

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 $E_{\text{xc}}(\Psi)$ be its indirect Coulomb (exchange–correlation) energy. Write $C_{\text{cell}} := \frac{3}{5}(4\pi/3)^{1/3} \approx 0.96720$ 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 $F : [0, \infty) \rightarrow [0, \infty)$ with $\limsup_{r \downarrow 0} F(r) < C_{\text{cell}}$ fails the natural local lower bound for some antisymmetric Ψ with N arbitrarily large. Since $C_{\text{cell}} > C_D(q)$ 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 $C_{\text{cell}} > C_D(q)$ that blocks the limit.

For a normalized N -fermion wavefunction Ψ we set

$$\rho_\Psi(x) = N \int |\Psi(x, x_2, \dots, x_N)|^2 dx_2 \cdots dx_N, \quad (1)$$

$$T_\Psi(x) = N \int |\nabla_x \Psi(x, x_2, \dots, x_N)|^2 dx_2 \cdots dx_N, \quad (2)$$

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

The indirect Coulomb energy of Ψ is

$$E_{\text{xc}}(\Psi) = \left\langle \Psi, \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|} \Psi \right\rangle - \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_\Psi(x)\rho_\Psi(y)}{|x - y|} dx dy. \quad (4)$$

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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*

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

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 $F : [0, \infty) \rightarrow [0, \infty)$ be bounded above. If*

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

then the bound

$$E_{\text{xc}}(\Psi) \geq - \int_{\mathbb{R}^3} F(\mathcal{R}_\Psi(x)) \rho_\Psi(x)^{4/3} dx \quad (6)$$

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

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

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

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

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 ,

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

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

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

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

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

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

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

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

$$\Psi_N = u_1 \wedge \dots \wedge u_N$$

is an antisymmetric N -fermion wavefunction. Disjoint supports give

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

so the local ratio \mathcal{R}_{Ψ_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

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

By Equation (7),

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

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

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

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

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

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

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

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

$$\text{Var}_\Psi(N_f) \text{Var}_\Psi(J_f) \geq \frac{1}{4} \left(\int_{\mathbb{R}^3} \rho_\Psi(x) |\nabla f(x)|^2 dx \right)^2. \quad (11)$$

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

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

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

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

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

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

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

Then

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

where the fraction is set to 0 on the set $\text{Var}_\Psi(J_{g_{s,z}}) = 0$. 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

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

yields

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

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

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

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

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

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