# Explicit quantitative gaps for low-particle Lieb–Oxford constants

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**Abstract**

We give explicit, highly nonsharp lower bounds for two successive low-particle-number gaps in the three-dimensional Coulomb Lieb–Oxford inequality. Assuming the fixed-particle attainment theorem stated in a 2026 preprint, we prove $C_3 - C_2 \geq e^{-1769000}$. A complete Coulomb-specific reconstruction of compatible potentials and compact support is included. More generally, if $0 < g \leq 1$ and $C_3 - C_2 \geq g$, then

$$C_4 - C_3 \geq \frac{g^{211}}{2 \cdot 30^{25} \cdot 10^{395}} \exp\left(-\frac{4 \cdot 10^{12}}{g^9}\right).$$

The argument quantifies an existing strict-extension mechanism using normalized optimizer bounds, localization from a saturated triple, and exterior Coulomb variance that survives deletion of an arbitrary small-volume set. An elementary radial witness independently supplies $C_2 > 1.2515$. These bounds have no practical decimal precision; no exact constant, numerical record, priority, or all-particle-number recursion is claimed.

**Authorship and review status.** This manuscript was prepared with substantial AI assistance in deriving, organizing, typesetting, and checking the arguments. The accompanying scripts check finite arithmetic only. The manuscript has not undergone external mathematical peer review. Appendix B reconstructs the compatible-potential and compact-support package in three-dimensional Coulomb form; fixed-particle attainment and the other identified literature inputs remain assumed and are not machine-verified here.

## Contents

**1 Definitions, prior work, and the quantitative statements** **2**
1.1 Relationship with prior work . . . . . 3
1.2 Proof dependency graph . . . . . 4

**2 External inputs and shared estimates** **4**

**3 An explicit gap between two and three particles** **7**
3.1 A compatible dual normalization and an essential core . . . . . 8
3.2 A quantitative dual gap and occupied-volume bound . . . . . 10
3.3 Two-atom identifiability and a conditional covariance bound . . . . . 11
3.4 Shell harmonics under an arbitrary deterministic mask . . . . . 13
3.5 The exact interaction and a positive marginal-preserving coupling . . . . . 15
3.6 The sharp three-particle comparison and its explicit balance . . . . . 16

**4 Three-particle localization and the chemical gap** **18**
4.1 A joint core event from the energetic gap . . . 18
4.2 Localization from a saturated triple . . . 21
4.3 The compatible potential and the chemical gap . . . 24

**5 Harmonic moments of three points and exterior covariance** **27**
5.1 A quantitative inverse estimate . . . 27
5.2 Variance from a single bounded marginal . . . 29
5.3 Irregular shell masks and the exact Coulomb potential . . . 30

**6 An explicit transfer from three to four particles** **32**

**A An elementary independent lower witness** **37**

**B Compatible Coulomb potentials and compact support** **38**
B.1 Variational inequality and a precise feasible representative . . . 39
B.2 A bounded feasible majorant by sequential transforms . . . 40
B.3 A monotone averaged transform and exact conjugacy . . . 41
B.4 The global positive part relation and continuous representatives . . . 43
B.5 The limit at infinity and the sign of the compatible gap . . . 43
B.6 Two-cycle monotonicity and qualitative dissociation . . . 44
B.7 Attaining the lower-particle energy and the global upper tail . . . 46
B.8 Compact support and the normalized shift . . . 46
B.9 The one-particle case . . . 47

**C Finite arithmetic and source provenance** **47**

# 1 Definitions, prior work, and the quantitative statements

For a nonnegative density $\rho \in L^1(\mathbb{R}^3) \cap L^{4/3}(\mathbb{R}^3)$ of mass $N \in \mathbb{N}$, define

$$D(f,k) = \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{f(x)k(y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y, \qquad H(f) = \tfrac{1}{2}D(f,f),$$
$$I(f) = \int_{\mathbb{R}^3} f^{4/3}, \qquad c_N(X) = \sum_{1\le i<j\le N} |x_i - x_j|^{-1}. \tag{1}$$

Let $\mathcal{P}_N(\rho)$ denote the symmetric probability measures on $(\mathbb{R}^3)^N$ whose every labeled marginal is $\rho/N$. Put

$$W_N(\rho) = \inf_{P\in\mathcal{P}_N(\rho)} \int c_N\,\mathrm{d}P, \qquad C_N = \sup_{\substack{\rho\ge 0\\ \int\rho = N}} \frac{H(\rho) - W_N(\rho)}{I(\rho)}.$$

The joint measures may be singular. Only the one-body densities have the stated integrability. In particular, $D$ is the full Coulomb double integral and $H$ has the factor $1/2$. Mass-preserving dilation $\rho_a(x) = a^3\rho(ax)$ multiplies $H, W_N, I$ by $a$, so a nonzero optimizer can be normalized by $I(\rho) = 1$.

### 1.1 Relationship with prior work

Rosenzweig's 2026 preprint [1] proves attainment and qualitative strict monotonicity of the fixed-particle constants. Its Sections 6.2–6.3 construct the non-product one-particle extension and diffuse completion used below. Its Section 7.2 leaves quantitative successive-gap estimates unevaluated. Attainment and qualitative monotonicity remain explicit literature inputs. The compatible dual-potential and compact-support framework of Di Marino and Lelotte [2] is reconstructed in Appendix B for the precise three-dimensional Coulomb setting used here, conditional on optimizer existence.

Several ingredients have close antecedents. Buttazzo, Champion, and De Pascale [4] obtain quantitative collision exclusion and regularity and bounds for Coulomb Kantorovich potentials. Thus explicit potential control in general is not a contribution asserted here. Lelotte's dissociation and binding analysis [5] motivates the lower-particle exchange argument. Appendix B reproduces the global upper-tail mechanism of its Section 3.1, equations (29)–(32), under a temporary unbounded-support assumption; it does not use a global two-sided asymptotic or impose connected support. Wang and Lü [6], Lemma 0.4.3, use configuration-dependent complex-isotropic projections, spherical-cap exclusion, and annihilating polynomials. The triple-moment argument below is a self-contained equal-weight specialization of that geometry, rather than a new reconstruction principle.

The proposed contribution is a quantitative refinement of the known strict-extension mechanism at two low particle numbers. Its specific estimates use occupied volume instead of a uniform bound on the diameter of the full support. The most specialized new bridge is the explicit saturated-triple localization argument; the exterior variance estimates are uniform after irregular deterministic deletion. The fourth-particle result is a worked continuation of the same mechanism. A focused primary-source check on 4 October 2026 located no matching explicit replacement bound, but it does not establish priority or an exhaustive literature clearance.

**Theorem 1.1** (Quantitative low-particle gaps)**.** *Assume the external attainment and standard analytic inputs identified in Proposition 2.1, with the compatible-potential package proved in Appendix B. For the constants defined above,*

$$C_3 - C_2 \geq \exp(-1769000). \tag{2}$$

*Moreover, for every* $0 < g \leq 1$ *satisfying* $C_3 - C_2 \geq g$*,*

$$\begin{aligned} C_4 - C_3 \geq G(g) &:= \frac{g^{211}}{2 \cdot 30^{25} \cdot 10^{395}} \exp\left(-\frac{4 \cdot 10^{12}}{g^9}\right) \\ &\geq \exp\left(-\frac{5 \cdot 10^{12}}{g^9}\right). \end{aligned} \tag{3}$$

*In particular,*

$$C_4 - C_3 \geq \exp[-\exp(15921030)]. \tag{4}$$

*No attainment result for* $N = 4$ *is needed.*

The informative quantitative statement is the transfer function $G(g)$; the nested exponential is only a convenient weakening. The constants are far too small to improve useful decimal digits. Neither the exact value of $C_2$, radiality or uniqueness of an optimizer, a numerical record, nor an all-$N$ quantitative recursion follows.

### 1.2 Proof dependency graph

The dependencies are acyclic. Here "external" refers to cited theorem inputs, not conclusions of the arithmetic scripts.

| Node | Required inputs and output |
|---|---|
| E | External attainment and qualitative monotonicity; published 1.58 upper bound; sharp Coulomb HLS |
| F | E's attainment + variational optimality $\longrightarrow$ compatible c-conjugated potential, positive-part relation, compact support (Appendix B) |
| L | Explicit radial trial plan $\longrightarrow C_2 > 1.2515 > 5/4$ (Appendix A) |
| U | E + F + L $\longrightarrow \rho < 12$, $U_\rho < 4$ for normalized $N = 2, 3$ optimizers |
| T2 | U + two-particle core and dual localization $\longrightarrow \kappa_2$ and occupied-volume bound |
| V2 | T2 + masked dipole/quadrupole variance + extension $\longrightarrow C_3 - C_2 \geq e^{-1769000}$ |
| T3 | E + F + U + $C_3 - C_2 \geq g \longrightarrow$ joint core, anchor-based dual-pair localization, $\kappa_3$, occupied volume |
| V3 | T3 + degree-three harmonic variance + extension $\longrightarrow C_4 - C_3 \geq G(g)$ |

The $N = 3$ attainment input does not depend on the quantitative $N = 4$ conclusion. The reconstruction F applies to an already existing optimizer and uses no numerical successive-gap estimate. We prove all arrows beyond E in the manuscript. The finite scripts reproduce selected numerical inequalities and do not certify infinite-dimensional analysis.

## 2 External inputs and shared estimates

The next proposition separates the remaining literature inputs from the compatible-potential conclusions reconstructed in Appendix B. The attainment input is taken from a 2026 preprint as of the manuscript date; neither that paper's full proof nor the entire cited literature is certified here.

**Proposition 2.1** (Attainment input and reconstructed compatible-potential package)**.** *For $N = 2, 3$, item 1 is an external input. Items 2–3 follow from the reconstruction in Appendix B, conditional on item 1.*

1. *The supremum defining $C_N$ is attained by a density $\rho \in L^1 \cap L^{4/3}$ of mass $N$. The fixed-particle constants are qualitatively increasing; only $C_3 \geq C_2$ is used before our quantitative proof [1, Theorem 1.1]. The density may be dilated so that $I(\rho) = 1$. Its Coulomb multimarginal problem has a symmetric optimal probability law $P$, by the weak-compactness argument recalled in Appendix B; see also [1, Lemma 2.1].*

2. *Such an optimizer has compact support. Set $\lambda = C_N$, $U = \rho * |\cdot|^{-1}$, $\beta = 4\lambda/3$, and $v = U - \beta\rho^{1/3}$. There is a bounded, globally Lipschitz, pointwise feasible and $c_N$-conjugated potential $\phi$, and a constant $c$, such that*

$$\sum_{i=1}^{N} \phi(x_i) \leq c_N(X), \qquad \int \phi\rho = W_N(\rho), \tag{5}$$

$$\phi(x) = \inf_{x_2,\dots,x_N} \left\{ c_N(x, x_2, \dots, x_N) - \sum_{i=2}^{N} \phi(x_i) \right\}, \tag{6}$$

$$\phi \geq v + c \text{ globally}, \qquad \phi = v + c \text{ on the density support.} \tag{7}$$

*The continuous representatives of $\rho$ and $U$ and boundary vanishing permit these relations to be used pointwise. Proposition B.1 proves this package using the variational framework of [2, Section 3].*

3. *Define*

$$E_k(f) = \inf_{z_1,\dots,z_k} \left\{ c_k(z_1,\dots,z_k) - \sum_{i=1}^{k} f(z_i) \right\}.$$

*For the same normalized representative, $E_N(\phi) = 0$, and*

$$C_\phi := \lim_{|x|\to\infty} \phi(x) = E_{N-1}(\phi). \tag{8}$$

*The global limit identity is proved directly in Appendix B; see also [2, Lemma 2] and [5, Lemma 4]. The compactness proof uses only the separately established global upper-tail estimate under a temporary unbounded-support assumption, never a global two-sided asymptotic.*

*We also use the published universal estimate $C_N \le 1.58 < 8/5$ [3, Eq. (7)] and the sharp Hardy–Littlewood–Sobolev inequality [7, 8]. The pointwise dual feasibility, equality of primal and dual values for the constructed potential, and almost-sure saturation needed below are proved directly in Appendix B.*

**Lemma 2.2** (Compatible positive-part relation)**.** *For a normalized optimizer as above, put $\psi = \phi - C_\phi$ and $\kappa = C_\phi - c$. Then*

$$\psi \ge 0, \quad \psi(x) \longrightarrow 0 \quad (|x| \to \infty), \quad \kappa \ge 0, \tag{9}$$

$$c = -\frac{W_N(\rho)}{N} - \frac{2\lambda}{3N}, \qquad \rho = \left[ \frac{(U - \psi - \kappa)_+}{\beta} \right]^3. \tag{10}$$

*Proof.* The c-transform in (6) is at least $E_{N-1}(\phi) = C_\phi$, because the interactions with its fixed point are nonnegative. Thus $\psi \ge 0$, and its limit follows from (8). Integrate the compatible equality against $\rho$ and use $H = W_N + \lambda$ and $I = 1$:

$$W_N = 2H - \frac{4}{3}\lambda + Nc = 2W_N + \frac{2}{3}\lambda + Nc.$$

This gives the displayed $c$. On $\{\rho > 0\}$, compatibility is precisely $\beta\rho^{1/3} = U - \psi - \kappa$. At zero-density points the global majorization in (7) gives $U - \psi - \kappa \le 0$. This proves the positive-part identity, initially almost everywhere and then for the continuous representatives. If $\kappa < 0$, $\psi \to 0$ and $U \ge 0$ would force a positive density floor sufficiently far away, contradicting finite mass. Hence $\kappa \ge 0$. □

**Lemma 2.3** (HLS and interpolation)**.** *For $f \ge 0$ in $L^1 \cap L^{4/3}$,*

$$H(f) \le a \left( \int f \right)^{2/3} I(f), \qquad a = \frac{2}{3} \left( \frac{4}{\sqrt{\pi}} \right)^{2/3} < \frac{23}{20}. \tag{11}$$

*More generally, for nonnegative $f, k$,*

$$D(f,k) \le 2a \left( \int f \right)^{1/3} \left( \int k \right)^{1/3} I(f)^{1/2} I(k)^{1/2}.$$

*Proof.* The sharp Coulomb HLS inequality has diagonal constant $2a$ in dimension three. Interpolation yields $\|f\|_{6/5} \le \|f\|_1^{1/3}\|f\|_{4/3}^{2/3}$, so its square is at most $(\int f)^{2/3} I(f)$. Applying the bilinear form gives both assertions. Finally $a^3 = 128/(27\pi) < (23/20)^3$, using $\pi > 333/106$; Appendix A supplies elementary rational bounds on $\pi$. □

**Proposition 2.4** (Uniform normalized density and potential caps)**.** *For $N = 2, 3$, a normalized optimizer satisfies $5/4 \le \lambda \le 8/5$ and*

$$\|\rho\|_\infty < 12, \qquad \|U\|_\infty < 4.$$

*Proof.* The lower bound for $C_2$ follows from Proposition A.1; qualitative monotonicity from [1, Theorem 1.1] gives $C_3 \ge C_2$. The published universal bound gives the upper bound. Continuity and compact support imply $B = \|\rho\|_\infty < \infty$.

For any nonnegative $f \le B$ with $I(f) = 1$, an elementary capped variational inequality gives

$$\|f * |\cdot|^{-1}\|_\infty \le KB^{1/9}, \qquad K = 6\pi\left(\frac{3}{16\pi}\right)^{2/3}, \quad K^3 = \frac{243\pi}{32}. \tag{12}$$

Here is a direct proof. At the origin compare with

$$f_*(r) = B\min\{1, (b/r)^3\}, \qquad b = \left(\frac{3}{16\pi}\right)^{1/3} B^{-4/9}.$$

Radial integration gives $I(f_*) = (16\pi/3)B^{4/3}b^3 = 1$. Choose the positive multiplier $\mu$ with $(4\mu/3)B^{1/3} = b^{-1}$. For each $r > 0$, the concave function $t/r - \mu t^{4/3}$ on $[0, B]$ is maximized by $t = f_*(r)$. Integrating this pointwise inequality and using the equal power integrals shows that the potential of $f$ at the origin is at most that of $f_*$. A translation proves the same assertion at every point. The latter potential is $6\pi Bb^2 = KB^{1/9}$. The comparison profile has infinite mass, which is permissible because the mass constraint was dropped in this upper comparison; all integrals used in the comparison are finite.

From Lemma 2.2, $\beta\rho^{1/3} \le U$ and $\beta \ge 5/3$. Therefore

$$B \le \left(\frac{K}{5/3}\right)^{9/2}, \qquad \|U\|_\infty^2 \le \frac{K^3}{5/3} = \frac{729\pi}{160} < 16.$$

Also $B^2 \le (K^3/(5/3)^3)^3 < 144$. Both strict rational comparisons follow from $\pi < 22/7$. □

**Lemma 2.5** (Marginal-preserving one-particle extension)**.** *Let $\rho$ be a normalized compactly supported $N$-particle optimizer with optimal law $P$. Let $\nu$ be a boundedly supported probability density in $L^{4/3}$, with $\rho\nu = 0$ almost everywhere, and $A = I(\nu)$. Suppose a coupling $\Gamma$ of the entire old law $P$ and the new marginal $\nu$ reduces the old–new pair cost by $\Delta > 0$ relative to $P \otimes \nu$, all costs being finite. Then, for every $0 < \varepsilon < 1$,*

$$C_{N+1} - C_N \ge \varepsilon\Delta - C_{N+1}A\varepsilon^{4/3}. \tag{13}$$

*Proof.* Take a smooth compactly supported probability density $\zeta$ and dilate and translate it to $\zeta_L$ with support disjoint from those of $\rho$ and $\nu$ and with $I(\zeta_L) = L^{-1}I(\zeta) \to 0$. Compactness suffices; no uniform support radius is needed. Symmetrize the $(N+1)$-particle probability law

$$\Pi_L = \varepsilon\Gamma + (1-\varepsilon)(P \otimes \zeta_L).$$

It has one-body density $\rho + \sigma_L$, where $\sigma_L = \varepsilon\nu + (1-\varepsilon)\zeta_L$. Each configuration has exactly one additional particle. Preserving the whole old law gives the exact trial cost

$$\int c_{N+1}\,\mathrm{d}\Pi_L = W_N(\rho) + D(\rho, \sigma_L) - \varepsilon\Delta.$$

The Hartree expansion and $H(\sigma_L) \geq 0$ imply

$$H(\rho + \sigma_L) - \int c_{N+1}\,\mathrm{d}\Pi_L = C_N + \varepsilon\Delta + H(\sigma_L) \geq C_N + \varepsilon\Delta.$$

Disjointness almost everywhere gives

$$I(\rho + \sigma_L) = 1 + \varepsilon^{4/3}A + (1-\varepsilon)^{4/3}I(\zeta_L).$$

Since $W_{N+1}$ is no larger than the trial cost, the defining inequality for $C_{N+1}$ bounds this numerator by $C_{N+1}I(\rho + \sigma_L)$. Pass to $L \to \infty$ and rearrange to obtain (13). The cross Hartree term cancels exactly before the limit. There is no extra quotient denominator and no need for an $(N+1)$-particle optimizer. □

This is the non-product extension and diffuse-completion mechanism of [1, Sections 6.2–6.3]. The task below is to make $\Delta$ and an admissible $\varepsilon$ explicit.

## 3 An explicit gap between two and three particles

We now quantify the two-particle instance of the strict-extension mechanism of [1]. The optimizer and the compatible potential used below are supplied by Proposition 2.1; the Euler–Lagrange and compact-support framework of [2] is reconstructed in Appendix B. Throughout this section, let

$$\int_{\mathbb{R}^3} \rho = 2, \qquad I(\rho) = 1, \qquad \lambda = C_2 = H(\rho) - W_2(\rho), \qquad \frac{5}{4} \leq \lambda \leq \frac{8}{5}, \qquad \beta = \frac{4\lambda}{3}. \tag{14}$$

Here $\rho$ is a normalized optimizer and $P$ is a symmetric optimal two-particle probability measure, with each labeled marginal $\rho/2$. The lower numerical input in (14) follows from Proposition A.1 in Appendix A; the upper input follows from the universal bound of [3]. Set

$$U(x) = \int_{\mathbb{R}^3} \frac{\rho(y)}{|x-y|}\,\mathrm{d}y, \qquad \mathcal{O} = \{x : \rho(x) > 0\}.$$

The set $\mathcal{O}$ is understood up to Lebesgue-null sets. All volume and masking statements concern this occupied set, rather than a topological notion of support. The compactly supported continuous representative provided by Appendix B will be used when pointwise statements are convenient. Proposition 2.4 gives

$$0 \leq \rho \leq 12, \qquad 0 \leq U \leq 4. \tag{15}$$

No symmetry, connectedness, uniqueness, or uniform bound on the diameter of the support is assumed.

### 3.1 A compatible dual normalization and an essential core

**Lemma 3.1** (The two-particle dual level)**.** *There is a bounded, globally Lipschitz, c-conjugated compatible potential $\phi$ satisfying*

$$\phi(x) + \phi(y) \le \frac{1}{|x-y|}, \qquad \int \phi\rho = W_2(\rho). \tag{16}$$

*Writing*

$$\phi_\rho = U - \beta\rho^{1/3}, \qquad c = \frac{1}{2}E_2(\phi_\rho), \qquad S_\phi = \sup_{\mathbb{R}^3}\phi, \qquad \psi = \phi + S_\phi, \qquad \kappa = -S_\phi - c,$$

*one has*

$$c = -\frac{1}{2}W_2(\rho) - \frac{\lambda}{3}, \qquad 0 \le \kappa \le \frac{\lambda}{3} \le \frac{8}{15}, \qquad \psi \ge 0, \tag{17}$$

*and*

$$\rho(x) = \left(\frac{(U(x) - \psi(x) - \kappa)_+}{\beta}\right)^3. \tag{18}$$

*Moreover, $\psi(x) \longrightarrow 0$ as $|x| \longrightarrow \infty$.*

*Proof.* Use the particular compatible potential from Proposition 2.1, not an arbitrary dual maximizer. The cited construction gives

$$\phi = \phi_\rho + c \quad \text{on the support of } \rho, \qquad U + c \le \phi \quad \text{off that support.}$$

The shift in these relations indeed equals $E_2(\phi_\rho)/2$: global compatibility gives $\phi_\rho \le \phi - c$, so feasibility implies $E_2(\phi_\rho) \ge 2c$. Conversely, complementary slackness and compatibility on the two occupied coordinates give $|x-y|^{-1} - \phi_\rho(x) - \phi_\rho(y) = 2c$ for $P$-almost every pair, and hence $E_2(\phi_\rho) \le 2c$. Its two-particle asymptotic level is $-\sup\phi = -S_\phi$, which proves the asserted limit for $\psi$. Integrating the first relation against $\rho$ and using $I(\rho) = 1$ yields

$$W_2(\rho) = 2H(\rho) - \beta + 2c = 2W_2(\rho) + 2\lambda - \frac{4\lambda}{3} + 2c.$$

This proves the formula for $c$. The two compatible relations also show that $U + c - \phi = \beta\rho^{1/3}$ wherever $\rho > 0$, and that $U + c - \phi \le 0$ wherever $\rho = 0$. Consequently (18) holds almost everywhere, and then everywhere for the continuous representatives.

The $c_2$-conjugacy relation gives

$$\phi(x) = \inf_y \{|x-y|^{-1} - \phi(y)\} \ge -\sup_y \phi(y) = -S_\phi.$$

Thus $\psi \ge 0$. If $\kappa < 0$, then for all sufficiently large $|x|$ the limit $\psi(x) \to 0$, together with $U \ge 0$, would give

$$U(x) - \psi(x) - \kappa \ge -\kappa/2 > 0.$$

Equation (18) would impose a strictly positive density floor on an infinite-volume exterior region, contrary to $\int\rho = 2$. Thus $\kappa \ge 0$. Finally, (16) implies $2S_\phi \ge \int\phi\rho = W_2(\rho)$, and hence

$$\kappa = -S_\phi + \frac{1}{2}W_2(\rho) + \frac{\lambda}{3} \le \frac{\lambda}{3}.$$

□

**Lemma 3.2** (A ball containing more than one particle of mass)**.** *After a translation, one has*

$$\int_{B_R} \rho > \frac{11}{10}, \qquad R = 150. \tag{19}$$

*Proof.* Lemma 2.3, namely the sharp Hardy–Littlewood–Sobolev inequality [7] followed by interpolation, gives, for every nonnegative $f \in L^1 \cap L^{4/3}(\mathbb{R}^3)$,

$$H(f) \le K \left( \int f \right)^{2/3} \int f^{4/3}, \qquad K = \frac{2}{3} \left( \frac{4}{\sqrt{\pi}} \right)^{2/3} < \frac{23}{20}. \tag{20}$$

In fact, the interpolation step is $\|f\|_{6/5} \le \|f\|_1^{1/3} \|f\|_{4/3}^{2/3}$, so that the square of the interpolated bound has exactly the powers displayed in (20).

Partition space into half-open cubes of side length $\ell$, and average their common translation uniformly over $[0, \ell)^3$. A pair with displacement $z$ belongs to the same cube with probability

$$w_\ell(z) = \prod_{j=1}^{3} (1 - |z_j|/\ell)_+.$$

The elementary product estimate gives

$$1 - w_\ell(z) \le \sum_{j=1}^{3} \min\{1, |z_j|/\ell\} \le \frac{|z_1| + |z_2| + |z_3|}{\ell} \le \frac{\sqrt{3}\,|z|}{\ell}.$$

Let $q_\ell$ be the supremum of $\int_Q \rho$ over all cubes of this side length. For each translated partition, (20) gives

$$\sum_Q H(\rho \mathbf{1}_Q) \le K q_\ell^{2/3} \sum_Q \int_Q \rho^{4/3} = K q_\ell^{2/3}.$$

Tonelli's theorem identifies its average with $\frac{1}{2} \iint \rho(x)\rho(y) w_\ell(x-y) |x-y|^{-1} \, \mathrm{d}x \, \mathrm{d}y$. The lost interaction is bounded by $\frac{1}{2} (\int \rho)^2 \sqrt{3}/\ell = 2\sqrt{3}/\ell$. Therefore

$$H(\rho) \le K q_\ell^{2/3} + \frac{2\sqrt{3}}{\ell}. \tag{21}$$

Take $\ell = 100\sqrt{3}$. If $q_\ell \le 11/10$, then

$$H(\rho) < \frac{23}{20} \left( \frac{11}{10} \right)^{2/3} + \frac{1}{50} < \frac{5}{4}.$$

For completeness, the last strict inequality is equivalent to $(11/10)^2 < (123/115)^3$, and follows from $121 \cdot 115^3 = 184025875 < 186086700 = 100 \cdot 123^3$. This contradicts $H(\rho) \ge H(\rho) - W_2(\rho) = \lambda \ge 5/4$. Thus some cube has mass greater than $11/10$. Its circumscribed ball has radius $\sqrt{3}\ell/2 = 150$. Translate its center to the origin. □

**Lemma 3.3** (Localization of a dual maximizer)**.** *The potential $\phi$ attains its maximum at a point $y_0 \in B_{3R}$, and*

$$S_\phi \ge \frac{1}{4R} > 0, \qquad 0 \le \psi(z) \le \frac{1}{|z - y_0|} \quad (z \ne y_0). \tag{22}$$

*Proof.* Since both labeled marginals of $P$ equal $\rho/2$, the union bound yields

$$p := P(B_R \times B_R) \geq \int_{B_R} \rho - 1 > \frac{1}{10}. \tag{23}$$

Complementary slackness holds $P$-almost everywhere: $\phi(x) + \phi(y) = |x-y|^{-1}$. On the positive-probability event $B_R \times B_R$, this sum is at least $1/(2R)$. There is consequently a point $x \in B_R$ with $\phi(x) \geq 1/(4R)$, and the same lower bound holds for $S_\phi$.

Choose a maximizing sequence $y_j$ with $\phi(y_j) \to S_\phi$. If $y_j = x$ infinitely often, then $x$ itself is a maximizer and there is nothing to prove. Otherwise dual feasibility, with a positive denominator for all sufficiently large $j$, gives

$$|y_j - x| \leq \frac{1}{\phi(y_j) + \phi(x)}.$$

It follows that $\limsup_j |y_j - x| \leq 1/(S_\phi + \phi(x)) \leq 2R$. A subsequence converges to a point $y_0 \in B_{3R}$ (with closed balls used at their boundaries), and continuity gives $\phi(y_0) = S_\phi$. Feasibility with $y_0$ then gives $\psi(z) = \phi(z) + \phi(y_0) \leq |z - y_0|^{-1}$. Its nonnegativity was proved in Lemma 3.1. □

### 3.2 A quantitative dual gap and occupied-volume bound

**Proposition 3.4** (An explicit lower bound for the dual gap)**.** *Every optimizer and compatible potential above satisfy*

$$\kappa \geq \kappa_0 := \frac{\exp(-104000)}{852000} > 0. \tag{24}$$

*Proof.* Write $m_0 = 11/10$. For $s = |z| > 3R$, the core mass bound and Lemma 3.3 imply

$$U(z) - \psi(z) \geq \frac{m_0}{s+R} - \frac{1}{s-3R}.$$

For $s \geq 6R$ one has

$$\frac{1}{s+R} \geq \frac{1}{s} - \frac{R}{s^2}, \qquad \frac{1}{s-3R} = \frac{1}{s} + \frac{3R}{s(s-3R)} \leq \frac{1}{s} + \frac{6R}{s^2}.$$

Consequently

$$U(z) - \psi(z) \geq \frac{m_0 - 1}{s} - \frac{(m_0+6)R}{s^2} \geq \frac{m_0 - 1}{2s} \quad \text{for } s \geq s_0, \tag{25}$$

where

$$s_0 = \max\left\{6R, \frac{2(m_0+6)R}{m_0 - 1}\right\} = 21300.$$

If $\kappa = 0$, equations (18) and (25) force a positive multiple of $s^{-3}$ as a density lower bound on the entire exterior region $s \geq s_0$. Its radial mass integral is a positive multiple of $\int_{s_0}^{\infty} s^{-1}\,\mathrm{d}s$, contrary to the finite mass of $\rho$. Thus $\kappa > 0$.

On the annulus

$$s_0 \leq |z| \leq \frac{m_0 - 1}{4\kappa},$$

one has $\kappa \leq (m_0 - 1)/(4|z|)$, and hence

$$\rho(z) \geq \left(\frac{m_0 - 1}{4\beta|z|}\right)^3 \geq \left(\frac{3}{256|z|}\right)^3,$$

where the last inequality uses $\beta \le 32/15$. If the annulus is empty, then $\kappa \ge (m_0 - 1)/(4s_0) = 1/852000$, which is stronger than the conclusion. Otherwise radial integration gives

$$2 = \int \rho \ge 4\pi \left(\frac{3}{256}\right)^3 \log\left(\frac{m_0 - 1}{4\kappa s_0}\right).$$

Rearranging,

$$\kappa \ge \frac{1}{852000} \exp\left(-\frac{256^3}{54\pi}\right). \tag{26}$$

The elementary bound $\pi > 3$ gives $256^3/(54\pi) < 256^3/162 < 104000$, proving (24). We deliberately use the full mass 2 in the annular estimate; no sharper estimate for the remaining exterior mass is needed. □

**Proposition 3.5** (Occupied volume)**.** *The occupied set satisfies*

$$|\mathcal{O}| \le 36\pi\kappa^{-3} \le 36\pi\kappa_0^{-3} =: V. \tag{27}$$

*Proof.* Equation (18), together with $\psi \ge 0$, implies $\mathcal{O} \subset \{U \ge \kappa\}$ up to null sets. Let $F$ be a bounded measurable subset of the latter set. For every $y$, radial rearrangement of the decreasing kernel gives

$$\int_F \frac{\mathrm{d}x}{|x - y|} \le \int_{B_a} \frac{\mathrm{d}x}{|x|} = 2\pi a^2, \qquad a = \left(\frac{3|F|}{4\pi}\right)^{1/3}.$$

Tonelli's theorem and $\int \rho = 2$ therefore give

$$\kappa|F| \le \int_F U \le 4\pi \left(\frac{3|F|}{4\pi}\right)^{2/3}.$$

For $|F| > 0$, division by $|F|^{2/3}$ and cubing yield $|F| \le 36\pi\kappa^{-3}$; the assertion is immediate when $|F| = 0$. Apply this to $F = \{U \ge \kappa\} \cap B_a$ and let $a \to \infty$. Monotone convergence proves the asserted bound for $\mathcal{O}$. This is a volume estimate, and asserts no diameter or connectedness bound. □

### 3.3 Two-atom identifiability and a conditional covariance bound

Set

$$\mathcal{C} = B_R \times B_R, \qquad Q = P(\,\cdot \mid \mathcal{C}), \qquad r = \frac{1}{100}, \qquad \eta = \frac{r^2}{100R}. \tag{28}$$

The conditional law is well-defined by (23). For $X = (x_1, x_2)$ define the dipole and traceless quadrupole

$$d(X) = x_1 + x_2, \qquad q(X) = \sum_{i=1}^{2} \left(x_i x_i^{\mathsf{T}} - \frac{|x_i|^2}{3}\mathrm{Id}\right). \tag{29}$$

Matrix norms below are Frobenius norms, and $\mathrm{Var}_Q(q) = \mathbf{E}_Q\|q - \mathbf{E}_Q q\|^2$.

**Lemma 3.6** (A quantitative inverse estimate for two atoms)**.** *If $X, X' \in \mathcal{C}$ and*

$$|d(X) - d(X')|^2 + R^{-2}\|q(X) - q(X')\|^2 < \eta^2, \tag{30}$$

*then* $\mathrm{dist}(x_1, \{x_1', x_2'\}) < r$.

*Proof.* Put $F(v) = vv^{\mathsf{T}} - |v|^2\mathrm{Id}/3$. We first establish

$$\min_{\sigma\in\{-1,1\}} |u - \sigma v|^2 \le \sqrt{3}\,\|F(u) - F(v)\|. \tag{31}$$

Choose the sign of $v$ so that $c_0 = u\cdot v \ge 0$, and write $a_0 = |u|^2$, $b_0 = |v|^2$, and $A = uu^{\mathsf{T}} - vv^{\mathsf{T}}$. Then

$$\|A\|^2 = a_0^2 + b_0^2 - 2c_0^2,$$

and

$$2\|A\|^2 - |u - v|^4 = (a_0 - b_0)^2 + 4c_0(a_0 + b_0 - 2c_0) \ge 0.$$

Also $\|A\|^2 - (\operatorname{tr} A)^2 = 2(a_0b_0 - c_0^2) \ge 0$. Since taking the traceless part is an orthogonal projection,

$$\|F(u) - F(v)\|^2 = \|A\|^2 - \frac{1}{3}(\operatorname{tr} A)^2 \ge \frac{2}{3}\|A\|^2 \ge \frac{1}{3}|u - v|^4,$$

which proves (31).

Now write

$$m = \frac{x_1 + x_2}{2}, \quad u = \frac{x_1 - x_2}{2}, \qquad m' = \frac{x_1' + x_2'}{2}, \quad u' = \frac{x_1' - x_2'}{2}.$$

Then $d = 2m$, $q = 2F(m) + 2F(u)$, and similarly for the primed variables. Since $|m|, |m'| \le R$, the contraction property of the traceless projection and the rank-one identity imply

$$\|F(m) - F(m')\| \le \|mm^{\mathsf{T}} - m'm'^{\mathsf{T}}\| \le (|m| + |m'|)|m - m'| \le R|d - d'|.$$

Under (30), it follows that

$$\|F(u) - F(u')\| \le \frac{1}{2}\|q - q'\| + R|d - d'| < \frac{3}{2}R\eta = \frac{3r^2}{200}.$$

By (31), one of the two possible matchings has

$$\operatorname{dist}(x_1, \{x_1', x_2'\}) \le |m - m'| + \min_{\sigma\in\{-1,1\}} |u - \sigma u'| < \frac{\eta}{2} + \left(\frac{3\sqrt{3}}{200}\right)^{1/2} r.$$

As $r \le R$, the first term is at most $r/200$, and $1/200 + (3\sqrt{3}/200)^{1/2} < 1$. This proves the claim. □

**Proposition 3.7** (Conditional moment variance)**.** *One has*

$$\operatorname{Var}_Q(d) + R^{-2}\operatorname{Var}_Q(q) \ge \frac{r^4}{40000R^2}. \tag{32}$$

*Proof.* For every measurable $A \subset \mathbb{R}^3$, the first marginal of $Q$ satisfies

$$Q(x_1 \in A) = \frac{P(x_1 \in A,\, X \in \mathcal{C})}{p} \le \frac{1}{2p}\int_A \rho \le 60|A|,$$

by (15) and $p > 1/10$; the same holds for the second marginal. Thus, for each fixed $X' \in \mathcal{C}$,

$$Q\{\operatorname{dist}(x_1, \{x_1', x_2'\}) < r\} \le 120\frac{4\pi}{3}r^3 < \frac{1}{2}.$$

Let $X$ and $X'$ be independent with law $Q$. The contrapositive of Lemma 3.6 therefore implies

$$\mathbf{P}\left\{|d(X) - d(X')|^2 + R^{-2}\|q(X) - q(X')\|^2 \ge \eta^2\right\} \ge \frac{1}{2}.$$

Taking expectations and using the independent-copy variance identity,

$$2(\operatorname{Var}_Q(d) + R^{-2}\operatorname{Var}_Q(q)) = \mathbf{E}\left[|d(X) - d(X')|^2 + R^{-2}\|q(X) - q(X')\|^2\right] \ge \frac{\eta^2}{2}.$$

Substitution of $\eta = r^2/(100R)$ gives (32). □

### 3.4 Shell harmonics under an arbitrary deterministic mask

Choose the explicit exterior scale and the shell

$$T = 10^9 \kappa_0^{-1}, \qquad \mathcal{S} = \{y : T < |y| < 2T\}, \qquad E = \mathcal{S} \setminus \mathcal{O}, \qquad \nu_0 = \frac{\mathbf{1}_{\mathcal{S}}}{|\mathcal{S}|}, \qquad \nu = \frac{\mathbf{1}_E}{|E|}. \tag{33}$$

We will prove below that $|E| > 0$. The mask $\mathcal{O} \cap \mathcal{S}$ may have arbitrary measurable geometry; no angular regularity or independence assumption is imposed on it.

**Lemma 3.8** (Exact low-order shell estimates)**.** *For $X \in \mathcal{C}$ and $y = sn \in \mathcal{S}$, where $|n| = 1$, write the cross-interaction as*

$$\mathcal{W}(X, y) := \sum_{i=1}^{2} \frac{1}{|y - x_i|} = \frac{2}{s} + \frac{n \cdot d(X)}{s^2} + \frac{3}{2} \frac{n^{\mathsf{T}} q(X) n}{s^3} + e(X, y). \tag{34}$$

*For $T \geq 2R$, its exact remainder satisfies*

$$|e(X, y)| \leq \frac{4R^3}{T^4}. \tag{35}$$

*With $d_c = d - \mathbf{E}_Q d$, $q_c = q - \mathbf{E}_Q q$, and*

$$f(X, y) = \frac{n \cdot d_c(X)}{s^2} + \frac{3}{2} \frac{n^{\mathsf{T}} q_c(X) n}{s^3}, \tag{36}$$

*one has $\mathbf{E}_{\nu_0} f(X, \cdot) = 0$ for every $X$, and*

$$\|f\|^2_{L^2(Q \otimes \nu_0)} = \frac{\mathrm{Var}_Q(d)}{14T^4} + \frac{3 \,\mathrm{Var}_Q(q)}{80T^6} \geq \frac{3r^4}{3200000T^6}, \tag{37}$$

$$\sup_{y \in \mathcal{S}} |f(X, y)|^2 \leq 120 \|f(X, \cdot)\|^2_{L^2(\nu_0)}. \tag{38}$$

*Proof.* For $|x| < s$, the convergent Legendre expansion is

$$\frac{1}{|sn - x|} = \frac{1}{s} \sum_{k=0}^{\infty} \left( \frac{|x|}{s} \right)^k P_k \left( \frac{n \cdot x}{|x|} \right),$$

with the evident interpretation at $x = 0$. Its terms of orders zero, one, and two are respectively

$$\frac{1}{s}, \qquad \frac{n \cdot x}{s^2}, \qquad \frac{3(n \cdot x)^2 - |x|^2}{2s^3}.$$

Summing over the two atoms gives (34). The bound $|P_k(t)| \leq 1$ on $[-1, 1]$ shows that its remainder is bounded by

$$\sum_{i=1}^{2} \frac{|x_i|^3}{s^4 (1 - |x_i|/s)} \leq \frac{4R^3}{T^4},$$

which proves (35) without discarding any interaction term.

Under $\nu_0$, the direction $n$ is uniform on the sphere and independent of $s$, whose density on $(T, 2T)$ is $3s^2/(7T^3)$. The spherical moment identities

$$\mathbf{E}_n(n_i n_j) = \frac{\delta_{ij}}{3}, \qquad \mathbf{E}_n(n_i n_j n_k n_l) = \frac{\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}}{15}$$

give, for a traceless symmetric matrix $q$,

$$\mathbf{E}_n(n\cdot d)^2=\frac{|d|^2}{3},\quad \mathbf{E}_n(n^{\mathsf{T}}qn)^2=\frac{2\|q\|^2}{15},\quad \mathbf{E}_n[(n\cdot d)(n^{\mathsf{T}}qn)]=0.$$

The mixed term vanishes by oddness. Likewise, $\mathbf{E}_n(n\cdot d)=0$ and $\mathbf{E}_n(n^{\mathsf{T}}qn)=\operatorname{tr}(q)/3=0$, proving the mean-zero assertion. Direct radial integration gives

$$\mathbf{E}_{\nu_0}s^{-4}=\frac{3}{7T^3}\int_T^{2T}s^{-2}\,\mathrm{d}s=\frac{3}{14T^4},\qquad \mathbf{E}_{\nu_0}s^{-6}=\frac{3}{7T^3}\int_T^{2T}s^{-4}\,\mathrm{d}s=\frac{1}{8T^6}.$$

Combining these identities proves the equality in (37). Because $T\ge R$,

$$\frac{1}{14T^4}\ge\frac{3R^2}{80T^6}.$$

Factoring $3R^2/(80T^6)$ and applying (32) gives the lower bound in (37).

Finally, for each fixed $X$, the inequality $(a+b)^2\le 2a^2+2b^2$ and the Frobenius bound $|n^{\mathsf{T}}q_cn|\le\|q_c\|$ give

$$\sup_{\mathcal{S}}|f(X,\cdot)|^2\le\frac{2|d_c(X)|^2}{T^4}+\frac{9\|q_c(X)\|^2}{2T^6}.$$

The fixed-$X$ version of the preceding exact integral formula is

$$\|f(X,\cdot)\|^2_{L^2(\nu_0)}=\frac{|d_c(X)|^2}{14T^4}+\frac{3\|q_c(X)\|^2}{80T^6}.$$

The ratios of the respective coefficients are 28 and 120, proving (38). □

**Lemma 3.9** (Variance after arbitrary measurable deletion)**.** *Let a measurable set of $\nu_0$-measure $\theta<1$ be deleted from $\mathcal{S}$, and let $\nu$ be the normalized restriction to its complement. If $g$ has $\nu_0$-mean zero and $\sup_{\mathcal{S}}|g|^2\le 120\|g\|^2_{L^2(\nu_0)}$, then*

$$\operatorname{Var}_\nu(g)\ge\frac{1-121\theta}{(1-\theta)^2}\|g\|^2_{L^2(\nu_0)}.\tag{39}$$

*For the set $E$ in* (33)*, one has*

$$\theta\le\frac{27}{7\cdot 10^{27}}<\frac{1}{1000},\qquad A:=I(\nu)=|E|^{-1/3}\le T^{-1},\tag{40}$$

*and*

$$\|f-\mathbf{E}_\nu f\|^2_{L^2(Q\otimes\nu)}\ge\frac{3r^4}{6400000T^6}.\tag{41}$$

*Proof.* Denote the deleted set by $D_0$, and put $G=\|g\|^2_{L^2(\nu_0)}$. The removed second moment is at most $120\theta G$, so

$$\mathbf{E}_\nu g^2\ge\frac{1-120\theta}{1-\theta}G.$$

Since $\mathbf{E}_{\nu_0}g=0$,

$$\mathbf{E}_\nu g=-\frac{\int_{D_0}g\,\mathrm{d}\nu_0}{1-\theta},\qquad |\mathbf{E}_\nu g|^2\le\frac{\theta^2\sup_{\mathcal{S}}|g|^2}{(1-\theta)^2}\le\frac{120\theta^2}{(1-\theta)^2}G.$$

Subtracting proves (39). In particular, if $\theta \le 1/1000$, the coefficient is at least $1/2$.

In our application, $|\mathcal{S}| = (28\pi/3)T^3$, and (27) gives

$$\theta = \frac{|\mathcal{S} \cap \mathcal{O}|}{|\mathcal{S}|} \le \frac{36\pi\kappa_0^{-3}}{(28\pi/3)T^3} = \frac{27}{7 \cdot 10^{27}} < \frac{1}{1000}.$$

Thus $|E| \ge (1 - 10^{-3})(28\pi/3)T^3 > T^3$, which proves that $\nu$ is well-defined and that $A = |E|^{-1/3} \le T^{-1}$. Apply (39) separately to $g = f(X, \cdot)$, using Lemma 3.8, and then integrate over $Q$. The factor $1/2$ together with (37) proves (41). The proof used only the volume of the deleted set, not its shape. □

### 3.5 The exact interaction and a positive marginal-preserving coupling

**Proposition 3.10** (A uniform exterior coupling improvement)**.** *There is a coupling $\Gamma$ of the old configuration law $P$ and the new particle density $\nu$ such that*

$$\int \mathcal{W} \, \mathrm{d}\Gamma \le \int U\nu - \delta_0, \qquad \delta_0 = 10^{-18}T^{-5}. \tag{42}$$

*Its Radon–Nikodym density relative to $P \otimes \nu$ is everywhere between $1/2$ and $3/2$, up to null sets.*

*Proof.* On $\mathcal{C} \times E$ define the exact joint-centered interaction

$$h(X, y) = \mathcal{W}(X, y) - \mathbf{E}_Q \mathcal{W}(\cdot, y) - \mathbf{E}_\nu \mathcal{W}(X, \cdot) + \mathbf{E}_{Q\otimes\nu} \mathcal{W}. \tag{43}$$

In $L^2(Q \otimes \nu)$, the operators $I - \mathbf{E}_Q$ and $I - \mathbf{E}_\nu$ are commuting orthogonal projections, and their product has norm at most one. The monopole in (34) is independent of $X$ and is annihilated. The $Q$-centered sum of the dipole and quadrupole is $f$, and $\mathbf{E}_Q f(\cdot, y) = 0$. Thus

$$h = f - \mathbf{E}_\nu f + (I - \mathbf{E}_Q)(I - \mathbf{E}_\nu)e.$$

The triangle inequality, the contraction property, and (35)–(41) give

$$\|h\|_{L^2(Q\otimes\nu)} \ge \left(\frac{3r^4}{6400000T^6}\right)^{1/2} - \frac{4R^3}{T^4}. \tag{44}$$

Our choice of $T$ satisfies

$$T \ge 2R, \qquad T \ge \frac{20000R^3}{r^2} = 6.75 \cdot 10^{14};$$

indeed $T = 10^9 \cdot 852000 \exp(104000) > 8.52 \cdot 10^{14}$. The second inequality ensures

$$\frac{4R^3}{T^4} \le \frac{r^2}{5000T^3} \le \frac{1}{2}\left(\frac{3r^4}{6400000T^6}\right)^{1/2}.$$

Therefore

$$\|h\|^2_{L^2(Q\otimes\nu)} \ge \frac{3r^4}{25600000T^6}. \tag{45}$$

For $X \in \mathcal{C}$ and $y \in E$, each old particle lies in $B_R$ and $|y| > T$, so

$$0 \le \mathcal{W}(X, y) \le \frac{2}{T - R} \le \frac{4}{T}.$$

All four terms in (43) are consequently bounded in absolute value by $4/T$, and $|h| \le 16/T$. Extend $h$ by zero outside $\mathcal{C}$ in the $X$ variable and set

$$t = \frac{T}{32}, \qquad \mathrm{d}\Gamma(X,y) = (1 - t\mathbf{1}_{\mathcal{C}}(X)h(X,y))\,\mathrm{d}P(X)\,\nu(y)\,\mathrm{d}y. \tag{46}$$

The density lies in $[1/2, 3/2]$. Since $\mathbf{E}_\nu h(X,\cdot) = 0$ on $\mathcal{C}$, integration in $y$ preserves the marginal $P$. Similarly,

$$\int_{\mathcal{C}} h(X,y)\,\mathrm{d}P(X) = p\,\mathbf{E}_Q h(\cdot,y) = 0,$$

so integration in $X$ preserves the marginal $\nu$. In particular, $\Gamma$ is a probability measure.

The exact gain against the product coupling is

$$\begin{aligned}\int \mathcal{W}\,\mathrm{d}(P\otimes\nu) - \int \mathcal{W}\,\mathrm{d}\Gamma &= tp\,\mathbf{E}_{Q\otimes\nu}(\mathcal{W}h)\\ &= tp\,\|h\|^2_{L^2(Q\otimes\nu)}.\end{aligned}$$

For the second equality, subtract (43) from $\mathcal{W}$: the difference is a sum of an $X$-only function, a $y$-only function, and a constant. Each is orthogonal to $h$ because its two conditional means vanish. By $p > 1/10$ and (45), the gain is at least

$$\frac{3r^4}{81920000000T^5} > 10^{-18}T^{-5} = \delta_0,$$

where $r = 1/100$. Finally, the product interaction is finite because

$$\int \mathcal{W}\,\mathrm{d}(P\otimes\nu) = \int U(y)\nu(y)\,\mathrm{d}y \le 4.$$

Thus all energy differences are legitimate, including contributions from configurations outside $\mathcal{C}$. In particular, no positive distance between $E$ and the full support of $\rho$ was required. □

### 3.6 The sharp three-particle comparison and its explicit balance

**Theorem 3.11** (Explicit successive-particle gap)**.** *For the sharp canonical three-dimensional Coulomb constants in the admissible class of this manuscript,*

$$C_3 - C_2 \ge \exp(-1769000). \tag{47}$$

*The proof does not require a three-particle optimizer.*

*Proof.* We apply Lemma 2.5 to the density $\nu$ and coupling $\Gamma$ constructed above. Here $\rho\nu = 0$ almost everywhere because $E \subset \mathbb{R}^3 \setminus \mathcal{O}$, and $A = I(\nu) \le T^{-1}$. We spell out the specialization in order to make clear that the comparison constant is the sharp $C_3$ itself.

Choose a nonnegative smooth probability density $\zeta$ supported in $B_1$, and set

$$\zeta_L(x) = L^{-3}\zeta((x - a_L)/L),$$

where $a_L$ is chosen so that the support of $\zeta_L$ is disjoint from both the compact support of $\rho$ and the bounded shell $\mathcal{S}$. Such translations exist for each $L$ without any uniform support-radius estimate for $\rho$. Then $I(\zeta_L) = L^{-1}I(\zeta) \to 0$.

For $0 < \varepsilon < 1$, form $\varepsilon\Gamma + (1-\varepsilon)(P \otimes \zeta_L)$ and symmetrize the three particles. Call the resulting three-particle law $\Pi_{\varepsilon,L}$, and write

$$a_{\varepsilon,L} = \varepsilon\nu + (1-\varepsilon)\zeta_L, \qquad \rho_{\varepsilon,L} = \rho + a_{\varepsilon,L}.$$

Its one-particle density is $\rho_{\varepsilon,L}$, of mass three. Symmetrization changes neither the density nor the symmetric Coulomb cost. The two old particles have law $P$, while (42) controls their interaction with the added particle. Using the full-double-integral convention for $D$, this gives

$$\int c_3 \, \mathrm{d}\Pi_{\varepsilon,L} \le W_2(\rho) + D(\rho, a_{\varepsilon,L}) - \varepsilon\delta_0.$$

On the other hand, the Hartree identity is

$$H(\rho_{\varepsilon,L}) = H(\rho) + D(\rho, a_{\varepsilon,L}) + H(a_{\varepsilon,L}).$$

The cross terms cancel exactly, and the last Hartree term is nonnegative. Consequently

$$H(\rho_{\varepsilon,L}) - \int c_3 \, \mathrm{d}\Pi_{\varepsilon,L} \ge \lambda + \varepsilon\delta_0. \tag{48}$$

All interactions here are finite: the old and exterior interaction was bounded in Proposition 3.10, the interaction with $\zeta_L$ is bounded by $\|U\|_\infty$, and the remaining Hartree energies are finite by (20).

The three summands of the density have disjoint occupied sets up to null sets. Thus local-power additivity is exact:

$$I(\rho_{\varepsilon,L}) = 1 + \varepsilon^{4/3}A + (1-\varepsilon)^{4/3} I(\zeta_L). \tag{49}$$

By the supremum definition of $C_3$ and the minimizing property of $W_3(\rho_{\varepsilon,L})$,

$$H(\rho_{\varepsilon,L}) - \int c_3 \, \mathrm{d}\Pi_{\varepsilon,L} \le H(\rho_{\varepsilon,L}) - W_3(\rho_{\varepsilon,L}) \le C_3 I(\rho_{\varepsilon,L}).$$

Combine this with (48) and (49), and let $L \to \infty$. Since $I(\zeta_L) \to 0$, one obtains

$$C_3 - C_2 \ge \varepsilon\delta_0 - C_3 A \varepsilon^{4/3}. \tag{50}$$

No attainment assertion for $C_3$ appears in this argument. The universal estimate of [3], already included in Proposition 2.1, supplies the only further fact needed about it: $C_3 \le 8/5$.

Choose

$$\varepsilon = 10^{-57} T^{-12}. \tag{51}$$

This lies in $(0,1)$ because $T > 1$. By (40),

$$C_3 A \varepsilon^{1/3} \le \frac{8}{5}\, T^{-1}\, 10^{-19} T^{-4} = \frac{8}{5}\, 10^{-19} T^{-5} < \frac{1}{2}\, 10^{-18} T^{-5} = \frac{\delta_0}{2}.$$

Equation (50) therefore implies

$$\begin{aligned} C_3 - C_2 &\ge \frac{\varepsilon\delta_0}{2} = \frac{1}{2 \cdot 10^{75} T^{17}} \\ &= \frac{\exp(-1768000)}{2 \cdot 10^{228} \cdot 852000^{17}}. \end{aligned} \tag{52}$$

To round this down to a simple exponential, use $2 < e$, $10 < e^3$, and $852000 < 10^6$. The denominator in the last line is strictly less than

$$e \cdot e^{3 \cdot 228} \cdot e^{3 \cdot 6 \cdot 17} = e^{991}.$$

Thus the last line of (52) is greater than $\exp(-1768991)$, and in particular greater than $\exp(-1769000)$. This proves (47). □

The estimate quantifies a successive-particle separation. Its size is far too small to change a useful numerical digit, and it is not a reduction of the universal all-particle Lieb–Oxford constant. The quantitative bridge is the conditional two-atom covariance estimate, its persistence under an arbitrary small-volume mask, and the controlled passage from the truncated harmonics to the exact Coulomb interaction. The optimizer-existence input remains external; compatible potentials and compact support are reconstructed in Appendix B.

# 4 Three-particle localization and the chemical gap

This section converts a positive lower-particle energetic gap into an explicit joint core event, localizes a two-point dual minimizer, and then uses the Euler–Lagrange equation to bound the three-particle chemical gap. The resulting volume estimate concerns the occupied set $\mathcal{O} = \{\rho > 0\}$, understood up to null sets. The qualitative optimizer and compatible-dual inputs are those stated in Proposition 2.1; the normalized bounds are recorded in Proposition 2.4. The sector completion and localization framework is related to [1]. The compatible potential and its asymptotic level follow from Appendix B, within the framework of [2]. The finite-configuration comparisons below are written out directly; [5] provides the prior dissociation and binding framework. In particular, the strict completion theorem in [1] is not being used as a quantitative localization-radius theorem.

## 4.1 A joint core event from the energetic gap

For a grand-canonical probability law $\Gamma$, let $\mathcal{W}(\Gamma)$ denote the expectation of the sum of the Coulomb interactions over unordered pairs in its configuration, and let $f$ be its one-body density. Set

$$\mathcal{G}(\Gamma) = H(f) - \mathcal{W}(\Gamma).$$

For a canonical optimal three-particle law $P$ with density $\rho$, this notation gives $\mathcal{W}(P) = W_3(\rho)$. All densities in the next three statements are nonnegative and belong to $L^1(\mathbb{R}^3) \cap L^{4/3}(\mathbb{R}^3)$, and all laws have finite expected interaction.

**Lemma 4.1** (Completion of sectors of size at most two)**.** *If $\Gamma$ is a grand-canonical probability law supported on the sectors $K \in \{0, 1, 2\}$, with density $f$, then*

$$H(f) - \mathcal{W}(\Gamma) \le C_2 I(f). \tag{53}$$

*Proof.* Choose a smooth compactly supported probability density $\eta$ and put $\eta_S(x) = S^{-3}\eta(x/S)$. In every $k$-particle sector, add $2 - k$ independent particles of law $\eta_S$, independently also of the original configuration, and symmetrize. This produces a canonical two-particle probability law $P_S$ with density

$$f_S = f + (2 - \mathbb{E}_\Gamma K)\eta_S.$$

Since

$$\|\eta_S * |\cdot|^{-1}\|_\infty = O(S^{-1}), \qquad H(\eta_S) = O(S^{-1}), \qquad \|\eta_S\|_{4/3} \longrightarrow 0,$$

all interactions involving added particles tend to zero. Thus $\mathcal{W}(P_S) \to \mathcal{W}(\Gamma)$, while the Coulomb expansion of $H(f_S)$ gives $H(f_S) \to H(f)$. The convergence $f_S \to f$ in $L^{4/3}$ gives $I(f_S) \to I(f)$. The canonical two-particle inequality yields

$$H(f_S) - \mathcal{W}(P_S) \le H(f_S) - W_2(f_S) \le C_2 I(f_S).$$

Taking $S \to \infty$ proves (53); the case $f = 0$ is immediate. The construction uses the sector restriction $K \le 2$, rather than merely a bound on $\mathbb{E}K$. □

**Lemma 4.2** (Deletion of the three-particle sector)**.** *Let $P$ be a symmetric canonical three-particle law of density $\rho$, with $\int \rho = 3$, and let $Q \subset \mathbb{R}^3$ be measurable. Retaining only the coordinates in $Q$ gives a localized grand-canonical law $\Gamma_Q$, whose density is $\rho_Q = \rho \mathbf{1}_Q$. If $p_Q = P(Q^3)$, then*

$$\mathcal{G}(\Gamma_Q) \le (C_2 + 5p_Q^{1/3}) I(\rho_Q). \tag{54}$$

*Proof.* Delete the $K = 3$ sector of $\Gamma_Q$ and add its probability $p_Q$ to the vacuum sector. The resulting law $\Gamma'_Q$ is still a probability law and has sectors of size at most two. Let $t_Q$ be the one-body density of the removed sector and set $f_Q = \rho_Q - t_Q$. Then

$$0 \le t_Q \le \rho_Q, \qquad \int t_Q = 3p_Q, \qquad \rho_{\Gamma'_Q} = f_Q.$$

The interaction of the removed sector is nonnegative. Applying Lemma 4.1, expanding the Hartree term, and using $C_2 \ge 0$, we obtain

$$\begin{aligned} \mathcal{G}(\Gamma_Q) &\le H(\rho_Q) - \mathcal{W}(\Gamma'_Q) \\ &\le C_2 I(f_Q) + D(f_Q, t_Q) + H(t_Q) \\ &\le C_2 I(\rho_Q) + D(\rho_Q, t_Q). \end{aligned} \tag{55}$$

The last line follows from $I(f_Q) \le I(\rho_Q)$ and $D(f_Q, t_Q) + H(t_Q) \le D(\rho_Q, t_Q)$. No normalization by $1 - p_Q$ is made.

Set

$$A = \frac{2}{3} \left( \frac{4}{\sqrt{\pi}} \right)^{2/3} < \frac{23}{20}. \tag{56}$$

The sharp Coulomb Hardy–Littlewood–Sobolev inequality [7] and interpolation give

$$D(a, b) \le 2A \left( \int a \right)^{1/3} \left( \int b \right)^{1/3} \sqrt{I(a) I(b)}. \tag{57}$$

Indeed, the sharp bilinear bound is $D(a,b) \le 2A \|a\|_{6/5} \|b\|_{6/5}$, and $\|a\|_{6/5} \le \|a\|_1^{1/3} \|a\|_{4/3}^{2/3} = (\int a)^{1/3} I(a)^{1/2}$, with the same estimate for $b$. Using $\int \rho_Q \le 3$, $\int t_Q = 3p_Q$, and $I(t_Q) \le I(\rho_Q)$, we find

$$D(\rho_Q, t_Q) \le 2A \, 3^{2/3} p_Q^{1/3} I(\rho_Q) < 5 p_Q^{1/3} I(\rho_Q).$$

The numerical inequality follows from

$$\left( \frac{23}{10} 3^{2/3} \right)^3 = \frac{109503}{1000} < 125.$$

Combining this with (55) proves the claim. □

**Proposition 4.3** (Explicit three-particle core event)**.** *Let $P$ be a symmetric canonical three-particle law with density $\rho$, normalized by $\int \rho = 3$ and $I(\rho) = 1$. If*

$$H(\rho) - \mathcal{W}(P) \ge C_2 + g, \qquad g > 0,$$

*then there is a center $o \in \mathbb{R}^3$ such that*

$$R = \frac{27}{2g}, \qquad P(B_R(o)^3) \ge \frac{g^3}{1000}. \tag{58}$$

*Proof.* Partition $\mathbb{R}^3$ into cubes of side $\ell$, and average the partition over translations uniformly distributed in $[0,\ell)^3$. The probability that two points at displacement $z$ lie in the same cube is

$$w_\ell(z) = \prod_{j=1}^{3} \left(1 - \frac{|z_j|}{\ell}\right)_+ .$$

The elementary product bound and $\sum_j |z_j| \le \sqrt{3}|z|$ imply

$$\frac{1 - w_\ell(z)}{|z|} \le \frac{\sqrt{3}}{\ell}. \tag{59}$$

For every partition the sum of the within-cube interactions does not exceed the full interaction. The averaged omitted Hartree term is at most $3^2\sqrt{3}/(2\ell)$. Consequently

$$\mathcal{G}(P) \le \mathbb{E}_{\text{shift}} \sum_Q \mathcal{G}(\Gamma_Q) + \frac{9\sqrt{3}}{2\ell}. \tag{60}$$

All sums and averages can be separated into nonnegative Hartree and interaction terms, each with finite total, so Tonelli's theorem justifies these operations.

Let $p_*$ be the supremum of $P(Q^3)$ over all translates of a cube of side $\ell$. Since $\sum_Q I(\rho \mathbf{1}_Q) = I(\rho) = 1$, Lemma 4.2 gives

$$\mathcal{G}(P) \le C_2 + 5p_*^{1/3} + \frac{9\sqrt{3}}{2\ell}.$$

With $\ell = 9\sqrt{3}/g$, the hypothesis implies $p_* \ge (g/10)^3$.

For completeness, this positive supremum is attained. If the cube centers converge, the corresponding event indicators converge $P$-almost everywhere except when a coordinate lies on the boundary of the limiting cube. Each labeled marginal is absolutely continuous, so this exceptional set has probability zero. Dominated convergence therefore proves continuity of the event probability in the center. Moreover,

$$P(Q^3) \le \frac{1}{3}\int_Q \rho \longrightarrow 0$$

as the cube center tends to infinity. Hence a maximizing cube exists. Its circumscribed ball has radius $\sqrt{3}\ell/2 = 27/(2g)$. The boundary spheres and cube faces have zero marginal mass, so the same probability bound holds for the open ball in (58). □

*Remark* 4.4 (Direct localization by balls). The radius in (58) may be replaced by $27/(4g)$, without changing the probability bound. Indeed, the sector-deletion argument applies to balls. Average over all centers with measure $do/|B_R|$. Fubini's theorem gives exactly $I(\rho)$ for the integrated local power, and the normalized intersection volume of two radius-$R$ balls at distance $s$ is

$$w_R(s) = \begin{cases} 1 - \dfrac{3s}{4R} + \dfrac{s^3}{16R^3}, & 0 \le s \le 2R, \\ 0, & s \ge 2R. \end{cases}$$

This formula follows by adding the volumes of the two spherical caps. It implies $(1 - w_R(s))/s \le 3/(4R)$, so the missing Hartree term is at most $27/(8R)$. The preceding proof now gives

$$\mathcal{G}(P) \le C_2 + 5p_*^{1/3} + \frac{27}{8R}.$$

Taking $R = 27/(4g)$ proves the assertion; attainment follows from the same boundary-nullity and vanishing-at-infinity argument. We retain $R = 27/(2g)$ in the subsequent constants.

**Corollary 4.5** (Conditional marginal bound)**.** *For a normalized three-particle optimizer, suppose $C_3 - C_2 \geq g > 0$, and use the ball in Proposition 4.3. The first labeled marginal of $P(\cdot \mid B_R(o)^3)$ has a density bounded above by*

$$L \leq 4000 g^{-3}. \tag{61}$$

*In particular, with $r = g/100$,*

$$4\pi L r^3 \leq \frac{16\pi}{1000} < \frac{1}{2}. \tag{62}$$

*Proof.* Write $q = P(B_R(o)^3) \geq g^3/1000$. Symmetry gives the unconditioned labeled marginal $\rho/3$, and conditioning yields the measure domination

$$(\pi_1)_{\#} P(\cdot \mid B_R(o)^3) \leq \frac{\rho}{3q} \leq \frac{4}{q}.$$

Here $\|\rho\|_\infty < 12$ is supplied by Proposition 2.4. This proves both inequalities. □

## 4.2 Localization from a saturated triple

We use the configuration-energy convention

$$c_k(z_1, \dots, z_k) = \sum_{i<j} |z_i - z_j|^{-1}, \qquad E_k(f) = \inf_{z_1,\dots,z_k} \left( c_k(z_1, \dots, z_k) - \sum_{i=1}^{k} f(z_i) \right). \tag{63}$$

A collision has cost $+\infty$; in particular $c_1 = 0$. The next statement is purely geometric.

**Lemma 4.6** (Three-point Coulomb geometry)**.** *Let $x_1, x_2, x_3$ be distinct points of diameter $D > 0$. For $b \in \mathbb{R}^3$, define*

$$S_i = \sum_{j \neq i} |x_i - x_j|^{-1}, \qquad G_i(b) = S_i - |x_i - b|^{-1},$$

*with $G_i(b) = -\infty$ when $b = x_i$. Then*

$$\max_i G_i(b) > \frac{1}{20D}. \tag{64}$$

*Proof.* Scale so that $D = 1$, suppose every $G_i(b) \leq 1/20$, and put $r_i = |x_i - b|$. Since $S_i \geq 2$, the assumed inequalities give

$$r_i \leq \frac{1}{S_i - 1/20},$$

including the case $r_i = 0$. If the shortest side is at most $9/10$, relabel so that $|x_1 - x_2| = 1$ is a longest side and $|x_1 - x_3| \leq 9/10$ is a shortest side. These sides share a vertex. Then $S_1 \geq 19/9$ and $S_2 \geq 2$, whence

$$1 \leq r_1 + r_2 \leq \frac{180}{371} + \frac{20}{39} = \frac{14440}{14469} < 1,$$

a contradiction. Otherwise all three sides exceed $9/10$, and $r_i \leq 20/39$ for every $i$. The Euclidean identity

$$\sum_{i<j} |x_i - x_j|^2 = 3 \sum_i |x_i - b|^2 - \left| \sum_i (x_i - b) \right|^2$$

would then imply

$$3 \left( \frac{9}{10} \right)^2 < \sum_{i<j} |x_i - x_j|^2 \leq 9 \left( \frac{20}{39} \right)^2 < 3 \left( \frac{9}{10} \right)^2,$$

again a contradiction. Rescaling proves the lemma. □

**Proposition 4.7** (Anchor localization and binding)**.** *Let $\phi : \mathbb{R}^3 \to \mathbb{R}$ be finite valued, pointwise feasible, and Coulomb c-conjugated, in the following precise sense:*

$$\sum_{i=1}^{3} \phi(z_i) \le c_3(z_1, z_2, z_3) \qquad \text{for all } z_1, z_2, z_3, \tag{65}$$

$$\phi(x) = \inf_{a,b}\{c_3(x, a, b) - \phi(a) - \phi(b)\} \qquad \text{for all } x. \tag{66}$$

*Assume that its limit at infinity is finite and satisfies*

$$C = \lim_{|x|\to\infty} \phi(x) = \inf_{a,b}\{|a - b|^{-1} - \phi(a) - \phi(b)\}. \tag{67}$$

*Assume also that $R > 0$, $o \in \mathbb{R}^3$, and a distinct triple $X = (x_1, x_2, x_3) \in B_R(o)^3$ satisfy*

$$c_3(X) = \phi(x_1) + \phi(x_2) + \phi(x_3). \tag{68}$$

*Set $\psi = \phi - C$, $e = 3C$, and $d_0 = 1/(40R)$. Then the following conclusions hold.*

1. *The function $\phi$ is bounded and upper semicontinuous, $C \le \phi \le -2C$, and*

$$\psi \ge 0, \qquad E_3(\psi) = E_2(\psi) = e. \tag{69}$$

2. *If $0 \le \varepsilon < d_0$ and*

$$|a - b|^{-1} - \phi(a) - \phi(b) \le C + \varepsilon, \tag{70}$$

*then both $a$ and $b$ belong to $\overline{B}_{L_\varepsilon}(o)$, where*

$$L_\varepsilon = R + \frac{2}{d_0 - \varepsilon}. \tag{71}$$

*In particular, errors at most $1/(80R)$ give radius $161R$. An exact minimizing pair exists and lies in $\overline{B}_{81R}(o)^2$.*

3. *The one-to-two dual binding gap satisfies*

$$\Delta := E_1(\psi) - E_2(\psi) = -\sup \psi - e \ge d_0. \tag{72}$$

*For an exact minimizing pair $(a_0, b_0)$,*

$$0 \le \psi(z) \le |z - a_0|^{-1} + |z - b_0|^{-1} \le \frac{2}{|z - o| - 81R} \quad \text{if } |z - o| > 81R. \tag{73}$$

4. *Every distinct finite triple saturated for $\phi$ has at least two coordinates in $B_{241R}(o)$. If, additionally, $P$ is a symmetric canonical three-particle probability law of finite expected interaction, has an absolutely continuous one-body density $\rho$, is concentrated on saturated triples, and satisfies $P(B_R(o)^3) \ge p > 0$, then*

$$\int_{B_{241R}(o)} \rho \ge 2 + p. \tag{74}$$

*Proof. Normalization and regularity.* The identity (67) and (66) immediately give $\phi \geq C$. In (65), keep one point fixed and send the other two to infinity with their mutual distance also tending to infinity. This proves $\phi \leq -2C$. Feasibility and the saturated anchor give $E_3(\phi) = 0$, while (67) gives $E_2(\phi) = C$. Shifting the one-body potential by $-C$ adds $kC$ to the $k$-particle energy, proving (69).

To prove upper semicontinuity without an additional hypothesis, fix $x$ and $\delta > 0$. Test its $c$-transform with a finite $\delta$-minimizing pair. Its two entries are distinct from each other and from $x$; otherwise its cost would be infinite. The test expression is continuous near $x$ and bounds $\phi$ from above there. It follows that $\limsup_{y\to x} \phi(y) \leq \phi(x) + \delta$. Letting $\delta \downarrow 0$ proves upper semicontinuity.

*Exchange and localization.* Use $S_i, G_i$ from Lemma 4.6 for the anchor. Its diameter is at most $2R$, so

$$\max_i G_i(b) > d_0 \quad \text{for every } b. \tag{75}$$

Compare the saturated triple $(x_i, x_j, x_k)$ and the approximate pair $(a, b)$ with the new triple $(a, x_j, x_k)$ and pair $(x_i, b)$. The latter triple satisfies feasibility, and the latter pair has unshifted energy at least $C$. Cancellation of the potential values gives

$$S_i + |a-b|^{-1} \leq |a-x_j|^{-1} + |a-x_k|^{-1} + |x_i-b|^{-1} + \varepsilon. \tag{76}$$

Suppose $|a-o| > R$. Choose an index maximizing $G_i(b)$. It satisfies $b \neq x_i$, since the maximum in (75) is positive; the two terms involving $a$ and anchor points are also finite. Dropping $|a-b|^{-1} \geq 0$ in (76) yields

$$d_0 < G_i(b) \leq \frac{2}{|a-o| - R} + \varepsilon.$$

Thus $|a-o| < R + 2/(d_0 - \varepsilon)$. If $|a-o| \leq R$, the asserted bound is immediate. Interchanging $a$ and $b$ proves (71) for both entries.

*Attainment.* The pair infimum $C$ is finite. A minimizing sequence with errors tending to zero is eventually contained in $\overline{B}_{161R}(o)^2$, by the preceding estimate. Since $\phi$ is bounded, its pair costs remain bounded above; therefore the pair separations are bounded away from zero. After passing to a subsequence, the entries converge to a distinct pair. The function $Q(a,b) = |a-b|^{-1} - \phi(a) - \phi(b)$ is lower semicontinuous at that pair, because $-\phi$ is lower semicontinuous. Its value at the limit is at most $C$, and hence is exactly $C$. Applying the localization estimate with $\varepsilon = 0$ gives the radius $81R$. This argument requires no continuity beyond what $c$-conjugacy already supplies.

*Binding and the exterior majorant.* For convenience write $h_k^\psi(Z) = c_k(Z) - \sum_{z\in Z} \psi(z)$. Append an arbitrary singleton $b$ to the anchor, and split the four entries into the pairs $(x_i, b)$ and $(x_j, x_k)$. For any index with $b \neq x_i$, direct cancellation gives

$$h_3^\psi(X) - \psi(b) - h_2^\psi(x_i, b) - h_2^\psi(x_j, x_k) = G_i(b).$$

Each pair energy is at least $e$, and the anchor energy equals $e$, so

$$-\psi(b) - e \geq G_i(b).$$

The maximizing index in (75) is admissible even if $b$ coincides with an anchor point. Thus $-\psi(b) - e > d_0$ for every $b$. Taking a sequence for which $\psi(b) \to \sup \psi$ proves (72).

Now compare an arbitrary third point $z$ with the exact minimizing pair $(a_0, b_0)$. Since $E_3(\psi) = E_2(\psi) = e$,

$$e \leq h_3^\psi(z, a_0, b_0) = e + |z-a_0|^{-1} + |z-b_0|^{-1} - \psi(z).$$

Together with $\psi \geq 0$ and the pair location, this proves (73); at pair entries the intermediate upper bound is interpreted as $+\infty$.

*Occupation and mass excess.* Put $S = \sup \psi$ and $A = 241R$. If a distinct saturated triple had two coordinates outside the open ball $B_A(o)$, the sum of their potential values would be at most

$$\frac{4}{A - 81R} = \frac{1}{40R} = d_0.$$

The third potential value is at most $S$. The triple has strictly positive Coulomb cost, and therefore its energy would be strictly greater than $-S - d_0 \geq e$, contradicting saturation. Thus its occupation number $K_A$ is at least two. For the law $P$ in the statement this holds almost surely, while $K_A = 3$ on $B_R(o)^3$. The definition of the one-body density then gives

$$\int_{B_A(o)} \rho = \mathbb{E}_P K_A \geq 2 + P(B_R(o)^3) \geq 2 + p.$$

□

*Remark* 4.8 (Diameter constants and the role of the event). Retaining the anchor diameter $D$ in Lemma 4.6 gives $d_0 = 1/(20D)$, exact-pair radius $R + 40D$, and occupation radius $R + 120D$, by the same computations. The positive probability of the core event is used to select a saturated anchor; its numerical size is not needed for pair localization. It re-enters in the mass excess (74). A joint event by itself would give only $\int_{B_R(o)} \rho \geq 3P(B_R(o)^3)$; the lower bound above two uses the exchange and binding argument.

### 4.3 The compatible potential and the chemical gap

Let $\rho$ be a normalized three-particle optimizer and $P$ an optimal symmetric canonical law for it. Write

$$I(\rho) = 1, \qquad \int \rho = 3, \qquad \lambda = C_3 = H(\rho) - W_3(\rho), \qquad \beta = \frac{4\lambda}{3}, \qquad U = \rho * |\cdot|^{-1}.$$

By Propositions 2.1 and 2.4, we use the bounded regular $c$-conjugated compatible representative $\phi$ reconstructed in Appendix B within the framework of [2], with pointwise feasibility, $\int \phi\rho = W_3(\rho)$, and

$$C_\phi = \lim_{|x| \to \infty} \phi(x) = E_2(\phi), \qquad \phi \geq C_\phi. \tag{77}$$

Its compatibility is

$$\phi = U - \beta\rho^{1/3} + c \quad \text{on the occupied set}, \qquad \phi \geq U - \beta\rho^{1/3} + c \quad \text{globally}. \tag{78}$$

The appropriate continuous representatives give the same equality on the density support. Integrating against $\rho$ gives

$$\begin{aligned} 3c &= W_3(\rho) - 2H(\rho) + \beta = -W_3(\rho) - \frac{2\lambda}{3}, \\ c &= -\frac{W_3(\rho)}{3} - \frac{2\lambda}{9}. \end{aligned} \tag{79}$$

Qualitative compact support and the exterior inequality $\phi \geq U + c$ imply $c \leq C_\phi$, by taking the limit at infinity. Define

$$\psi = \phi - C_\phi \geq 0, \qquad \kappa = C_\phi - c \geq 0. \tag{80}$$

The global positive-part equation is

$$\rho(x) = \left( \frac{(U(x) - \psi(x) - \kappa)_+}{\beta} \right)^3 . \tag{81}$$

The range $5/4 \le \lambda \le 8/5$ gives $5/3 \le \beta \le 32/15$.

*Remark* 4.9 (Two different dual quantities). For the compatible representative, $E_3(\phi) = 0$ and $E_2(\psi) = E_3(\psi) = 3C_\phi$. The auxiliary gap $\Delta = E_1(\psi) - E_2(\psi)$ in (72) is different from $\kappa = C_\phi - c$. To make the distinction explicit, put $v = U - \beta\rho^{1/3}$. Then $\phi \ge v + c$ everywhere, with equality at $P$-almost every coordinate. Feasibility gives $E_3(v + c) \ge 0$, and complementary slackness supplies a saturated triple with coordinates in that equality set, so $E_3(v+c) = 0$ and $E_3(v) = 3c$. However, the equality $E_2(v+c) = E_2(\phi)$ is not supplied by compatibility. Thus it cannot be used to identify the chemical gap. The exact identity used here is $\kappa = E_2(\phi) - c$.

**Proposition 4.10** (Chemical gap from a joint core event)**.** *In the normalized optimizer setting above, suppose that, for some $R > 0$, $o \in \mathbb{R}^3$, and $0 < p \le 1$, $P(B_R(o)^3) \ge p$. Then an exact $E_2(\phi)$-minimizing pair lies in $\overline{B}_{81R}(o)^2$, and $P$-almost every configuration has at least two coordinates in $B_{241R}(o)$. Moreover,*

$$\int_{B_{241R}(o)} \rho \ge 2 + p, \qquad \kappa \ge \frac{p^2}{8376R} \exp\left( -\frac{156}{p^3} \right) > 0. \tag{82}$$

*Proof.* Feasibility makes $c_3 - \sum_i \phi$ nonnegative, and dual equality makes its integral against $P$ zero. Hence it vanishes $P$-almost surely. Finite expected interaction excludes collisions almost surely. The positive core event therefore contains a distinct saturated triple, and all hypotheses of Proposition 4.7 hold. That proposition gives the pair localization, occupation statement, (74), and the exact exterior majorant.

Set

$$m = 2 + p, \qquad L = 81R, \qquad A = 241R, \qquad r_0 = \frac{2094R}{p}.$$

For $r = |x - o| \ge r_0$, the mass in $B_A(o)$ and the pair majorant give

$$\begin{aligned} U(x) - \psi(x) &\ge \frac{m}{r + A} - \frac{2}{r - L} \\ &\ge \frac{p}{r} - \frac{mA + 4L}{r^2} \ge \frac{p}{2r}. \end{aligned} \tag{83}$$

Indeed, $r_0 \ge 2L$, $1/(r + A) \ge 1/r - A/r^2$, and $2/(r - L) \le 2/r + 4L/r^2$ for $r \ge 2L$. Also $m \le 3$, so

$$2(mA + 4L) \le 2(723 + 324)R = 2094R = pr_0.$$

If $\kappa = 0$, equations (81) and (83) imply $\rho(x) \ge (p/(2\beta r))^3$ throughout the exterior $r \ge r_0$. This lower bound has divergent integral in three dimensions, contradicting $\int \rho = 3$. Thus $\kappa > 0$. On the annulus $r_0 \le r \le p/(4\kappa)$, when nonempty,

$$U(x) - \psi(x) - \kappa \ge \frac{p}{4r}, \qquad \rho(x) \ge \left( \frac{p}{4\beta r} \right)^3 \ge \left( \frac{15p}{128r} \right)^3 .$$

Integration in spherical coordinates about $o$ yields

$$3 \ge 4\pi \left( \frac{15p}{128} \right)^3 \log\left( \frac{p}{4\kappa r_0} \right).$$

Consequently

$$\kappa \geq \frac{p}{4r_0} \exp\left(-\frac{3 \cdot 128^3}{4\pi \cdot 15^3 p^3}\right). \tag{84}$$

If the annulus is empty, then $\kappa > p/(4r_0)$, which is stronger than this bound; equality of its two radii causes no difficulty either. Finally,

$$\frac{3 \cdot 128^3}{4\pi \cdot 15^3} < \frac{128^3}{4 \cdot 15^3} = \frac{524288}{3375} < 156, \qquad \frac{p}{4r_0} = \frac{p^2}{8376R}.$$

These inequalities prove (82). □

**Corollary 4.11** (Explicit three-particle chemical gap)**.** *If $0 < g \leq 1$ and $C_3 - C_2 \geq g$, then every normalized three-particle optimizer satisfies*

$$\kappa \geq \kappa_0(g) := \frac{g^7}{10^{12}} \exp\left(-\frac{160000000000}{g^9}\right). \tag{85}$$

*Proof.* Apply Proposition 4.3 with $R = 27/(2g)$ and $p = g^3/1000$, and then Proposition 4.10. Direct substitution gives

$$\kappa \geq \frac{g^7}{113076000000} \exp\left(-\frac{156000000000}{g^9}\right). \tag{86}$$

Increasing the denominator to $10^{12}$ and the exponent coefficient to 160000000000 weakens the bound and proves the claim. □

**Proposition 4.12** (Occupied volume)**.** *For the normalized three-particle optimizer,*

$$|\mathcal{O}| \leq \frac{243\pi}{2\kappa^3}. \tag{87}$$

*In particular, under the hypotheses of Corollary 4.11, the right-hand side may be replaced by $243\pi/(2\kappa_0(g)^3)$.*

*Proof.* Since $\psi \geq 0$, the positive-part equation places $\mathcal{O}$ in $\{U > \kappa\}$, up to a null set. For any finite-measure measurable set $F \subset \{U \geq \kappa\}$, Tonelli's theorem and the rearrangement bound for the radially decreasing Coulomb kernel give

$$\begin{aligned} \kappa|F| &\leq \int_F U(x)\,dx \\ &= \int \rho(y) \left(\int_F \frac{dx}{|x-y|}\right) dy \\ &\leq 3 \cdot 2\pi \left(\frac{3|F|}{4\pi}\right)^{2/3}. \end{aligned}$$

Here the inner integral is maximized by a ball centered at $y$ of volume $|F|$; its value is $2\pi a^2$, where $a = (3|F|/(4\pi))^{1/3}$. If $|F| > 0$, divide by $|F|^{2/3}$ and cube to obtain

$$|F| \leq \frac{3^3(2\pi)^3}{\kappa^3} \left(\frac{3}{4\pi}\right)^2 = \frac{243\pi}{2\kappa^3}.$$

The case $|F| = 0$ is immediate. Take $F = \mathcal{O} \cap B_n(0)$, after discarding a null set, and let $n \to \infty$. This proves (87) without a diameter, connectedness, or symmetry assumption on $\mathcal{O}$. □

**Corollary 4.13** (Explicit shell data)**.** *Under the hypotheses of Corollary 4.11, retain the core center $o$ and set*

$$R = \frac{27}{2g}, \qquad r = \frac{g}{100}, \qquad T = \frac{30}{\kappa_0(g)}, \qquad \mathcal{S} = \{x : T < |x - o| < 2T\}, \qquad E = \mathcal{S} \setminus \mathcal{O}.$$

*Then*

$$\frac{|\mathcal{S} \setminus E|}{|\mathcal{S}|} \le \frac{729}{56 \cdot 30^3} < \frac{1}{2000}, \qquad T > 10^{15} g^{-7} > \max\left\{2R, \frac{7200R^4}{r^3}\right\}. \tag{88}$$

*The conditional core marginal also satisfies* (61)–(62)*.*

*Proof.* The shell volume is $(28\pi/3)T^3$, so Proposition 4.12 gives

$$\frac{|\mathcal{S} \cap \mathcal{O}|}{|\mathcal{S}|} \le \frac{243\pi/(2\kappa_0(g)^3)}{(28\pi/3)T^3} = \frac{729}{56 \cdot 30^3} = \frac{27}{56000} < \frac{1}{2000}.$$

Furthermore,

$$\frac{T}{10^{15} g^{-7}} = \frac{3}{100} \exp\left(\frac{160000000000}{g^9}\right) > 1,$$

using $0 < g \le 1$ and $\exp(t) \ge 1 + t$. Finally,

$$\frac{7200R^4}{r^3} = 239148450000000\, g^{-7} < 10^{15} g^{-7}, \qquad 2R = 27 g^{-1} < 10^{15} g^{-7}.$$

The marginal assertions were proved in Corollary 4.5. □

# 5 Harmonic moments of three points and exterior covariance

The complex-isotropic projection and annihilating-polynomial argument used below specializes the method of Wang–Lü [6, Lemma 0.4.3 and its proof] to three equal-weight points. The resulting estimates hold without a separation assumption, including collinear configurations and configurations with repeated points. The argument is given in full because its uniformity at collisions and its stability under an irregular shell deletion are needed in the next section.

## 5.1 A quantitative inverse estimate

For a real symmetric tensor, let STF denote its orthogonal projection onto the trace-free subspace, with respect to the full Frobenius inner product. Given triples $X = (x_1, x_2, x_3)$ and $Y = (y_1, y_2, y_3)$ in $(B_R)^3$, where $R > 0$, define

$$M_k(X) = \sum_{i=1}^{3} \mathrm{STF}(x_i^{\otimes k}), \qquad k = 1, 2, 3, \tag{89}$$

and

$$e(X, Y)^2 = \|M_1(X) - M_1(Y)\|^2 + R^{-2}\|M_2(X) - M_2(Y)\|^2 + R^{-4}\|M_3(X) - M_3(Y)\|^2. \tag{90}$$

In particular,

$$M_1(X) = \sum_i x_i,$$

$$M_2(X) = \sum_i \left(x_i x_i^{\mathsf{T}} - \frac{|x_i|^2}{3}\mathrm{Id}_{\mathbb{R}^3}\right),$$

$$[\mathrm{STF}(x^{\otimes 3})]_{abc} = x_a x_b x_c - \frac{|x|^2}{5}(x_a \delta_{bc} + x_b \delta_{ac} + x_c \delta_{ab}).$$

Thus these are homogeneous harmonic moments, rather than unrestricted polynomial moments.

**Lemma 5.1** (Three-point harmonic inverse estimate)**.** *For all $X, Y \in (B_R)^3$,*

$$\max_{1\le i\le 3} \operatorname{dist}(x_i, \{y_1, y_2, y_3\})^3 \le 30R^2 e(X, Y). \tag{91}$$

*The analogous estimate holds with $X$ and $Y$ interchanged. Moreover, equality of $M_k(X)$ and $M_k(Y)$ for $k = 1, 2, 3$ implies equality of the unordered point multisets, including multiplicities.*

*Proof.* Fix $i$ and put $v_j = x_i - y_j$. If any $v_j = 0$, the corresponding point-to-set distance is zero. Otherwise put $u_j = v_j/|v_j|$. For a uniformly distributed unit normal $n \in \mathbb{S}^2$, the set $|n \cdot u_j| > 1/\sqrt{2}$ has normalized area $1 - 1/\sqrt{2}$. Since $3(1 - 1/\sqrt{2}) < 1$, the union bound gives a normal $n$ such that $|n \cdot u_j| \le 1/\sqrt{2}$ for all $j$. Choose real orthonormal vectors $a, b$ spanning $n^\perp$ and set $z = a + \mathrm{i}b$. Using the complex bilinear dot product for $z \cdot z$ and the Hermitian norm for $|z|$,

$$z \cdot z = 0, \qquad |z|^2 = 2, \qquad |z \cdot v_j|^2 = |v_j|^2 - |n \cdot v_j|^2 \ge \frac{|v_j|^2}{2}.$$

In particular, $|z \cdot x| \le |x|$ for real $x$, and

$$\prod_{j=1}^{3} |z \cdot (x_i - y_j)| \ge \frac{\operatorname{dist}(x_i, \{y_1, y_2, y_3\})^3}{2\sqrt{2}}. \tag{92}$$

The polynomials $x \mapsto (z \cdot x)^k$ are harmonic because $z \cdot z = 0$. Hence their power sums are

$$p_k(X) := \sum_i (z \cdot x_i)^k = z^{\otimes k} : M_k(X), \qquad k = 1, 2, 3.$$

All projected nodes lie in $\{|t| \le R\}$, so $|p_k(X)|, |p_k(Y)| \le 3R^k$. We also have, for any real rank-$k$ tensor $A$,

$$|z^{\otimes k} : A| \le 2^{(k-1)/2} \|A\|. \tag{93}$$

Indeed, write $z^{\otimes k} = A_0 + \mathrm{i}B_0$ with real tensors $A_0, B_0$. The identity $(z \cdot z)^k = 0$ implies $A_0 \perp B_0$ and $\|A_0\| = \|B_0\|$, while $\|A_0\|^2 + \|B_0\|^2 = |z|^{2k} = 2^k$. Bessel's inequality for these orthogonal real tensors proves (93).

Consider the monic root polynomial

$$F_X(t) = \prod_{i=1}^{3} (t - z \cdot x_i) = t^3 - e_1(X)t^2 + e_2(X)t - e_3(X).$$

Newton's identities give

$$e_1 = p_1, \qquad e_2 = \frac{p_1^2 - p_2}{2}, \qquad e_3 = \frac{p_1^3 - 3p_1p_2 + 2p_3}{6}.$$

Write $\Delta$ for the difference between the $X$ and $Y$ quantities. The preceding disk bounds yield

$$\begin{aligned} |\Delta e_2| &\le 3R|\Delta p_1| + \tfrac{1}{2}|\Delta p_2|, \\ |\Delta e_3| &\le 6R^2|\Delta p_1| + \tfrac{3R}{2}|\Delta p_2| + \tfrac{1}{3}|\Delta p_3|. \end{aligned}$$

Consequently, for $|t| \le R$,

$$\begin{aligned} |F_X(t) - F_Y(t)| &\le 10R^2|\Delta p_1| + 2R|\Delta p_2| + \tfrac{1}{3}|\Delta p_3| \\ &\le R^2\left(10\|\Delta M_1\| + 2\sqrt{2}R^{-1}\|\Delta M_2\| + \tfrac{2}{3}R^{-2}\|\Delta M_3\|\right) \\ &\le \frac{4\sqrt{61}}{3}R^2 e(X,Y). \end{aligned} \tag{94}$$

Here the last constant is $\sqrt{10^2 + (2\sqrt{2})^2 + (2/3)^2} = 4\sqrt{61}/3$. Evaluate (94) at $t = z \cdot x_i$, where $F_X(t) = 0$, and combine it with (92). This gives

$$\operatorname{dist}(x_i, \{y_1, y_2, y_3\})^3 \le \frac{8\sqrt{122}}{3}R^2 e(X,Y) < 30R^2 e(X,Y),$$

proving (91). Interchanging $X$ and $Y$ gives the reverse point-to-set estimate.

For the multiplicity assertion, suppose that the three moment tensors agree. Their power sums, and therefore their root polynomials, agree for every complex null vector $z$. Choose a projection plane that is injective on the finite set of distinct points occurring in either triple: it is enough to choose its normal not parallel to any nonzero pairwise difference of these points. Equality of the projected root multisets then gives equality of the original multisets, with multiplicities. This last argument is needed because a Hausdorff-distance statement alone would not identify multiplicities. □

### 5.2 Variance from a single bounded marginal

For a tensor-valued random variable $M$, write $\operatorname{Var}_Q(M) = \mathbb{E}_Q\|M - \mathbb{E}_Q M\|^2$.

**Lemma 5.2** (Bounded-marginal moment variance)**.** *Let $Q$ be a probability law on $(B_R)^3$ whose first labeled marginal has a Lebesgue density bounded by $L$. If $r > 0$ satisfies $4\pi L r^3 \le 1/2$, then*

$$\operatorname{Var}_Q(M_1) + R^{-2}\operatorname{Var}_Q(M_2) + R^{-4}\operatorname{Var}_Q(M_3) \ge \frac{r^6}{3600R^4}. \tag{95}$$

*Neither symmetry, independence of the three coordinates, nor collision separation is required.*

*Proof.* For a fixed triple $Y$, the union of its three radius-$r$ balls has first-marginal probability at most $3L(4\pi/3)r^3 \le 1/2$. Thus, with $Q$-probability at least $1/2$, $x_1$ has distance at least $r$ from $\{y_1, y_2, y_3\}$. By Lemma 5.1,

$$Q\left\{e(X,Y) \ge \frac{r^3}{30R^2}\right\} \ge \frac{1}{2}.$$

Average over an independent copy $Y$ of $X$. Then $\mathbb{E}_{Q\otimes Q} e(X,Y)^2 \ge r^6/(1800R^4)$. The independent-copy identity $\mathbb{E}\|M(X) - M(Y)\|^2 = 2\operatorname{Var}_Q(M)$ applied separately to the three moment tensors proves (95). □

For later use, suppose that $P$ is a symmetric three-particle probability law with one-body density $\rho \le B$ and $\int \rho = 3$. If $C = (B_R)^3$ and $q = P(C) > 0$, then the first marginal of $Q = P(\cdot \mid C)$ is bounded by

$$L = \frac{B}{3q}. \tag{96}$$

Indeed, restricting the positive measure $P$ to $C$ can only decrease its first marginal, which before restriction is $\rho/3$; conditioning then divides by $q$. In particular, every $r$ with $r^3 \le 3q/(8\pi B)$ is admissible in Lemma 5.2.

### 5.3 Irregular shell masks and the exact Coulomb potential

Let $S = \{y : T < |y| < 2T\}$, with $T \geq R$, and let $\nu_0$ be uniform probability on $S$. Write $y = sn$, with $n \in \mathbb{S}^2$, and let $M_{k,c} = M_k - \mathbb{E}_Q M_k$. Define the centered truncated potential

$$f(X, y) = \frac{n : M_{1,c}}{s^2} + \frac{3}{2}\frac{n^{\otimes 2} : M_{2,c}}{s^3} + \frac{5}{2}\frac{n^{\otimes 3} : M_{3,c}}{s^4}. \tag{97}$$

**Lemma 5.3** (Stability under an arbitrary small-volume deletion)**.** *Under the assumptions of Lemma 5.2, let $E \subset S$ be measurable and suppose*

$$\theta := \frac{|S \setminus E|}{|S|} \leq \frac{1}{2000}.$$

*Let $\nu$ be uniform probability on $E$. Then*

$$\|f - \mathbb{E}_\nu f\|^2_{L^2(Q\otimes\nu)} \geq \frac{r^6}{320000T^8}. \tag{98}$$

*The deletion may be irregular; no rotational symmetry of $E$ is assumed.*

*Proof.* Different homogeneous harmonic degrees are orthogonal on the sphere. For a real symmetric trace-free rank-$k$ tensor $A_k$, the angular second moment is

$$\frac{1}{4\pi}\int_{\mathbb{S}^2} (n^{\otimes k} : A_k)^2 \, dn = \frac{k!}{(2k+1)!!}\|A_k\|^2.$$

To see the factor, the normalized spherical average of $n^{\otimes 2k}$ is $(2k+1)!!^{-1}$ times the sum of all Kronecker-delta pairings. Trace-freeness eliminates any pairing within one copy of $A_k$, leaving the $k!$ pairings between its two copies. For $k = 1, 2, 3$, the resulting factors are $1/3$, $2/15$, and $2/35$. The radial density of $\nu_0$ is $3s^2/(7T^3)$ on $(T, 2T)$, and hence

$$\mathbb{E}_{\nu_0} s^{-4} = \frac{3}{14T^4}, \qquad \mathbb{E}_{\nu_0} s^{-6} = \frac{1}{8T^6}, \qquad \mathbb{E}_{\nu_0} s^{-8} = \frac{93}{1120T^8}.$$

Using these formulas and the coefficients in (97) gives the exact identity

$$\|f\|^2_{L^2(Q\otimes\nu_0)} = \frac{\mathrm{Var}_Q(M_1)}{14T^4} + \frac{3\,\mathrm{Var}_Q(M_2)}{80T^6} + \frac{93\,\mathrm{Var}_Q(M_3)}{3136T^8}. \tag{99}$$

Since $T \geq R$, each weight dominates the corresponding weight in (95) times $93R^4/(3136T^8)$. It follows that

$$\|f\|^2_{L^2(Q\otimes\nu_0)} \geq \frac{93r^6}{3136 \cdot 3600T^8} \geq \frac{r^6}{160000T^8}. \tag{100}$$

For each fixed $X$, the sum-of-three-squares inequality, followed by $|n^{\otimes k} : M_{k,c}| \leq \|M_{k,c}\|$, gives

$$\sup_{y\in S} |f(X, y)|^2 \leq 700\|f(X, \cdot)\|^2_{L^2(\nu_0)}. \tag{101}$$

Indeed, the three ratios between the resulting supremum coefficients and the exact shell coefficients are 42, 180, and 58800/93, each less than 700.

Set $B_X = \|f(X, \cdot)\|^2_{L^2(\nu_0)}$. The $\nu_0$-mean of $f(X, \cdot)$ is zero, because all its angular degrees are positive. Deleting a fraction $\theta$ loses at most $700\theta B_X$ of its second moment. Therefore

$$\mathbb{E}_\nu f(X, \cdot)^2 \geq \frac{1 - 700\theta}{1 - \theta} B_X.$$

Since the integral on $E$ is the negative of that on $S \setminus E$,

$$|\mathbb{E}_\nu f(X,\cdot)|^2 \le \frac{700\theta^2}{(1-\theta)^2} B_X.$$

Subtracting the squared mean yields

$$\mathrm{Var}_\nu(f(X,\cdot)) \ge \frac{1-701\theta}{(1-\theta)^2} B_X \ge \frac{1}{2} B_X,$$

where the last inequality holds for $0 \le \theta \le 1/2000$. Average this bound over $Q$ and use (100) to prove (98). □

**Proposition 5.4** (Exact exterior Coulomb covariance)**.** *Let $Q, L, r, R, E, \nu$ be as in Lemma 5.3, and assume in addition*

$$T \ge \max\left\{2R, \frac{7200R^4}{r^3}\right\}. \tag{102}$$

*For*

$$V(X,y) = \sum_{i=1}^{3} \frac{1}{|y-x_i|}, \qquad h = (\mathrm{Id} - \mathbb{E}_Q)(\mathrm{Id} - \mathbb{E}_\nu)V,$$

*one has*

$$\|h\|^2_{L^2(Q\otimes\nu)} \ge \frac{r^6}{1280000T^8}. \tag{103}$$

*Proof.* For $s = |y| > |x_i|$, the convergent Legendre expansion is

$$\frac{1}{|y-x_i|} = \frac{1}{s}\sum_{k=0}^{\infty} \left(\frac{|x_i|}{s}\right)^k P_k\left(n \cdot \frac{x_i}{|x_i|}\right),$$

with its continuous interpretation at $x_i = 0$. Its monopole is $3/s$. The next three terms, after $Q$-centering, are exactly (97), as follows from $P_1(u) = u$, $P_2(u) = (3u^2-1)/2$, and $P_3(u) = (5u^3-3u)/2$. Since $|P_k(u)| \le 1$ for $|u| \le 1$, the sum $b$ of the remaining terms satisfies, when $T \ge 2R$,

$$|b(X,y)| \le \sum_{i=1}^{3} \frac{|x_i|^4}{s^5(1-|x_i|/s)} \le \frac{6R^4}{T^5}. \tag{104}$$

The two centering operators are commuting orthogonal projections on $L^2(Q\otimes\nu)$, so their product does not increase the norm of $b$. The monopole vanishes under $Q$-centering and the retained terms become $f - \mathbb{E}_\nu f$. Thus (98) and (104) imply

$$\|h\|_{L^2(Q\otimes\nu)} \ge \frac{r^3}{\sqrt{320000}T^4} - \frac{6R^4}{T^5}.$$

Because $\sqrt{320000} < 600$, condition (102) makes the second term at most half the first. Squaring the resulting lower bound proves (103) for the exact Coulomb potential. □

# 6 An explicit transfer from three to four particles

We now apply the covariance estimate of Proposition 5.4 to the non-product one-particle extension and diffuse-completion construction of Rosenzweig [1, Sections 6.2–6.3]. The proof keeps track of the whole original three-particle law, the conditional-event probability, and the cancellation of all old–new Hartree cross terms. Throughout, $D$ is the full Coulomb bilinear form, $H(f) = D(f,f)/2$, $W_N(f)$ is the minimum pair cost for a symmetric probability law with one-body density $f$ of mass $N$, and $I(f) = \int f^{4/3}$.

**Theorem 6.1** (Quantitative three-to-four-particle transfer)**.** *Let $0 < g \le 1$ and suppose $C_3 - C_2 \ge g$. Set*

$$\kappa_0 = \frac{g^7}{10^{12}} \exp\!\left(-\frac{160000000000}{g^9}\right), \qquad T = \frac{30}{\kappa_0}. \tag{105}$$

*Then*

$$\begin{aligned} C_4 - C_3 \ge G(g) &:= \frac{g^{36}}{2 \cdot 10^{95} T^{25}} \\ &= \frac{g^{211}}{2 \cdot 30^{25} \cdot 10^{395}} \exp\!\left(-\frac{4000000000000}{g^9}\right). \end{aligned} \tag{106}$$

*In particular,*

$$C_4 - C_3 \ge \exp\!\left(-\frac{5000000000000}{g^9}\right). \tag{107}$$

*With the preceding three-particle gap $g = \exp(-1769000)$, this gives*

$$C_4 - C_3 \ge \exp[-5000000000000 \exp(15921000)] \ge \exp[-\exp(15921030)]. \tag{108}$$

*No four-particle optimizer is required.*

*Proof.* We separate the proof into the geometric construction, the coupling, and the final energy balance.

*Optimizer data and the shell mask.* By the preceding existence and normalization results and Proposition 2.4, choose a normalized three-particle optimizer $\rho$ and a symmetric optimal probability law $P$ such that

$$\int \rho = 3, \qquad I(\rho) = 1, \qquad H(\rho) - W_3(\rho) = C_3, \qquad \rho \le 12, \qquad U_\rho \le 4. \tag{109}$$

The density has compact support. Proposition 4.3 allows a translation for which

$$R = \frac{27}{2g}, \qquad C = (B_R)^3, \qquad q = P(C) \ge p := \frac{g^3}{1000}. \tag{110}$$

Proposition 4.10 and Corollary 4.11 give the compatible chemical gap $\kappa \ge \kappa_0$. Proposition 4.12 then gives the occupied-volume bound

$$|\mathcal{O}| \le \frac{243\pi}{2\kappa_0^3}, \qquad \mathcal{O} := \{\rho > 0\}. \tag{111}$$

Here $\kappa$ has the compatible normalization $E_2(\phi) - c$ from that proposition; no identification with $E_2(v) - E_3(v)$ is used.

Choose a measurable representative of $\rho$ and define

$$S = \{y : T < |y| < 2T\}, \qquad E = S \setminus \mathcal{O}, \qquad \nu = \frac{\mathbf{1}_E}{|E|}, \qquad \nu_0 = \frac{\mathbf{1}_S}{|S|}. \tag{112}$$

Thus $\mathcal{O}$ is the occupied set and $E$ is the available, unoccupied part of the shell. The use of the positive set avoids any dependence on the measure of a topological support boundary. Since $|S| = (28\pi/3)T^3$, equations (105) and (111) imply

$$\theta := \frac{|S \setminus E|}{|S|} \le \frac{243\pi/(2\kappa_0^3)}{(28\pi/3)(30/\kappa_0)^3} = \frac{729}{56 \cdot 30^3} = \frac{27}{56000} < \frac{1}{2000}. \tag{113}$$

In particular, $E$ has positive measure. As $\pi > 3$,

$$|E| \ge \left(1 - \frac{1}{2000}\right)|S| > \left(1 - \frac{1}{2000}\right) 28T^3 > T^3.$$

Consequently

$$\int \nu = 1, \qquad \rho\nu = 0 \quad \text{a.e.}, \qquad A := I(\nu) = |E|^{-1/3} \le \frac{1}{T}. \tag{114}$$

The mask $E$ is fixed by $\rho$ and does not depend on the random configuration $X$.

*Conditional density cap and the covariance scale.* Let $Q = P(\,\cdot \mid C)$ and set $r = g/100$. By (96), its first labeled marginal has density bounded by

$$L = \frac{12}{3q} \le \frac{4}{p} = 4000g^{-3}. \tag{115}$$

This follows directly by restricting the first marginal $\rho/3$ of $P$ to the event $C$ and dividing by $q$, and requires no independence of the three coordinates. The choice of $r$ gives

$$4\pi L r^3 \le \frac{2\pi}{125} < \frac{8}{125} < \frac{1}{2}. \tag{116}$$

Furthermore,

$$\frac{T}{10^{15}g^{-7}} = \frac{3}{100}\exp\!\left(\frac{160000000000}{g^9}\right) > 1,$$

where $e^a \ge 1 + a$ and $g \le 1$ already suffice. Direct substitution yields

$$\begin{aligned} \frac{7200R^4}{r^3} &= 239148450000000g^{-7} < 10^{15}g^{-7}, \\ 2R &= 27g^{-1} < 10^{15}g^{-7}. \end{aligned} \tag{117}$$

Thus (113), (116), and (117) verify every hypothesis of Proposition 5.4.

For $X \in C$ and $y \in E$, define

$$\begin{aligned} V(X, y) &= \sum_{i=1}^{3} \frac{1}{|y - x_i|}, \\ h(X, y) &= V(X, y) - \mathbb{E}_Q V(\cdot, y) - \mathbb{E}_\nu V(X, \cdot) + \mathbb{E}_{Q\otimes\nu} V. \end{aligned} \tag{118}$$

The expectations are taken under the conditional law $Q$ and the masked probability $\nu$. In particular,

$$\mathbb{E}_\nu h(X, \cdot) = 0 \quad (Q\text{-a.e. } X), \qquad \mathbb{E}_Q h(\cdot, y) = 0 \quad (\nu\text{-a.e. } y). \tag{119}$$

The exact-potential lower bound is

$$\|h\|^2_{L^2(Q\otimes\nu)} \geq \frac{r^6}{1280000T^8}. \tag{120}$$

For clarity, the proof of this estimate controls the degree-one through degree-three retained part by $r^6/(320000T^8)$ after deletion and centering, and the full Legendre remainder by $6R^4/T^5$ in supremum norm. Both centering operations are $L^2$ contractions, and (117) makes this remainder at most half the retained part's lower norm. Thus (120) is an estimate for the exact Coulomb potential.

*A positive coupling preserving the whole old law.* Since $T \geq 2R$, on $C \times E$ we have

$$0 \leq V(X,y) \leq \frac{3}{T-R} \leq \frac{6}{T}.$$

Bounding the four terms in (118) separately gives

$$|h(X,y)| \leq \frac{24}{T}. \tag{121}$$

Extend $\mathbf{1}_C h$ by zero outside $C$ and set

$$t = \frac{T}{48}, \qquad d\Gamma(X,y) = \big[1 - t\mathbf{1}_C(X)h(X,y)\big]\, dP(X)\, d\nu(y). \tag{122}$$

The bracket is between $1/2$ and $3/2$, so $\Gamma$ is nonnegative. Its $X$-marginal is $P$ by the first identity in (119). Its $y$-marginal is $\nu$ because

$$\int_C h(X,y)\, dP(X) = q\mathbb{E}_Q h(\cdot, y) = 0.$$

Thus $\Gamma$ has mass one. In particular, it preserves the entire three-particle law $P$, including all old pair correlations and the old pair energy; preservation of only its one-body density would not suffice for the accounting below.

The product cross energy is finite, even if the masked shell comes arbitrarily close to the full occupied support:

$$\int V\, d(P\otimes\nu) = \int U_\rho(y)\nu(y)\, dy \leq 4. \tag{123}$$

The perturbation is supported on $C \times E$, where $V$ is bounded, so all terms in the following subtraction are finite. Define the cross-energy reduction

$$\begin{aligned}\Delta &:= \int V\, d(P\otimes\nu) - \int V\, d\Gamma \\ &= tq\, \mathbb{E}_{Q\otimes\nu}(Vh) = tq\, \|h\|^2_{L^2(Q\otimes\nu)}.\end{aligned} \tag{124}$$

For the last equality, $V - h$ is a sum of an $X$-only and a $y$-only function and is therefore orthogonal to $h$ by (119). This is a positive reduction of the pair cost. The conditional-event probability $q$ occurs exactly once. Using (110) and (120) now gives

$$\begin{aligned}\Delta &\geq \frac{pr^6}{61440000T^7} = \frac{g^9}{614400000000000000000000T^7} \\ &> 10^{-23} g^9 T^{-7} =: \delta_0.\end{aligned} \tag{125}$$

No uniform radius for the whole support of $\rho$, nor a positive separation between that support and $E$, was needed. The factor $t$ has length dimension, so the right side of (124) has energy dimension, as does $pr^6/T^7$ in (125); the substitution $r = g/100$ uses the normalization $I(\rho) = 1$.

*Diffuse completion and four-label symmetrization.* Fix a smooth nonnegative compactly supported probability density $\zeta$. For each dilation scale $\ell \to \infty$, choose a translation $z_\ell$ so that

$$\zeta_\ell(x) = \ell^{-3}\zeta\Big(\frac{x - z_\ell}{\ell}\Big)$$

has support disjoint from both the compact support of $\rho$ and the bounded shell $S$. Such translations exist; no uniform numerical bound on the support of $\rho$ is needed. Then

$$\int \zeta_\ell = 1, \qquad I(\zeta_\ell) = \ell^{-1} I(\zeta) \longrightarrow 0. \tag{126}$$

For $0 < \varepsilon < 1$, form

$$\Pi_\ell = \varepsilon\Gamma + (1-\varepsilon)(P \otimes \zeta_\ell), \qquad \sigma_\ell = \varepsilon\nu + (1-\varepsilon)\zeta_\ell, \tag{127}$$

and then symmetrize all four coordinates of $\Pi_\ell$. The symmetrized probability law has one-body density $\rho + \sigma_\ell$, of total mass four. Each configuration contains the original three particles and exactly one fourth particle; there is no fourth–fourth pair cost. Symmetrization changes neither the total one-body density nor the sum of pair costs.

Let $c_4$ denote the sum of the six pair interactions. Both components in (127) preserve $P$ as their old-configuration marginal, and (124) is the entire non-product cross-energy reduction. Consequently the trial pair cost is exactly

$$\int c_4 \, d\Pi_\ell = W_3(\rho) + D(\rho, \sigma_\ell) - \varepsilon\Delta. \tag{128}$$

On the other hand, the full-double-integral convention for $D$ gives

$$H(\rho + \sigma_\ell) = H(\rho) + D(\rho, \sigma_\ell) + H(\sigma_\ell).$$

Subtracting (128) and using (109) gives

$$\begin{aligned} H(\rho + \sigma_\ell) - \int c_4 \, d\Pi_\ell &= C_3 + \varepsilon\Delta + H(\sigma_\ell) \\ &\geq C_3 + \varepsilon\delta_0. \end{aligned} \tag{129}$$

Here $H(\sigma_\ell) = D(\sigma_\ell, \sigma_\ell)/2 \geq 0$. Its cross contribution between $\nu$ and $\zeta_\ell$ is also nonnegative. It is not an additional pair cost: the single fourth particle is sampled from a mixture, rather than accompanied by a second added particle.

The occupied sets of $\rho$, $\nu$, and $\zeta_\ell$ are pairwise disjoint up to null sets. Thus the denominator is exactly

$$I(\rho + \sigma_\ell) = 1 + \varepsilon^{4/3}A + (1-\varepsilon)^{4/3} I(\zeta_\ell). \tag{130}$$

Since $W_4(\rho + \sigma_\ell) \leq \int c_4 \, d\Pi_\ell$, the definition of $C_4$, followed by (129)–(130), gives

$$C_3 + \varepsilon\delta_0 \leq C_4 \left[1 + \varepsilon^{4/3}A + (1-\varepsilon)^{4/3} I(\zeta_\ell)\right].$$

Let $\ell \to \infty$ and use (126). Rearrangement yields

$$C_4 - C_3 \geq \varepsilon\delta_0 - C_4 A \varepsilon^{4/3}. \tag{131}$$

There is no additional quotient denominator in this inequality. Attainment of $C_4$ is not required, and the diffuse cross energy need not tend to zero: it already cancels exactly in (129).

For the numerical balance, the Hardy–Littlewood–Sobolev and interpolation bound of Lemma 2.3 gives

$$H(f) \le a \left( \int f \right)^{2/3} I(f), \qquad a = \frac{2}{3} \left( \frac{4}{\sqrt{\pi}} \right)^{2/3} < \frac{23}{20}. \tag{132}$$

The interpolation step is $\|f\|_{6/5}^2 \le \|f\|_1^{2/3} \|f\|_{4/3}^{4/3}$. Since $W_4 \ge 0$, (132) implies

$$C_4 \le a\, 4^{2/3} < 3, \tag{133}$$

where the last inequality follows by cubing, $(23/20)^3 \cdot 16 < 27$. Thus no sharp numerical universal upper bound for $C_4$ is needed here.

*The explicit balance and exponent accounting.* Set

$$\varepsilon = 10^{-72} g^{27} T^{-18}, \qquad \varepsilon^{1/3} = 10^{-24} g^9 T^{-6}. \tag{134}$$

Since $g \le 1$ and $T > 1$, we have $0 < \varepsilon < 1$. Equations (114), (125), and (133) give

$$C_4 A \varepsilon^{1/3} < 3 \cdot 10^{-24} g^9 T^{-7} = \frac{3}{10} \delta_0 < \frac{1}{2} \delta_0. \tag{135}$$

Substitution into (131) proves

$$C_4 - C_3 \ge \frac{\varepsilon \delta_0}{2} = \frac{g^{36}}{2 \cdot 10^{95} T^{25}}.$$

Finally,

$$T = 30 \cdot 10^{12} g^{-7} \exp\!\left( \frac{160000000000}{g^9} \right).$$

Its twenty-fifth power accounts for all factors in (106): the power of $g$ is $36 + 7 \cdot 25 = 211$, the power of ten is $95 + 12 \cdot 25 = 395$, and $25 \cdot 160000000000 = 4000000000000$.

For the simpler estimate, $2 \cdot 30^{25} < 10^{38}$ gives

$$G(g) \ge g^{211} 10^{-433} \exp\!\left( -\frac{4000000000000}{g^9} \right).$$

For $x = 1/g \ge 1$, the elementary inequality $\log x \le (x^9 - 1)/9 \le x^9/9$, together with $\log 10 < 3$, yields

$$211 \log(1/g) + 433 \log 10 \le \frac{211/9 + 1299}{g^9} < \frac{1330}{g^9}.$$

As $4000000000000 + 1330 < 5000000000000$, this proves (107). At $g = \exp(-1769000)$, $g^{-9} = \exp(15921000)$. Finally, $e > 8/3$ and $(8/3)^{30} > 5000000000000$ imply $5000000000000 < \exp(30)$, proving (108). □

The estimates quantify this three-to-four-particle instance of the extension mechanism. They do not determine $C_3$, $C_4$, or the universal Lieb–Oxford constant, and they do not establish an all-$N$ quantitative recursion.

# A An elementary independent lower witness

**Proposition A.1.** *In the normalization of Section 1, $C_2 > 2503/2000 = 1.2515 > 5/4$.*

*Proof.* Set

$$\rho(x) = \frac{3}{2\pi}(1+|x|^3)^{-2}.$$

Substitution $t = r^3$ gives $\int \rho = 2$. The radial probability density for $\rho/2$ is $3r^2(1+r^3)^{-2}\,\mathrm{d}r$, invariant under $r \mapsto 1/r$. If $x_1$ has density $\rho/2$ and $x_2 = -x_1/|x_1|^2$, this involution preserves the marginal. The resulting two-particle law is symmetric and admissible, although singular. Its optimality is unnecessary.

The enclosed radial mass is $M(r) = 2r^3/(1+r^3)$. Newton's theorem and direct integration give

$$\begin{aligned} H(\rho) &= \int_0^\infty \frac{M(r)}{r}\,M'(r)\,\mathrm{d}r = 12\int_0^\infty \frac{r^4}{(1+r^3)^3}\,\mathrm{d}r \\ &= \frac{8\pi}{9\sqrt{3}}, \\ I(\rho) &= \frac{4\pi}{5}\left(\frac{3}{2\pi}\right)^{4/3}, \qquad I(\rho)^3 = \frac{324}{125\pi}. \end{aligned}$$

For an elementary evaluation of the Hartree integral, put $J = \int_0^\infty r/(1+r^3)\,\mathrm{d}r$. Integrating the derivatives of $r^2/(1+r^3)$ and $r^2/(1+r^3)^2$, whose endpoint values vanish, gives $\int_0^\infty r^4/(1+r^3)^3\,\mathrm{d}r = J/9$. Partial fractions give the antiderivative

$$-\tfrac{1}{3}\log(r+1) + \tfrac{1}{6}\log(r^2-r+1) + \frac{1}{\sqrt{3}}\arctan\frac{2r-1}{\sqrt{3}}$$

for $r/(1+r^3)$, so $J = 2\pi/(3\sqrt{3})$, as required. The pair separation is $r + r^{-1}$. Inverting the part $r > 1$ of the cost integral yields

$$W_{\mathrm{trial}} = 6\int_0^1 \frac{r^3}{(1+r^3)^2(1+r^2)}\,\mathrm{d}r.$$

We now enclose this integral by finite integer arithmetic, without numerical quadrature assumptions. Put $n = 10000$ and $s = 2^{80}$. On $[i/n, (i+1)/n]$, increase the numerator and decrease each denominator factor. The contribution to $W_{\mathrm{trial}}$ is at most

$$b_i = \frac{6(i+1)^3 n^4}{(n^3+i^3)^2(n^2+i^2)}.$$

Rounding each $b_i$ upward on the $s^{-1}$ grid gives the exact upper bound

$$\begin{aligned} W_{\mathrm{trial}} &\le s^{-1}\sum_{i=0}^{9999} \lceil s b_i \rceil \\ &= \frac{33091719716859063827679}{75557863725914323419136} =: W_+. \end{aligned} \tag{136}$$

For completeness, rational alternating-series brackets in Machin's identity

$$\pi = 16\arctan(1/5) - 4\arctan(1/239)$$

give $333/106 < \pi < 22/7$. Specifically, use 20 and 21 terms for the lower and upper brackets of $\arctan(1/5)$, and 4 and 5 terms for $\arctan(1/239)$. The identity itself follows from the tangent addition formula and the angle ranges. Also $(17321/10000)^2 > 3$. Thus

$$H(\rho) > \frac{1480000}{918013} =: H_-, \qquad I(\rho)^3 < \frac{3816}{4625} =: J_+.$$

The following are strict rational inequalities; clearing their positive denominators reduces them to integer comparisons:

$$H_- > W_+, \qquad (H_- - W_+)^3 > \left(\frac{2503}{2000}\right)^3 J_+.$$

Equations (136) and these comparisons are reproduced by the supplied standard-library script. They imply

$$\frac{H(\rho) - W_{\text{trial}}}{I(\rho)} > \frac{2503}{2000}.$$

Since $W_2(\rho) \le W_{\text{trial}}$, the variational definition proves the claim. □

This witness supplies only a convenient lower input. No claim that it is an optimizing density or an optimal transport plan is used. The proof does not depend on the stronger optional piecewise-radial certificate from earlier calculations.

# B Compatible Coulomb potentials and compact support

This appendix gives the foundational reconstruction used in the manuscript for the three-dimensional Coulomb problem at a fixed particle number. Existence of an optimizing density remains an external input, taken from [1]; it is not proved here. The variational framework follows [2, Section 3, equations (18)–(21)]. The dissociation and global upper-tail argument below reproduces the mechanism of [5, Theorem 3 and Section 3.1, equations (29)–(32)], whose journal publication appeared in 2025. The regular-potential results of [4] provide background, but the construction of the compatible representative is included here in full. No numerical successive-gap estimate is used, and no novelty is claimed for this reconstruction. Its checking was model-assisted; it is not external mathematical peer review or a certification of the cited papers.

**Proposition B.1** (Foundational reconstruction conditional on attainment)**.** *Fix $N \ge 2$ and suppose that $\rho \ge 0$ in $L^1(\mathbb{R}^3) \cap L^{4/3}(\mathbb{R}^3)$, with $\int \rho = N$, attains $C_N$. After a mass-preserving dilation, suppose $I(\rho) = 1$. Write*

$$\lambda = C_N, \qquad \beta = \frac{4\lambda}{3}, \qquad U = \rho * |\cdot|^{-1}, \qquad W = W_N(\rho), \qquad v = U - \beta\rho^{1/3}.$$

*Then $0 < \lambda < \infty$, an optimal symmetric probability law $P$ exists, and there are a bounded globally Lipschitz function $\phi$ and a real constant $c$ with the following properties:*

1. *The same representative $\phi$ is pointwise feasible, optimal, and $c_N$-conjugated:*

$$\sum_{i=1}^{N} \phi(x_i) \le c_N(X) \quad \text{for every } X \in (\mathbb{R}^3)^N, \qquad \int \phi\rho = W, \tag{137}$$

$$\phi(x) = \inf_{y_2,\dots,y_N} \left\{ c_N(x, y_2, \dots, y_N) - \sum_{i=2}^{N} \phi(y_i) \right\}. \tag{138}$$

2. *The functions $U$ and $\rho$ have continuous representatives on $\mathbb{R}^3$, the density has compact support and vanishes on its boundary, and*

$$\phi \geq v + c \quad \text{on } \mathbb{R}^3, \qquad \phi = v + c \quad \text{on } \operatorname{supp} \rho, \tag{139}$$

$$c = -\frac{W}{N} - \frac{2\lambda}{3N}. \tag{140}$$

3. *For $k \geq 1$ set*

$$E_k(f) = \inf_{z_1,\dots,z_k} \left\{ c_k(z_1, \dots, z_k) - \sum_{i=1}^{k} f(z_i) \right\}, \qquad E_0(f) = 0.$$

*Then*

$$E_N(\phi) = 0, \qquad C_\phi := \lim_{|x|\to\infty} \phi(x) = E_{N-1}(\phi), \qquad \phi \geq C_\phi, \tag{141}$$

$$\psi := \phi - C_\phi \geq 0, \qquad \psi(x) \longrightarrow 0, \qquad \kappa := C_\phi - c \geq 0, \tag{142}$$

$$\rho(x) = \left[ \frac{(U(x) - \phi(x) + c)_+}{\beta} \right]^3 = \left[ \frac{(U(x) - \psi(x) - \kappa)_+}{\beta} \right]^3 \quad (x \in \mathbb{R}^3). \tag{143}$$

*Moreover, $\rho \in L^4(\mathbb{R}^3)$ and $U(x) \to 0$ as $|x| \to \infty$.*

*The one-particle analogue, also conditional on attainment, holds with $\phi = 0$; its proof is given at the end of the appendix.*

## B.1 Variational inequality and a precise feasible representative

We prove the proposition in successive steps. The notation and normalizations are those of Section 1; the Coulomb cost is $+\infty$ at collisions. Interpolation gives $\rho \in L^{6/5}$, and the Hardy–Littlewood–Sobolev inequality [7] gives finite $H(\rho)$. More generally its bilinear form and interpolation give $H(\eta) \leq K_N I(\eta)$ for admissible mass-$N$ densities, with a finite constant $K_N$. Since $W_N \geq 0$, this also proves $C_N < \infty$. For any such nonzero density $\eta$, the product probability law $(\eta/N)^{\otimes N}$ has cost

$$\int c_N \, \mathrm{d}(\eta/N)^{\otimes N} = \binom{N}{2} \frac{D(\eta,\eta)}{N^2} = \frac{N-1}{N} H(\eta). \tag{144}$$

Consequently its indirect gain is exactly $H(\eta)/N > 0$, so $C_N > 0$ and $\beta > 0$.

The same product trial shows $W < \infty$. A minimizing sequence of admissible laws is tight: the mass outside $K^N$ is at most $N \int_{K^c} \rho/N = \int_{K^c} \rho$ for every compact set $K$. A weakly convergent subsequence retains each marginal and permutation symmetry. Since $c_N$ is nonnegative and lower semicontinuous, the limit $P$ is an optimal law. This is compactness of plans with a fixed marginal, and does not assert compact support of $\rho$.

By the defining inequality for $\lambda = C_N$, the functional

$$F(\eta) = W_N(\eta) - H(\eta) + \lambda I(\eta)$$

is nonnegative on nonnegative mass-$N$ densities and vanishes at $\rho$. Let $\eta$ be a bounded compactly supported mass-$N$ density and put $\rho_t = (1-t)\rho + t\eta$, $0 < t < 1$. Mixtures of admissible laws give convexity of $W_N$, and therefore

$$\begin{aligned} W_N(\eta) - W &\geq \frac{W_N(\rho_t) - W}{t} \\ &\geq \frac{H(\rho_t) - H(\rho) - \lambda(I(\rho_t) - I(\rho))}{t}. \end{aligned}$$

Differentiate only $H$ and $I$ along this segment. Their derivatives are $\int U(\eta-\rho)$ and $\frac{4}{3}\int \rho^{1/3}(\eta-\rho)$, respectively. These are finite by HLS and Hölder, and ordinary dominated differentiation for $t^{4/3}$ justifies the latter derivative. Thus

$$W_N(\eta) \geq W + \int v(\eta-\rho). \tag{145}$$

No differentiability of $W_N$ has been used. The HLS mapping estimate gives $U \in L^{12}(\mathbb{R}^3)$, and $\int U\rho = 2H(\rho) < \infty$; also $\int \rho^{1/3}\rho = I(\rho) < \infty$. It follows that $v \in L^1_{\mathrm{loc}}(\mathbb{R}^3) \cap L^1(\rho\,\mathrm{d}x)$.

Let $\mathcal{L}$ be the full-Lebesgue-measure set of finite Lebesgue points of $v$, using its precise Lebesgue representative there. Fix distinct $x_1, \dots, x_N \in \mathcal{L}$. For sufficiently small $\varepsilon > 0$, the balls $B_\varepsilon(x_i)$ are disjoint. Let $m_{i,\varepsilon}$ be the uniform probability density on the $i$th ball and set $\eta_\varepsilon = \sum_i m_{i,\varepsilon}$. The symmetrization of $\bigotimes_i (m_{i,\varepsilon}\,\mathrm{d}x)$ has one-body density $\eta_\varepsilon$. Because the balls remain mutually separated, its pair cost converges to $c_N(X)$; Lebesgue differentiation gives $\int v\eta_\varepsilon \to \sum_i v(x_i)$. Using this trial law in (145) yields

$$\sum_{i=1}^N v(x_i) \leq c_N(X) - W + \int v\rho. \tag{146}$$

Define

$$c = \frac{W - \int v\rho}{N}, \qquad h(x) = \begin{cases} v(x) + c, & x \in \mathcal{L}, \\ -\infty, & x \notin \mathcal{L}. \end{cases} \tag{147}$$

The sum of the $h$-values is unambiguously real or $-\infty$, never $+\infty$. Equation (146) proves its feasibility for distinct points in $\mathcal{L}$; collisions have infinite cost, and any point outside $\mathcal{L}$ makes the sum $-\infty$. Thus

$$\sum_{i=1}^N h(x_i) \leq c_N(X) \quad \text{for every } X, \qquad \int h\rho = W. \tag{148}$$

The integral uses the finite almost-everywhere representative of $h$. It is well defined because the one-body measure $\rho\,\mathrm{d}x$ is absolutely continuous and $v \in L^1(\rho\,\mathrm{d}x)$. In particular, we have not integrated an almost-everywhere tuple inequality against possibly singular $P$.

### B.2 A bounded feasible majorant by sequential transforms

First $h$ has a finite global upper bound. Choose two lists $A = (a_2, \dots, a_N)$ and $B = (b_2, \dots, b_N)$ in $\mathcal{L}$ such that all $2(N-1)$ points are distinct, and let $\delta > 0$ be their minimum mutual separation. For every $x$, at least one list has all its points at distance at least $\delta/3$ from $x$. Otherwise two selected points, one in each list, would be less than $2\delta/3$ apart. For the separated list $Z = (z_2, \dots, z_N)$, feasibility gives

$$h(x) \leq c_N(x, Z) - \sum_{i=2}^N h(z_i) \leq \frac{3(N-1) + \binom{N-1}{2}}{\delta} - \sum_{i=2}^N h(z_i). \tag{149}$$

Both lists have fixed finite $h$-values, so the larger of their right-hand bounds is a finite uniform bound. This remains valid if $x$ is a selected point, by using the other list, and is automatic when $h(x) = -\infty$.

Starting with the feasible tuple $(h, \dots, h)$, transform slots $j = 1, \dots, N$ in order. At step $j$, with the current functions $f_1, \dots, f_N$, replace $f_j$ by

$$\mathcal{T}_j(f)(x) = \inf_{(y_i)_{i\neq j}} \left\{ c_N(y_1, \dots, y_{j-1}, x, y_{j+1}, \dots, y_N) - \sum_{i\neq j} f_i(y_i) \right\}. \tag{150}$$

Whenever an untransformed slot equals $-\infty$, its objective value in (150) is defined to be $+\infty$. The old feasible inequality gives $\mathcal{T}_j(f) \geq f_j$ pointwise. The definition of the infimum gives feasibility after replacement; if another slot equals $-\infty$, that tuple inequality is automatic.

At each step all other slots have finite global upper bounds $M_i$. Since all pair interactions are nonnegative,

$$\mathcal{T}_j(f)(x) \geq -\sum_{i \neq j} M_i. \tag{151}$$

For an upper bound, use two separated test lists consisting of points of $\mathcal{L}$, assigned to the slots $i \neq j$. Every untransformed value on these lists is finite, and previously transformed slots are finite everywhere by induction. The same separation argument as in (149) gives a finite uniform upper bound $B$ for this transform. Hence every transformed slot is a bounded real-valued function on all of $\mathbb{R}^3$.

Measurability and regularity follow from a cost truncation, which we record explicitly. Choose

$$L > \max\left(0,\ B + \sum_{i \neq j} M_i\right), \quad w_L(z) = \begin{cases} \min\{L, |z|^{-1}\}, & z \neq 0, \\ L, & z = 0, \end{cases} \quad c_{N,L}(X) = \sum_{i<k} w_L(x_i - x_k). \tag{152}$$

If any original pair interaction exceeds $L$ (including a collision), both the original objective and the objective with $c_{N,L}$ are at least $L - \sum_{i \neq j} M_i > B$; they cannot lower an infimum bounded above by $B$. If all pair interactions are at most $L$, the two objectives agree. Tuples containing an untransformed $-\infty$ value have objective $+\infty$ in both versions and can be omitted. Therefore the transform is unchanged by this truncation. The function $w_L$ is globally Lipschitz with constant $L^2$. For every remaining choice of the other coordinates the truncated objective is Lipschitz in $x$, with constant $(N-1)L^2$ independent of those coordinates. A finite-valued infimum of such a family obeys the same Lipschitz bound: apply each member's bound, take its infimum, and interchange the two fixed points. This proves that every slot transform is globally Lipschitz, without appealing to measurability of an arbitrary uncountable infimum.

After all slots are transformed, call them $g_1, \dots, g_N$. They are bounded real-valued globally Lipschitz functions with $g_j \geq h$, and $(g_1, \dots, g_N)$ is pointwise feasible. Put

$$u_0 = \frac{1}{N} \sum_{j=1}^{N} g_j. \tag{153}$$

For each label permutation $\sigma$, feasibility gives $\sum_j g_j(x_{\sigma(j)}) \leq c_N(X)$. Averaging over all $N!$ permutations proves $\sum_i u_0(x_i) \leq c_N(X)$. Now bounded pointwise feasibility can legitimately be integrated against $P$, yielding

$$W = \int h\rho \leq \int u_0 \rho = \int \sum_{i=1}^{N} u_0(x_i)\, \mathrm{d}P \leq \int c_N \, \mathrm{d}P = W. \tag{154}$$

Thus $u_0$ is optimal and $u_0 = h$ $\rho\,\mathrm{d}x$-almost everywhere. No pointwise supremum of unrelated feasible symmetric potentials has been used.

### B.3 A monotone averaged transform and exact conjugacy

For any bounded pointwise feasible symmetric potential $u$, define

$$Tu(x) = \inf_{y_2, \dots, y_N} \left\{ c_N(x, y_2, \dots, y_N) - \sum_{i=2}^{N} u(y_i) \right\}. \tag{155}$$

The preceding bounds and truncation argument apply, so $Tu$ is a bounded globally Lipschitz function, and feasibility gives $Tu \geq u$. Set, inductively,

$$u_{n+1} = \frac{(N-1)u_n + Tu_n}{N}. \tag{156}$$

For every slot $i$, the tuple with $Tu_n$ in slot $i$ and $u_n$ in all other slots is feasible. Averaging these $N$ tuple inequalities shows that $u_{n+1}$ is a feasible symmetric potential. Thus $u_{n+1} \geq u_n$, and bounded weak duality together with (154) shows $\int u_n \rho = W$ for every $n$.

There are uniform bounds independent of $n$. The lower bound is $b := \inf u_0 > -\infty$. Use the two separated lists chosen above in the feasible inequality for $u_n$. Their costs are bounded by the same constant as in (149), while each of the $N-1$ subtracted values is at least $b$. Consequently $u_n(x) \leq B_*$ for a finite constant $B_*$ independent of $n$ and $x$. The increasing sequence therefore has a bounded real-valued pointwise limit $\phi$. This limit is measurable, pointwise feasible, and satisfies $\phi \geq u_0 \geq h$. Bounded convergence gives

$$\int \phi\rho = W, \qquad \phi = h \quad \rho\,\mathrm{d}x\text{-almost everywhere.} \tag{157}$$

For fixed $x$, the objectives in (155) for $u_n$ decrease pointwise. The following interchange is of two infima, and hence requires no compactness or attainment of the minimizing configurations:

$$\begin{aligned} \lim_{n\to\infty} Tu_n(x) &= \inf_n \inf_Y \left\{ c_N(x,Y) - \sum_{i=2}^N u_n(y_i) \right\} \\ &= \inf_Y \inf_n \left\{ c_N(x,Y) - \sum_{i=2}^N u_n(y_i) \right\} = T\phi(x). \end{aligned} \tag{158}$$

At colliding tuples both limiting objectives are $+\infty$, since the potentials are bounded. On the other hand, (156) gives $Tu_n = Nu_{n+1} - (N-1)u_n \to \phi$. Thus $\phi = T\phi$, proving (138). Neither uniform convergence on $\mathbb{R}^3$ nor a limit of increasing infima is being asserted.

Put $M = \|\phi\|_\infty$ and choose $L > NM$ with $L > 0$. If any pair interaction is greater than $L$, both its original and truncated objectives are at least $L - (N-1)M > M \geq T\phi(x)$. The same truncation argument gives

$$\phi(x) = \inf_Y \left\{ c_{N,L}(x,Y) - \sum_{i=2}^N \phi(y_i) \right\}, \qquad \mathrm{Lip}(\phi) \leq (N-1)L^2. \tag{159}$$

In particular, $\phi$ is feasible for the bounded continuous cost $c_{N,L}$ as well as for $c_N$. Together, (147) and (157) now give one and the same bounded globally Lipschitz representative satisfying

$$\phi \geq U - \beta\rho^{1/3} + c \quad \text{Lebesgue-a.e.}, \qquad \phi = U - \beta\rho^{1/3} + c \quad \rho\,\mathrm{d}x\text{-a.e.} \tag{160}$$

Finally, the nonnegative slack in (137) has integral zero against $P$. Hence

$$c_N(X) = \sum_{i=1}^N \phi(x_i) \quad P\text{-almost surely.} \tag{161}$$

Feasibility gives $E_N(\phi) \geq 0$, and any finite saturated tuple from this full-measure set gives the reverse inequality. Thus $E_N(\phi) = 0$.

### B.4 The global positive part relation and continuous representatives

A $\rho\,\mathrm{d}x$-null subset of $\{\rho > 0\}$ is Lebesgue-null: intersect it with $\{\rho \geq 1/k\}$, for $k \in \mathbb{N}$, and take the countable union. Consequently equality in (160) holds Lebesgue-almost everywhere on $\{\rho > 0\}$. On $\{\rho = 0\}$, its inequality reads $U - \phi + c \leq 0$ almost everywhere. Therefore

$$\rho = \left[\frac{(U - \phi + c)_+}{\beta}\right]^3 \quad \text{Lebesgue-almost everywhere on } \mathbb{R}^3. \tag{162}$$

This reasoning does not identify a measure-theoretic equality with an equality on an arbitrary topological support.

The HLS mapping estimate $U \in L^{12}$, boundedness of $\phi - c$, and (162) imply $\rho \in L^4_{\mathrm{loc}}$. We include the continuity argument. For a fixed compact set $K$ and $0 < r < 1$, Hölder gives, uniformly for $x \in K$,

$$\begin{aligned}\int_{|x-y|<r} \frac{\rho(y)}{|x-y|}\,\mathrm{d}y &\leq \|\rho\|_{L^4(K+B_1)} \left(\int_{|z|<r} |z|^{-4/3}\,\mathrm{d}z\right)^{3/4} \\ &= \left(\frac{12\pi}{5}\right)^{3/4} r^{5/4}\|\rho\|_{L^4(K+B_1)}.\end{aligned} \tag{163}$$

The convolutions $\rho * w_{1/r}$ are continuous, since $w_{1/r}$ is bounded Lipschitz and $\rho \in L^1$. The differences $U - \rho * w_{1/r}$ are nonnegative and bounded on $K$ by (163); hence the convolutions converge locally uniformly to $U$. Thus $U$ is finite and continuous everywhere.

The right side of (162) now defines a continuous representative of $\rho$ on all of $\mathbb{R}^3$; replacing $\rho$ by it does not change its Coulomb potential or any integrals. The positive-part identity holds everywhere for these representatives. The majorization in (160) extends everywhere by continuity, while equality holds on $\{\rho > 0\}$ and therefore on its closure. For a continuous nonnegative density, that closure is $\mathrm{supp}(\rho\,\mathrm{d}x)$, which we denote by $\mathrm{supp}\,\rho$. The density vanishes on the boundary of its positivity set and on the boundary of its closed support. This proves all pointwise representative claims before any compact-support conclusion is used.

### B.5 The limit at infinity and the sign of the compatible gap

Set

$$C_\phi = E_{N-1}(\phi) = \inf_{y_2,\dots,y_N} \left\{ c_{N-1}(y_2, \dots, y_N) - \sum_{i=2}^{N} \phi(y_i) \right\}. \tag{164}$$

This number is finite: boundedness of $\phi$ gives a finite lower bound, and any fixed finite distinct tuple gives a finite upper bound. Nonnegative interactions with the fixed point in (138) imply $\phi(x) \geq C_\phi$ for every $x$. For each fixed distinct tuple $Y = (y_2, \dots, y_N)$, feasibility gives

$$\phi(x) \leq c_{N-1}(Y) - \sum_{i=2}^{N} \phi(y_i) + \sum_{i=2}^{N} \frac{1}{|x - y_i|}. \tag{165}$$

First take $\limsup_{|x|\to\infty}$ and then the infimum over fixed $Y$. The preceding lower bound proves

$$\lim_{|x|\to\infty} \phi(x) = C_\phi, \qquad \phi(x) \geq C_\phi \quad (x \in \mathbb{R}^3). \tag{166}$$

No attainment of the lower-particle infimum has been assumed.

If $c > C_\phi$, then $U \geq 0$, (166), and the global positive-part identity would give, for all sufficiently large $|x|$,

$$\rho(x) \geq \left(\frac{c - C_\phi}{2\beta}\right)^3 > 0,$$

contradicting finite mass. Thus $\kappa = C_\phi - c \geq 0$. With $\psi = \phi - C_\phi \geq 0$, the identity becomes precisely (143), and implies

$$\beta\rho^{1/3} \leq U. \tag{167}$$

Since $U \in L^{12}$, it follows that $\rho^4 \leq \beta^{-12}U^{12}$ and $\rho \in L^4(\mathbb{R}^3)$.

This global integrability implies uniform decay of $U$ at infinity. For every fixed $R > 0$, split at distance $R$ from $x$ to obtain

$$U(x) \leq \left(\frac{12\pi}{5}\right)^{3/4} R^{5/4}\|\rho\|_{L^4(B_R(x))} + \frac{N}{R}. \tag{168}$$

As $|x| \to \infty$, the first term tends to zero uniformly outside large balls, by the vanishing $L^4$ tail. Thus $\limsup_{|x|\to\infty} U(x) \leq N/R$; now send $R \to \infty$. If $c < C_\phi$, then $\phi \geq C_\phi$ and $U \to 0$ imply $U - \phi + c < 0$ outside a large ball, so $\rho$ already has compact support. Consequently the contrary hypothesis of unbounded support can be used only with

$$c = C_\phi. \tag{169}$$

### B.6 Two-cycle monotonicity and qualitative dissociation

We give the full dissociation argument needed for the upper bound. It is the mechanism of [5, Theorem 3 and equations (29)–(32)] applied to the bounded truncation in (159). Write $\Gamma = \operatorname{supp} P$ and retain $M = \|\phi\|_\infty$. On the full-measure set in (161),

$$0 < c_N(X) = \sum_i \phi(x_i) \leq NM.$$

Here $N \geq 2$ and all coordinates are finite, so $M > 0$. In particular every pair distance on this set is at least

$$d_* := \frac{1}{NM} > 0. \tag{170}$$

The set of configurations satisfying this separation and saturation is closed: separation excludes collisions, and $c_N$ and $\phi$ are continuous there. It has full $P$-measure, so it contains $\Gamma$. Thus both separation and saturation hold at every $X \in \Gamma$.

Choose $L > NM$. On $\Gamma$, the truncation is inactive and $c_{N,L} = c_N$. Equation (159) gives pointwise feasibility for $c_{N,L}$. Integrating it against any law with the same labeled marginals gives cost at least $\int \phi\rho = W$, while $P$ has truncated cost $W$. Therefore $P$ is optimal for the bounded continuous cost $c_{N,L}$, even among laws not assumed symmetric. Equivalently one can symmetrize any such competitor without changing its cost or marginals.

For $X, Y \in \Gamma$, exchange their first coordinates. Optimality implies the following two-cycle inequality:

$$\begin{aligned} &c_{N,L}(X) + c_{N,L}(Y) \\ &\quad \leq c_{N,L}(y_1, x_2, \dots, x_N) + c_{N,L}(x_1, y_2, \dots, y_N). \end{aligned} \tag{171}$$

For completeness, a strict violation would persist, with a fixed positive improvement, on two sufficiently small neighborhoods of $X, Y$, by continuity. The neighborhoods can be chosen disjoint: a

violation is impossible if $X = Y$. Each has positive $P$-mass. Take equal-mass submeasures $\alpha, \gamma$ of those restrictions, each of mass $m > 0$. Remove $\alpha + \gamma$ from $P$. For $(X', Y')$ distributed according to $m^{-1}\alpha \otimes \gamma$, add both coordinate-swapped tuples. The resulting positive measure has total mass one and exactly the same marginal in each label, since each pair preserves the two values in every slot. Integrating the strict inequality lowers the cost. If desired, symmetrizing preserves this improvement. This contradicts optimality and proves (171) at every pair of support configurations. Cancellation of the pair terms not involving the first coordinate gives

$$\sum_{i=2}^{N} w_L(x_1 - x_i) + \sum_{i=2}^{N} w_L(y_1 - y_i) \\ \leq \sum_{i=2}^{N} w_L(y_1 - x_i) + \sum_{i=2}^{N} w_L(x_1 - y_i). \tag{172}$$

The same inequality holds with any label distinguished.

We claim that some fixed ball $B_{R_0}$ has the property

$$\#\{i : |x_i| > R_0\} \leq 1 \qquad \text{for every } X \in \Gamma. \tag{173}$$

Suppose otherwise. Choose support configurations with at least two coordinates outside balls of radii tending to infinity. Permutation symmetry and a subsequence allow these to be labels 1 and 2. Since there are finitely many labels, successive subsequence extraction makes each remaining coordinate either convergent in $\mathbb{R}^3$ or escaping to infinity. Relabel once more to obtain a sequence $Y^k \in \Gamma$ and an integer $2 \leq J \leq N$ such that

$$|y_i^k| \longrightarrow \infty \quad (1 \leq i \leq J), \qquad y_i^k \longrightarrow \bar{y}_i \quad (J < i \leq N). \tag{174}$$

Empty sums when $J = N$ have their usual value zero.

Fix any $X \in \Gamma$ in (172) and put $Y = Y^k$. Drop the nonnegative second sum on the left. All terms $w_L(y_1^k - x_i)$ tend to zero; the terms $w_L(x_1 - y_i^k)$ tend to zero for $i \leq J$ and to $w_L(x_1 - \bar{y}_i)$ for $i > J$. It follows that

$$\sum_{i=2}^{N} w_L(x_1 - x_i) \leq \sum_{i=J+1}^{N} w_L(x_1 - \bar{y}_i) \qquad \text{for every } X \in \Gamma. \tag{175}$$

This inequality is now valid for every fixed support configuration, so we may substitute $X = Y^k$ into it and multiply by $|y_1^k|$. For every nonescaping label $i > J$, boundedness of both $y_i^k$ and $\bar{y}_i$ implies

$$|y_1^k| w_L(y_1^k - y_i^k) \longrightarrow 1, \qquad |y_1^k| w_L(y_1^k - \bar{y}_i) \longrightarrow 1.$$

Their contributions on the two sides of (175) therefore cancel in the limit. All other left-hand terms are nonnegative, and hence for $2 \leq i \leq J$,

$$|y_1^k| w_L(y_1^k - y_i^k) \longrightarrow 0. \tag{176}$$

The truncation cannot be active along an infinite subsequence in (176), because then the expression would equal $L|y_1^k| \to \infty$. Consequently

$$\frac{|y_1^k|}{|y_1^k - y_i^k|} \longrightarrow 0.$$

The triangle inequality implies

$$\frac{|y_i^k|}{|y_1^k|} \geq \frac{|y_1^k - y_i^k|}{|y_1^k|} - 1 \longrightarrow \infty, \qquad \text{so} \qquad \frac{|y_1^k|}{|y_i^k|} \longrightarrow 0.$$

Repeat the same two-cycle argument with label $i$ distinguished in place of label 1. It gives the reciprocal limit $|y_i^k|/|y_1^k| \to 0$, a contradiction. This proves (173). The argument is qualitative and does not use compactness of the optimizing density, a gap estimate, or connectedness of its support.

### B.7 Attaining the lower-particle energy and the global upper tail

Temporarily suppose that $\rho$ has unbounded support. Its first labeled marginal is $\rho/N$, so for arbitrarily large radii there are points of $\Gamma$ whose first coordinate is beyond that radius. Choose $X^k = (x_1^k, \dots, x_N^k) \in \Gamma$ with $|x_1^k| \to \infty$. By (173), all other coordinates lie in the fixed closed ball $\overline{B}_{R_0}$ for large $k$. Passing to a subsequence gives $x_i^k \to \bar{y}_i$ for $2 \leq i \leq N$. The limits are distinct by (170). Saturation on $\Gamma$ reads

$$\phi(x_1^k) + \sum_{i=2}^{N} \phi(x_i^k) = c_{N-1}(x_2^k, \dots, x_N^k) + \sum_{i=2}^{N} \frac{1}{|x_1^k - x_i^k|}.$$

Use continuity, separation, and (166) to pass to the limit. With $\bar{Y} = (\bar{y}_2, \dots, \bar{y}_N)$, this proves

$$c_{N-1}(\bar{Y}) - \sum_{i=2}^{N} \phi(\bar{y}_i) = C_\phi. \tag{177}$$

Thus the lower-particle infimum is attained under this temporary unbounded-support hypothesis; its attainment was not needed earlier. Testing (138) with this single fixed tuple gives

$$\phi(x) \leq C_\phi + \sum_{i=2}^{N} \frac{1}{|x - \bar{y}_i|} \qquad (x \in \mathbb{R}^3), \tag{178}$$

where the right side is $+\infty$ at a test point. For $|x| \geq 2 \max_i |\bar{y}_i|$ and $x$ sufficiently large,

$$\left| \frac{1}{|x - \bar{y}_i|} - \frac{1}{|x|} \right| \leq \frac{2|\bar{y}_i|}{|x|^2}.$$

Hence the all-space upper estimate is, uniformly in direction,

$$\phi(x) - C_\phi \leq \frac{N-1}{|x|} + O(|x|^{-2}) \qquad (|x| \to \infty). \tag{179}$$

This is the global upper mechanism of [5, Section 3.1, equations (29)–(32)]. No support-restricted two-sided asymptotic is extended to the exterior of the density support.

### B.8 Compact support and the normalized shift

Continue the contrary hypothesis of unbounded support. By (169), $c = C_\phi$. Fix $0 < \varepsilon < 1/4$ and choose a ball $B_R$ containing mass at least $N - \varepsilon$. For all $x$,

$$U(x) \geq \int_{B_R} \frac{\rho(y)}{|x - y|} \, \mathrm{d}y \geq \frac{N - \varepsilon}{|x| + R}.$$

For sufficiently large $|x|$, this is at least $(N-2\varepsilon)/|x|$. Increase the radius further so that (179) gives $\phi(x) - C_\phi \le (N-1+\varepsilon)/|x|$ there. Consequently

$$U(x) - \phi(x) + c \ge \frac{1-3\varepsilon}{|x|}, \qquad \rho(x) \ge \left(\frac{1-3\varepsilon}{\beta}\right)^3 |x|^{-3} \quad \text{for every sufficiently large } |x|. \tag{180}$$

The right side is not integrable in $\mathbb{R}^3$, since its radial mass integral is a positive multiple of $\int^\infty r^{-1}\,\mathrm{d}r$. This contradicts $\int \rho = N$. Thus $\rho$ has compact support. The argument covers disconnected support and support equal to all of space; it does not require a boundary-approaching sequence.

It remains to check the normalization in (140). Since $I(\rho) = 1$ and $H(\rho) - W = \lambda$,

$$\int v\rho = 2H(\rho) - \beta I(\rho) = 2W + \frac{2\lambda}{3}.$$

Substitution into (147) gives $c = -W/N - 2\lambda/(3N)$. All conclusions of Proposition B.1 for $N \ge 2$ now follow. In particular, the same $\phi$ has the pointwise compatibility, exact conjugacy, and global limit used elsewhere in the manuscript.

### B.9 The one-particle case

Suppose a mass-one optimizer exists and normalize it by $I(\rho) = 1$. Then $W_1 = 0$, $c_1 = 0$, and $\lambda = C_1 = H(\rho) > 0$. The segment argument leading to (145) is unchanged. Testing with the normalized indicator of one shrinking ball gives, at every finite Lebesgue point,

$$v(x) + c \le 0, \qquad c = -\int v\rho = -2\lambda + \frac{4\lambda}{3} = -\frac{2\lambda}{3} < 0.$$

Moreover $\int (v+c)\rho = 0$, so the inequality is an equality $\rho\,\mathrm{d}x$-almost everywhere. Set $\phi = 0$. It is bounded, globally Lipschitz, pointwise feasible and exactly $c_1$-conjugated (the infimum over the empty tuple is zero). The null-set argument of §B.4 gives

$$\rho = \left[\frac{(U+c)_+}{\beta}\right]^3 \quad \text{almost everywhere,} \qquad \beta\rho^{1/3} \le U.$$

HLS therefore gives global $L^4$ integrability. The local continuity argument supplies continuous representatives and an everywhere positive-part identity, and (168) gives $U(x) \to 0$. Since $c < 0$, the positive part vanishes outside a large ball. Thus the density has compact support. Here $C_\phi = E_0(\phi) = 0$, $\psi = 0$, and $\kappa = -c > 0$. This base case needs no $N \ge 2$ dissociation argument.

## C Finite arithmetic and source provenance

The accompanying source archive contains the complete editable LaTeX manuscript, a mathematical supplement for the foundational reconstruction, and a small reproducibility directory. Its Python scripts use only the standard library and exact integers or rational arithmetic. They check the radial upper Riemann enclosure, normalization and geometric constants, harmonic sphere integrals, masking factors, powers in the coupling gains, and the final exponential weakenings. Exponential quantities are compared symbolically rather than evaluated as underflowing floating-point numbers.

The three-to-four-particle arithmetic script performs 49 selected exact checks. Separate scripts cover the two-particle proof and radial witness, the three-particle core, the dual localization, and

the harmonic bridge. The existence of these checks must not be confused with a formal proof certificate: they do not prove optimizer attainment, the compatible-potential reconstruction, the cited external theorems, or the analytic arguments connecting the finite inequalities.

For traceability, the archive includes unchanged mathematical source derivations, their hashes, a map from those derivations to the sections of this manuscript, and a transcription-change record. The record makes the following substantive notation choices explicit:

1. $D$ always denotes the full Coulomb double integral; $H = D/2$.
2. $E_k(f)$ always means $\inf(c_k - \sum f)$. An auxiliary sign-convention alias in the earlier standalone pair-localization derivation is removed, so its shifted energy is written $E_k(\psi)$ throughout.
3. Volume and mask statements use the occupied set $\mathcal{O} = \{\rho > 0\}$ up to null sets. No claim about the measure of a topological-support boundary is needed.
4. The earlier two-particle comparison is specialized from a universal trial-state upper bound to the sharp $C_3$, exactly as justified by the preserved successive-gap addendum. No three-particle attainment is needed for that particular comparison.
5. The simple independent witness in Appendix A replaces the optional stronger lower-bound certificate as the sole numerical lower input.
6. Revision 2 adds the complete three-dimensional Coulomb reconstruction in Appendix B. Its slot-transform regularization, global positive-part relation, dissociation argument, and global upper-tail estimate are written out. Attainment, qualitative monotonicity, sharp HLS, and the published universal cap remain identified literature inputs. No numerical gap is used in that reconstruction.

Duplicate arguments and historical statements that a later step was still pending have been removed from the manuscript; no frozen mathematical derivation is overwritten. Revision 1 is preserved, and the source archive records the mathematical changes for revision 2. The external inputs, the reconstructed foundations, the quantitative deductions, and the selected finite checks remain distinct. External expert review should examine the compatible-potential reconstruction, the saturated-triple localization and mass-excess argument, and the deletion-stable exterior covariance estimates. No external submission, publication, or human peer-review status is represented by this archive.

# References


[1] M. Rosenzweig, *Fixed-Particle-Number Optimizers for the Lieb–Oxford Inequality*, preprint, arXiv:2608.17155v1 (2026). arXiv record.

[2] S. Di Marino and R. Lelotte, *Absence of non-compactly supported minimisers for the Lieb–Oxford bound*, preprint, arXiv:2607.11440v1 (2026). arXiv record.

[3] M. Lewin, E. H. Lieb, and R. Seiringer, *Improved Lieb–Oxford bound on the indirect and exchange energies*, Letters in Mathematical Physics **112**, article 92 (2022). doi:10.1007/s11005-022-01584-5; arXiv:2203.12473v3.

[4] G. Buttazzo, T. Champion, and L. De Pascale, *Continuity and estimates for multimarginal optimal transportation problems with singular costs*, Applied Mathematics & Optimization **78**, 185–200 (2018). doi:10.1007/s00245-017-9403-7; arXiv:1608.08780v1.

[5] R. Lelotte, *Asymptotics of the Kantorovich Potential for the Optimal Transport with Coulomb Cost*, Archive for Rational Mechanics and Analysis **249**, article 68 (2025). doi:10.1007/s00205-025-02140-w; arXiv:2210.07830v2.

[6] Y. Wang and Q. Lü, *Stability Estimates for the Inverse Recovery of Drift and Diffusion Point Sources in Stochastic Parabolic Equations*, preprint, arXiv:2609.14009v1 (2026). arXiv record.

[7] E. H. Lieb, *Sharp constants in the Hardy–Littlewood–Sobolev and related inequalities*, Annals of Mathematics **118**, no. 2, 349–374 (1983). doi:10.2307/2007032.

[8] R. L. Frank and E. H. Lieb, *A new, rearrangement-free proof of the sharp Hardy–Littlewood–Sobolev inequality*, arXiv:1010.5821v3 (2011). arXiv record.