# A certified explicit Lieb–Oxford constant below 1.64

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**Abstract**

The Lieb–Oxford inequality provides a universal lower bound on the classical indirect Coulomb energy of an $N$-particle density, $E_{\mathrm{ind}}[\rho] \geq -C_{\mathrm{LO}} \int \rho^{4/3}$, with a constant $C_{\mathrm{LO}}$ of central importance in density functional theory. Lieb–Oxford's original estimate gave $C_{\mathrm{LO}} \leq 1.68$; subsequent work, in particular the variational reduction of Lewin–Lieb–Seiringer (LLS), has improved this in principle but has not produced a fully explicit, rationally certified value below the original. In this paper we close that gap. Using the LLS variational principle with the symmetric ball-smearing choice $\mu = \nu = B$, an explicit auxiliary function $g$ built from the closed-form expression for $\Psi_{BB}(a, b)$, and a finite-precision rational interval-arithmetic computation, we produce a machine-verifiable certificate $C_{\mathrm{LO}} \leq 1.64$. The constant is not claimed to be optimal: improving past the value 1.58 suggested by numerical optimization would require a richer pair of radial measures $(\mu, \nu)$ and a corresponding certified upper function, which we do not produce here.

## 1 Setting and main theorem

The Lieb–Oxford inequality [1] furnishes a universal lower bound on the classical indirect Coulomb energy of a density $\rho \geq 0$ with total mass $N \in \mathbb{N}$ in terms of the $L^{4/3}$ norm of $\rho$. The smallest constant for which the inequality holds is called the *Lieb–Oxford constant*, $C_{\mathrm{LO}}$. The original 1981 bound was 1.68; the LLS reformulation [2] expresses any explicit upper bound on $C_{\mathrm{LO}}$ as the value of a variational expression in two radial probability measures, opening the door to constructive improvements. Yet a fully proof-grade, rational, finite certificate below 1.68 is not present in the published literature in a directly verifiable form. The goal of this paper is to produce such a certificate.

Let

$$E_{\mathrm{ind}}[\rho] = \inf_{\mathbb{P} \mapsto \rho} \int_{\mathbb{R}^{3N}} \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|} \, \mathrm{d}\mathbb{P} - \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho(x)\rho(y)}{|x - y|} \, \mathrm{d}x \, \mathrm{d}y$$

be the classical indirect Coulomb energy, where $\rho \geq 0$, $\int \rho = N \in \mathbb{N}$.

**Theorem 1.1** (Certified explicit ball-smearing bound)**.** *For every admissible density $\rho$,*

$$E_{\mathrm{ind}}[\rho] \geq -1.64 \int_{\mathbb{R}^3} \rho(x)^{4/3} \, \mathrm{d}x.$$

*Consequently the exchange-correlation energy satisfies the same bound.*

*Remark* 1.2. This is not the optimal Lieb–Oxford constant. It is a proof-grade explicit certificate using the symmetric ball-smearing measure. The sharper value 1.58 requires optimizing over two radial measures $\mu, \nu$; the harder certificate is not produced here.

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**Plan of the paper.** Section 2 recalls the LLS reduction (Theorem 2.1) that expresses any upper bound on $C_{\mathrm{LO}}$ as the optimum of a variational principle over radial probability measures and admissible upper functions. Section 3 carries out the ball certificate. We construct the explicit admissible function $g$ associated to $\mu = \nu = B$ (Theorem 3.1), control the resulting radial integral by exact rational interval arithmetic (Theorem 3.2), and combine the pieces to prove Theorem 1.1. Section 4 delineates precisely what an analogous certificate would have to produce to beat 1.58.

## 2 The Lewin–Lieb–Seiringer reduction

For finite measures define

$$D(\alpha, \beta) = \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\mathrm{d}\alpha(x)\,\mathrm{d}\beta(y)}{|x-y|}.$$

For radial probability measures $\mu, \nu$ put

$$\Phi_{\mu\nu}(a,b) = a^3 b^3 \left(1 - 2D(\mu_{0,a}, \nu_{e_1,b})\right), \qquad \Psi_{\mu\nu} = \Phi_{\mu\nu} + \Phi_{\nu\mu} - \Phi_{\nu\nu},$$

where $\mu_{x,a} = a^3 \mu(a(\cdot - x))$. Let $F_{\mu\nu}$ be the set of continuous nonnegative functions $f$ on $[0,\infty)$ such that

$$\Psi_{\mu\nu}(a,b) \le f(a) + f(b) \qquad (a, b \ge 0),$$

and define

$$I(\mu,\nu) = \inf_{f \in F_{\mu\nu}} \int_{\mathbb{R}^3} \frac{f(|z|)}{|z|^7}\,\mathrm{d}z.$$

**Lemma 2.1** (LLS variational bound)**.** *For every radial probability measure $\mu$ with $D(\mu,\mu) < \infty$ and every radial probability measure $\nu$,*

$$C_{\mathrm{LO}} \le \frac{3}{2} \left(2I(\mu,\nu) D(\mu,\mu)^2\right)^{1/3}.$$

*Proof.* This is the Onsager-smearing argument. Replace each point charge at $x$ by $\mu_x$, subtract an auxiliary smeared density $\eta(y) = \int \rho(x)\nu_x(y)\,\mathrm{d}x$, and use positivity of the Coulomb quadratic form:

$$D(f,f) \ge -D(\eta,\eta) + 2D(f,\eta).$$

After symmetrization the two-body error is

$$\frac{1}{2} \iint \frac{\Psi_{\mu\nu}(|x-y|\rho(x)^{1/3}, |x-y|\rho(y)^{1/3})}{|x-y|^7}\,\mathrm{d}x\,\mathrm{d}y.$$

If $\Psi_{\mu\nu}(a,b) \le f(a) + f(b)$, the change of variables $z = (y-x)\rho(x)^{1/3}$ bounds this term by

$$\left(\int_{\mathbb{R}^3} \frac{f(|z|)}{|z|^7}\,\mathrm{d}z\right) \int_{\mathbb{R}^3} \rho(x)^{4/3}\,\mathrm{d}x.$$

The self-energy contribution is

$$D(\mu,\mu) \int \rho^{4/3}.$$

Finally one optimizes over the dilation of $\mu, \nu$; under $\mu_t = t^3 \mu(t\cdot)$, one has

$$D(\mu_t, \mu_t) = tD(\mu,\mu), \qquad I(\mu_t, \nu_t) = t^{-2} I(\mu,\nu).$$

Minimizing $tD + t^{-2}I$ gives the stated constant. □

## 3 The explicit ball certificate

Let

$$B(x) = \frac{3}{4\pi}\mathbf{1}_{|x|\le 1}$$

be the uniform probability measure on the unit ball, and choose $\mu = \nu = B$. Then

$$D(B,B) = \frac{3}{5}.$$

For this choice the function $\Psi_{BB}$ is explicit:

$$\begin{aligned}\Psi_{BB}(a,b) = {} & \frac{(a+b-ab)_+^4}{160}\left(a^2b^2 - 5a^2 - 5b^2 + 4ab^2 + 4ba^2 + 20ab\right)\\ & - \frac{(|a-b|-ab)_+^4}{160}\left(a^2b^2 - 5a^2 - 5b^2 + 4|a-b|ab - 20ab\right).\end{aligned}$$

**Lemma 3.1** (Explicit admissible function)**.** *Define*

$$g(a) = \max_{0\le b\le a}\left\{\Psi_{BB}(a,b) - \frac{1}{2}\Psi_{BB}(b,b)\right\}.$$

*Then $g \in F_{BB}$.*

*Proof.* The function $\Psi_{BB}$ is symmetric and nonnegative. Since $g(a) \ge 0$ and $g(a) \ge \Psi_{BB}(a,b) - \Psi_{BB}(b,b)/2$ whenever $b \le a$, symmetry gives, for $a \ge b$,

$$\Psi_{BB}(a,b) \le g(a) + \frac{1}{2}\Psi_{BB}(b,b) \le g(a) + g(b).$$

The case $b \ge a$ follows by symmetry. □

**Lemma 3.2** (Certified one-dimensional integral)**.** *For the above $g$,*

$$4\pi\int_0^\infty g(r)r^{-5}\,\mathrm{d}r < 1.8150.$$

*Proof.* This is a finite rational interval-arithmetic computation applied to the explicit polynomial formula for $\Psi_{BB}$. The accompanying script

`certify_lo_ball_1p64.py`

uses only exact rational arithmetic in the certification comparisons.

The interval $[0,\infty)$ is split into $[0,10^{-3}]$, $[10^{-3},4]$, and $[4,\infty)$.

On the first interval one uses $\Psi_{BB}(a,b) \le a^3b^3$, hence $g(a) \le a^6$. On the compact interval $[10^{-3},4]$, divide the $a$-axis into intervals of length $1/800$ and the $b$-axis into intervals of length $1/400$. On each rectangle in the $(a,b)$-plane, the displayed formula for $\Psi_{BB}$ gives an outward-rounded rational upper bound for

$$\Psi_{BB}(a,b) - \frac{1}{2}\Psi_{BB}(b,b).$$

The diagonal lower bound uses

$$\Psi_{BB}(b,b) = \frac{b^6(b-2)^4(b^2+8b+10)}{160} \qquad (0 \le b \le 2),$$

whose derivative is

$$\frac{3b^5(b-2)^3(b^3+6b^2-b-10)}{40}.$$

Thus the minimum of $\Psi_{BB}(b,b)$ on each subinterval is attained at an endpoint, except when the interval touches 0 or 2, where the lower bound 0 is exact.

Summing the resulting upper bounds times $\int_{r_j}^{r_{j+1}} r^{-5}\,\mathrm{d}r$ gives

$$4\pi \int_0^4 g(r) r^{-5}\,\mathrm{d}r < 1.65791.$$

For the tail $a \geq 4$, put $u = 1/a$. The nonzero region is split by

$$b \leq \frac{1}{1+u}, \qquad \frac{1}{1+u} \leq b \leq \frac{1}{1-u}.$$

In the first region,

$$\frac{\Psi_{BB}(a,b)}{a^3} = \frac{b^3}{10}\left(10 - 15b + 5b^3 + 3b^3u^2\right), \qquad 0 \leq u \leq \frac{1}{4}.$$

In the second region, with $t = us$,

$$\frac{\Psi_{BB}(a,b)}{a^3} = \frac{u^2 s^4\left(us^2(5u+1) - s(30u+6) + 30\right)}{160(1-u)}.$$

Exact rational interval subdivision verifies that both expressions are strictly below $1/20$. Hence

$$g(a) \leq \frac{a^3}{20} \qquad (a \geq 4),$$

and the tail contributes less than

$$4\pi \int_4^\infty \frac{1}{20} r^{-2}\,\mathrm{d}r = \frac{\pi}{20} < \frac{333}{2120}.$$

Using $\pi < 333/106$, the script obtains the certified rational bound

$$4\pi \int_0^\infty g(r) r^{-5}\,\mathrm{d}r < 1.81498 < 1.8150. \qquad \square$$

*Proof of Theorem 1.1.* By Theorems 2.1, 3.1 and 3.2,

$$C_{\mathrm{LO}} \leq \frac{3}{2}\left(2 \cdot 1.8150 \cdot \left(\frac{3}{5}\right)^2\right)^{1/3}.$$

The right side is $< 1.64$, proving the theorem. $\square$

## 4 What would be needed to beat 1.58

The same variational formula can produce 1.58 by optimizing over nontrivial radial measures $\mu, \nu$. A proof at the level of rigor of the Jellium/UEG papers would require the following finite certificate:

$$\text{explicit rational radial measures } \mu, \nu, \quad \text{an explicit rational piecewise upper function } f,$$

with

$$\Psi_{\mu\nu}(a,b) \leq f(a) + f(b) \quad \text{for all } a, b \geq 0,$$

and

$$\frac{3}{2}\left(2D(\mu,\mu)^2 \int_{\mathbb{R}^3} \frac{f(|z|)}{|z|^7}\,\mathrm{d}z\right)^{1/3} < 1.58.$$

Without such a certificate, a smaller number is only a numerical experiment, not a proof of a new Lieb–Oxford constant.

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## References


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

[2] 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.