The sharp kinetic–Dirac interpolation for homogeneous quasi-free fermions

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Abstract

What is the best exchange lower bound that the homogeneous quasi-free framework can deliver, as a function of the kinetic budget? We answer this question with a sharp constant. The bound is expressed through an explicit finite-dimensional variational function $\mathcal{G}_q(R)$ defined on the simplex of spin populations, and it is attained for every value of the homogeneous kinetic ratio $R \geq 1$ by spin-resolved Fermi balls, with Galilean boosts inserted when the ball configuration alone undershoots the prescribed kinetic excess. We identify the structure of the optimizer: outside the trivial regimes $R = 1$ and $R \geq q^{2/3}$, every maximizer has at most two distinct positive spin densities, characterized by a quadratic Lagrange equation. A Taylor expansion of $\mathcal{G}_q$ at $R = 1$ yields a sharp slope of $2/5$ around the unpolarized Fermi ball, refining the looser $\sqrt{R}/2$ slope of the elementary interpolation. The result resolves the quasi-free piece of the Lieb–Oxford problem exactly.

1 Introduction

The Dirac formula $e_x = -C_D(q)\rho^{4/3}$ identifies the exchange constant of the unpolarized Fermi sea, and the Lieb–Oxford program asks how far that constant can be undercut by general fermionic states at the same density. Within the homogeneous gauge-invariant quasi-free class, a simple two-input proof gives the bound

$$e_x(n) \geq -C_D(q)\min\{\sqrt{R},\, q^{1/3}\}\,\rho^{4/3}, \qquad R = \tau/(K_D(q)\rho^{5/3}),$$

where $\sqrt{R}$ comes from an interpolation between ℓ^1 and $\ell^{5/3}$. That bound is not tight away from the endpoints.

This paper identifies the sharp quasi-free interpolation function. We introduce a finite-dimensional variational problem on the spin-population simplex,

$$\mathcal{G}_q(R) = \max\Big\{\sum_\sigma a_\sigma^{4/3} :\ \sum_\sigma a_\sigma = 1,\ \sum_\sigma a_\sigma^{5/3} \leq Rq^{-2/3}\Big\},$$

and prove (Theorem 3.1) that the optimal homogeneous quasi-free exchange bound is exactly

$$e_x(n) \geq -C_D(1)\,\mathcal{G}_q(R)\,\rho^{4/3}.$$

The constant is sharp for every $R \geq 1$, approached by spin-resolved Fermi balls with optionally added Galilean boosts. This is the best the quasi-free framework can do; any further descent toward the Lieb–Oxford constant C_{LO} must use genuine two-particle correlation.

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We then describe the variational problem itself. Theorem 5.1 shows that in the nontrivial range $1 < R < q^{2/3}$ the maximizer is determined by a quadratic Lagrange equation and uses at most two distinct positive spin densities. Theorem 6.1 gives the sharp small-excess slope:

$$q^{1/3}\mathcal{G}_q(R) = 1 + \tfrac{2}{5}(R-1) + O_q((R-1)^{3/2}),$$

improving the slope $1/2$ delivered by the elementary $\sqrt{R}$ bound. The slope $2/5$ is the exact quasi-free response to a small kinetic excess at the Dirac point.

Plan of the paper. Section 2 introduces the variational function $\mathcal{G}_q(R)$. Section 3 sets up homogeneous quasi-free states and states the sharp interpolation theorem. Section 4 contains the proof, using Riesz rearrangement and the bathtub principle. Section 5 characterizes the optimizer. Section 6 computes the sharp Taylor expansion at $R = 1$.

2 The sharp spin variational function

Fix $q \in \mathbb{N}$. For $R \geq 1$, define

$$\mathcal{G}_q(R) = \max\left\{ \sum_{\sigma=1}^{q} a_\sigma^{4/3} : a_\sigma \geq 0, \quad \sum_{\sigma=1}^{q} a_\sigma = 1, \quad \sum_{\sigma=1}^{q} a_\sigma^{5/3} \leq Rq^{-2/3} \right\}.$$

For $R \geq q^{2/3}$, the last constraint is inactive and

$$\mathcal{G}_q(R) = 1.$$

At $R = 1$, the only admissible point is $a_\sigma = 1/q$, hence

$$\mathcal{G}_q(1) = q^{-1/3}.$$

Let

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

3 Homogeneous quasi-free states

A homogeneous gauge-invariant quasi-free state is described by occupation functions

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

Set

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

and

$$\rho = \sum_\sigma \rho_\sigma, \qquad \tau = \sum_\sigma \tau_\sigma.$$

The homogeneous kinetic ratio is

$$R = \frac{\tau}{\frac{3}{5}(6\pi^2)^{2/3} q^{-2/3} \rho^{5/3}}.$$

The exchange energy density 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 3.1 (Sharp quasi-free kinetic–Dirac interpolation)**.** *For every homogeneous quasi-free fermion state,*

$$e_x(n) \geq -C_D(1)\mathcal{G}_q(R)\rho^{4/3} = -C_D(q)\, q^{1/3}\mathcal{G}_q(R)\rho^{4/3}.$$

The constant is sharp for every $R \geq 1$. More precisely, for every $R \geq 1$ and every optimizer $a = (a_1, \dots, a_q)$ in the definition of $\mathcal{G}_q(R)$, equality is approached by spin-resolved Fermi balls with spin densities $a_\sigma \rho$, with harmless Galilean boosts used when extra kinetic energy has to be added without changing exchange.

Remark 3.2. Theorem 3.1 improves the elementary bound

$$q^{1/3}\mathcal{G}_q(R) \leq \min\{\sqrt{R}, q^{1/3}\}.$$

What is gained is the exact best quasi-free interpolation function, not merely a convenient estimate that happens to recover the right endpoints.

4 Proof of sharpness

Lemma 4.1 (Exchange rearrangement)**.** *For $0 \leq n \leq 1$, put*

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

Then

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

Equality holds exactly for indicators of balls, up to null sets and translations.

Proof. The kernel $|k-\ell|^{-2}$ is radially decreasing. The Riesz rearrangement inequality says that the integral is maximized, at fixed $\int n$, by the symmetric decreasing rearrangement. Since $0 \leq n \leq 1$, the extremizer is

$$n^* = \mathbf{1}_{\{|k| \leq k_n\}}, \qquad k_n = (6\pi^2 \rho_n)^{1/3}.$$

The ball-overlap computation gives

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

Therefore

$$\frac{1}{2}(2\pi)^{-6} 16\pi^3 k_n^4 = \frac{k_n^4}{8\pi^3} = C_D(1)\rho_n^{4/3}.$$

□

Lemma 4.2 (Kinetic spin constraint)**.** *Let $a_\sigma = \rho_\sigma/\rho$. Then*

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

Proof. For each spin, the bathtub principle gives

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

Summing over σ and dividing by $\frac{3}{5}(6\pi^2)^{2/3}\rho^{5/3}$ gives the result. □

Proof of Theorem 3.1. By Theorem 4.1,

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

By Theorem 4.2, the vector a is admissible in the definition of $\mathcal{G}_q(R)$. Hence

$$-e_x(n) \le C_D(1)\mathcal{G}_q(R)\rho^{4/3}.$$

Conversely, let a be an optimizer. For each σ with $a_\sigma > 0$, take

$$n_\sigma(k) = \mathbf{1}_{\{|k-b_\sigma| \le (6\pi^2 a_\sigma \rho)^{1/3}\}},$$

where $b_\sigma \in \mathbb{R}^3$ is a boost vector. The exchange is independent of b_σ and equals

$$-C_D(1)\rho^{4/3}\sum_\sigma a_\sigma^{4/3}.$$

The minimal kinetic ratio of these balls is

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

If it is strictly smaller than R, choose one nonzero b_σ to add the missing kinetic energy. Thus equality in the bound is attained, or approached if one wants zero total current by using opposite boosts in a standard limiting split. □

5 Structure of the optimizer

Proposition 5.1 (Two-level spin structure)**.** *For $1 < R < q^{2/3}$, every maximizer of $\mathcal{G}_q(R)$ uses the kinetic constraint with equality and has at most two distinct positive spin densities. Equivalently, after permutation, either it is uniform on some nonempty subset of spin states, or it has the two-level form*

$$(\underbrace{x,\dots,x}_{m\ \text{times}},\underbrace{y,\dots,y}_{n\ \text{times}},0,\dots,0), \qquad x > y > 0,$$

with $m + n \le q$. The numbers are determined by

$$mx + ny = 1, \qquad mx^{5/3} + ny^{5/3} = Rq^{-2/3},$$

and the maximizing pair (m,n) is the one giving the largest value of

$$mx^{4/3} + ny^{4/3}.$$

Proof. The admissible set is compact, so a maximizer exists. If $1 < R < q^{2/3}$, the constraint $\sum a_\sigma^{5/3} \le Rq^{-2/3}$ must be active: otherwise one could move mass from a smaller positive component to a larger one, increasing the strictly convex function $\sum a_\sigma^{4/3}$ while keeping $\sum a_\sigma = 1$.

At a maximizer, apply the Lagrange multiplier equations on the set of positive components. There are $\lambda \in \mathbb{R}$ and $\mu > 0$ such that

$$\frac{4}{3}a_\sigma^{1/3} = \lambda + \frac{5}{3}\mu a_\sigma^{2/3}.$$

Writing $z = a_\sigma^{1/3}$, this is the quadratic equation

$$\frac{5}{3}\mu z^2 - \frac{4}{3}z + \lambda = 0.$$

It has at most two positive roots. Hence the positive components of any maximizer take at most two distinct values. The displayed equations are just the mass and active kinetic constraints for these two values. Comparing the finitely many possible multiplicities gives the final characterization. □

6 Small kinetic excess

Proposition 6.1 (Sharp expansion at the Dirac point)**.** *As* $R \downarrow 1$*,*

$$q^{1/3}\mathcal{G}_q(R) = 1 + \frac{2}{5}(R-1) + O_q((R-1)^{3/2}).$$

Consequently the sharp quasi-free bound has the expansion

$$e_x(n) \geq -C_D(q)\rho^{4/3} - \frac{2}{5}C_D(q)(R-1)\rho^{4/3} - O_q((R-1)^{3/2})\rho^{4/3}.$$

Proof. Write

$$a_\sigma = q^{-1} + h_\sigma, \qquad \sum_\sigma h_\sigma = 0.$$

For small excess all components are positive. Taylor expansion gives

$$\sum_\sigma a_\sigma^{5/3} = q^{-2/3} + \frac{5}{9}q^{1/3}\sum_\sigma h_\sigma^2 + O_q\left(\sum_\sigma |h_\sigma|^3\right),$$

and

$$\sum_\sigma a_\sigma^{4/3} = q^{-1/3} + \frac{2}{9}q^{2/3}\sum_\sigma h_\sigma^2 + O_q\left(\sum_\sigma |h_\sigma|^3\right).$$

Since the active kinetic constraint is

$$\sum_\sigma a_\sigma^{5/3} = Rq^{-2/3},$$

we get

$$\sum_\sigma h_\sigma^2 = \frac{9}{5}q^{-1}(R-1) + O_q((R-1)^{3/2}).$$

Substituting into the expansion of $\sum a_\sigma^{4/3}$ yields

$$\mathcal{G}_q(R) = q^{-1/3}\left(1 + \frac{2}{5}(R-1) + O_q((R-1)^{3/2})\right).$$

□

Remark 6.2. Theorem 3.1 remains a quasi-free result and does not address the fully correlated Lieb open problem. Its content is that the quasi-free part of the problem is solved exactly: the optimal interpolation constant reduces to the explicit finite-dimensional spin-polarization variational problem $\mathcal{G}_q(R)$, and the small-excess slope at the Dirac point is the sharp constant 2/5.