A local integer-variance lower bound for indirect Coulomb energy

Dong Bai*

May 13, 2026

Abstract

The Lieb–Oxford program asks for universal lower bounds on the indirect Coulomb energy of a many-body state in terms of its one-particle density alone. We give such a bound that uses only one nonperturbative fact: the number of particles in a ball is an integer-valued random variable. Starting from the Fefferman–de la Llave representation of the Coulomb kernel, the indirect Coulomb energy is rewritten as an exact integral of variances of local ball counts minus their means. The integer-valued constraint then gives the sharp single-variable variance bound $\operatorname{Var} X \geq \theta(m)(1-\theta(m))$, which produces a closed-form local density functional lower bound involving only the local ball mass. The resulting universal constant is $C_{\mathrm{IV}} = 1.569\ldots$, lying below the Lieb–Oxford constant 1.68 and above the Dirac constant. The bound is exact for one particle and isolates a clean number-quantization contribution to the Lieb–Oxford problem.

1 Introduction

The Lieb–Oxford program seeks a universal lower bound on the indirect Coulomb energy of an N-body fermionic or bosonic state in terms only of its one-particle density. The classical Lieb–Oxford bound gives such a constant roughly $1.68\,\rho^{4/3}$; the Dirac lower bound, valid for the closed-shell Fermi sea, has the smaller constant $C_D(q)\rho^{4/3}$. Bridging the two has been a longstanding open problem.

This note isolates one structural input to the universal problem. We use no exchange information, no quasi-free assumption, and no Slater determinant. We use only the elementary fact that the number of particles in a ball is an integer-valued random variable, and the Fefferman–de la Llave representation of the Coulomb kernel as a superposition of indicator overlaps. The combination yields an exact identity (Theorem 4.1) expressing the indirect Coulomb energy as an integral over balls of $\operatorname{Var} N_{z,r} - m_{\rho_\Psi}(z,r)$, where $N_{z,r}$ is the integer-valued local count. Applying the sharp variance bound for integer-valued random variables of Theorem 5.1 converts this identity into the closed-form density-functional lower bound of Theorem 2.1.

The resulting bound is universal: it applies to any normalized many-body state, symmetric or antisymmetric, with bounded compactly supported density and finite Coulomb energies. It is exact for $N = 1$ (Theorem 6.1), and on a constant density it produces the universal constant

$$C_{\mathrm{IV}} = \frac{1}{6\pi}\left(\frac{4\pi}{3}\right)^{4/3}\int_0^\infty \Phi(t)t^{-7/3}\,\mathrm{d}t = 1.569\ldots,$$

with $\Phi(t) = t - \theta(t)(1-\theta(t))$ recording the deficit between t and the sharp integer variance.

The constant $C_{\mathrm{IV}} = 1.569\ldots$ lies below the Lieb–Oxford constant 1.68 but above the Dirac constants, so the result does not settle the kinetic Dirac problem. Its significance is structural: it captures exactly the one-particle self-interaction obstruction and improves automatically as soon as local number quantization forces nonzero variance above the Bernoulli value.

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

Plan of the paper. Section 2 states the main bound. Section 3 records the Fefferman–de la Llave ball representation of the Coulomb kernel. Section 4 derives the exact variance identity for the indirect Coulomb energy. Section 5 states the sharp integer-variance inequality and uses it to prove the main theorem. Section 6 contains two checks: exact equality for $N = 1$ and the homogeneous constant C_{IV}.

2 The bound

For $t \geq 0$, let

$$\theta(t) = t - \lfloor t \rfloor \in [0, 1), \qquad \Phi(t) = t - \theta(t)(1 - \theta(t)).$$

Thus $\Phi(t) = t^2$ for $0 \leq t \leq 1$, and $\Phi(t) \leq t$ for all t.

For a density ρ, define the local ball mass

$$m_\rho(z, r) = \int_{B(z,r)} \rho(x)\, \mathrm{d}x.$$

Theorem 2.1 (Integer-variance lower bound)**.** *Let Ψ be a normalized N-particle wavefunction on $\mathbb{R}^3$, symmetric or antisymmetric, with density ρ_Ψ. Assume that ρ_Ψ is bounded and compactly supported, and that the Coulomb quantities below are finite. Then*

$$E_{\mathrm{xc}}(\Psi) \geq -\frac{1}{2\pi} \int_0^\infty \frac{\mathrm{d}r}{r^5} \int_{\mathbb{R}^3} \Phi(m_{\rho_\Psi}(z, r))\, \mathrm{d}z.$$

Remark 2.2. Theorem 2.1 is a universal many-body bound. It is not quasi-free, not perturbative, and uses no Slater determinant. Beyond the exact Coulomb identity, the only input is that the number of particles in a ball is an integer-valued random variable.

3 Fefferman–de la Llave representation

Lemma 3.1 (Ball representation of Coulomb)**.** *For $x \neq y$,*

$$\frac{1}{|x - y|} = \frac{1}{\pi} \int_0^\infty \frac{\mathrm{d}r}{r^5} \int_{\mathbb{R}^3} \mathbf{1}_{B(z,r)}(x) \mathbf{1}_{B(z,r)}(y)\, \mathrm{d}z.$$

Proof. Let $s = |x - y|$. The inner integral is the volume of the intersection of two balls of radius r whose centers are distance s apart. It vanishes for $r < s/2$, and for $r \geq s/2$ equals

$$\frac{\pi}{12}(4r + s)(2r - s)^2.$$

Therefore

$$\begin{aligned} \int_0^\infty \frac{\mathrm{d}r}{r^5} \int_{\mathbb{R}^3} \mathbf{1}_{B(z,r)}(x) \mathbf{1}_{B(z,r)}(y)\, \mathrm{d}z &= \int_{s/2}^\infty \frac{\pi}{12}(4r + s)(2r - s)^2 r^{-5}\, \mathrm{d}r \\ &= \frac{\pi}{s}. \end{aligned}$$

□

4 Exact variance identity

For a ball $B(z, r)$, let

$$N_{z,r} = \sum_{j=1}^N \mathbf{1}_{B(z,r)}(x_j)$$

be the random number of particles in that ball. Its mean is

$$\mathbb{E}_\Psi N_{z,r} = m_{\rho_\Psi}(z, r).$$

Lemma 4.1 (Exact variance formula)**.** *For every normalized N-particle wavefunction for which the following integrals are finite,*

$$E_{\rm xc}(\Psi) = \frac{1}{2\pi} \int_0^\infty \frac{{\rm d}r}{r^5} \int_{\mathbb{R}^3} \left(\operatorname{Var}_\Psi N_{z,r} - m_{\rho_\Psi}(z,r)\right) {\rm d}z.$$

Proof. By Theorem 3.1,

$$\left\langle \Psi, \sum_{i<j} \frac{1}{|x_i - x_j|} \Psi \right\rangle = \frac{1}{2\pi} \int_0^\infty \frac{{\rm d}r}{r^5} \int_{\mathbb{R}^3} \mathbb{E}_\Psi \left(N_{z,r}^2 - N_{z,r}\right) {\rm d}z.$$

Similarly,

$$\frac{1}{2} \iint \frac{\rho_\Psi(x)\rho_\Psi(y)}{|x-y|} \,{\rm d}x\,{\rm d}y = \frac{1}{2\pi} \int_0^\infty \frac{{\rm d}r}{r^5} \int_{\mathbb{R}^3} m_{\rho_\Psi}(z,r)^2 \,{\rm d}z.$$

Subtracting and using

$$\mathbb{E} N_{z,r}^2 - m_{\rho_\Psi}(z,r)^2 = \operatorname{Var} N_{z,r}$$

gives the identity. □

5 Integer-valued variance

Lemma 5.1 (Sharp variance of an integer random variable)**.** *Let X be an integer-valued random variable with mean m. Then*

$$\operatorname{Var} X \geq \theta(m)(1 - \theta(m)).$$

The constant is sharp.

Proof. Write $m = n + \theta$, where $n = \lfloor m \rfloor$ and $\theta \in [0,1)$. Since X is integer-valued,

$$(X-n)(X-n-1) \geq 0$$

pointwise. Taking expectations gives

$$\mathbb{E}(X-n)^2 \geq \mathbb{E}(X-n) = \theta.$$

Therefore

$$\operatorname{Var} X = \mathbb{E}(X-m)^2 = \mathbb{E}(X-n)^2 - \theta^2 \geq \theta(1-\theta).$$

Sharpness is attained by the two-point law

$$\mathbb{P}(X = n) = 1 - \theta, \qquad \mathbb{P}(X = n+1) = \theta.$$

□

Proof of Theorem 2.1. Apply Theorem 5.1 to $X = N_{z,r}$. Since

$$m_{\rho_\Psi}(z,r) - \theta(m_{\rho_\Psi}(z,r))(1 - \theta(m_{\rho_\Psi}(z,r))) = \Phi(m_{\rho_\Psi}(z,r)),$$

Theorem 4.1 gives the result. □

6 Two checks

Proposition 6.1 (Exact one-particle self-interaction)**.** *For $N = 1$, Theorem 2.1 is an equality:*

$$E_{\mathrm{xc}}(\Psi) = -\frac{1}{2\pi} \int_0^\infty \frac{\mathrm{d}r}{r^5} \int_{\mathbb{R}^3} m_{\rho_\Psi}(z, r)^2 \, \mathrm{d}z.$$

Proof. If $N = 1$, then $N_{z,r} \in \{0, 1\}$, so

$$\operatorname{Var} N_{z,r} = m_{\rho_\Psi}(z, r)(1 - m_{\rho_\Psi}(z, r)).$$

Since $0 \le m_{\rho_\Psi}(z, r) \le 1$, $\Phi(m) = m^2$. The identity follows from Theorem 4.1. □

Proposition 6.2 (Homogeneous constant produced by the bound)**.** *For a constant density ρ, the thermodynamic density of the right side is*

$$-C_{\mathrm{IV}} \rho^{4/3},$$

where

$$C_{\mathrm{IV}} = \frac{1}{6\pi} \left(\frac{4\pi}{3}\right)^{4/3} \int_0^\infty \Phi(t) t^{-7/3} \, \mathrm{d}t = 1.569 \ldots .$$

Proof. For a constant density,

$$m_\rho(z, r) = \rho |B(0, r)| = \frac{4\pi}{3} \rho r^3.$$

The bound per unit volume is therefore

$$-\frac{1}{2\pi} \int_0^\infty \Phi\left(\frac{4\pi}{3} \rho r^3\right) r^{-5} \, \mathrm{d}r.$$

With $t = (4\pi/3)\rho r^3$,

$$r^{-5} \, \mathrm{d}r = \frac{1}{3} \left(\frac{4\pi}{3} \rho\right)^{4/3} t^{-7/3} \, \mathrm{d}t.$$

This gives the formula for C_{IV}. The numerical value follows by summing the absolutely convergent interval integrals

$$\int_n^{n+1} \Phi(t) t^{-7/3} \, \mathrm{d}t.$$

□

Remark 6.3. The constant $C_{\mathrm{IV}} = 1.569 \ldots$ lies below the standard Lieb–Oxford constant 1.68 but above the Dirac constants, so the result does not solve Lieb's kinetic Dirac problem. Its significance is different: it provides a universal correlated many-body lower bound that captures the one-particle self-interaction obstruction exactly and improves as soon as local number quantization forces nonzero variance above the Bernoulli value.