A no-go theorem for purely local (ρ, T) Dirac interpolation

Dong Bai*

May 13, 2026

Abstract

We prove a sharp impossibility result for local Lieb–Oxford-type lower bounds on the indirect Coulomb energy of antisymmetric fermionic states. For a normalized N-fermion wavefunction Ψ write ρ_Ψ for its one-particle density, T_Ψ for its local kinetic energy density, and $E_{\mathrm{xc}}(\Psi)$ for its indirect (exchange-correlation) energy. Let $\mathcal{R}_\Psi$ be the dimensionless local kinetic ratio. Two constants control the discussion: the Dirac exchange constant $C_D(q) = \frac{3}{4}(6/\pi)^{1/3}q^{-1/3}$ and the *one-cell self-interaction constant* $C_{\mathrm{cell}} = \frac{3}{5}(4\pi/3)^{1/3}$, which is strictly larger than $C_D(q)$ for every spin multiplicity $q \geq 1$. We show that any bounded function F with $\limsup_{r\downarrow 0} F(r) < C_{\mathrm{cell}}$ cannot serve as the integrand of a universal pointwise lower bound $E_{\mathrm{xc}}(\Psi) \geq -\int F(\mathcal{R}_\Psi)\rho_\Psi^{4/3}$ for arbitrarily large N. The proof constructs antisymmetric many-cell states whose local data (ρ_Ψ, T_Ψ) look like a flat Fermi sea but whose indirect energy is dominated by one-particle self-interaction. Consequently, no universal pointwise bound depending only on (ρ_Ψ, T_Ψ) can have $C_D(q)$ as its small-$\mathcal{R}$ limit.

1 Setting and statement

A long-standing goal in density-functional analysis is to refine the Lieb–Oxford inequality [2] into a *pointwise* lower bound whose integrand depends only on local densities and whose small-kinetic-ratio limit reproduces the Dirac exchange constant $C_D(q)$ [1]. Various ansätze in the physics literature take the natural form

$$E_{\mathrm{xc}}(\Psi) \geq -\int F\big(\mathcal{R}_\Psi(x)\big)\,\rho_\Psi(x)^{4/3}\,\mathrm{d}x,$$

with F bounded and $F(r) \to C_D(q)$ as $r \downarrow 0$. The main theorem of this paper rules out every such ansatz: there is a hard *cell self-interaction constant* $C_{\mathrm{cell}} > C_D(q)$ such that no F with $\limsup_{r\downarrow 0} F(r) < C_{\mathrm{cell}}$ can give a universal bound.

For a normalized N-fermion wavefunction Ψ, write

$$\rho_\Psi(x) = N\int |\Psi(x, x_2, \dots, x_N)|^2\,\mathrm{d}x_2 \cdots \mathrm{d}x_N$$

and

$$T_\Psi(x) = N\int |\nabla_x \Psi(x, x_2, \dots, x_N)|^2\,\mathrm{d}x_2 \cdots \mathrm{d}x_N.$$

Let

$$\mathcal{R}_\Psi(x) = \frac{T_\Psi(x)}{\frac{3}{5}(6\pi^2)^{2/3}q^{-2/3}\rho_\Psi(x)^{5/3}}.$$

The indirect Coulomb energy is

$$E_{\mathrm{xc}}(\Psi) = \left\langle \Psi, \sum_{1\leq i<j\leq N} \frac{1}{|x_i - x_j|}\Psi \right\rangle - \frac{1}{2}\iint \frac{\rho_\Psi(x)\rho_\Psi(y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y.$$

*College of Mechanics and Engineering Science, Hohai University, Nanjing 211100, China. E-mail: bydonfancy@gmail.com.

Let

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

be the Dirac constant and define the one-cell self-interaction constant

$$C_{\mathrm{cell}} = \frac{3}{5}\left(\frac{4\pi}{3}\right)^{1/3}.$$

Numerically,

$$C_{\mathrm{cell}} = 0.967\ldots, \qquad C_D(1) = 0.930\ldots,$$

so $C_{\mathrm{cell}} > C_D(q)$ for every $q \geq 1$.

Theorem 1.1 (No purely local Dirac interpolation)**.** *Let $F : [0,\infty] \to [0,\infty)$ be bounded above and suppose*

$$\limsup_{r\downarrow 0} F(r) < C_{\mathrm{cell}}.$$

Then the bound

$$E_{\mathrm{xc}}(\Psi) \geq -\int_{\mathbb{R}^3} F(\mathcal{R}_\Psi(x))\rho_\Psi(x)^{4/3}\,\mathrm{d}x$$

cannot hold for all antisymmetric N-fermion wavefunctions, even if N is allowed to be arbitrarily large.

In particular, no universal pointwise local bound depending only on $\rho_\Psi(x)$ and $T_\Psi(x)$ can have the Dirac constant $C_D(q)$ as its small-$\mathcal{R}$ local limit.

Plan of the paper. Section 2 carries out the one-cell computation that identifies C_{cell} and constructs a smooth approximating sequence with controlled boundary error. Section 3 translates that single cell into a many-cell Slater determinant whose density and kinetic profile place each cell deep in the regime $F \leq a < C_{\mathrm{cell}}$, and deduces the contradiction that proves Theorem 1.1.

2 The one-cell computation

Let $B \subset \mathbb{R}^3$ be the unit ball and

$$\rho_B(x) = \frac{\mathbf{1}_B(x)}{|B|}, \qquad |B| = \frac{4\pi}{3}.$$

Then

$$\int \rho_B^{4/3} = |B|^{-1/3}.$$

The Coulomb self-energy of the uniform unit ball of total charge one is

$$\frac{1}{2}\iint \frac{\rho_B(x)\rho_B(y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y = \frac{3}{5}.$$

Hence

$$\frac{\frac{1}{2}\iint |x-y|^{-1}\rho_B(x)\rho_B(y)\,\mathrm{d}x\,\mathrm{d}y}{\int \rho_B^{4/3}} = \frac{3}{5}\left(\frac{4\pi}{3}\right)^{1/3} = C_{\mathrm{cell}}.$$

We shall use smooth approximations to ρ_B. Choose $\varphi_\varepsilon \in C_c^\infty(B)$, $\|\varphi_\varepsilon\|_2 = 1$, such that

$$|\varphi_\varepsilon|^2 \to \rho_B \quad \text{in } L^{4/3}(\mathbb{R}^3)$$

and in Coulomb energy. Additionally, choose it so that φ_ε is constant on $|x| \leq 1-\varepsilon$. Then

$$\frac{1}{2}\iint \frac{|\varphi_\varepsilon(x)|^2|\varphi_\varepsilon(y)|^2}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y = C_{\mathrm{cell}}\int |\varphi_\varepsilon|^{8/3} + o_\varepsilon(1),$$

The contribution of the boundary layer

$$\{1-\varepsilon < |x| < 1\}$$

to $\int |\varphi_\varepsilon|^{8/3}$ is $o_\varepsilon(1)$.

3 Many disjoint cells

Proof of Theorem 1.1. Let $M = \sup F < \infty$. By assumption, choose $a < C_{\text{cell}}$ and $\delta > 0$ such that

$$F(r) \le a \qquad 0 < r \le \delta.$$

If $M = 0$, the contradiction is immediate. Otherwise choose $\varepsilon > 0$ so small that the boundary-layer contribution to $\int |\varphi_\varepsilon|^{8/3}$ is less than

$$\frac{C_{\text{cell}} - a}{4M} \int |\varphi_\varepsilon|^{8/3},$$

and the Coulomb self-energy ratio of φ_ε is larger than

$$\frac{C_{\text{cell}} + a}{2}.$$

Choose a vector $\kappa \in \mathbb{R}^3$ so small that, on the plateau where φ_ε is constant,

$$\frac{|\kappa|^2}{\frac{3}{5}(6\pi^2)^{2/3} q^{-2/3} |\varphi_\varepsilon|^{4/3}} \le \delta.$$

Replace φ_ε by

$$e^{i\kappa\cdot x}\varphi_\varepsilon(x).$$

This does not change its density or Coulomb self-energy. On the plateau, however, the ratio $\mathcal{R}$ is now a positive number not exceeding δ, so the estimate $F(\mathcal{R}) \le a$ applies there.

Place N translated copies of φ_ε in pairwise disjoint balls whose mutual distances tend to infinity. Denote these orbitals by

$$u_1, \dots, u_N.$$

Because their supports are disjoint, they are orthonormal. Put

$$\Psi_N = u_1 \wedge \cdots \wedge u_N.$$

This is an antisymmetric N-fermion wavefunction.

On each cell, the one-particle density is $|u_j|^2$, and the cells are disjoint. Therefore

$$\rho_{\Psi_N} = \sum_{j=1}^{N} |u_j|^2, \qquad T_{\Psi_N} = \sum_{j=1}^{N} |\nabla u_j|^2.$$

Since the supports are disjoint, the local ratio $\mathcal{R}_{\Psi_N}$ is exactly the one-cell ratio on each cell. Thus, on the plateau part of every cell, $\mathcal{R}_{\Psi_N} \le \delta$.

The pair density between different cells is exactly the product of the corresponding one-cell densities. Hence all inter-cell Coulomb terms cancel against the inter-cell Hartree terms in E_{xc}. What remains is only the self-interaction subtraction in each cell:

$$E_{\text{xc}}(\Psi_N) = -N\,\frac{1}{2} \iint \frac{|\varphi_\varepsilon(x)|^2 |\varphi_\varepsilon(y)|^2}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y.$$

Consequently,

$$E_{\text{xc}}(\Psi_N) \le -N\,\frac{C_{\text{cell}} + a}{2} \int |\varphi_\varepsilon|^{8/3}.$$

On the other hand,

$$\begin{aligned}
\int F(\mathcal{R}_{\Psi_N}) \rho_{\Psi_N}^{4/3} &= N \int F(\mathcal{R}_{\varphi_\varepsilon}) |\varphi_\varepsilon|^{8/3} \\
&\le Na \int |\varphi_\varepsilon|^{8/3} + NM \int_{\text{boundary layer}} |\varphi_\varepsilon|^{8/3} \\
&\le N\frac{3a + C_{\text{cell}}}{4} \int |\varphi_\varepsilon|^{8/3}.
\end{aligned}$$

Since

$$\frac{C_{\mathrm{cell}} + a}{2} > \frac{3a + C_{\mathrm{cell}}}{4},$$

we obtain

$$E_{\mathrm{xc}}(\Psi_N) < -\int F(\mathcal{R}_{\Psi_N})\rho_{\Psi_N}^{4/3}$$

for large enough cell separation. This contradicts the proposed universal bound. □

Remark 3.1. The construction uses arbitrarily many fermions, not merely $N = 1$. The obstruction is local: every cell contains a single electron, so the kinetic ratio is small on most of the cell, yet the indirect Coulomb energy is dominated by one-particle self-interaction whose sharp local constant is C_{cell}, strictly larger than the Dirac constant.

Remark 3.2. A true local Dirac theorem must therefore include an additional datum that excludes this construction. Natural candidates are: a local many-particle condition, a subtraction of one-particle self-interaction, or a pair- or number-variance datum on a controlled spatial scale. Without such an addition, the pair (ρ_Ψ, T_Ψ) is insufficient.

Acknowledgements. LaTeX typesetting and bibliographic copy-editing were carried out with assistance from Claude Opus 4.7 (Anthropic). All mathematical content and proofs are the author's own.

References

[1] P. A. M. Dirac. Note on exchange phenomena in the Thomas atom. *Math. Proc. Cambridge Philos. Soc.* **26** (1930), 376–385.

[2] E. H. Lieb and S. Oxford. Improved lower bound on the indirect Coulomb energy. *Int. J. Quantum Chem.* **19** (1981), 427–439.