions $0 \le n \le 1$ with fixed integral, by the symmetric decreasing rearrangement $n^* = \mathbf{1}_{B_{k_n}}$, where

$$\frac{|B_{k_n}|}{(2\pi)^3} = \rho_n, \qquad k_n = (6\pi^2 \rho_n)^{1/3}.$$

For this ball,

$$\iint_{B_{k_n} \times B_{k_n}} \frac{4\pi}{|k-\ell|^2}\, \mathrm{d}k\, \mathrm{d}\ell = 16\pi^3 k_n^4.$$

Therefore

$$\begin{aligned} \frac{1}{2}(2\pi)^{-6} 16\pi^3 k_n^4 &= \frac{k_n^4}{8\pi^3} \\ &= \frac{3}{4}\left(\frac{6}{\pi}\right)^{1/3} \rho_n^{4/3} = C_D(1)\rho_n^{4/3}. \end{aligned}$$

□

4 Kinetic moment constraint

Lemma 4.1 (Spin-density moment bound)**.** *For each spin component,*

$$\tau_\sigma \ge K_D(1)\rho_\sigma^{5/3}, \qquad K_D(1) = \frac{3}{5}(6\pi^2)^{2/3}.$$

Consequently, with $a_\sigma = \rho_\sigma/\rho$,

$$\sum_{\sigma=1}^{q} a_\sigma^{5/3} \le R q^{-2/3}.$$

Proof. Among all $0 \le n \le 1$ with fixed integral, the moment $\int |k|^2 n(k)\, \mathrm{d}k$ is minimized by filling a ball centered at the origin. This is the bathtub principle. Thus

$$\tau_\sigma \ge (2\pi)^{-3} \int_{|k| \le (6\pi^2 \rho_\sigma)^{1/3}} |k|^2\, \mathrm{d}k = K_D(1)\rho_\sigma^{5/3}.$$

Summing over σ gives

$$\tau \ge K_D(1)\rho^{5/3} \sum_\sigma a_\sigma^{5/3}.$$

Since $K_D(q) = K_D(1)q^{-2/3}$, this is equivalent to

$$\sum_\sigma a_\sigma^{5/3} \le R q^{-2/3}.$$

□

5 Proof of the theorem

Proof of Theorem 2.1. By Theorem 3.1,

$$-e_x(n) \le C_D(1) \sum_{\sigma=1}^{q} \rho_\sigma^{4/3} = C_D(1)\rho^{4/3} \sum_{\sigma=1}^{q} a_\sigma^{4/3}.$$

The elementary interpolation inequality between ℓ^1 and $\ell^{5/3}$ gives

$$\sum_{\sigma=1}^{q} a_\sigma^{4/3} \le \left(\sum_{\sigma=1}^{q} a_\sigma^{5/3} \right)^{1/2}, \qquad \sum_{\sigma} a_\sigma = 1, \quad a_\sigma \ge 0.$$

Indeed,

$$\|a\|_{4/3} \le \|a\|_1^{3/8} \|a\|_{5/3}^{5/8},$$

and raising to the 4/3 power gives the displayed inequality. Using Theorem 4.1,

$$\sum_{\sigma=1}^{q} a_\sigma^{4/3} \le \sqrt{R}\, q^{-1/3}.$$

Since always

$$\sum_{\sigma=1}^{q} a_\sigma^{4/3} \le 1,$$

we obtain

$$-e_x(n) \le C_D(1)\rho^{4/3} \min\{\sqrt{R}\, q^{-1/3}, 1\}.$$

Finally $C_D(q) = C_D(1)q^{-1/3}$, and hence

$$e_x(n) \ge -C_D(q) \min\{\sqrt{R}, q^{1/3}\}\rho^{4/3}.$$

The expansion at $R = 1$ follows from

$$\sqrt{R} = 1 + \frac{1}{2}(R-1) + O((R-1)^2).$$

□

Remark 5.1. The equality case at $R = 1$ is the unpolarized Fermi ball:

$$\rho_1 = \cdots = \rho_q = \rho/q, \qquad n_\sigma = \mathbf{1}_{\{|k| \le (6\pi^2\rho/q)^{1/3}\}}.$$

The theorem also clarifies the source of difficulty in the correlated Lieb problem. In the quasi-free class, kinetic excess inflates the exchange constant only through spin polarization, and the inflation obeys the explicit $\sqrt{R}$ law of Theorem 2.1. Any descent from the Dirac constant toward C_{LO} therefore requires genuine two-particle correlation; it cannot arise from one-particle phase-space rearrangement alone.