A sharp obstruction to local (ρ, T) Dirac interpolation and an exact fluctuation–current bridge

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Abstract

A long-standing question in the Lieb–Oxford programme asks whether the universal lower bound on the indirect Coulomb energy of fermions admits a pointwise local refinement whose low-kinetic-ratio limit reproduces the Dirac exchange constant. We show that the answer is no, in a sharp form. Let $\rho_\Psi(x)$ and $T_\Psi(x)$ denote the one-particle density and local kinetic energy density of a normalized antisymmetric N-fermion wavefunction Ψ, and let $E_{\mathrm{xc}}(\Psi)$ be its indirect Coulomb (exchange-correlation) energy. Write $C_{\mathrm{cell}} := \frac{3}{5}(4\pi/3)^{1/3} \approx 0.96720$ and let $C_D(q) := \frac{3}{4}(6/\pi)^{1/3}q^{-1/3}$ be the Dirac constant for spin multiplicity q. We prove that any bounded $F : [0,\infty) \to [0,\infty)$ with $\limsup_{r\downarrow 0} F(r) < C_{\mathrm{cell}}$ fails the natural local lower bound for some antisymmetric Ψ with N arbitrarily large. Since $C_{\mathrm{cell}} > C_D(q)$ for every $q \geq 1$, no universal local lower bound depending only on (ρ_Ψ, T_Ψ) can converge to $C_D(q)$ in the low-$\mathcal{R}$ regime. As a positive companion we establish a Gaussian scale-window identity that rewrites the indirect energy of an admissible kernel family exactly in terms of local number variances, and combine it with a canonical-commutator uncertainty inequality to bound it from below by a conjugate-current variance.

1 The obstruction

The Lieb–Oxford inequality [2] and its modern refinements [3] furnish a universal lower bound on the indirect Coulomb energy of any N-fermion state in terms of the $L^{4/3}$ norm of its one-particle density. A natural project is to sharpen that inequality into a *pointwise* statement whose integrand depends on local densities and whose low-kinetic-ratio limit recovers the Dirac exchange constant $C_D(q)$. Many proposals in the density-functional literature aspire to such a local form. Our first result shows that no purely (ρ_Ψ, T_Ψ)-local prescription can achieve this: there is a hard cell-self-interaction constant $C_{\mathrm{cell}} > C_D(q)$ that blocks the limit.

For a normalized N-fermion wavefunction Ψ we set

$$\rho_\Psi(x) = N \int |\Psi(x, x_2, \ldots, x_N)|^2 \, \mathrm{d}x_2 \cdots \mathrm{d}x_N, \tag{1}$$

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

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

The indirect Coulomb energy of Ψ is

$$E_{\mathrm{xc}}(\Psi) = \Big\langle \Psi, \sum_{1\leq i<j\leq N} \frac{1}{|x_i - x_j|} \Psi \Big\rangle - \frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_\Psi(x)\rho_\Psi(y)}{|x-y|} \, \mathrm{d}x \, \mathrm{d}y. \tag{4}$$

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Two constants control the discussion: the Dirac exchange constant [1]

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

and what we call the *one-cell self-energy constant*

$$C_{\text{cell}} = \frac{3}{5}\left(\frac{4\pi}{3}\right)^{1/3} = 0.967195\ldots;$$

elementary inspection shows $C_{\text{cell}} > C_D(q)$ for every spin multiplicity $q \geq 1$. The Lieb–Oxford constant sits slightly above C_{cell}; the obstruction we identify is therefore a qualitative gap between the local Lieb–Oxford regime and the Dirac regime, present in the *local* formulation alone.

Plan of the paper. Section 1 states and proves the obstruction (Theorem 1.1) by constructing a many-cell antisymmetric state on which every (ρ, T)-local candidate functional with subcritical low-$\mathcal{R}$ limit must fail. Section 2 provides the positive companion: a Gaussian scale-window identity (Theorem 2.2) that rewrites a kernel-mollified indirect energy exactly as an integral of local number variances, together with a canonical-commutator uncertainty inequality (Theorem 2.1) showing that the same quantity is controlled below by a conjugate-current variance. The two results together identify, in precise terms, the *extra* local datum a successful Dirac interpolation must carry: fluctuations on the test scale.

Theorem 1.1 (Sharp one-cell obstruction)**.** *Let $F : [0, \infty) \to [0, \infty)$ be bounded above. If*

$$\limsup_{r \downarrow 0} F(r) < C_{\text{cell}}, \tag{5}$$

then the bound

$$E_{\text{xc}}(\Psi) \;\geq\; -\int_{\mathbb{R}^3} F(\mathcal{R}_\Psi(x))\rho_\Psi(x)^{4/3}\,\mathrm{d}x \tag{6}$$

cannot hold for all antisymmetric N-fermion wavefunctions, even allowing arbitrarily large N.

Consequently, a universal pointwise local lower bound depending only on $\rho_\Psi(x)$ and $T_\Psi(x)$ cannot have the Dirac constant $C_D(q)$ as its low-$\mathcal{R}$ local limit.

Proof. Let B denote the closed unit ball in $\mathbb{R}^3$ and let $\rho_B = |B|^{-1}\mathbf{1}_B$ be the uniform density of total charge one. Then

$$\int_{\mathbb{R}^3} \rho_B^{4/3} = |B|^{-1/3}, \qquad \frac{1}{2}\iint \frac{\rho_B(x)\rho_B(y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y = \frac{3}{5},$$

where the second identity is Newton's theorem [5] for the self-energy of a uniform unit ball of total charge one. The ratio of these two quantities is exactly C_{cell}.

Choose $a < C_{\text{cell}}$ and $\delta > 0$ so that $F(r) \leq a$ on $(0, \delta]$, and set $M := \sup F$. Pick a sequence $\varphi_\varepsilon \in C_c^\infty(B)$ with $\|\varphi_\varepsilon\|_2 = 1$, each φ_ε constant on $|x| \leq 1 - \varepsilon$, such that

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

together with their Coulomb self-energies. Such a sequence is obtained by smoothing the constant density only inside the boundary layer $1 - \varepsilon < |x| < 1$. For all sufficiently small ε,

$$\frac{1}{2}\iint \frac{|\varphi_\varepsilon(x)|^2|\varphi_\varepsilon(y)|^2}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y > \frac{C_{\text{cell}} + a}{2}\int |\varphi_\varepsilon|^{8/3}, \tag{7}$$

$$M\int_{1-\varepsilon<|x|<1} |\varphi_\varepsilon(x)|^{8/3}\,\mathrm{d}x < \frac{C_{\text{cell}} - a}{4}\int |\varphi_\varepsilon|^{8/3}. \tag{8}$$

Multiplying φ_ε by the plane-wave phase $e^{i\kappa\cdot x}$ leaves the density and Coulomb self-energy unchanged but produces

$$T(x) = |\kappa|^2\, |\varphi_\varepsilon(x)|^2 \quad \text{on the plateau } |x| \le 1-\varepsilon.$$

Choosing $|\kappa| > 0$ small enough yields

$$0 < \mathcal{R}(x) \le \delta \quad \text{on } |x| \le 1-\varepsilon,$$

so the cell sits in the regime where $F \le a$.

Translate this one-particle orbital to N pairwise disjoint cells and call the translates $u_1, \dots, u_N$. They are orthonormal, and

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

is an antisymmetric N-fermion wavefunction. Disjoint supports give

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

so the local ratio $\mathcal{R}_{\Psi_N}$ inside each cell is just the translated one-cell ratio. The exchange term between two different cells vanishes (the one-body density matrix has disjoint support there), and the resulting inter-cell pair energy equals the inter-cell Hartree energy and cancels in E_{xc}. Hence

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

By Equation (7),

$$E_{\mathrm{xc}}(\Psi_N) < -N\, \frac{C_{\mathrm{cell}} + a}{2} \int |\varphi_\varepsilon|^{8/3}. \tag{9}$$

On the other hand, using $F \le a$ on the plateau and $F \le M$ in the boundary layer,

$$\begin{aligned} \int F(\mathcal{R}_{\Psi_N}) \rho_{\Psi_N}^{4/3} &= N \int F(\mathcal{R}_{\varphi_\varepsilon}) |\varphi_\varepsilon|^{8/3} \\ &\le Na \int |\varphi_\varepsilon|^{8/3} + NM \int_{1-\varepsilon<|x|<1} |\varphi_\varepsilon|^{8/3}\, \mathrm{d}x \\ &< N\, \frac{3a + C_{\mathrm{cell}}}{4} \int |\varphi_\varepsilon|^{8/3}. \end{aligned} \tag{10}$$

Since $\frac{C_{\mathrm{cell}}+a}{2} > \frac{3a+C_{\mathrm{cell}}}{4}$, Equations (9) and (10) contradict Equation (6). The construction works for arbitrarily large N by simply adding more disjoint one-electron cells. □

Remark 1.2. The obstruction is structural, not technical. On most of each cell the density is flat and the local kinetic ratio is arbitrarily small, yet the *local* self-interaction constant is C_{cell}, strictly above the Dirac constant. Equivalently, the variables (ρ_Ψ, T_Ψ) cannot distinguish a sparse one-electron cell from a many-particle Fermi sea of comparable density.

2 The exact bridge that remains possible

Theorem 1.1 says what cannot be true. The next theorem delivers the positive counterpart: an exact identity isolating the local fluctuation datum that any successful local refinement must carry.

For a real Schwartz function f on $\mathbb{R}^3$, set

$$N_f = \sum_{j=1}^{N} f(x_j), \qquad J_f = \frac{1}{2} \sum_{j=1}^{N} (\nabla f(x_j) \cdot p_j + p_j \cdot \nabla f(x_j)),$$

with $p_j = -i\nabla_{x_j}$.

Lemma 2.1 (Number–current uncertainty)**.** *For every normalized finite-kinetic-energy state* Ψ*,*

$$\mathrm{Var}_\Psi(N_f)\ \mathrm{Var}_\Psi(J_f)\ \geq\ \frac{1}{4}\Big(\int_{\mathbb{R}^3}\rho_\Psi(x)|\nabla f(x)|^2\,\mathrm{d}x\Big)^2. \tag{11}$$

Proof. The canonical commutation relations give the quadratic-form identity

$$i[J_f,N_f]=\sum_{j=1}^N|\nabla f(x_j)|^2.$$

Taking the expectation in Ψ yields

$$\langle i[J_f,N_f]\rangle_\Psi=\int_{\mathbb{R}^3}\rho_\Psi(x)|\nabla f(x)|^2\,\mathrm{d}x,$$

and the Robertson uncertainty inequality [4] applied to the self-adjoint operators N_f and J_f gives the claim. ☐

For a nonnegative even kernel w, define its indirect energy by

$$E_w(\Psi)=\Big\langle\Psi,\sum_{1\leq i<j\leq N}w(x_i-x_j)\Psi\Big\rangle-\frac{1}{2}\iint\rho_\Psi(x)\rho_\Psi(y)w(x-y)\,\mathrm{d}x\,\mathrm{d}y.$$

Theorem 2.2 (Gaussian scale-window bridge)**.** *For* $0<\alpha<\beta<\infty$*, set*

$$w_{\alpha,\beta}(x)=\frac{2}{\sqrt{\pi}}\int_\alpha^\beta e^{-s^2|x|^2}\,\mathrm{d}s,\qquad g_{s,z}(x)=\left(\frac{4s^2}{\pi}\right)^{3/4}e^{-2s^2|x-z|^2}.$$

Then

$$\begin{aligned}E_{w_{\alpha,\beta}}(\Psi)&=\frac{1}{\sqrt{\pi}}\int_\alpha^\beta\int_{\mathbb{R}^3}\Big[\mathrm{Var}_\Psi(N_{g_{s,z}})-\int_{\mathbb{R}^3}g_{s,z}(x)^2\rho_\Psi(x)\,\mathrm{d}x\Big]\,\mathrm{d}z\,\mathrm{d}s\\&\geq-\frac{1}{\sqrt{\pi}}\int_\alpha^\beta\int_{\mathbb{R}^3}\left[\int g_{s,z}^2\rho_\Psi-\frac{\left(\int\rho_\Psi|\nabla g_{s,z}|^2\right)^2}{4\ \mathrm{Var}_\Psi(J_{g_{s,z}})}\right]\mathrm{d}z\,\mathrm{d}s,\end{aligned}\tag{12}$$

where the fraction is set to 0 *on the set* $\mathrm{Var}_\Psi(J_{g_{s,z}})=0$*. On that set Theorem 2.1 forces* $\int\rho_\Psi|\nabla g_{s,z}|^2=0$*, so the convention loses no positive information.*

Proof. The normalized Gaussian convolution identity

$$\int_{\mathbb{R}^3}g_{s,z}(x)g_{s,z}(y)\,\mathrm{d}z=e^{-s^2|x-y|^2}$$

yields

$$w_{\alpha,\beta}(x-y)=\frac{2}{\sqrt{\pi}}\int_\alpha^\beta\int_{\mathbb{R}^3}g_{s,z}(x)g_{s,z}(y)\,\mathrm{d}z\,\mathrm{d}s.$$

For each fixed pair (s,z),

$$\sum_{i<j}g_{s,z}(x_i)g_{s,z}(x_j)=\frac{1}{2}(N_{g_{s,z}}^2-N_{g_{s,z}^2}).$$

Subtracting the Hartree contribution therefore gives the exact identity

$$E_{w_{\alpha,\beta}}(\Psi)=\frac{1}{\sqrt{\pi}}\int_\alpha^\beta\int_{\mathbb{R}^3}\Big[\mathrm{Var}_\Psi(N_{g_{s,z}})-\int g_{s,z}^2\rho_\Psi\Big]\,\mathrm{d}z\,\mathrm{d}s.$$

Applying Theorem 2.1 to $f=g_{s,z}$ gives the lower bound. ☐

Corollary 2.3. *Any genuine replacement for the impossible local (ρ, T)-only Dirac interpolation must add information that controls the conjugate current variance $\mathrm{Var}_\Psi(J_{g_{s,z}})$ or, equivalently, the local number variance $\mathrm{Var}_\Psi(N_{g_{s,z}})$. By Theorem 1.1 the pair (ρ_Ψ, T_Ψ) alone cannot supply this information universally.*

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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.

[3] M. Lewin, E. H. Lieb, and R. Seiringer. Improved Lieb–Oxford bound and its application to density functional theory. *Pure Appl. Anal.* **2**, no. 1 (2020), 35–73. arXiv:1707.07664.

[4] H. P. Robertson. The uncertainty principle. *Phys. Rev.* **34** (1929), 163–164.

[5] I. Newton. *Philosophiæ Naturalis Principia Mathematica.* Book I, Proposition LXXI (1687).