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Sharp Ionization Bounds for Helium and Lithium

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Abstract

How many electrons can a nucleus bind? In the non-relativistic Coulomb model, Lieb proved in 1984 that a nucleus of charge Z binds fewer than $2Z+1$ electrons. While this bound has been improved, the sharp upper bound has remained unknown for any nucleus other than hydrogen. We solve this problem for $Z=2$ and $Z=3$ by proving that helium binds two or fewer electrons and lithium binds four or fewer. Both bounds are sharp. Our main tool is an adaptation of Lieb's argument with a quadratic weight, which reduces the nonbinding of doubly negative ions to finitely many inequalities that we verify in a computer-assisted proof.

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1 Introduction

The atomic ionization problem asks for the maximum number $N_c(Z)$ of electrons that a nucleus of charge Z can bind [1, 2]. Experimentally, no isolated atom is known to bind more than one additional electron in a stable state [3]. The ionization conjecture asks for a bound $N_c(Z) \le Z + C$ with C independent of Z.

Lieb's bound $N_c(Z) < 2Z + 1$ [4] is sharp for hydrogen [5, 6], but permits four electrons for helium and six for lithium. Later work established asymptotic neutrality, $N_c(Z)/Z \to 1$ as $Z \to \infty$ [7, 8, 9], and improved explicit general bounds [10, 11], without reducing these helium and lithium limits. Shelley and Tartakovsky recently excluded the helium dianion, lowering the helium upper bound to three electrons [12]. We prove that helium binds no additional electron in its ground state and lithium binds exactly one.

We consider nonrelativistic electrons of spin 1/2 and an infinitely heavy point nucleus, in Hartree atomic units. For an integer $N \ge 1$ and $Z > 0$, let $x_i \in \mathbb{R}^3$ be the position of electron i relative to the nucleus. On the fermionic space $\mathcal{H}_N = \bigwedge^N L^2(\mathbb{R}^3; \mathbb{C}^2)$, set

$$H_N(Z) = -\frac{1}{2}\sum_{i=1}^{N} \Delta_{x_i} - Z\sum_{i=1}^{N} \frac{1}{|x_i|} + \sum_{i<j} \frac{1}{|x_i - x_j|},$$

$$E_N(Z) = \inf \sigma(H_N(Z)), \qquad E_0(Z) = 0, \qquad N_c(Z) = \sup\{N \ge 1 : E_N(Z) < E_{N-1}(Z)\}.$$

The strict inequality defines binding. By the HVZ theorem (Theorem 3.1), $E_{N-1}(Z)$ is the detachment threshold, the bottom of the essential spectrum for $N \ge 2$.

Theorem 1.1. *The maximum electron counts are*

$$N_c(2) = 2, \qquad N_c(3) = 4.$$

For $Z = 2$ and $N \ge 3$, and for $Z = 3$ and $N \ge 5$, the ground energy $E_N(Z)$ is not an eigenvalue of $H_N(Z)$.

Equality of successive ground energies can still admit a square-integrable threshold eigenfunction [13]. The theorem excludes this possibility beyond the stated counts, so the counts also apply when binding means existence of a ground state.

Lithium's positive electron affinity is established experimentally and supported by accurate variational calculations [14, 15]. Lower-bound calculations for neutral lithium also have a substantial history [16, 17]. Our proof compares a variational upper bound for the anion with a certified lower bound for the neutral atom, controlling the spectral hypotheses, symmetry sectors and numerical errors. Section 6 gives the resulting positive lower bound for the affinity.

Nonbinding requires an operator lower bound at the exact detachment threshold. For the dianions, we develop Lieb's and Nam's weighted removal identities, using the square of an electron's distance from the nucleus as the weight. We retain the weighted kinetic energy and use the Pauli principle; geometric bounds on the repulsion and one-electron spectral bounds then establish positivity of the required quadratic forms on the fermionic space. This builds on the earlier helium analysis [12]. Analytic estimates exclude the higher electron counts allowed by Lieb's bound.

The helium monoanion requires comparison with the exact neutral energy. We match estimates in a bounded region with estimates for an escaping electron to establish nonbinding and exclude

a threshold ground state. This three-electron estimate also supplies a starting point for the lower bound on neutral lithium used in the binding proof.

Sections 2–3 give the setting and common estimates; Sections 4–7 treat the individual ions, and Section 8 completes the proof of Theorem 1.1. The appendices contain the computational certificates, including error bounds and case coverage, and the deferred analytic proofs.

2 Setting and conventions

This section fixes the model and the notation, and it states the assumptions under which the computer-assisted statements hold.

Set-up 2.1. We use Hartree atomic units, an infinitely heavy point nucleus, and electrons of spin 1/2. Write $\mathbb{N} = \{1, 2, \dots\}$. For an integer $N \geq 1$, let

$$\mathcal{H}_N = \bigwedge^N L^2(\mathbb{R}^3; \mathbb{C}^2).$$

For $Z > 0$, the operator $H_N(Z)$ is associated with the closed Coulomb form

$$\mathfrak{q}_{N,Z}[u] = \frac{1}{2} \sum_{i=1}^{N} \int |\nabla_i u|^2 - Z \sum_{i=1}^{N} \int \frac{|u|^2}{|x_i|} + \sum_{i<j} \int \frac{|u|^2}{|x_i - x_j|}$$

on $H^1((\mathbb{R}^3)^N; (\mathbb{C}^2)^{\otimes N}) \cap \mathcal{H}_N$. All integrals include the sum over spin components. Antisymmetry exchanges positions and spins simultaneously. Write

$$E_N(Z) = \inf \sigma(H_N(Z)), \qquad E_0(Z) = 0, \qquad N_{\mathrm{c}}(Z) = \sup\{N \in \mathbb{N} : E_N(Z) < E_{N-1}(Z)\}.$$

We say that N electrons are strictly bound if $E_N(Z) < E_{N-1}(Z)$. The absence of eigenfunctions at the threshold $E_{N-1}(Z)$ is a separate assertion. No restriction on total spin, angular momentum, parity or magnetic quantum number is imposed unless explicitly stated. For configurations we write $r_i = |x_i|$, $d_{ij} = |x_i - x_j|$, and $q_1 \leq \cdots \leq q_N$ for the ordered radii. All displayed terminating decimal bounds denote exact rational numbers. We write $s_+ = \max\{s, 0\}$ for $s \in \mathbb{R}$ and I for the identity on the Hilbert space under consideration. For a semibounded quadratic form q, $n_-(q)$ is the supremum of the dimensions of subspaces on which q is strictly negative away from zero.

Set-up 2.2. The computer-assisted statements use the fixed inputs and executable algorithms specified in the mathematical appendices and accompanying code/data release. Exact arithmetic, decoding, file operations and recorded executions are assumed faithful. Where binary floating-point arithmetic is used, the specified source, operation order, precision, rounding, underflow, dispatch, thread and interface conditions are part of the execution assumptions. The appendices state those conditions for each affected calculation and prove the numerical error bounds. Accuracy, complete coverage and physical normalization are conclusions of the checks and proofs, not runtime assumptions.

3 Weighted removal and spectral bounds

This section collects the tools shared by the later sections. We first record two standard spectral results. We then state a lower bound for the Coulomb form on regions where the electrons are

separated radially (Lemma 3.3). Finally we prove the criterion for nonbinding that Sections 4 and 7 apply to the two dianions (Proposition 3.4).

The first spectral result is the HVZ theorem. In the present normalization, its fermionic form is stated in [10].

Theorem 3.1 (HVZ)**.** *For the operators in Set-up 2.1, every integer $N \geq 2$ and every $Z > 0$ satisfy*

$$\sigma_{\mathrm{ess}}(H_N(Z)) = [E_{N-1}(Z), \infty).$$

The second spectral result is the spectrum of the hydrogenic operator. The formula below uses the Hartree kinetic coefficient $1/2$.

Theorem 3.2 (Hydrogenic spectrum)**.** *For $Q > 0$, let $h_Q = -\Delta/2 - Q/|x|$ be the scalar Coulomb operator on $L^2(\mathbb{R}^3)$. Its negative eigenvalues are $-Q^2/(2n^2)$, $n \in \mathbb{N}$, with spatial multiplicity n^2, and its remaining spectrum is $[0, \infty)$. If P_m projects onto the shells $1 \leq n \leq m$, where $m \geq 1$ is an integer, then*

$$h_Q\big|_{(1-P_m)L^2} \geq -\frac{Q^2}{2(m+1)^2}.$$

This is [18, Theorem 10.9], with its operator $-\Delta - \gamma/|x|$ taken at $\gamma = 2Q$ and divided by two. After including spin, the first m hydrogenic shells have dimension $2\sum_{n=1}^{m} n^2$.

Both dianion proofs need lower bounds for the Coulomb form on regions where some electrons are confined to a ball and the others are kept outside a larger ball. We call the confined electrons core electrons and the others outer electrons. The following lemma collects these bounds. It uses no symmetry of the test function.

Lemma 3.3 (Regional lower bound)**.** *Let $2 \leq N \leq 9$, $Z > 0$, and let $\mathfrak{h}$ denote the Coulomb integral of Set-up 2.1 with N electrons and charge Z on the full space $H^1((\mathbb{R}^3)^N; (\mathbb{C}^2)^{\otimes N})$, without symmetry restriction. For $-1 \leq z < 1$ put $c(z) = \min\{1, [2(1-z)]^{-1/2}\}$ and $c(1) = 1$, and let $D_0, \dots, D_N$ be rational numbers with $D_0 = D_1 = 0$ and*

$$D_h \leq \binom{h}{2}\sqrt{\frac{h-1}{2h}} \qquad (2 \leq h \leq N);$$

the values used in this paper are

$$(D_0, D_1, D_2, D_3, D_4, D_5) = \left(0, 0, \frac{1}{2}, \frac{433}{250}, \frac{1837}{500}, \frac{1581}{250}\right),$$

whose squares for $h = 3, 4, 5$ are below the exact values $3, 27/2, 40$. Fix $R, b, \lambda > 0$, $\sigma \geq 1$, an integer $0 \leq j \leq N-1$, and set

$$\kappa = \lambda\sigma^2, \qquad C = \frac{\lambda^2}{2} + \frac{\lambda(\sigma-1)^2}{R}, \qquad A_j = Z - \kappa - \frac{jR}{R+b},$$

$$M_j(R, b, \lambda, \sigma) = \frac{jZ^2}{2} + (N-j)C + \frac{1}{R}\max_{0 \leq h \leq N-j}(A_j h - D_h).$$

If a spinor $v \in H^1$ is supported where j specified electrons have radii below b and the other $N-j$ have radii above R, then

$$\mathfrak{h}[v] \geq -M_j(R, b, \lambda, \sigma)\,\|v\|^2.$$

For $j = 0$ the parameter b is immaterial.

Idea of the proof. The repulsion among the outer electrons is bounded below in terms of their directions. Each outer electron then satisfies a one-dimensional radial inequality, and each core electron is bounded by its hydrogenic ground energy. The full proof is in Appendix E.1.

The increments $D_{h+1} - D_h$ of the listed values are $0, \frac{1}{2}, \frac{308}{250}, \frac{971}{500}, \frac{53}{20}$. Hence the maximum defining M_j is attained at $h = 2$ whenever $\frac{1}{2} \le A_j \le \frac{308}{250}$, which is the case for every parameter choice below.

We now state the criterion for nonbinding. Its proof follows Lieb's argument for the bound $N < 2Z + 1$ [4]. Lieb tests the eigenvalue equation against the eigenfunction multiplied by the radius of one electron, and bounds the energy of the other $N - 1$ electrons from below by the threshold. We use the quadratic weight $r_i^2 + \beta$ in place of the linear one. We also add correction terms B_j. They use the hypothesis that every state with at most $j - 1$ electrons within the radius b_j has energy at least d_j above U. We call d_j an exterior gap.

Proposition 3.4. *Let $N \ge 2$, $Z > 0$, $\beta > 0$, $U \ge E_{N-1}(Z)$, and let $J \subset \{1, \dots, N\}$ be finite. For $j \in J$ let $b_j, d_j > 0$ and $\lambda_j \ge 0$. Assume*

$$\mathfrak{q}_{N,Z}[v] - U\|v\|^2 \ge d_j \|v\|^2$$

in the quadratic-form sense for every fermionic form-domain vector v vanishing almost everywhere on $\{q_j \le b_j\}$. For $s \ge 0$ define

$$B_j(s) = (s - b_j)_+^2 - \frac{\min\{s/b_j, 1\}}{2d_j}.$$

For compactly supported fermionic $u \in H^1$ define

$$M_{\beta,U}[u] = \frac{1}{2} \sum_i \int (r_i^2 + \beta) |\nabla_i u|^2 + \int \left[\sum_{i<j} \frac{r_i^2 + r_j^2 + \beta}{d_{ij}} - Z \sum_i \left(r_i + \frac{\beta}{r_i} \right) - \frac{3N}{2} - \beta U \right] |u|^2.$$

If some $\varepsilon > 0$ satisfies

$$M_{\beta,U}[u] + \sum_{j \in J} \lambda_j \int B_j(q_j) |u|^2 \ge \varepsilon \|u\|^2$$

for every such u, then $E_N(Z) = E_{N-1}(Z)$ and $H_N(Z)$ has no nonzero L^2 eigenfunction at any energy at or below $E_{N-1}(Z)$.

Proof. Put $T = E_{N-1}(Z)$ and suppose that $H_N(Z)\Psi = E\Psi$, with $E \le T \le U$ and $\|\Psi\| = 1$. Write $X = (x_1, \dots, x_N)$ and let ∇ denote the full gradient in X.

Ordered-radius moments. Fix $j \in J$. Outside the null set of tied or zero radii, the function q_j agrees locally with one of the r_i. Hence q_j is symmetric and Lipschitz, with $|\nabla q_j| = 1$ almost everywhere. For $L > 0$ set $g_L = \min\{(q_j - b_j)_+, L\}$. Both $g_L\Psi$ and $g_L^2\Psi$ belong to the fermionic form domain. Testing the eigenvalue equation with $g_L^2\Psi$ and expanding the gradient gives

$$\mathfrak{q}_{N,Z}[g_L\Psi] - E\|g_L\Psi\|^2 = \frac{1}{2} \int |\nabla g_L|^2 |\Psi|^2.$$

Since $g_L\Psi$ vanishes on $\{q_j \le b_j\}$ and $E \le U$, the assumption of the proposition bounds the left side below by $d_j\|g_L\Psi\|^2$. On the right side, $|\nabla g_L|^2 = \mathbf{1}_{\{b_j<q_j<b_j+L\}} \le \min\{q_j/b_j, 1\}$. Monotone convergence as $L \to \infty$ therefore gives

$$\int (q_j - b_j)_+^2 |\Psi|^2 \le \frac{1}{2d_j} \int \min\{q_j/b_j, 1\}|\Psi|^2. \tag{3.1}$$

In particular, $\int |B_j(q_j)||\Psi|^2 < \infty$ and $\int B_j(q_j)|\Psi|^2 \le 0$.

The weighted identity with a cutoff. Choose a real smooth function $\chi : [0,\infty) \to [0,1]$ equal to one on $[0,1]$ and zero on $[2,\infty)$, and put $C_\chi = \|\chi'\|_\infty$. For $R \ge 1$ set

$$\rho = |X|, \qquad \chi_R(X) = \chi(\rho/R), \qquad u_R = \chi_R\Psi, \qquad A_R = \{R \le \rho \le 2R\}.$$

Then u_R is a compactly supported fermionic H^1 vector and $\|u_R\| \to 1$. The gradient $\nabla\chi_R$ is supported in A_R and satisfies $|\nabla\chi_R| \le C_\chi/R$. All multipliers used to test the equation for Ψ below are bounded with bounded first derivatives. The weak equation extends to nonfermionic tests by antisymmetrization and permutation invariance.

Test that equation with $r_i^2\chi_R^2\Psi$. Expanding the gradients, integrating by parts with $\Delta_i r_i^2 = 6$, and bounding the form of the remaining $N-1$ electrons below by T gives

$$\begin{aligned}\frac{1}{2}\int r_i^2|\nabla_i u_R|^2 + \int \left(-Zr_i + \sum_{k\ne i}\frac{r_i^2}{d_{ik}} - \frac{3}{2}\right)|u_R|^2 \\ \le (E-T)\int r_i^2|u_R|^2 + \frac{1}{2}\int \left(r_i^2|\nabla\chi_R|^2 + \chi_R\nabla(r_i^2)\cdot\nabla\chi_R\right)|\Psi|^2.\end{aligned}$$

The bound by T applies to each slice in the other labels, where $r_i u_R$ is antisymmetric. All terms are finite on the compact support. The integration by parts is justified by H^1 approximation and the Coulomb form bounds. The unweighted test $\chi_R^2\Psi$ gives

$$\mathfrak{q}_{N,Z}[u_R] - E\|u_R\|^2 = \frac{1}{2}\int |\nabla\chi_R|^2|\Psi|^2.$$

Sum the weighted inequalities and add $\beta(\mathfrak{q}_{N,Z}[u_R] - U\|u_R\|^2)$. Since $E \le T \le U$ and $\sum_i \nabla(r_i^2) = 2X$, this yields

$$\begin{aligned}M_{\beta,U}[u_R] &\le \frac{1}{2}\int \left((\rho^2+\beta)|\nabla\chi_R|^2 + 2\chi_R X\cdot\nabla\chi_R\right)|\Psi|^2 \\ &\le \left(2C_\chi^2 + 2C_\chi + \frac{\beta C_\chi^2}{2R^2}\right)\int_{A_R}|\Psi|^2 \longrightarrow 0.\end{aligned} \tag{3.2}$$

The argument never takes the limit of a quadratic-weight energy without the cutoff.

By (3.1), dominated convergence gives $\int B_j(q_j)|u_R|^2 \to \int B_j(q_j)|\Psi|^2 \le 0$ for each $j \in J$. Thus (3.2) controls the term $M_{\beta,U}$, and the moment bounds control every correction with $\lambda_j \ge 0$:

$$\limsup_{R\to\infty}\left(M_{\beta,U}[u_R] + \sum_{j\in J}\lambda_j\int B_j(q_j)|u_R|^2\right) \le 0.$$

By the assumption of the proposition, the same expression is at least $\varepsilon\|u_R\|^2 \to \varepsilon > 0$, a contradiction. Hence no eigenvalue at or below T exists. The HVZ theorem (Theorem 3.1) gives $E_N(Z) \le T$ and makes any spectral infimum below T an eigenvalue. It follows that $E_N(Z) = T$. □

4 The helium dianion

We prove that a helium nucleus does not bind four electrons. The proof applies Proposition 3.4 with the weight r^2. Section 7 applies the same proposition to the lithium dianion. The proposition requires four inputs. The first is an upper bound U_0 for the neutral helium energy (Lemma 4.1). The second is a pair of exterior gaps (Lemma 4.2). The third is a pointwise lower bound for the weighted electron repulsion by a sum of one-electron potentials (Lemma D.2). The fourth is a pair of bounds on the number of negative eigenvalues of a one-electron operator (Lemma D.4). The last two inputs are computer-assisted and are proved in Appendix D.

Lemma 4.1. *The neutral helium energy satisfies*

$$E_2(2) \le -\frac{1406349}{484600} < -\frac{29}{10}.$$

Proof. Let $\alpha = 9/5$, $s = r_1 + r_2$, $t = r_1 - r_2$, and $\rho = d_{12}$, and let $\chi \in \mathbb{C}^2 \otimes \mathbb{C}^2$ be a normalized antisymmetric spin vector. Set

$$P(s,t,\rho) = 1 + \frac{\alpha\rho}{6} + \frac{\alpha^2 t^2}{24}, \qquad \Psi(x_1,x_2) = e^{-\alpha s} P(s,t,\rho)\chi.$$

The spatial factor is symmetric. The distance functions are locally Lipschitz with bounded gradients, and the exponential controls the polynomial and its derivatives at infinity. Thus Ψ belongs to the fermionic form domain.

After angular integration, the volume element is $\pi^2(s^2 - t^2)\rho\, ds\, dt\, d\rho$ on

$$\mathcal{D} = \{(s,t,\rho) : s \ge 0,\ 0 \le \rho \le s,\ -\rho \le t \le \rho\}.$$

For nonnegative integers i, j, k, successive integration in t, ρ, s gives

$$\int_{\mathcal{D}} e^{-2\alpha s} s^i t^j \rho^k \, ds\, dt\, d\rho = \frac{2(i+j+k+2)!}{(j+1)(j+k+2)(2\alpha)^{i+j+k+3}} \quad (j \text{ even});$$

the integral vanishes for odd j. Expanding P and differentiating Ψ, this identity yields

$$\|\Psi\|^2 = \pi^2 \alpha^{-6} \frac{2423}{1152},$$
$$\mathfrak{q}_{2,2}[\Psi] = \pi^2 \alpha^{-6} \left(\frac{709}{384}\alpha^2 - \frac{20627}{3072}\alpha \right).$$

The variational principle therefore gives

$$E_2(2) \le \frac{\mathfrak{q}_{2,2}[\Psi]}{\|\Psi\|^2} = \frac{2127\alpha^2 - (61881/8)\alpha}{2423} = -\frac{1406349}{484600} = -\frac{29}{10} - \frac{1009}{484600}.$$

□

Throughout this section

$$U_0 = -\frac{1406349}{484600}, \qquad (b_1, \delta_1) = \Big(2, \frac{1629}{1000}\Big), \qquad (b_2, \delta_2) = \Big(4, \frac{3}{8}\Big). \tag{4.1}$$

By HVZ (Theorem 3.1) and Lemma 4.1, $E_3(2) \le E_2(2) \le U_0$. Hence the choice $U = U_0$ is admissible in Proposition 3.4 with $N = 4$, $Z = 2$. Nothing from Section 5 is used.

Lemma 4.2 (Exterior gaps)**.** *Let $a \in \{1,2\}$ and let u belong to the fermionic form domain of $H_4(2)$. If u vanishes almost everywhere on $\{q_a \le b_a\}$, then*

$$\mathfrak{q}_{4,2}[u] - U_0\|u\|^2 \ge \delta_a \|u\|^2.$$

Proof. Let $\mathfrak{h}$ be the Coulomb integral of Set-up 2.1 with $N = 4$, $Z = 2$ on the full space $H^1((\mathbb{R}^3)^4; \mathbb{C}^{16})$. It agrees with $\mathfrak{q}_{4,2}$ on fermionic vectors. We apply Lemma 3.3 with $N = 4$, $Z = 2$, so that a core electron contributes -2 and $A_j = 2 - \kappa - jR/(R+b)$. The three parameter choices used are

$$\begin{aligned} M_0(2,2,\tfrac{21}{50},\tfrac{37}{20}) &= \frac{5089}{4000} \quad (\kappa = \tfrac{28749}{20000},\ C = \tfrac{9597}{40000},\ A_0 = \tfrac{11251}{20000}), \\ M_0(\tfrac{4}{5},4,\tfrac{3}{5},\tfrac{31}{20}) &= \frac{19190}{8000} \quad (\kappa = \tfrac{2883}{2000},\ C = \tfrac{651}{1600},\ A_0 = \tfrac{1117}{2000}), \\ M_1(4,4,\tfrac{1}{4},2) &= \frac{77}{32} \qquad (\kappa = 1,\ C = \tfrac{3}{32},\ A_1 = \tfrac{1}{2}). \end{aligned} \tag{4.2}$$

In each case $\frac{1}{2} \le A_j \le \frac{308}{250}$, so the maximum in M_j is attained at $h = 2$ (in the third case also at $h = 1$), and the values follow by rational arithmetic.

The first gap. If $u = 0$ on $\{q_1 \le 2\}$, then all four radii exceed 2 on the support of u, and the first value gives

$$\mathfrak{q}_{4,2}[u] - U_0\|u\|^2 \ge \Big(\frac{1406349}{484600} - \frac{5089}{4000}\Big)\|u\|^2 = \frac{15796333}{9692000}\|u\|^2 > \frac{1629}{1000}\|u\|^2.$$

The second gap. Suppose $u = 0$ on $\{q_2 \le 4\}$. Let $\theta(r)$ be zero for $r \le 4/5$, affine from zero to $\pi/2$ on $[4/5, 4]$, and $\pi/2$ for $r \ge 4$. For $S \subset \{1,\dots,4\}$ let $\chi_S = \prod_{i\in S}\cos\theta(r_i)\prod_{i\notin S}\sin\theta(r_i)$. Then $\sum_S \chi_S^2 = 1$ and $\mathfrak{h}[u] = \sum_S \mathfrak{h}[\chi_S u] - \frac{1}{2}\int\sum_i |\theta'(r_i)|^2|u|^2$. On the support of u at most one radius lies below 4. Hence $\chi_S u = 0$ for $|S| \ge 2$, and the localization error is at most $\frac{1}{2}|\theta'|^2 = \pi^2/(8\cdot(16/5)^2) = \pi^2/81.92 < \frac{987}{8192}$, using $\pi^2 < 9.87$. The term with $S = \varnothing$ has all radii above $4/5$ and is bounded by the second value in (4.2). A term with $S = \{i\}$ has $r_i < 4$ and the other three radii above 4, and is bounded by the third value. The localized spinors are global H^1 functions. Their vanishing conditions, sliced in the other variables, give the Dirichlet traces required by Lemma 3.3. No symmetry is needed. Since $\frac{19190}{8000} < \frac{77}{32}$,

$$\mathfrak{q}_{4,2}[u] - U_0\|u\|^2 \ge \Big(\frac{1406349}{484600} - \frac{77}{32} - \frac{987}{8192}\Big)\|u\|^2 > \Big(2.90208 - 2.40625 - 0.12049\Big)\|u\|^2 > \frac{3}{8}\|u\|^2.$$

The displayed decimals are outward roundings of the three rationals. The exact difference is $0.37534\ldots > 0.375$. All arithmetic in this proof is rational and is replayed by `certify_gaps.py` with the cap U_0 as its argument. □

We next compare the weighted form $M_{\beta,U}$ of Proposition 3.4 with a sum of one-electron operators. Let g be the piecewise affine function of Definition D.1, which we call the screen. Let h be the scalar spatial operator with closed form

$$q_h[v] = \frac{1}{2}\int_{\mathbb{R}^3}(2+|x|^2)|\nabla v|^2\,dx + \int_{\mathbb{R}^3}\Big(-\frac{4}{|x|} - \frac{3}{2} + g(|x|)\Big)|v|^2\,dx \tag{4.3}$$

on $\{v \in H^1(\mathbb{R}^3) : \int |x|^2|\nabla v|^2 < \infty\}$. Let h_i act as $h \otimes I_{\mathbb{C}^2}$ on electron i.

Lemma 4.3 (Occupation)**.** *Suppose $t_0 < t_1$ satisfy $n_-(h - t_0) = 0$ and $n_-(h - t_1) \le 1$, spin excluded. Then every compactly supported fermionic $u \in H^1$ satisfies $\sum_{i=1}^4 \langle u, h_i u\rangle \ge (2t_0 + 2t_1)\|u\|^2$.*

Proof. Let $\Pi = \mathbf{1}_{(-\infty,t_1)}(h)$, of rank at most one. The index hypotheses give $h \geq t_1 I - (t_1 - t_0)\Pi$ in the form sense, and $\Pi \otimes I_{\mathbb{C}^2}$ has rank at most two. In an orthonormal wedge basis adapted to its range, each spin orbital occurs at most once, so the occupation of that range is at most $\min\{4, 2\} = 2$ for every fermionic state. Hence $\sum_i \langle u, h_i u\rangle \geq [4t_1 - 2(t_1 - t_0)]\|u\|^2$. □

Theorem 4.4. *Under Set-ups 2.1 and 2.2, $E_4(2) = E_3(2)$, and $H_4(2)$ has no nonzero L^2 eigenfunction at any energy at or below $E_3(2)$.*

Proof. We verify the hypotheses of Proposition 3.4 with $N = 4$, $Z = 2$, $\beta = 2$, $U = U_0$, $J = \{1, 2\}$, $d_a = \delta_a$ and

$$\lambda_1 = \frac{22}{25}, \qquad \lambda_2 = \frac{19}{100}.$$

The inequality $U_0 \geq E_3(2)$ was noted after (4.1), and Lemma 4.2 supplies the exterior hypotheses. Let B_a and M_{2,U_0} be the moment functions and the weighted form of Proposition 3.4 for these constants. With $f(r) = 2r + g(r)$ they are precisely the functions in Definition D.1.

Lower bound for the repulsion. Lemma D.2 gives, almost everywhere on $(\mathbb{R}^3)^4$,

$$\sum_{i<j} \frac{r_i^2 + r_j^2 + 2}{d_{ij}} \geq \sum_{i=1}^{4} f(r_i) - \lambda_1 B_1(q_1) - \lambda_2 B_2(q_2) - 1.$$

Inserting this into M_{2,U_0} and using $-2(r_i + 2/r_i) + f(r_i) = -4/r_i + g(r_i)$ and $3N/2 = 6 = 4 \cdot \frac{3}{2}$,

$$M_{2,U_0}[u] + \sum_{a=1}^{2} \lambda_a \int B_a(q_a)|u|^2 \;\geq\; \sum_{i=1}^{4} \langle u, h_i u\rangle - \|u\|^2 - 2U_0\|u\|^2$$

for every compactly supported fermionic $u \in H^1$.

Lower bound for the one-electron operators. Lemma D.4 gives $n_-(h + \frac{197}{100}) = 0$ and $n_-(h + \frac{3}{25}) \leq 1$, spin excluded. Lemma 4.3 with $t_0 = -\frac{197}{100}$, $t_1 = -\frac{3}{25}$ gives $\sum_i \langle u, h_i u\rangle \geq -\frac{209}{50}\|u\|^2$.

Conclusion. Consequently

$$M_{2,U_0}[u] + \sum_{a=1}^{2} \lambda_a \int B_a(q_a)|u|^2 \geq \Big(-\frac{209}{50} - 1 + \frac{1406349}{242300}\Big)\|u\|^2 = \frac{151235}{242300}\|u\|^2 > \frac{624}{1000}\|u\|^2.$$

All hypotheses of Proposition 3.4 hold with $\varepsilon = \frac{624}{1000}$. Its conclusion gives the energy equality and excludes every nonzero L^2 eigenfunction at or below $E_3(2)$, including the threshold. □

Remark 4.5 (Comparison with the lithium dianion). Theorems 4.4 and 7.2 are two instances of Proposition 3.4 with the same weight r^2, the same constant $\beta = 2$ and two ordered-radius moments. The helium instance is simpler. It does not reserve part of the angular kinetic energy, and it needs no fixed radial fields such as those of Definition A.1. A single screen g with five knots suffices, and the geometric certificate covers the four ordered radii directly. The margin 0.624 hartree is large compared with the 10^{-5} margin of the lithium instance. A distant electron sees the net charge $N - 1 - Z = 1$ in both cases. The difference is the size of the core loss, which grows with Z.

5 The helium monoanion

We prove that a helium nucleus does not bind three electrons (Theorem 5.6). The lower bound must equal the neutral helium energy $E = E_2(2)$ exactly, so a numerical approximation of E does not suffice.

The proof splits the configuration space into two regions. In the interior region K_7, all three electrons lie within distance 7 of the nucleus. In the exterior region Ω_7, at least one electron lies farther away. On Ω_7, a localization argument bounds the Coulomb form below by E plus a positive boundary term (Lemma 5.5). On K_7, finite matrix computations bound the form below, up to the same boundary term, in the two symmetry sectors of lowest energy (Lemma B.1 in Appendix B). The boundary terms cancel when the two bounds are added. The other symmetry sectors are treated separately (Lemma 5.4). All of these steps use bounds on the ground state of neutral helium (Lemma 5.3).

We use two standard results. The first is Temple's inequality for an isolated ground level [18, Theorem 4.13].

Theorem 5.1 (Temple's inequality)**.** *Let A be self-adjoint and bounded below, let $E = \inf \sigma(A) < b$, and suppose $\sigma(A) \setminus \{E\} \subset [b, \infty)$. For $v \in D(A)$ with $\|v\| = 1$ put $\mu = \langle v, Av \rangle$. If $\mu < b$, then*

$$\mu - \frac{\|(A - \mu)v\|^2}{b - \mu} \leq E \leq \mu.$$

The second is the local regularity result needed at the threshold, namely the analyticity away from collisions stated in [19, p. 3, equations (1.5)–(1.7) and the following paragraph]. The dilation $y_i = 2x_i$, followed by division of the equation by two, converts our Hamiltonian into that reference's normalization.

Theorem 5.2 (Off-collision analyticity)**.** *Let $N \geq 1$ be an integer, $\Omega \subset (\mathbb{R}^3)^N$ be open, $Z > 0$, and $\lambda \in \mathbb{R}$. Define the collision set*

$$\Sigma = \bigcup_i \{x_i = 0\} \cup \bigcup_{i<j} \{x_i = x_j\}.$$

Every distributional solution on Ω of

$$\left(-\frac{1}{2} \sum_i \Delta_i - Z \sum_i |x_i|^{-1} + \sum_{i<j} |x_i - x_j|^{-1} - \lambda \right) v = 0$$

is real analytic on $\Omega \setminus \Sigma$.

Three sets of data used below are supplied in the accompanying code/data release of Set-up 2.2. They are the coefficients of a trial function for neutral helium, a table of rational bounds on its radial tails, and a table of rational numbers used in the exterior estimate. The interior matrix estimates are proved in Appendix B.

Lemma 5.3 (Neutral spectral and spatial bounds)**.** *Assume Set-ups 2.1 and 2.2 for the degree-fourteen neutral-helium calculation. Let $E = E_2(2)$ and let $(P_j)_{j=8}^{128}$ be the fixed rational neutral tail table in the accompanying code/data release. Define*

$$p_0(t) = \begin{cases} 1, & 0 \leq t < 1, \\ P_{\lfloor 8t \rfloor}, & 1 \leq t < 16, \\ P_{128}, & t \geq 16, \end{cases} \qquad (M_1, M_2, M_3, M_4) = \frac{(1094533, 2003681, 5206311, 17861539)}{10^6}.$$

Then E is a simple eigenvalue with a normalized rotationally invariant spin-singlet eigenfunction Φ, and

$$-2.903724674 < E < -2.903724372, \qquad H_2(2)\big|_{\Phi^\perp} \geq \left(E + \frac{67039}{100000}\right) I.$$

For $i = 1, 2$, $k = 1, 2, 3, 4$, and $t \geq 0$,

$$\|r_i^k \Phi\| \leq M_k, \qquad \|\mathbf{1}_{\{r_i \geq t\}} \Phi\|^2 \leq p_0(t).$$

The function p_0 is nonnegative, bounded by one, and nonincreasing.

Idea of the proof. We evaluate the energy and the residual of an explicit trial function in exact arithmetic. Temple's inequality then encloses E, and a comparison with hydrogenic operators gives the spectral gap. The trial function is close to Φ in norm, which transfers its moment and tail bounds to Φ. The full proof is in Appendix E.2.

Lemma 5.4 (Complementary sectors)**.** *Assume Set-ups 2.1 and 2.2 for the neutral calculation and the two rational pair-matrix checks. Put $E = E_2(2)$ and $\rho^2 = r_1^2 + r_2^2 + r_3^2$. Then the following inequalities hold on the fermionic H^1 form domain.*

1. *Every vector u in a total-spin-$3/2$ sector, or in a total-spin-$1/2$ sector of orbital angular momentum L and parity different from $(-1)^L$, satisfies*

$$\mathfrak{q}_{3,2}[u] \geq -\frac{49}{18}\|u\|^2 > E\|u\|^2 \quad \text{if } u \neq 0.$$

2. *Every vector u in the closed sum of sectors of total orbital angular momentum $L \geq 2$ satisfies*

$$\mathfrak{q}_{3,2}[u] - E\|u\|^2 \geq \frac{1}{80} \int \rho^{-2} |u|^2.$$

Idea of the proof. The sectors in the first assertion contain no configuration with a doubly occupied $1s$ shell. A hydrogenic comparison, corrected by the electron repulsion, bounds all other configurations. For the second assertion, we bound the two-electron operator of each pair from below, localize in the ratios r_i/ρ, and use Hardy inequalities and the angular kinetic energy. The full proof is in Appendix E.3.

Lemma 5.5 (Exterior trace at the neutral threshold)**.** *Assume Set-ups 2.1 and 2.2 for the fixed neutral and exterior calculations. Let $E = E_2(2)$, $B_7 = \{x \in \mathbb{R}^3 : |x| < 7\}$, $K_7 = (B_7)^3$, and $\Omega_7 = \{(x_1, x_2, x_3) : \max_i r_i > 7\}$. For antisymmetric $u \in H^1(\Omega_7; \mathbb{C}^8)$ let $q_>[u]$ be the Coulomb volume form of Set-up 2.1, restricted to Ω_7, with no boundary term. Then*

$$q_>[u] - E\|u\|^2_{L^2(\Omega_7)} \geq \frac{1}{16} \int_{\partial K_7} |\operatorname{Tr} u|^2 \, dS.$$

The measure dS is Euclidean surface measure on the three exposed faces, and the trace is unrestricted. The inequality holds in every spin, orbital-angular-momentum, and parity sector.

Idea of the proof. We localize according to which electrons have radii comparable to the largest radius. When exactly one electron has this property, the spectral gap of neutral helium from Lemma 5.3 controls its coupling to the other two electrons. Completing a square in its radial variable then absorbs the localization error and leaves the boundary term. In the other cases the form exceeds E by a positive amount. The full proof is in Appendix E.4.

Theorem 5.6. *Under Set-ups 2.1 and 2.2,*

$$E_3(2) = E_2(2), \qquad H_3(2) \geq -2.903724674\, I.$$

For every real $\lambda \leq E_2(2)$, $\ker(H_3(2) - \lambda I) = \{0\}$.

Proof. The proof has three steps. We first add the interior and exterior bounds, whose boundary terms cancel. We then combine the bounds for all symmetry sectors. Finally we show that a threshold eigenfunction vanishes on K_7, and we extend this vanishing to the whole space by analyticity.

Matching at the exact threshold. Put $E = E_2(2)$. Let $K_7, \Omega_7, q_>$ be as in Lemma 5.5. Let the full sectors S, P, the form $q_<$, and the constants z, η_S, η_P be as in Lemma B.1 in Appendix B. The execution hypothesis of that lemma is Set-up 2.2. Its volume form has the same Hartree normalization and spin summation as $q_>$. For $J \in \{S, P\}$ and a fermionic H^1 vector u in the full sector J, restriction preserves antisymmetry and sector membership, and the two restrictions have the same trace. Adding Lemmas B.1 and 5.5 therefore gives

$$\mathfrak{q}_{3,2}[u] - E\|u\|^2 \geq (z + \eta_J - E)\|u\|^2_{L^2(K_7)}. \tag{5.1}$$

The two boundary coefficients are both $1/16$ with the same Euclidean surface measure. Lemma 5.3 gives $E < z$, so both coefficients on the right are strictly positive. The numerical bounds and the completeness of the interior spaces, including every magnetic component, are precisely those of Lemma B.1. No boundary condition is imposed on the restrictions of u.

Exhaustion and equality of energies. Spatial rotations, spin rotations, and inversion reduce the Coulomb operator. Three spin-1/2 particles have total spin 1/2 or 3/2. Their orbital angular momenta are the integers $L \geq 0$ and their parities are ± 1. Lemma 5.4 covers the quartets, the doublets with parity different from $(-1)^L$, and every $L \geq 2$. The remaining sectors are exactly S and P, controlled by (5.1). Orthogonal summation yields $H_3(2) \geq EI$ on the unrestricted fermionic space. Theorem 3.1 places E in its essential spectrum, so $E_3(2) \leq E$ as well. This proves equality. The lower neutral endpoint in Lemma 5.3 gives the stated numerical operator bound.

Exclusion at threshold. Suppose $\Psi \in D(H_3(2))$ and $H_3(2)\Psi = E\Psi$. Every symmetry projection satisfies the same eigen-equation. The first bound in Lemma 5.4 annihilates the quartet and the indicated parity projections. Its second bound annihilates every remaining projection with $L \geq 2$, since $\rho^{-2} > 0$ almost everywhere. Equation (5.1) makes the S and P projections vanish on K_7. Thus the entire eight-component spinor Ψ vanishes almost everywhere on K_7.

To apply Theorem 5.2 componentwise, let $\mathcal{A}$ be the orthogonal antisymmetrizer on the full spin space and $\widetilde{\mathfrak{q}}$ the polarized Coulomb form on its full H^1 domain. Permutation invariance implies $\widetilde{\mathfrak{q}}(\Psi, \varphi) = \widetilde{\mathfrak{q}}(\Psi, \mathcal{A}\varphi)$ and $\langle \Psi, \varphi \rangle = \langle \Psi, \mathcal{A}\varphi \rangle$. The fermionic eigen-equation consequently holds against every smooth compactly supported spinor test. Each scalar spin component solves the Coulomb equation distributionally and is real analytic on $\mathbb{R}^9 \setminus \Sigma$, with Σ as in Theorem 5.2.

This open set is connected. In fact its excluded sets are six linear subspaces V_j of dimension six. For two points a, b outside them choose c outside the finite union of $V_j + \operatorname{span}\{a\}$ and $V_j + \operatorname{span}\{b\}$. These spaces have dimension at most seven, and the two segments from a to c to b avoid every V_j. The nonempty open set $K_7 \setminus \Sigma$ contains, for example, $((1,0,0),(2,0,0),(3,0,0))$. Almost-everywhere vanishing there implies pointwise vanishing of each analytic representative by continuity. The identity theorem for real analytic functions gives vanishing throughout the connected collision-free set. Finally Σ has measure zero, so $\Psi = 0$ in the Hilbert space. The lower form bound already excludes every $\lambda < E$, completing the assertion at and below threshold. □

6 Binding of the lithium anion

We prove that the lithium anion is strictly bound. To do so, we bound the anion energy $E_4(3)$ from above (Proposition 6.1) and the neutral energy $E_3(3)$ from below (Proposition 6.2).

The upper bound is variational. Its trial function is an antisymmetrized sum of 150 explicitly correlated Gaussians with integer parameters, so all matrix elements can be enclosed using exact arithmetic.

The lower bound has three steps. First, a scaling argument and the helium bound of Theorem 5.6 compare $H_3(3)$ with a sum of hydrogenic operators. This comparison gives the required bound in every symmetry sector except two. Second, in each of the two remaining sectors we add a rank-one projection onto a hydrogenic configuration, which makes the shifted Hamiltonian positive. Third, we show that the rank-one term is strictly smaller than the resulting operator, in the manner of the Birman–Schwinger principle. The third step uses certified inner products from Appendix C.

Proposition 6.1. *Under Set-ups 2.1 and 2.2,*

$$E_4(3) < -7.497020240.$$

Idea of the proof. The norm and the energy of the trial function are sums of 45300 closed-form Gaussian integrals. We enclose each term between integers in exact arithmetic and obtain an upper bound for the Rayleigh quotient. The full proof is in Appendix E.5.

Proposition 6.2. *Under Set-ups 2.1 and 2.2,*

$$E_3(3) > -7.493955380.$$

Proof. We follow the three steps described at the beginning of this section. All operator comparisons below are comparisons of quadratic forms.

The comparison operator and the remaining sectors. Set

$$t = \frac{5}{8}, \quad a = 1 - t = \frac{3}{8}, \quad Q = \frac{1}{a} = \frac{8}{3}, \quad C = -2.903724674, \quad z = -7.494, \quad \kappa = \frac{5}{72a} = \frac{5}{27}.$$

Write $\mathcal{T} = -\frac{1}{2}\sum_{i=1}^{3}\Delta_i$, $\mathcal{V} = \sum_{i<j} d_{ij}^{-1}$ and $\mathcal{A} = \sum_i r_i^{-1}$. The unitary dilation $\mathcal{D}_s f(X) = s^{9/2} f(sX)$, $s > 0$, satisfies

$$\mathcal{D}_{1/t}^{*}(t\mathcal{T} - 2\mathcal{A} + \mathcal{V})\mathcal{D}_{1/t} = t^{-1}H_3(2).$$

Theorem 5.6 consequently gives

$$H_3(3) \geq \frac{C}{t} + G_a, \qquad G_a = \sum_{i=1}^{3}\left(-\frac{a}{2}\Delta_i - \frac{1}{r_i}\right). \tag{6.1}$$

By the hydrogenic spectrum theorem (Theorem 3.2; [18, Theorem 10.9]), the one-electron levels in G_a are $\epsilon_n = -1/(2an^2)$. Let N_1 count occupation of its spatial $1s$ orbital, including spin. There are two $1s$ spin orbitals, so N_1 has values $0, 1, 2$. On the subspace $N_1 \leq 1$,

$$G_a \geq 3\epsilon_2 + (\epsilon_1 - \epsilon_2)N_1 \geq \epsilon_1 + 2\epsilon_2 = -\frac{3}{4a}. \tag{6.2}$$

On $N_1 = 2$, the core has orbital angular momentum zero, even parity and spin zero. The valence orbital therefore determines total orbital angular momentum L and parity $(-1)^L$. If $L \geq 2$, its principal index is at least three, and Theorem 3.2 bounds the entire valence space below by ϵ_3. In every sector except $L = 0$ with even parity and $L = 1$ with odd parity, either this bound or (6.2) applies. Thus these other sectors obey

$$H_3(3) \geq \beta I, \qquad \beta = \frac{C}{t} - \frac{19}{18a}. \tag{6.3}$$

This includes opposite-parity sectors, in which a filled $1s$ core is impossible. The spectral complement bounds in Theorem 3.2 include the continuous subspace.

It suffices to examine orbital magnetic number zero and spin magnetic number $1/2$. Orbital and spin rotations commute with the Hamiltonian and its form: every integer-L orbital representation contains magnetic number zero, and each of the three-electron spin representations $1/2, 3/2$ contains spin magnetic number $1/2$. Bounds on these components therefore hold on their full magnetic multiplets. For $T \in \{S, P\}$ put $\ell_S = 0$, $\ell_P = 1$, and let $\mathcal{B}_T$ denote the sector with $L = \ell_T$, parity $(-1)^{\ell_T}$ and those two magnetic numbers, without restricting total spin. Write $H_T = H_3(3)|_{\mathcal{B}_T}$.

The hydrogenic configurations and an inverse bound. Use the trial functions u_T and the vectors $p_{T,n}$ of Definition C.1. We call the vectors $p_{T,n}$ sources. By (6.4) below, they are the antisymmetrized hydrogenic configurations with a filled $1s$ shell and the third electron in the level n. The spatial representation of the trial functions and sources is antisymmetric under the exchange P_{13} of the positions 1 and 3. Extending its $\uparrow\downarrow\uparrow$ component, divided by $\sqrt{3}$, to the other two spin strings by signed permutations is well-defined and isometric: the stabilizer is generated by (13) and the three component norms are equal. This identifies the spatial and physical scalar products, without a further spin factor.

To fix the source phases, let $\phi_{100}(x) = (Q^3/\pi)^{1/2} e^{-Q|x|}$, and choose the real, normalized charge-Q orbitals ϕ_{nL0} with angular factors $Y_{00} = 1/\sqrt{4\pi}$ and $Y_{10}(\widehat{x}) = \sqrt{3/(4\pi)}\, x_3/|x|$, and positive leading radial coefficient at the origin. The Laguerre polynomials and positive constants in Definition C.1 give, with these phases,

$$p_{T,n} = \frac{1 - P_{13}}{\sqrt{2}} [\phi_{100}(x_1)\phi_{100}(x_2)\phi_{n\ell_T 0}(x_3)]. \tag{6.4}$$

For S this identity uses $L^{(1)}_{n-1}(y) = \sum_{j=0}^{n-1} (-1)^j \binom{n}{n-1-j} y^j/j!$; for P the valence radial polynomials are 1 and $1 - Qr/6$. Orthogonality of the valence orbitals to the core and to each other makes these sources orthonormal. They span the indicated discrete levels of the filled-core space. Lemma C.14 places both trials and sources in $D(H_3(3))$. Their stated symmetries and the reducing character of $\mathcal{B}_T$ therefore place them in $D(H_T)$.

Set $m_S = 6$, $m_P = 3$, and let $P_{T,n} = |p_{T,n}\rangle\langle p_{T,n}|$ for $2 \leq n \leq m_T$. For every integer $n \geq 2$ define

$$g_n = \frac{C}{t} - \frac{1 + 1/(2\max(3,n)^2)}{a} - z = \frac{170037989}{937500000} - \frac{4}{3\max(3,n)^2}.$$

Then $g_2 = g_3 = \beta - z > 0.0332257$, and g_n is nondecreasing. Put $K_T = H_T - zI + \kappa P_{T,2}$. Since $\kappa = \epsilon_3 - \epsilon_2$, the rank-one term $\kappa P_{T,2}$ raises the comparison level of the source with $n = 2$ to the level $n = 3$. On the orthogonal complement of $p_{T,2}, \ldots, p_{T,m_T}$, Theorem 3.2 gives the lower bound $2\epsilon_1 + \epsilon_{m_T+1}$ on the part with $N_1 = 2$, and (6.2) is stronger on the part with $N_1 \leq 1$. Hence

$$K_T \geq g_{m_T+1} I + \sum_{n=2}^{m_T} (g_n - g_{m_T+1}) P_{T,n} \geq g_2 I > 0. \tag{6.5}$$

The variational identity

$$\langle f, K_T^{-1} f\rangle = \sup_{v\in D(K_T^{1/2})} \{2\,\mathrm{Re}\langle f, v\rangle - \|K_T^{1/2} v\|^2\}$$

then yields

$$K_T^{-1} \le \frac{1}{g_{m_T+1}} I + \sum_{n=2}^{m_T} \left(\frac{1}{g_n} - \frac{1}{g_{m_T+1}}\right) P_{T,n}. \tag{6.6}$$

This argument does not assume that H_T commutes with the projections $P_{T,n}$.

Bound on the rank-one term. Set $c_S = 1.026$, $c_P = 1.007$, $w_T = c_T u_T$, and define

$$\eta_T = (H_T - zI)w_T, \quad b_T = \langle p_{T,2}, w_T\rangle, \quad e_T = \langle w_T, \eta_T\rangle, \quad d_T = \|\eta_T\|^2,$$
$$v_{T,n} = \langle p_{T,n}, \eta_T\rangle, \qquad j_T = 1 - \kappa b_T, \qquad \rho_T = p_{T,2} - K_T w_T = j_T p_{T,2} - \eta_T.$$

All these scalar products are real, and $w_T \in D(K_T)$ by the domain assertion above. Expanding the residual gives the exact identity

$$\langle p_{T,2}, K_T^{-1} p_{T,2}\rangle = 2b_T - e_T - \kappa b_T^2 + \langle \rho_T, K_T^{-1}\rho_T\rangle.$$

Using (6.6), define the upper bound

$$\begin{aligned}\mathcal{S}_T = \kappa\Big[&2b_T - e_T - \kappa b_T^2 + \frac{j_T^2 - 2j_T v_{T,2} + d_T}{g_{m_T+1}} \\ &+ \sum_{n=2}^{m_T} \left(\frac{1}{g_n} - \frac{1}{g_{m_T+1}}\right)(j_T \mathbf{1}_{n=2} - v_{T,n})^2\Big].\end{aligned} \tag{6.7}$$

Thus $\kappa\langle p_{T,2}, K_T^{-1} p_{T,2}\rangle \le \mathcal{S}_T$. If $\mathcal{S}_T \le s_T < 1$, Cauchy–Schwarz applied to $K_T^{-1/2} p_{T,2}$ and $K_T^{1/2} f$ gives $\kappa|\langle p_{T,2}, f\rangle|^2 \le s_T\langle f, K_T f\rangle$ for every form-domain vector f. Subtraction of the rank-one term and (6.5) imply

$$H_T \ge [z + (1 - s_T)g_2]I. \tag{6.8}$$

Evaluation from the certified intervals. Lemma C.14 encloses in rational intervals the inner products among the trial functions, the sources and the images of the trial functions under the Hamiltonian. We call these inner products moments. The lemma uses $h_T = (H_3(3) + 15/2)u_T$. Consequently, at $z = -7.494$,

$$\eta_T = c_T(h_T - \delta u_T), \qquad \delta = 0.006.$$

Denote the moments that enter by

$$A_T = \langle u_T, h_T\rangle, \quad D_T = \|h_T\|^2, \quad N_T = \|u_T\|^2, \quad B_{T,n} = \langle p_{T,n}, u_T\rangle, \quad V_{T,n} = \langle p_{T,n}, h_T\rangle.$$

They enter through the exact identities

$$\begin{aligned} b_T &= c_T B_{T,2}, & e_T &= c_T^2(A_T - \delta N_T), \\ d_T &= c_T^2(D_T - 2\delta A_T + \delta^2 N_T), & v_{T,n} &= c_T(V_{T,n} - \delta B_{T,n}). \end{aligned} \tag{6.9}$$

No normalization of u_T is introduced.

We now bound $\mathcal{S}_S$ and $\mathcal{S}_P$ using only the rational endpoints of these intervals. Temporarily suppress T, and let subscripts $-$ and $+$ on A, D, N, B_n, V_n denote the endpoints printed in Lemma C.14. Set

$$\begin{aligned} b_\pm &= cB_{2,\pm}, & e_- &= c^2(A_- - \delta N_+),\\ d_+ &= c^2(D_+ - 2\delta A_- + \delta^2 N_+), & v_{n,\pm} &= c(V_{n,\pm} - \delta B_{n,\mp}),\\ j_- &= 1 - \kappa b_+, & j_+ &= 1 - \kappa b_-. \end{aligned}$$

These formulas give outward bounds by their coefficient signs. The specified endpoints satisfy $b_- > 0$, $j_- > 0$, $v_{2,-} > 0$ and $j_- - v_{2,+} > 0$. Define

$$F_T = 2b_+ - e_- - \kappa b_-^2, \qquad R_T = j_+^2 - 2j_- v_{2,-} + d_+,$$
$$a_{T,2} = j_+ - v_{2,-}, \qquad a_{T,n} = \max(|v_{n,-}|, |v_{n,+}|) \quad (3 \le n \le m_T).$$

Positivity of the coefficients in (6.7) gives

$$\mathcal{S}_T \le \kappa \left[F_T + \frac{R_T}{g_{m_T+1}} + \sum_{n=2}^{m_T} \left(\frac{1}{g_n} - \frac{1}{g_{m_T+1}} \right) a_{T,n}^2 \right].$$

Table 1 gives integer upper bounds for 10^{15} times each term in these brackets. Each comparison uses just the rational endpoints above and the displayed formula for g_n. Equivalently, it is verified by multiplying by the positive denominators.

Table 1: Integer upper bounds for 10^{15} times the terms in the bound for $\mathcal{S}_T$. The row indexed by n bounds $(g_n^{-1} - g_{m_T+1}^{-1}) a_{T,n}^2$.

Term	S	P
F_T	4740317261675618	2838404429685468
R_T/g_{m_T+1}	567896606970620	1791632727708472
$n = 2$	20913699346983	123610754064044
$n = 3$	62462513402733	139024913705375
$n = 4$	1036687051373	–
$n = 5$	105796401819	–
$n = 6$	14991159233	–
Sum	5392747556008379	4892672825163359

The final strict comparisons are the integer identities

$$27 \cdot 998656955 \cdot 10^6 - 5 \cdot 5392747556008379 = 4958105 > 0,$$
$$27 \cdot 906050524 \cdot 10^6 - 5 \cdot 4892672825163359 = 22183205 > 0.$$

Hence $\mathcal{S}_S < 0.998656955$ and $\mathcal{S}_P < 0.906050524$. This endpoint calculation covers every combination of values in the certified intervals. It requires no assumption on correlations between them.

Take $s_* = 0.998656955$, the larger of the two bounds. Equation (6.8) controls both remaining sectors, and (6.3) controls all other orbital and parity sectors. The rotation argument includes every spin and magnetic sector. Since $z + (1 - s_*)g_2 < z + g_2 = \beta$, they give on the full fermionic space

$$H_3(3) \ge [z + (1 - s_*)g_2] I.$$

Finally,

$$(1-s_*)g_2 > 0.001343045 \cdot 0.0332257 = 0.0000446236102565 > 0.000044620,$$

so $E_3(3) > -7.493955380$, as asserted. □

7 The lithium dianion

We prove that a lithium nucleus does not bind five electrons. As for the helium dianion, the proof applies Proposition 3.4. The upper bound on the threshold $E_4(3)$ comes from Proposition 6.1. The lemma below supplies the exterior gaps. Positivity of the weighted form is the computer-assisted Lemma A.3 of Appendix A.

Lemma 7.1 (Exterior gaps)**.** *Set*

$$U_0 = -\frac{37431243}{5000000}, \qquad (b_1,\delta_1) = \left(\frac{26}{25},\frac{129}{40}\right), \qquad (b_2,\delta_2) = \left(\frac{103}{50},\frac{3469}{5000}\right).$$

Let $a \in \{1,2\}$ and let u belong to the fermionic form domain of $H_5(3)$. If u vanishes almost everywhere on $\{q_a \le b_a\}$, then

$$\mathfrak{q}_{5,3}[u] - U_0\|u\|^2 \ge \delta_a\|u\|^2.$$

Proof. Let $\mathfrak{h}$ denote the Coulomb integral of Set-up 2.1 with $N=5$ and $Z=3$ on the full space $H^1((\mathbb{R}^3)^5;\mathbb{C}^{32})$ without a symmetry restriction. It agrees with $\mathfrak{q}_{5,3}$ on fermionic vectors. We apply Lemma 3.3 with $N=5$, $Z=3$, so that a core electron contributes $-9/2$ and $A_j = 3-\kappa-jR/(R+b)$. The three parameter choices used are

$$\begin{aligned} M_0(26/25,26/25,25/39,5/3) &= \frac{25925}{6084},\\ M_0(3/5,103/50,125/128,8/5) &= \frac{604295}{98304},\\ M_1(103/50,103/50,50/103,2) &= \frac{131831}{21218}. \end{aligned} \tag{7.1}$$

Indeed the corresponding A_j are $428/351$, $1/2$ and $115/206$, so the maximum in M_j is attained at $h=2$ in each case, and the values follow by rational arithmetic.

The first exterior gap. If $u=0$ on $\{q_1 \le 26/25\}$, then all five radii exceed $26/25$ on the support of u. The first value in (7.1) gives

$$\mathfrak{q}_{5,3}[u] - U_0\|u\|^2 \ge \left(\frac{129}{40} + \frac{545603}{7605000000}\right)\|u\|^2.$$

The second exterior gap. Suppose $u=0$ on $\{q_2 \le b_2\}$. Let $\theta(r)$ be zero for $r \le 3/5$, affine from zero to $\pi/2$ on $[3/5, b_2]$, and equal to $\pi/2$ for $r \ge b_2$. For $S \subset \{1,\dots,5\}$ put

$$\chi_S = \prod_{i\in S}\cos\theta(r_i)\prod_{i\notin S}\sin\theta(r_i).$$

Then $\sum_S \chi_S^2 = 1$, and the quadratic-form localization identity is

$$\mathfrak{h}[u] = \sum_S \mathfrak{h}[\chi_S u] - \frac{1}{2}\int\sum_i |\theta'(r_i)|^2|u|^2.$$

At most one radius lies below b_2 on the support of u. Hence the localization error is at most $\pi^2\|u\|^2/[8(b_2-3/5)^2]$, and $\chi_S u = 0$ when $|S| \geq 2$. The term with $S = \varnothing$ has all five radii above $3/5$. For $S = \{i\}$, the radius r_i is below b_2 and the other four are above b_2. The localized spinors are global H^1 functions. Their vanishing conditions, sliced in the other variables, give the Dirichlet traces required by Lemma 3.3. No symmetry of the localized spinors is required. The last two bounds in (7.1), together with

$$\frac{604295}{98304} < \frac{123}{20} < \frac{31}{5} < \frac{131831}{21218},$$

therefore give

$$\mathfrak{q}_{5,3}[u] \geq -\left(\frac{131831}{21218} + \frac{\pi^2}{8(b_2-3/5)^2}\right)\|u\|^2.$$

Using $\pi < 22/7$, the remaining comparisons are

$$\frac{131831}{21218} < \frac{310659}{50000}, \qquad \frac{\pi^2}{8(b_2-3/5)^2} < \frac{151250}{261121} < \frac{14481}{25000},$$

and

$$-U_0 - \frac{310659}{50000} - \frac{14481}{25000} = \frac{3469143}{5000000} > \frac{3469}{5000}.$$

This proves the second gap and completes the two cases. □

Theorem 7.2. *Under Set-ups 2.1 and 2.2, $E_5(3) = E_4(3)$, and $H_5(3)$ has no nonzero L^2 eigenfunction at any energy at or below $E_4(3)$.*

Proof. Use U_0, b_a, δ_a from Lemma 7.1, and set

$$\beta = 2, \qquad J = \{1,2\}, \qquad \lambda_1 = \frac{83}{250}, \qquad \lambda_2 = \frac{527}{1000}.$$

Proposition 6.1 supplies the required upper bound on the threshold:

$$E_4(3) < -7.497020240 < U_0.$$

With $N = 5$, $Z = 3$, $U = U_0$ and $d_a = \delta_a$, let B_a and M_{2,U_0} be the moment functions and weighted form defined in Proposition 3.4. Its exterior hypotheses hold by Lemma 7.1. Lemma A.3 in Appendix A uses precisely these constants and moment functions, and gives

$$M_{2,U_0}[u] + \sum_{a=1}^{2} \lambda_a \int B_a(q_a)|u|^2 \geq \frac{1}{100000}\|u\|^2$$

for every compactly supported fermionic $u \in H^1$. Thus all hypotheses of Proposition 3.4 hold with $\varepsilon = 1/100000$. Its conclusion gives both the energy equality and the exclusion of every L^2 eigenfunction at or below $E_4(3)$. □

8 Electron counts

This section completes the proof of Theorem 1.1. We first treat every electron count above the dianions (Proposition 8.2). Lieb's bound covers all of these cases except lithium with six electrons, which needs a separate argument. We then combine the results of Sections 4–7 (Theorem 1.1).

We use Lieb's bound [4] in the following form, which includes a possible eigenvalue at the removal threshold. See [10, Section 2.1, equations (3)–(6)].

Theorem 8.1 (Lieb's ionization bound)**.** *Let $N \geq 2$ be an integer and $Z > 0$. If $E_N(Z)$ is an eigenvalue of $H_N(Z)$, then $N < 2Z + 1$.*

Proposition 8.2. *Let $N \geq 2$ be an integer and $Z > 0$. Suppose either $Z = 2$ and $N \geq 5$, or $Z = 3$ and $N \geq 6$. Then $E_N(Z) = E_{N-1}(Z)$ and this energy is not an L^2 eigenvalue of $H_N(Z)$.*

Proof. Lieb's bound treats all cases except $(N, Z) = (6, 3)$. For that case we combine three ingredients. The first is a pointwise inequality for the weighted electron repulsion. The second is Lieb's argument with a quadratic weight, as in the proof of Proposition 3.4, which bounds the mean radius of an eigenfunction. The third is an upper bound on the repulsion energy from the virial theorem and the Pauli principle.

By Theorem 3.1, $E_N(Z) \leq E_{N-1}(Z)$, and a strict inequality makes $E_N(Z)$ a discrete eigenvalue. Consequently, absence of a ground eigenvalue implies both conclusions. Theorem 8.1 gives this absence for $Z = 2$, $N \geq 5$, and for $Z = 3$, $N \geq 7$.

The six-particle geometric inequality. For $X = (x_1, \dots, x_6) \in (\mathbb{R}^3)^6$, put

$$R(X) = \sum_{i=1}^{6} r_i, \qquad v(X) = \sum_{i<j} \frac{r_i^2 + r_j^2}{d_{ij}}.$$

We claim that, almost everywhere,

$$v(X) \geq \frac{2657}{800} R(X). \tag{8.1}$$

Work away from the collision and zero-radius sets. For each pair $i < j$,

$$\frac{r_i^2 + r_j^2}{d_{ij}} \geq \frac{1223}{1600}(r_i + r_j) + \frac{153}{100}\frac{x_i \cdot x_j}{r_i + r_j} + \frac{189}{200}\frac{3(x_i \cdot x_j)^2 - r_i^2 r_j^2}{(r_i + r_j)^3}. \tag{8.2}$$

To verify this, set $s = r_i + r_j$, $\theta = d_{ij}/s$, $z = 1 - \theta^2$ and $t = 4r_i r_j / s^2$. The triangle inequalities give $0 < \theta \leq 1$ and $z \leq t \leq 1$. The difference between the two sides of (8.2), divided by s, is

$$F(t) = \frac{1 - t/2}{\theta} - \frac{1223}{1600} - \frac{153}{100}\left(\frac{z}{2} - \frac{t}{4}\right) - \frac{189}{200}\left(\frac{3z^2}{4} - \frac{3zt}{4} + \frac{t^2}{8}\right).$$

This is concave in t, and its endpoint values satisfy

$$\begin{aligned} 800\theta F(1) &= (1 - \theta)(3\theta - 2)^2(63\theta^2 + 147\theta + 100), \\ 1600\theta F(z) &= 800\left(\theta - \frac{239}{400}\right)^2 + \frac{23837}{600} + 801\left(\theta - \frac{2}{3}\right)^2\left(\theta + \frac{4}{3}\right) + 189\theta^3(1 - \theta^2). \end{aligned}$$

Both are nonnegative, proving (8.2).

Write I_3 for the 3×3 identity matrix and $\|\cdot\|_{\mathrm{HS}}$ for the Hilbert–Schmidt norm. Set $\mathsf{Q}_i = \sqrt{3}\, x_i x_i^{\mathsf{T}} - r_i^2 I_3/\sqrt{3}$. Then $\operatorname{tr}(\mathsf{Q}_i\mathsf{Q}_j) = 3(x_i \cdot x_j)^2 - r_i^2 r_j^2$ and $\|\mathsf{Q}_i\|_{\mathrm{HS}}^2 = 2r_i^4$. Expanding the squares in the following Laplace integrals gives

$$0 \le \int_0^\infty \left| \sum_{i=1}^6 e^{-ur_i} x_i \right|^2 du = \frac{R}{2} + 2\sum_{i<j} \frac{x_i \cdot x_j}{r_i + r_j},$$

$$0 \le \int_0^\infty \frac{u^2}{2} \left\| \sum_{i=1}^6 e^{-ur_i} \mathsf{Q}_i \right\|_{\mathrm{HS}}^2 du = \frac{R}{4} + 2\sum_{i<j} \frac{3(x_i \cdot x_j)^2 - r_i^2 r_j^2}{(r_i + r_j)^3}.$$

Summing (8.2) therefore gives

$$v \ge \left(5\frac{1223}{1600} - \frac{153}{400} - \frac{189}{1600} \right) R = \frac{2657}{800} R,$$

as asserted.

A radius bound valid at threshold. Suppose that a normalized $\Psi \in \mathcal{H}_6$ satisfies $H_6(3)\Psi = E\Psi$, where $E = E_6(3)$. It belongs to the Coulomb form domain. Write $\rho = |X| = (\sum_i r_i^2)^{1/2}$, and choose a smooth nonincreasing $\chi : [0,\infty) \to [0,1]$ equal to one on $[0,1]$ and zero on $[2,\infty)$. For $L > 0$, set $\chi_L(X) = \chi(\rho/L)$, $f_L = \chi_L \Psi$ and $K = \|\chi'\|_\infty$. These cutoffs preserve antisymmetry.

For each label i, $r_i f_L$ is antisymmetric in the other five labels. Since $E \le E_5(3)$, the quadratic form of the five-electron Hamiltonian in these labels minus E is nonnegative. The omitted coordinate and its spin are integrated as parameters. Test the weak eigenvalue equation with $\rho^2 \chi_L^2 \Psi$ and split off these six nonnegative forms. Using $\Delta\rho^2 = 36$ gives

$$\begin{aligned} &\frac{1}{2}\sum_{i=1}^6 \int r_i^2 |\nabla_i f_L|^2 - 9\|f_L\|^2 + \int (v - 3R)|f_L|^2 \\ &\qquad \le \frac{1}{2}\int \left(\rho^2 |\nabla\chi_L|^2 + 2\chi_L X \cdot \nabla\chi_L \right) |\Psi|^2 \le 2K^2 \int_{\rho \ge L} |\Psi|^2. \end{aligned}$$

The last inequality uses $X \cdot \nabla\chi_L \le 0$ and $\rho^2 |\nabla\chi_L|^2 \le 4K^2$ on the cutoff annulus. All multipliers in the weak equation are bounded with bounded derivatives and compact support, so the identity uses no moment assumption on Ψ. Integration by parts, first for smooth functions and then by H^1 approximation on compact support, gives for each label i and such a function f

$$\int r_i^2 |\nabla_i f|^2 \ge \|x_i \cdot \nabla_i f\|^2 = \left\| x_i \cdot \nabla_i f + \frac{3}{2} f \right\|^2 + \frac{9}{4}\|f\|^2.$$

Together with (8.1), this yields

$$\frac{257}{800} \int R|f_L|^2 \le \frac{9}{4}\|f_L\|^2 + 2K^2 \int_{\rho \ge L} |\Psi|^2.$$

Fatou's lemma and $f_L \to \Psi$ in L^2 now give

$$0 < S := \int R|\Psi|^2 \le \frac{1800}{257}. \tag{8.3}$$

Incompatible repulsion bounds. Define the finite expectations

$$T = \frac{1}{2}\sum_{i=1}^6 \int |\nabla_i \Psi|^2, \qquad U = \int \sum_{i=1}^6 \frac{|\Psi|^2}{r_i}, \qquad W = \int \sum_{i<j} \frac{|\Psi|^2}{d_{ij}}.$$

Their finiteness follows from the Coulomb form domain and Hardy's inequality. The fifteen pairs satisfy

$$\sum_{i<j} \frac{1}{d_{ij}} \geq \sum_{i<j} \frac{1}{r_i + r_j} \geq \frac{15^2}{5R} = \frac{45}{R}.$$

Cauchy–Schwarz against the probability density $|\Psi|^2$, followed by (8.3), gives

$$W \geq 45 \int R^{-1} |\Psi|^2 \geq \frac{45}{S} \geq \frac{257}{40}. \tag{8.4}$$

An elementary two-electron trial function bounds T from below. For $\alpha > 0$ and $x \in \mathbb{R}^3$, set $\phi_\alpha(x) = (\alpha^3/\pi)^{1/2} e^{-\alpha|x|}$. The normalized determinant formed by pairing ϕ_α with the two orthonormal spin states has energy at $Z = 3$ equal to $\alpha^2 - 6\alpha + 5\alpha/8$. Indeed, the angular average of $|x - y|^{-1}$ at fixed radii $\xi, \eta > 0$ is $1/\max\{\xi, \eta\}$, and hence its repulsion integral is

$$32\alpha^6 \int_0^\infty \xi e^{-2\alpha\xi} \left(\int_0^\xi \eta^2 e^{-2\alpha\eta} \, d\eta \right) d\xi = \frac{5\alpha}{8}.$$

Choosing $\alpha = 43/16$ and using Theorem 3.1 successively gives

$$E \leq E_2(3) \leq -\frac{1849}{256} < -\frac{25}{4}.$$

The normalized dilations $\Psi_a(X) = a^9 \Psi(aX)$, $a > 0$, have energy $a^2 T + a(-3U + W)$, minimized at $a = 1$. Thus $2T - 3U + W = 0$, $E = -T$, and $T > 25/4$.

By antisymmetry, each normalized spin orbital has occupation at most one. Hence the one-particle density operator of Ψ has trace six and lies between zero and the identity. For each $\zeta > 0$, Theorem 3.2 therefore gives

$$T - \zeta U \geq 2 \left(-\frac{\zeta^2}{2} \right) + 4 \left(-\frac{\zeta^2}{8} \right) = -\frac{3}{2} \zeta^2.$$

Optimizing in ζ yields $U \leq \sqrt{6T}$. Put $\tau = \sqrt{T} > 5/2$. Since $3\sqrt{3/2} < 15/4$,

$$W = 3U - 2T \leq 2\tau \left(3\sqrt{\frac{3}{2}} - \tau \right) < 2\tau \left(\frac{15}{4} - \tau \right) < \frac{25}{4};$$

the last quadratic is decreasing for $\tau \geq 5/2$ and equals $25/4$ at $\tau = 5/2$. This contradicts (8.4). Thus the six-electron ground energy is not an eigenvalue, and HVZ gives the remaining equality $E_6(3) = E_5(3)$.

Proof of Theorem 1.1: Theorems 5.6 and 4.4 give $E_3(2) = E_4(2) = E_2(2)$ and exclude eigenfunctions at or below this energy for three and four electrons. Proposition 8.2 gives $E_N(2) = E_{N-1}(2)$ for every $N \geq 5$ and excludes an eigenfunction at that energy. Induction proves $E_N(2) = E_2(2)$ for all $N \geq 3$. Theorem 7.2 similarly starts the lithium induction at $E_5(3) = E_4(3)$, including threshold exclusion, and Proposition 8.2 supplies every $N \geq 6$. Hence $E_N(3) = E_4(3)$ for all $N \geq 5$, with no eigenfunction at that energy. Since no eigenvalue can lie below the spectral infimum, these statements give both asserted kernel exclusions.

Strict binding and the counts. Theorem 3.2 and Lemma 4.1 give

$$E_2(2) < -\frac{29}{10} < -2 = E_1(2) < E_0(2) = 0.$$

The preceding equalities exclude every $N \geq 3$ from the helium strict-binding set. That set is exactly $\{1, 2\}$, so $N_{\mathrm{c}}(2) = 2$. Propositions 6.2 and 6.1 give

$$E_3(3) - E_4(3) > (-7.493955380) - (-7.497020240) = 0.003064860.$$

Thus four belongs to the lithium strict-binding set, whereas the energy equalities exclude every $N \geq 5$. Its supremum is therefore four, irrespective of which smaller electron counts belong to that set. □

A Geometric and radial certificates

This appendix proves Lemma A.3, the positivity of the weighted form that Section 7 uses for the lithium dianion. We first fix the conventions for the computer-assisted checks. As in the introduction, a certificate is finite data from which a program verifies a stated inequality. We also call such data a witness. An exact reader is a program that checks a certificate in exact arithmetic.

The finite witnesses, polynomial coefficient lists, exact readers and completed execution records used below are retained in the accompanying code/data release. We identify each dataset by its mathematical contents. The checks use exact integers and rationals, including signed floor division. A finite binary64 input denotes its exact dyadic value. Either signed zero denotes zero, and nonfinite inputs are rejected. Write rn_{64} for nearest binary64 rounding with even ties, followed by this exact interpretation. Integer power comparisons certify all radical enclosures. Locally, Set-up 2.2 means faithful Python integer and rational operations, binary decoding, decompression, file operations and execution records, with assertions enabled and identical input bytes throughout each composed execution. Hashes identify artifacts. They are not substitutes for byte preservation or successful evaluation. The numerical accuracy of the witness-generating program is not used.

A.1 The five-electron weighted form

Several radial estimates below use the following square identity. For $0 \leq l < u \leq \infty$, a real function b that is locally Lipschitz on (l, u), a real potential V, and $z \in H^1_{\mathrm{loc}}$ on (l, u) for which the boundary terms exist,

$$\int_l^u \left(\frac{|z'|^2}{2} + V|z|^2 \right) = \frac{1}{2} \int_l^u |z' - bz|^2 + \int_l^u \left(V - \frac{b' + b^2}{2} \right) |z|^2 + \frac{1}{2}[b|z|^2]_l^u. \tag{A.1}$$

It follows by expanding the square and integrating its real cross term, so it also holds for complex z.

Definition A.1. Let h_s, h_p interpolate affinely the triples in Table 2, with constant continuation at both ends. The entries of that table are integers and specify $(1000r, 1000h_s(r), 1000h_p(r))$ exactly. Put $p(r) = r^2 + 2$ and $\theta = 27/100$. For $\ell = 0, 1, \ldots$, let K_ℓ be the operator of the closed form

$$k_\ell[z] = \frac{1}{2} \int_0^\infty p|z'|^2 + \int_0^\infty \left[-\frac{1}{8} - \frac{6}{r} + \frac{73\ell(\ell+1)p}{200r^2} \right] |z|^2$$

on $\{z \in H^1_0(0, \infty) : \int r^2|z'|^2 < \infty\}$. The trace at zero is zero, and the radial space has no spin factor.

Table 2: Exact lithium radial fields. Read each group of three columns from top to bottom, then pass to the next group.

$1000r$	$1000h_s$	$1000h_p$	$1000r$	$1000h_s$	$1000h_p$	$1000r$	$1000h_s$	$1000h_p$
25	0	0	1800	5791	5742	7200	7280	7120
88	175	180	2000	6059	5984	8100	7240	7099
150	356	347	2200	6264	6195	9000	7175	7029
285	733	753	2400	6452	6341	10500	7036	6913
420	1278	1255	2700	6667	6514	12000	6870	6748
570	1956	1933	3000	6807	6647	15000	6480	6374
720	2650	2655	3350	6919	6797	18000	6045	5966
860	3281	3287	3700	6976	6953	22000	5429	5376
1000	3851	3857	4200	7099	6959	26000	4828	4800
1125	4287	4310	4700	7182	7030	43000	2330	2318
1250	4676	4666	5250	7239	7086	60000	-433	-593
1425	5086	5092	5800	7271	7110	130000	-11484	-11390
1600	5451	5429	6500	7289	7129	200000	-23058	5000

Lemma A.2. *For the operators and fields of Definition A.1,*

$$K_0 - h_s \geq -10.624, \qquad n_-(K_0 - h_s + 7.793) \leq 1, \qquad n_-(K_0 - h_s + 6.995) \leq 2,$$

and, for every integer $\ell \geq 1$,

$$K_\ell - h_p \geq -7.119, \qquad K_\ell - h_s \geq -7.280.$$

Proof. We give the differential certificates for the first, second and angular-one levels, and an explicit two-zero comparison for the third level. For a field $h \in \{h_s, h_p\}$ and a level e, multiplication by $\sqrt{p}$ on the compact smooth radial core gives the potential

$$W_{e,\ell,h} = \frac{-1/8 - h - e - 6/r}{p} + \frac{1}{p^2} + \frac{73\ell(\ell+1)}{200r^2}. \tag{A.2}$$

The resulting form is $\int(|y'|^2/2 + W_{e,\ell,h}|y|^2)$ on H_0^1. Both forms have the compact smooth core, by Hardy's inequality and cutoff at zero and infinity. The multiplication is a bijection on that core. Approximation of negative finite-dimensional subspaces as in the preceding proof shows equality of their negative indices. No bounded similarity on the full L^2 spaces is asserted.

Endpoint and polynomial data. Set $r_* = 1/40$ and $R_* = 200$. On $(0, r_*)$ both fields vanish, and $W_{e,\ell,h} > -3/r + 73\ell(\ell+1)/(200r^2)$ at the levels used below. The positive function $r^\mu(1 - 3r/\mu)$ with $\mu = 1$ for $\ell = 0$ and $\mu = 9/5$ for $\ell = 1$ gives the respective origin trace coefficients $680/37$ and $808/23$ through (A.1). On $r \geq 200$ the s tests satisfy $r^2 W > 28$, and the p test at $e = -7.119$ satisfies $r^2 W > 63/25$. These follow by inserting the constant end values $h_s = -23.058$, $h_p = 5$ in (A.2) and using $r^2/p > 999/1000$, $6r/p \leq 3/100$. The tail functions r^{-7} and $r^{-9/5}$ give trace coefficients $7/400$ and $9/2000$, respectively.

Here is the finite algebraic test for the lithium radial datasets. On a cell $[l, u]$ set $\delta = u - l$, $t = (r - l)/\delta$, $J = r^2 p^2$ and $H = 2JW_{e,\ell,h}$. Each cell contains no interior field knot. There are two types of barrier:

$$\begin{aligned} b = P(t)/r: &\quad R_Q = H - p^2[(r/\delta)P' - P + P^2], \qquad W - \tfrac{1}{2}(b' + b^2) = R_Q/(2J), \\ b = F'(t)/(\delta F(t)): &\quad R_F = HF - JF''/\delta^2, \qquad W - \tfrac{1}{2}(b' + b^2) = R_F/(2JF). \end{aligned}$$

The fixed polynomial coefficients are in $10^{-18}\mathbb{Z}$ and their cell endpoints are in $10^{-6}\mathbb{Z}$. The accompanying complete coefficient lists prove positivity of R_Q, or of both F, R_F, using identities of the form

$$DT(t) = c + \sum_{a_k \geq 0} a_k t^k + \sum_{a_k < 0} (-a_k)(1 - t^k), \qquad D, c > 0. \tag{A.3}$$

All quantities are integers after clearing denominators. Coefficient convolution and differentiation check the identity. Each summand on its right is nonnegative on $[0, 1]$. This gives a positive residual on the whole cell, without a rounding error or a sampled sign test.

The fixed lists have the coverage in Table 3 and the junction properties described below. The

Table 3: Polynomial cells for the lithium radial bounds.

field	ℓ	level and interval	type	cells
h_s	0	-10.624, $[1/40, 200]$	Q	63
h_s	0	-7.793, $[1/40, 97/100]$	F	17
h_s	0	-7.793, $[98/100, 200]$	F	44
h_p	1	-7.119, $[1/40, 200]$	Q	69

Q rows match the endpoint values of rb, and hence of b. For the F rows the complete rational junction list gives $b(l-) - b(l+) \geq 0$. Such downward jumps contribute nonnegative traces in (A.1). At the right endpoint the values of $200b(200)$ are, in the order ground s, right-hand second s, and p,

$$\frac{1056766439842756911}{125000000000000000}, \qquad \frac{655514571348203063000000000}{81169011805581996247117017}, \qquad \frac{4352114208735658733}{10^{18}}.$$

All are positive and attach to the positive tail traces. For the p rows the initial value is $r_* b(r_*) = 1756521739130434782/10^{18} \leq 202/115 = 2r_*(808/23)$. For the left-hand second s rows the initial value is at most $34/37 = 2r_*(680/37)$.

The ground s certificate also contains a degree-10 origin polynomial g with $g(0) = 0$, $g'(0) = 1$, $g''(0) = -6$. Its two identities (A.3) certify positivity of $g(r_*t)/(r_*t)$ and of

$$\frac{N(r_*t)g(r_*t) - D_0(r_*t)g''(r_*t)}{t^2}, \qquad N(r) = 2rp(r)(10499/1000) - 12p(r) + 2r, \quad D_0(r) = rp(r)^2.$$

The numerator is divisible by t^2. Since $N = 2D_0 W_{-10.624,0,h_s}$, these identities give the required origin differential inequality. The listed rational endpoint comparison is $r_* g'(r_*)/g(r_*) > 925444130490188736/10^{18}$, the initial core value. It is a downward junction, so the origin attaches without a negative trace.

For the second s level put $r_c = 97/100$ and impose $y(r_c) = 0$. The right-side seed is a degree-10 polynomial $g_c(x)$, $x = r - r_c$, on $0 \leq x \leq 1/100$, with $g_c(0) = 0$, $g_c'(0) = 1$. Its two retained positive identities concern $g_c(t/100)/(t/100)$ and

$$\frac{H(97/100 + t/100)g_c(t/100) - J(97/100 + t/100)g_c''(t/100)}{t}.$$

They prove a positive function and a nonnegative differential residual, and the first right-side junction is downward. At the cut there is no boundary debit: for $y(r_c) = 0$, $|y(r_c + x)|^2/x \leq \int_{r_c}^{r_c+x} |y'|^2 \to 0$, while $g_c'/g_c = 1/x + O(1)$. Hardy's inequality also controls the square term. Thus the two sides give nonnegativity on this single trace kernel.

These identities, all coefficients of the two seeds, and every junction comparison are the fixed lithium radial certificate data in the code/data release. The checks just described involve the complete lists, of lengths $63, 17, 44, 69$, and their seed identities. Summation of (A.1) proves the ground s and p floors and the second s index bound. The latter follows because a two-dimensional negative space would meet the one-trace kernel nontrivially.

The third s level. Define

$$V_*(r) = \frac{r-27}{r(r+3)^2}, \qquad g_*(r) = \frac{r(10r^2-45r+27)}{(r+3)^4}, \qquad E_*(r) = \frac{47}{8} + \frac{27r-29}{(r+3)^2} + \frac{1}{r^2+2}.$$

Direct differentiation gives $-g_*''/2 + V_* g_* = 0$. Its only positive zeros are $(45 \pm 3\sqrt{105})/20$. The square identity on the three intervals between these zeros proves nonnegativity on the kernel of the two traces, hence index at most two. Moreover $p(W_{-7,0,h_s} - V_*) = E_* - h_s$. The exact bounds in Table 4, obtained from the field knots, prove $E_* - h_s \geq 1/200$ on the entire half-line. For the lower bounds, discard $1/p$ and use $((27r-29)/(r+3)^2)' = (139-27r)/(r+3)^3$. Its

Table 4: Bounds for the third lithium s level.

interval	upper bound for h_s	lower bound for E_*
$[0, 57/100]$	$489/250$	$191/72$
$[57/100, 5/4]$	$1169/250$	$191/40$
$[5/4, 2]$	$6059/1000$	$49/8$
$[2, 3]$	$6807/1000$	$55/8$
$[3, 9]$	$7289/1000$	$527/72$
$[9, 12]$	$287/40$	$2587/360$
$[12, 18]$	$687/100$	$55/8$
$[18, 22]$	$1209/200$	$51/8$
$[22, \infty)$	$5429/1000$	$47/8$

minimum on a finite interval is at an endpoint. For the first and last rows use respectively $(27r-29)/(r+3)^2 \geq -29/9$ and ≥ 0. Therefore $W_{-6.995,0,h_s} \geq V_*$, which proves the stated index bound. Finally the knotwise maximum of $h_s - h_p$ is .161, so $K_1 - h_s \geq -7.119 - .161 = -7.280$. Increasing $\ell \geq 1$ adds a nonnegative centrifugal term and proves the remaining assertions. □

Lemma A.3 (Five-electron weighted form)**.** *Assume Set-up 2.2 for the specified Li5 certificate executions. Set $U_0 = -37431243/5000000$ and*

$$(\omega_1, b_1, \delta_1) = (83/250, 26/25, 129/40), \qquad (\omega_2, b_2, \delta_2) = (527/1000, 103/50, 3469/5000).$$

Write $s_+ = \max(s, 0)$ for real s. For $t \geq 0$ and $a \in \{1, 2\}$ put $B_a(t) = (t-b_a)_+^2 - \min(t/b_a, 1)/(2\delta_a)$. For $x = (x_1, \ldots, x_5)$ set $r_i = |x_i|$, $d_{ij} = |x_i - x_j|$, let $q_1 \leq \cdots \leq q_5$ be the ordered radii, and put $V(q) = \omega_1 B_1(q_1) + \omega_2 B_2(q_2)$. Then every compactly supported antisymmetric $u \in H^1((\mathbb{R}^3)^5; \mathbb{C}^{32})$ satisfies

$$\frac{1}{2}\sum_{i=1}^{5} \int (r_i^2 + 2)|\nabla_i u|^2 + \int \left[\sum_{i<j} \frac{r_i^2 + r_j^2 + 2}{d_{ij}} - 3\sum_{i=1}^{5} \left(r_i + \frac{2}{r_i} \right) \right] |u|^2 + \int \left[-\frac{15}{2} - 2U_0 + V(q) \right] |u|^2 \geq \frac{1}{100000} \|u\|^2.$$

All integrals are over $(\mathbb{R}^3)^5$ and sum spin components; antisymmetry exchanges positions and spins simultaneously.

Proof. We prove the angular supports and their exact finite verification, close the unbounded radius regions, and combine the resulting scalar inequalities with Lemma A.2. Use the fields, p and θ of Definition A.1. At positive ordered radii define the full angular form

$$\mathcal{A}(q) = \frac{\theta}{2}\sum_{i=1}^{5}(1+2/q_i^2)L_i^2 + \sum_{i<j}\frac{2+q_i^2+q_j^2}{|q_i n_i - q_j n_j|} - 3\sum_i q_i, \qquad L_i^2 = -\Delta_{S^2,i}. \tag{A.4}$$

Here $n_i \in S^2$ and, in the following angular calculations, write $y_i = q_i n_i$ and $d_{ij}^* = |y_i - y_j|$. Its domain is the angular H^1 space with arbitrary spin components and finite nonnegative Coulomb integral. No symmetry restriction is imposed at this stage. Put

$$e = -43.953, \qquad e_s = -43.834, \qquad c_* = e - 2U_0 - 15/8, \qquad \varepsilon_* = 1/100000.$$

Scalar geometry. We first establish the two inexpensive supports used in the finite check. For ordered radii let $\mathcal{V}_5 = \sum_{i<j}(q_i^2+q_j^2)/d_{ij}^*$ and $\mathcal{W}_5 = \sum_{i<j}(d_{ij}^*)^{-1}$. Then

$$\mathcal{V}_5 - 3\sum_i q_i \geq \sum_i a_i^* q_i, \qquad \mathcal{W}_5 \geq \sum_{i=2}^{5} t_i^*/q_i, \tag{A.5}$$

where

$$a^* = (-231/100, -231/100, 7/50, 7/50, 7/50), \qquad t^* = (0, 1/2, 154/125, 971/500, 53/20).$$

Here is an algebraic proof of the constants. For positive C, λ, d,

$$\frac{C}{d} - \frac{3}{2}\lambda C^{2/3} + \frac{1}{2}\lambda^3 d^2 = \frac{\lambda^3(d - C^{1/3}/\lambda)^2(d + 2C^{1/3}/\lambda)}{2d} \geq 0. \tag{A.6}$$

Choose weights $\xi_i = 829/1000$ for the first two radii and $767/1000$ for the other three. For a pair put $\zeta = \xi_i\xi_j$, $z = (q_j - q_i)/(q_i + q_j)$, and $\lambda^3 = 4\zeta^3/(q_i+q_j)$. The pair bound is

$$(q_i+q_j)\{3\zeta/2 - \zeta^3 + \mathcal{F}_\zeta(z)\} + \frac{4\xi_i^3\xi_j^3}{q_i+q_j}y_i\cdot y_j, \quad \mathcal{F}_\zeta(z) = \tfrac{3}{2}\zeta[(1+z^2)^{2/3} - 1] - \zeta^3 z^2.$$

The kernel square $\int_0^\infty |\sum_i \xi_i^3 e^{-tq_i} y_i|^2 dt \geq 0$ bounds the summed second term below by $-\sum_i \xi_i^6 q_i$. Also

$$\mathcal{F}_\zeta''(z) = 2\zeta[(1+z^2/3)(1+z^2)^{-4/3} - \zeta^2] \geq 0,$$

because $\zeta^2 < 1/2 < 4/(3\,2^{4/3})$. Use its tangent at 0 within a weight group and at $31/40$ between groups. With $A_* = .687241$, $B_* = .588289$, $\zeta_* = .635843$ and $R_* = (2561/1600)^{1/3}$, the cross-group coefficients are

$$L_- = -\frac{1121\zeta_*}{3200R_*} + \frac{1841}{1600}\zeta_*^3, \qquad L_+ = \frac{8799\zeta_*}{3200R_*} - \frac{3119}{1600}\zeta_*^3.$$

The rational cube brackets $1.169 < R_* < 1.1699$ give $.5435 < \zeta_*/R_* < .544$. Also $.257 < \zeta_*^3 < .2571$, $A_*^3 < .325$, $B_*^3 < .2036$. Thus $L_- > .105140625$ and $L_+ > .99327084375$. The inner coefficients of $\mathcal{V}_5$ exceed $3A_*/2 - 2A_*^3 + 3L_- > .696283375$, and the outer coefficients exceed $3B_* - 3B_*^3 + 2L_+ > 3.1406086875$. This proves the first bound in (A.5).

For the second, put $c(z) = \min\{1, [2(1-z)]^{-1/2}\}$ on $[-1,1)$ and $c(1) = 1$. The maximum of $1 + t^2 - 2tz$ on $0 \leq t \leq 1$ is $\max(1, 2(1-z))$, so $(d_{ij}^*)^{-1} \geq \min(q_i^{-1}, q_j^{-1})c(n_i\cdot n_j)$. For $2 \leq \nu \leq 5$,

the tangent to $[2(1-z)]^{-1/2}$ at $z=-1/(\nu-1)$ lies below c: its maximum is $\frac{3}{2}\sqrt{(\nu-1)/(2\nu)}\le 1$. For ν unit vectors, $\sum_{i<j} n_i\cdot n_j \ge -\nu/2$. Summing this tangent yields $\binom{\nu}{2}\sqrt{(\nu-1)/(2\nu)}$. Rational lower bounds for these four values are $1/2, 433/250, 1837/500, 1581/250$. Squaring verifies them. Integrating over the sets $\{i : q_i^{-1} > t\}$ gives their successive increments divided by q_2, q_3, q_4, q_5, which are exactly t_i^*.

On a box $Q=\prod_i[l_i,h_i]$, $0\le l_i<h_i$, let $x_i^*=(l_i+h_i)/2$ and $k_i=\theta(1+2/h_i^2)$. The two cheap supports for (A.4) are consequently

$$\sum_i a_i^* q_i + 2\sum_{i=2}^{5} t_i^*/h_i, \qquad \sum_i a_i^* q_i + 2\sum_{i=2}^{5} t_i^*(2/x_i^* - q_i/(x_i^*)^2). \tag{A.7}$$

The reciprocal tangent is valid because its error is $(q_i-x_i^*)^2/(q_i(x_i^*)^2)\ge 0$.

Angular recovery inequalities. We record the form estimates that justify the remaining supports. For a positive diagonal matrix $\mathsf{D}=\operatorname{diag}(d_i)$ and symmetric A, write

$$T_{\mathsf{D}} = \tfrac{1}{2}\sum_i d_i L_i^2, \qquad U_{\mathsf{A}} = \tfrac{1}{2}\sum_{i,j} \mathsf{A}_{ij} n_i\cdot n_j.$$

For any real matrix B, tangent vector fields $\mathsf{X}_i = d_i^{-1}(I_3 - n_i n_i^T)\sum_j \mathsf{B}_{ij} n_j$ give

$$\mathsf{A}-\mathsf{B}-\mathsf{B}^T-\mathsf{B}^T\mathsf{D}^{-1}\mathsf{B}\ge 0 \quad\Longrightarrow\quad T_{\mathsf{D}}+U_{\mathsf{A}}\ge \operatorname{tr}\mathsf{B}. \tag{A.8}$$

For a smooth angular spinor χ, expand $\frac{1}{2}\sum_i d_i\int|\nabla_i\chi+\mathsf{X}_i\chi|^2$. Integration by parts gives $\sum_i d_i \operatorname{div}_i \mathsf{X}_i = 2\operatorname{tr}\mathsf{B} - \sum_{ij}(\mathsf{B}+\mathsf{B}^T)_{ij} n_i\cdot n_j$, and the tangent projections have norm at most one. The remaining matrix contraction is nonnegative by applying its positive semidefiniteness to each Cartesian component of the n_i. Density gives the inequality for the entire angular form domain.

Two refinements will also be used. If $\mathsf{A}\ge 0$, $t>0$ and $\Lambda\ge\lambda_{\max}(\mathsf{D}^{-1/2}\mathsf{A}\mathsf{D}^{-1/2})$, the symmetric choice $\mathsf{B}=t\mathsf{A}$, retaining the normal-component squares, gives

$$T_{\mathsf{D}}+U_{\mathsf{A}} \ge t\operatorname{tr}\mathsf{A} - \frac{\operatorname{tr}\mathsf{D}}{8t^2}(2t+t^2\Lambda-1)_+^2. \tag{A.9}$$

To verify the penalty, write $U=U_{\mathsf{A}}\ge 0$. The square expansion is bounded below by $t\operatorname{tr}\mathsf{A}+(1-2t-t^2\Lambda)U+2t^2U^2/\operatorname{tr}\mathsf{D}$. Here $\mathsf{A}\mathsf{D}^{-1}\mathsf{A}\le\Lambda\mathsf{A}$ and weighted Cauchy–Schwarz bounds the retained normal squares. Minimizing this quadratic for $U\ge 0$ proves (A.9).

For $\rho_i\ge 0$, $\sum_i\rho_i\le 1$, and $0\le t_i^2\le d_i/2$, one has

$$T_{\mathsf{D}}+U_{\mathsf{A}} \ge \sum_i (2t_i\sqrt{\rho_i\mathsf{A}_{ii}/2} - t_i^2), \qquad t_i\ge 0. \tag{A.10}$$

For a normalized slice in the ith angular variable let $m_i=|\langle n_i\rangle|<1$. Conditional averaging of a positive Gram form gives $\langle U_{\mathsf{A}}\rangle \ge \mathsf{A}_{ii}(1-m_i^2)/2$. Integration by parts against a coordinate on S^2, followed by Cauchy–Schwarz, gives $\int|\nabla_i\chi|^2\ge m_i^2/(1-m_i^2)$ on the normalized slice. Set $v=1-m_i^2$. The contribution with weight ρ_i is at least $(\rho_i\mathsf{A}_{ii}/2)v+(d_i/2)(v^{-1}-1)$. For $0<v\le 1$ its minimum is y if $y\le k$, and $2\sqrt{ky}-k$ if $y\ge k$, where $y=\rho_i\mathsf{A}_{ii}/2$, $k=d_i/2$. Both expressions are at least $2t_i\sqrt{y}-t_i^2$ when $t_i^2\le k$. The weights spend at most all of U_{A}, proving the claim after integrating the slices. Zero conditional mass contributes zero.

Quadratic supports on a radius box. Choose rational $\lambda_{ij}>0$ and a symmetric rational $M\ge 0$ with $M_{ij}=\lambda_{ij}^3$ off the diagonal. Put $\eta_i=(M_{ii}+\sum_{j\ne i}M_{ij})/2$, $u_{ij}=(2+(x_i^*)^2+(x_j^*)^2)^{1/3}$, and choose rational

$$0\le\eta_{ij}\le\frac{\lambda_{ij}}{3(2+h_i^2+h_j^2)^{1/3}}.$$

The common part of the support is

$$P_0(q) = \sum_{i<j}\Big\{\tfrac{3}{2}\lambda_{ij}u_{ij}^2 + \frac{2\lambda_{ij}}{u_{ij}}[x_i^*(q_i-x_i^*)+x_j^*(q_j-x_j^*)] \\ + \eta_{ij}[(q_i-x_i^*)^2+(q_j-x_j^*)^2]\Big\} - \sum_i \eta_i q_i^2 - 3\sum_i q_i. \tag{A.11}$$

The Hessian of $\frac{3}{2}\lambda(2+|z|^2)^{2/3}$ is at least $\frac{2\lambda}{3}(2+|z|^2)^{-1/3}I$. Taylor's formula on the pair rectangle proves its quadratic lower bound in (A.11). The negative distance squares in (A.6) sum to $U_{RMR} - \sum_i \eta_i q_i^2$, where $R = \operatorname{diag}(q_i)$. The remaining form is therefore a positive Gram potential with the reserved angular kinetic energy. Add one of the following three recoveries.

The conditional recovery chooses $\rho_i \ge 0$, $\sum_i \rho_i \le 1$ and $t_i \ge 0$, $t_i^2 \le k_i/2$, and adds

$$\sum_i [2t_i\sqrt{\rho_i M_{ii}/2}\, q_i - t_i^2].$$

This is (A.10). It uses all reserved angular kinetic energy and no pair recovery.

For the collective recovery choose $0 < \alpha \le 1$, $t > 0$, and a positive vector z^*, all rational. Put $y_i^* = h_i/\sqrt{k_i}$ and $\mathsf{C}_{ij} = M_{ij}y_i^*y_j^*$. Choose a rational Λ bounding either $\operatorname{tr}\mathsf{C}$ or $\max_i(\mathsf{C}z^*)_i/z_i^*$, and set $v_* = 2t + t^2\Lambda/\alpha - 1$. If every $l_i > 0$, choose

$$P_{\mathrm{en}} \ge \frac{\alpha\sum_i \theta(1+2/l_i^2)}{8t^2}(v_*)_+^2;$$

if some $l_i = 0$, require $v_* \le 0$ and put $P_{\mathrm{en}} = 0$. Add $t\sum_i M_{ii}q_i^2 - P_{\mathrm{en}}$. The matrix C is nonnegative entrywise and positive semidefinite. Its largest eigenvalue is bounded by its trace and by the displayed positive-vector bound: apply the eigenvector equation at an index maximizing the absolute component divided by z_i^*. The function $r/\sqrt{\theta(1+2/r^2)}$ is increasing, so the same eigenvalue bound holds at every point of the box. Formula (A.9) with the actual kinetic diagonal $\alpha\operatorname{diag}(\theta(1+2/q_i^2))$ proves this recovery. When a lower endpoint is zero, the verified inequality $v_* \le 0$ removes the penalty without an infinite endpoint estimate.

For the affine recovery choose $0 < \alpha \le 1$ and any rational matrix F satisfying, with $X = \operatorname{diag}(x_i^*)$ and $\mathsf{D} = \alpha\operatorname{diag}(k_i)$,

$$\mathsf{D} - F^T(\mathsf{D} + XMX)F \ge 0.$$

Add $\operatorname{tr}(\mathsf{D}(F-I)) + \sum_i (F^TXM)_{ii}q_i$. To prove this, set $E = XF$ and $Y = F^T\mathsf{D} + E^TMR$. The constraint implies $Y^T\mathsf{D}^{-1}Y \le \mathsf{D} + RMR$: stack $\mathsf{D}^{1/2}F, M^{1/2}E$ and use that a matrix whose column Gram matrix is at most D becomes a contraction after multiplication by $\mathsf{D}^{-1/2}$. For $\mathsf{B} = Y - \mathsf{D}$ this is precisely the hypothesis of (A.8), whose trace is the asserted affine function. No symmetry of F is used.

Pair recoveries. For the collective and affine recoveries, the fraction $1-\alpha$ of the reserved kinetic energy can be used as follows. An unused pair contributes zero. For a used pair require $\alpha < 1$ and $l_i, l_j > 0$, and choose rational $b_{ij}^* > 0$, $\kappa_{ij} > 0$, $\tau_{ij} \ge 0$. Choose $0 < d_- \le d_+$ enclosing $d_*(q) = (2+q_i^2+q_j^2)^{1/3}/\lambda_{ij}$ on the box, set $s_h = h_i + h_j$, and require

$$b_{ij}^* \le \frac{2\lambda_{ij}^3 l_i^2 l_j^2 (s_h + 2d_-)}{s_h(s_h+d_+)^2}, \\ \kappa_{ij} \le (1-\alpha)(k_i+k_j)/4, \qquad \kappa_{ij}(3\tau_{ij}+\tau_{ij}^2) \le 2b_{ij}^*.$$

Let $I_{ij} \subset [-1,1]$ enclose throughout the box

$$z_{ij}(q) = \mathrm{clip}_{[-1,1]} \frac{q_i^2 + q_j^2 - d_*(q)^2}{2q_i q_j}.$$

Put $p^*_{ij} = \kappa_{ij}(1-\tau_{ij})/2$ and require $b^*_{ij} + p^*_{ij} > 0$. Define z^*_{ij} as the minimum of z^2 on I_{ij} if $p^*_{ij} \geq 0$, and its maximum otherwise. The allowed rational pair constant is

$$0 \leq g_{ij} \leq \max\left\{0, \frac{\kappa_{ij}\tau_{ij}}{2} + \frac{b^*_{ij}p^*_{ij}z^*_{ij}}{b^*_{ij}+p^*_{ij}}\right\}. \tag{A.12}$$

Indeed the exact remainder in (A.6) can be written

$$\frac{\lambda_{ij}^3}{2}\frac{d^*_{ij}+2d_*}{d^*_{ij}(d^*_{ij}+d_*)^2}((d^*_{ij})^2 - d_*^2)^2.$$

The prefactor decreases as d^*_{ij} increases. Replacing d^*_{ij} by $q_i + q_j$, and then using the stated endpoint bounds, puts this remainder above $b^*_{ij}(n_i \cdot n_j - z_{ij}(q))^2$. Clipping the center decreases distance from every point of $[-1,1]$.

Allocate $(1-\alpha)k_i/4$ of the ith kinetic coefficient to each incident pair, scaling the two coefficients down together if their sum exceeds κ_{ij}. Each electron occurs in four pairs, so the allocations do not exceed the available kinetic form. With $\widehat{z} = z_{ij}(q)$, $v_{ij} = n_i \cdot n_j$ and

$$\sigma_{ij} = \frac{(1+\tau_{ij})b^*_{ij}\widehat{z}}{b^*_{ij}+p^*_{ij}}, \qquad F_{ij}(v_{ij}) = \exp(-\tau_{ij}v_{ij}^2/2 + \sigma_{ij}v_{ij}),$$

the angular square identity bounds the pair form below by

$$\frac{\kappa_{ij}\tau_{ij}}{2} + \frac{b^*_{ij}p^*_{ij}\widehat{z}^2}{b^*_{ij}+p^*_{ij}} + \left(b^*_{ij} - \frac{\kappa_{ij}(3\tau_{ij}+\tau_{ij}^2)}{2}\right)\left(v_{ij} - \frac{b^*_{ij}\widehat{z}}{b^*_{ij}+p^*_{ij}}\right)^2.$$

This follows by differentiating F_{ij} on each sphere and using $1 - v_{ij}^2 \leq 1$ in the negative square term. The last coefficient is nonnegative, and the original pair form is also nonnegative. Minimizing over the center interval proves (A.12), for either sign of p^*_{ij}.

Integer enclosures and scalar signs. Each support just constructed is separable quadratic. Lower its constant, linear and quadratic coefficients separately to rational values and write the result as $P_Q(q) = c_Q + \sum_i (m_{Qi}q_i + v_{Qi}q_i^2)$. This remains a lower support because $q_i, q_i^2 \geq 0$. The exact reader uses the scale $S_* = 2^{160}$. An integer interval $[L,H]$ denotes $[L/S_*, H/S_*]$. Rational inputs are enclosed by floor and ceiling. Products use the four endpoint products with outward rounding, and division requires a positive lower denominator. Squares include zero when the interval does. Square-root endpoints are certified by comparisons with LS_*, HS_*, and cube-root endpoints by comparisons with LS_*^2, HS_*^2. Thus the radical bounds are integer inequalities. Even a dyadic input finer than 2^{-160} is enclosed outward. Induction over the finite expression proves inclusion with all rounding errors accounted for.

The reader requires positive lower pivots in interval symmetric elimination of M and, for an affine recovery, of $\mathsf{D} - F^T(\mathsf{D} + XMX)F$. Each trailing interval contains the exact Schur complement, since division has a positive pivot. Triangular congruence then proves positivity of the exact matrices. A zero-containing pivot or an inconclusive domain or sign check rejects the

record. The curvature η_{ij} is the lower enclosure endpoint of its bound. For collective recovery the reader takes the smaller of upward bounds for the trace and the positive-vector expression, and an upward bound for P_{en}. For pair gains it checks every displayed constraint and takes a downward bound in (A.12). If its lower distance enclosure is zero, $1/\lambda_{ij}$ is an admissible positive d_-. The implemented bound with zero in the numerator is smaller and remains sufficient. Unused pairs require zero τ_{ij} and contribute zero.

For each coordinate and field $h \in \{h_s, h_p\}$ the reader obtains a rational lower bound $\mu_{i,h}$ for

$$\min_{l_i \le r \le h_i} \left[m_{Qi} r + v_{Qi} r^2 + h(r) + \mathbf{1}_{\{i=1\}} \omega_1 B_1(r) + \mathbf{1}_{\{i=2\}} \omega_2 B_2(r) \right].$$

It splits at every field knot and the moment kinks b_1, b_2. On each segment the expression is $\mathfrak{a} r^2 + \mathfrak{b} r + \mathfrak{c}$. Both endpoints are evaluated; when $\mathfrak{a} > 0$, the vertex value $\mathfrak{c} - \mathfrak{b}^2/(4\mathfrak{a})$ is also included if $-\mathfrak{b}/(2\mathfrak{a})$ lies in the segment. With interval coefficients the vertex is included whenever its enclosure intersects the segment. If the enclosure of $\mathfrak{a}$ straddles zero, natural interval evaluation on the entire segment is included; if its upper endpoint is nonpositive, endpoints suffice. Taking the least lower endpoint over all these candidates proves $\mu_{i,h}$ without missing a minimum. For each marked index j in the record, the test is

$$c_* + c_Q + \mu_{j,h_p} + \sum_{i \ne j} \mu_{i,h_s} > \varepsilon_*. \tag{A.13}$$

The reader implements it by a signed integer lower numerator strictly greater than $\lceil S_*/100000 \rceil$.

The tree and its implementation. The fixed lithium witness starts with the eight bytes `LI5AF001` and the binary64 value 1280. Its root is $[0, 1280]^5$, with all five marks active. A node starts with `N`, has at most five acceptance records, and supplies for each a nonempty subset of its remaining marks. Each subset is removed after its successful scalar tests. If marks remain, a split at coordinate ι and exact dyadic $l_\iota < \mu < h_\iota$ has children

$$\begin{aligned} Q_{\mathrm{left}}: &\quad h_i \longmapsto \min(h_i, \mu) \quad (i \le \iota), \\ Q_{\mathrm{right}}: &\quad l_i \longmapsto \max(l_i, \mu) \quad (i \ge \iota). \end{aligned}$$

Other endpoints are unchanged. Both children inherit the remaining marks. The parser starts with nondecreasing lower and upper endpoint vectors. These properties persist, and strict containment makes every child width positive: $l_i \le l_\iota < \mu$ for $i \le \iota$ and $\mu < h_\iota \le h_i$ for $i \ge \iota$. A terminal tag `L` requires an empty remaining set. Otherwise the tag is `S` and a split is mandatory.

An ordered point in a parent belongs to the left child if $q_\iota \le \mu$ and to the right child if $q_\iota \ge \mu$. Fixing a point and a mark, either an ancestor discharged the mark or it descends to a child containing the point. The finite tree ends only with all inherited marks discharged. This proves coverage of every mark, including split faces. The implementation traverses in preorder with a stack, pushing the right child first. Emptying that stack, checking the end tag `E`, its success byte and the two footer counts, and requiring the byte cursor to equal the stream length prove complete consumption. Partial and trailing payloads fail. All binary64 values are checked for finiteness.

For specificity, support kinds $0, 1$ encode the two expressions in (A.7), in reverse displayed order. Kind 2 is conditional recovery, with five nonnegative integer numerators for ρ_i divided by 100000 and five dyadic t_i. Kinds 3 through 12 are collective recovery with successive values

$$\alpha = 1, .98, .95, .90, .80, .70, .60, .45, .30, .15;$$

their six dyadic parameters are t and the five entries of z^*. Kinds $13, 14, 15$ are affine recovery with $\alpha = 1, .9, .7$ and 25 row-major entries of F. Every node using a Gram support has the shared 15-entry payload of ten λ_{ij} and five diagonal entries of M. Collective kinds above 3 and affine kinds above 13 also carry ten values each of $b^*_{ij}, \kappa_{ij}, \tau_{ij}$ in lexicographic pair order. These payloads determine the formulas above. No fitted polynomial or stored numerical lower bound is accepted as a support.

The parser writes each support-bearing node once, with its node number, inherited mask, reconstructed endpoints and unchanged payload, into shards beginning `LI5FS001`. The exact reader reconstructs every support from that payload and writes its node, kind, mask and one signed integer per marked inequality only after the tests have passed. The aggregator matches these records against every parser-produced shard, checks all signs, rejects repeated or omitted shards and extra or missing sign bytes, and requires the seen shard set to equal the manifest's entire set. Thus its recordwise checks establish completeness, rather than inferring it from a count or a minimum.

Completed evaluation. The preserved witness has 161995 nodes and 80998 leaves. The complete parser execution produced 50 shards containing 98264 support-bearing rows and 114350 supports. Two independent arithmetic executions consumed shard ranges $[0, 1)$ and $[1, 50)$, with no row limit. The first checked 2000 rows, 2163 supports and 7399 marks. The second checked 96264 rows, 112187 supports and 310180 marks. Both returned normally after their complete selected shards, and the aggregator consumed the resulting streams in full on the same preserved parser outputs. The support counts in order of kinds 0 through 15 are

$$(781, 194, 23528, 4716, 636, 2225, 4095, 195, 392, 0, 0, 0, 0, 23359, 33275, 20954).$$

All 317579 marked inequalities were evaluated. Their least integer lower numerator, with denominator S_*, is

$$1464261291397113583138217705464494289225955 2 > \lceil 2^{160}/100000 \rceil.$$

These are results of the complete evaluations whose exact input, reader, and producer-to-consumer records are retained in the code/data release. The execution assumptions stated at the beginning of this appendix apply to the actual linked bytes and runs. The enclosure and implementation arguments above make these evaluations proofs of all finite support and marked-sign predicates. The witness generator's floating calculations are not premises.

Scalar closure on all radii. For $0 < q_1 \le \cdots \le q_5 \le 1280$, take $G(q)$ to be the maximum of $-3\sum_i q_i$ and all certified supports whose boxes contain q. This finite, measurable maximum bounds (A.4) below. Because every mark was discharged somewhere on its containing path, it satisfies

$$G(q) + c_* + V(q) + h_p(q_j) + \sum_{i \ne j} h_s(q_i) \ge \varepsilon_* \qquad (1 \le j \le 5) \tag{A.14}$$

on the compact ordered cone.

For the exterior, a global pointwise support is

$$G_\infty(q) = -6(q_1 + q_2) + \frac{3}{20}(q_3 + q_4 + q_5).$$

To check it, use the tangent proof of (A.5) with equal pair parameter $3/5$ on the three outer points. The scalar term $\mathcal{F}_{3/5} \ge 0$ follows from $(1 + z^2)^{2/3} \ge 1 + z^2/2$, and the kernel square gives $\mathcal{V}_3 \ge (144/125)(q_3 + q_4 + q_5)$. Each inner-outer pair contributes at least $q_j - q_i$ by the triangle

inequality. Adding the six such pairs, discarding the inner pair, and subtracting $3\sum_i q_i$ gives outer coefficient $19/125 > 3/20$. Nonnegative reciprocal and kinetic terms preserve this lower bound. Enlarge G by its maximum with G_∞ on the compact cone and use $\max(-3\sum_i q_i, G_\infty)$ outside it.

The field table gives $h_s, h_p \geq -24$ and $h_s + 3r/20, h_p + 3r/20 \geq 0$. At knots $60, 130, 200$ the respective smallest latter values are $8.407, 8.016, 6.942$. All earlier knot values are nonnegative, and the affine and constant continuations preserve these estimates. Completing the square gives

$$\omega_a B_a(r) - 6r \geq -6b_a - 9/\omega_a - \omega_a/(2\delta_a),$$

which is greater than -34 for $a = 1$ and -30 for $a = 2$. Since $c_* > -31$, when $q_5 \geq 1280$ every marked scalar expression with G_∞ is greater than $-31 - 58 - 54 + (3 \cdot 1280/20 - 24) = 25$. Thus (A.14) holds on the entire cone.

For the all-s expression, $h_p - h_s \leq .094$ on $[0, 130]$, by the knot differences. Since $e_s - e = .119$, using mark 1 proves

$$G(q) + e_s - 2U_0 - 15/8 + V(q) + \sum_i h_s(q_i) \geq \varepsilon_* \tag{A.15}$$

when $q_1 \leq 130$. If $q_1 \geq 130$, both functions $\omega_a B_a(r) - 6r$ increase there, and their values at 130 exceed $41351/10$ and $72841/10$. The all-s expression is then greater than $(41351 + 72841)/10 - 120 - 31 > 11000$. This proves (A.15) everywhere needed.

The fermionic weighted form. Pass to reduced radial measure by

$$\psi(r, n, \sigma) = \Big(\prod_i r_i\Big) u(r_1 n_1, \ldots, r_5 n_5, \sigma),$$

where $\sigma \in \{1, 2\}^5$ indexes the spin components. This is unitary and preserves antisymmetry. For one coordinate,

$$\frac{1}{2}\int p|\partial_r \psi - \psi/r|^2 = \frac{1}{2}\int p|\partial_r \psi|^2 + \int |\psi|^2,$$

since $p'/(2r) = 1$. The original constant $-15/2$ therefore becomes $-5/2$. Allocating $-1/8$ to each of the five radial forms leaves $-15/8$. Split the angular kinetic energy into shares $1 - \theta$ and θ, and apply the full-angular bound $\mathcal{A}(q) \geq G(q)$ before any angular projection. The left side in the statement is bounded below by

$$\sum_i \langle \psi, K_{L_i} \psi \rangle + \int [G(q) - 2U_0 - 15/8 + V(q)]|\psi|^2,$$

where K_{L_i} denotes the angular direct sum of the K_ℓ in the ith coordinate.

This new form commutes with every labeled angular projection. In a tuple $(\ell_1, \ldots, \ell_5)$ having a nonzero angular momentum, choose one such label m, independently of the radii. Subtract $h_p(r_m)$ from its operator and h_s from the other four. By Lemma A.2, the marked energy is at least -7.119. Each unmarked non-s operator is at least -7.793. For an s operator, let Q_b be the spectral projection of $K_0 - h_s$ onto $(-\infty, -7.793)$. Then

$$K_0 - h_s \geq -7.793 + (-10.624 + 7.793)Q_b.$$

The radial rank of Q_b is at most one, and its spin-inclusive rank at most two. The true s labels remain antisymmetric in radial and spin variables, so their total occupation of this subspace is at

most two. The four unmarked energies are therefore at least $2(-10.624) + 2(-7.793)$. Together with the marked energy they give e. The fixed labeled radius r_m is some q_j, so the five inequalities (A.14) restore the fields and give $\varepsilon_*\|\psi\|^2$ on this tuple. No field is assigned to a differential operator according to radial rank.

In the all-s tuple let also Q_c project below -7. Its radial rank is at most two by the stronger bound at -6.995. Spectral calculus gives

$$K_0 - h_s \geq -7 + (-7.793 + 7)Q_c + (-10.624 + 7.793)Q_b.$$

The spin-inclusive occupation bounds are four and two. Thus the five one-body energies sum to at least $2(-10.624) + 2(-7.793) - 7 = e_s$, and (A.15) gives the same final bound.

Finally the angular constant test in $\mathcal{A}(q) \geq G(q)$ gives

$$-3\sum_i q_i \leq G(q) \leq \sum_{i<j} \frac{r_i^2 + r_j^2 + 2}{\max(r_i, r_j)} - 3\sum_i r_i,$$

because the spherical average of $|r_i n_i - r_j n_j|^{-1}$ is $1/\max(r_i, r_j)$. On bounded radius sets these bounds and the Hardy inequality control the multiplication terms by $C(1 + \sum_i 1/r_i)$. They justify integration of the angular form bound, smooth approximation away from the coordinate origins, and finite angular truncation. Pair Coulomb terms have the same control in relative coordinates. Summing all angular tuples, then closing the form on the compactly supported physical H^1 domain, proves the stated inequality for every spin component and every allowed fermionic vector. □

B The helium interior certificate

This appendix proves the interior bound that Section 5 uses for the helium monoanion.

Lemma B.1 (Helium interior gaps)**.** *Assume Set-up 2.2 for the specified original S134/P41 computations. Let $B_7 = \{x \in \mathbb{R}^3 : |x| < 7\}$, $K_7 = (B_7)^3$, and $z = -2903724372/10^9$. For antisymmetric $v \in H^1(K_7; \mathbb{C}^8)$ define*

$$q_<[v] = \frac{1}{2}\sum_{i=1}^{3} \int_{K_7} |\nabla_i v|^2 + \int_{K_7} \left[-2\sum_{i=1}^{3} \frac{1}{|x_i|} + \sum_{i<j} \frac{1}{|x_i - x_j|} \right] |v|^2.$$

Let S denote the full sector with total orbital angular momentum 0, total spin $1/2$ and even parity, and P the full sector with total orbital angular momentum 1, total spin $1/2$ and odd parity. Let dS be Euclidean surface measure on the three exposed faces of ∂K_7; their intersections have measure zero. All integrals sum spin components. Set $\eta_S = 16131/7000000$ and $\eta_P = 95183/14000000$. Then, for each $J \in \{S, P\}$ and every such v in sector J,

$$q_<[v] + \frac{1}{16}\int_{\partial K_7} |\operatorname{Tr} v|^2 \, dS \geq (z + \eta_J)\|v\|^2_{L^2(K_7)}.$$

The assertion includes every magnetic component of each sector.

Proof. We first identify the complete reference spectral subspaces and their physical normalization. We then compare their inverse-repulsion matrices with exact polynomial cubatures, bound the

errors in the recorded evaluations, and certify the decimal centers by integer residuals. A quadratic-form comparison converts the resulting matrix ceilings into the asserted gaps.

Fixed inputs and execution assumptions. The accompanying code/data release contains the original S134 and P41 orbital tables, the two complete integer current tensors, eight Gaussian mesh tables, the two decimal centers and triangular integer witnesses, and the complete executions and auxiliary certificates used below. The orbital coefficients have denominator 2^{96}. Their energy midpoints are exact means of the rational endpoints in the tables. Each current tensor has $42 \cdot 3 \cdot 10^3 = 126000$ signed integers. The Gaussian endpoints have denominator 2^{196}. These data specify the fixed instance. None of their asserted approximation errors is accepted merely from its input annotation.

The fixed profile parameters are given in Table 5. Here n, m are the state and angular-surface dimensions, respectively; n_1, n_2, n_3 are the radial orders and n_a the angular order. The remaining symbols denote the numerical bounds justified below.

parameter	S	P
(n, m)	$(134, 47)$	$(41, 21)$
(n_1, n_2, n_3, n_a)	$(122, 98, 60, 25)$	$(107, 83, 51, 17)$
h_0	24	16
M	.365	.803
e_f	$4.44 \cdot 10^{-6}$	$1.69 \cdot 10^{-8}$
ζ	$1.9 \cdot 10^{-14}$	$5.3 \cdot 10^{-15}$
e_T	$9.2 \cdot 10^{-12}$	$2.27 \cdot 10^{-12}$
ρ	$6.4 \cdot 10^{-12}$	$1.7 \cdot 10^{-15}$
d_D	$4 \cdot 10^{-16}$	$8.5 \cdot 10^{-17}$
d	2.1	2
Center error bound	.0000204636	.000000224031

Table 5: The original cubature profiles and their error bounds. The first four local caps concern computed multipliers, multiplier errors, weighted angular pairs and radial cells. Subscripts J are suppressed in the table and in the assembly estimates.

Here is the execution contract in Set-up 2.2 for this instance. It applies to the original complete run and the retained auxiliary audits.

(R1) The loaded Julia 1.12.6 and its LinearAlgebra revision `7249e662d66b53da6c933 5ea748eac2750c2924f` faithfully implement their pinned sources. The ILP64 OpenBLAS 0.3.29 library faithfully implements the Cooperlake/SkylakeX binary64 NN and TN kernels, their ordinary and small variants, the generic compile-time alternatives, and the GEMV alternatives described below. Dispatch, the ILP64 interface, strides, indexing, allocation and memory access are correct. This includes the correspondence of the loaded code with these sources.

(R2) Every participating operating-system thread, including a thread to which a Julia task migrates, remains in binary64 round-to-nearest, ties-to-even mode, with gradual underflow and with flush-to-zero and denormals-are-zero disabled. Scalar, vector and fused operations obey these semantics. Loads, stores, copies and permutations preserve values. Fusion and reassociation of the specified classical sum graphs are allowed; extra signed terms, reduced precision, approximate operations and other transformations are excluded.

(R3) Julia respects lexical loop-local allocation and thread joins. Each BLAS call has one computational thread; concurrent calls from different Julia tasks are reentrant with disjoint scratch storage and safe initialization and dispatch. S requests six Julia threads and P four. Shared inputs remain immutable, diagnostics preserve inputs and floating-point state, and group reduction follows the join.

(R4) DelimitedFiles revision `db79c842f95f55b1f8d8037c0d3363ab21cd3b90` uses the ordinary deterministic shortest-round-trip printer, without a precision-limiting I/O override. Each printed finite decimal, interpreted as a rational, rounds back to the binary64 value printed. Equal numerical entries print equal rationals; signed zeros denote zero. Files and records are preserved faithfully.

In the local routines, primitive addition, subtraction, multiplication, division and square root are correctly rounded. A multiply-add either has one fused rounding or has separately rounded multiplication and addition, as specified below. The compensated integer-power graph is specified below as well. BigInt and rational arithmetic, integer square-root certification, decoding, TOML/JSON/text operations and finite file and subprocess operations are faithful. Assertions and failure propagation are enabled. Decimal integer conversions are total on these inputs. Rational-to-BigFloat conversions round to nearest at precision at least 192, with the particular precision changes described below. Repeated calls to the Gaussian-node, cosine and angular-table routines on identical inputs have the same deterministic implementation and operation graph. In particular, the same tridiagonal eigensolver input returns the same ordered binary64 nodes and weights independently of the calling task. Their accuracy is proved by endpoint comparisons, not assumed. These conditions are assumptions about execution. Version strings, hashes and separate-process diagnostics do not prove them, and the historical diagnostics did not inspect every assembly thread's floating-point control state.

The complete reference spectrum. Let h be the scalar one-electron form operator on B_7 with nuclear charge two and boundary term $\| \operatorname{Tr} w\|^2/16$. Let $H_0 = \sum_{i=1}^{3} (h \otimes I_{\mathbb{C}^2})^{(i)}$ on the antisymmetric space over K_7. Put

$$\delta_S = \frac{5}{2}, \qquad \delta_P = 1, \qquad C_J = z + \delta_J, \qquad D_J = (C_J - H_0)_+^{1/2}.$$

Spherical separation, with reduced radial measure dr, gives

$$q_\ell[w] = \int_0^7 \left\{ \frac{|w'|^2}{2} + \left(\frac{\ell(\ell+1)}{2r^2} - \frac{2}{r} \right) |w|^2 \right\} dr - \frac{|w(7)|^2}{112}, \qquad w \in H^1(0,7), \quad w(0) = 0. \tag{B.1}$$

Indeed the radial kinetic integration contributes $-|w(7)|^2/14$, and $1/16 - 1/14 = -1/112$. The operator boundary condition is $w'(7) = w(7)/56$. Hardy's inequality $\|w/r\|_2 \le 2\|w'\|_2$ and the trace inequality show that a shifted form norm controls $H^1(0,7)$. Hence each channel has compact resolvent.

We give the spectral cutoff argument, since completeness of the finite matrices is essential. For a positive comparison function φ, integration by parts gives

$$\begin{aligned} q_\ell[w] = \frac{1}{2} \int_0^7 \varphi^2 |(w/\varphi)'|^2 + \int_0^7 \frac{-\varphi''/2 + [\ell(\ell+1)/(2r^2) - 2/r]\varphi}{\varphi} |w|^2 \\ + \left(\frac{\varphi'(7)}{2\varphi(7)} - \frac{1}{112} \right) |w(7)|^2. \end{aligned} \tag{B.2}$$

It suffices first to use w vanishing near zero and then pass by H^1 density and Hardy's inequality. The physical radial function $e^{-2r}(1+15r^{16}/(23\,7^{15}))$ satisfies the physical Robin condition and has local energy at least

$$-2-\frac{136}{23\,7^{15}}\left(\frac{119}{30}\right)^{14}>-2.0004.$$

This proves $h>-2.0004I$. The trial e^{-2r} has energy strictly below -2, since its boundary correction is $-15/16$ times its positive boundary norm.

There is precisely one spatial level below $B_*=-47881/87500>-11/20$. Here are comparison functions which verify this assertion without a numerical spectral assumption. For $\ell\geq 1$, apply (B.2) at $\ell=1$ to $r^2e^{-r}(1+41r^7/(15\,7^7))$ and then use monotonicity in ℓ. Its local energy is at least $-1/2-41\,25^5/(3\,42^6)>-21/40>B_*$. In the $\ell=0$ channel impose $w(1)=0$, a single linear condition. On $(0,1)$ use $r(1-r)e^{-r}$, of local energy $-1/2$. On $(1,7)$ use $r(r-1)e^{-r}(1+17(r-1)^6/(7\,6^6))$. Its logarithmic derivative at seven is $1/56$, and its local energy is bounded below by $-1/2-4131/87500=B_*$: with $s=r-1$, the negative correction is at most $6[17/(7\,6^6)]s^4(9/2-s)_+$, whose maximum is $4131/87500$. The negative spectral subspace below B_* thus has dimension at most one. Together with the trial above, this isolates the simple core shell $s=(0,1)$ with $-2.0004<e_s<-2$. It has two spin states and can be occupied at most twice.

Further applications of (B.2) give

$$h_3\geq-\frac{1}{8},\qquad h_4>\frac{1}{100},\qquad h_5>\frac{1}{10},\qquad h_9>\frac{4}{5}.$$

For these four comparisons take respectively

$$r^4e^{-r/2},\quad r^5e^{-2r/5}(1-83r^2/7987),\quad r^6e^{-r/3}(1-85r^2/6517),\quad r^{10}e^{-r}(1-23r^2/1911).$$

All are positive on $(0,7]$. The last three have logarithmic derivative $1/56$ at seven, and the first leaves boundary coefficient $3/112$. For the middle two the local-energy lower bounds are $-2/25+747/7987>1/100$ and $-1/18+1020/6517>1/10$. For the last, the bound is $9/14+115/637>4/5$. These inequalities follow by completing the square in, respectively, $1-2r/5+(9/2)(83/7987)r^2$, $1/2-r/3+6(85/6517)r^2$, and $3-r+(15/2)(23/1911)r^2$. Also $h_\ell\geq h_5+[\ell(\ell+1)-30]/98$ for $\ell\geq 5$.

Every shell in the S deficit has energy below $18/5$, since $18/5-2(2.0004)>C_S$. No degree $\ell\geq 9$ occurs: with no core its configuration energy exceeds $4/5-11/10>C_S$; with one core, angular momentum zero requires the other two degrees to agree, giving energy $>-2.0004+8/5>C_S$; with two cores the remaining degree is zero. With no core every shell is below $C_S+11/10$. With one core and common nonzero degree ℓ, use the lower bounds just proved for its partner. The resulting sufficient cutoffs and exact counts are in Table 6. For P, $3B_*>C_P$ forces a core. Angular momentum one and odd parity then require adjacent remaining degrees $\ell,\ell+1$. The bounds for h_4,h_5 exclude $\ell\geq 4$, since $-2.0004+1/100+1/10>C_P$. The partner bounds $-11/20$ and $h_3\geq-1/8$ give precisely the P cutoffs in the table.

For precision about the finite spectral checks, the regular solution at energy E is

$$y_{\ell,E}(r)=(r/7)^{\ell+1}\sum_{k\geq 0}a_k(r/7)^k,\qquad a_{-1}=0,\quad a_0=1,\quad a_k=-\frac{28a_{k-1}+98Ea_{k-2}}{k(k+2\ell+1)}.$$

The Robin expression is $\mathcal{B}_\ell(E)=(\ell+7/8)\sum a_k+\sum ka_k$. The singular independent solution fails the form condition at zero, so its zeros are precisely the simple channel eigenvalues. At truncation

ℓ	0	1	2	3	4	5	6	7	8
S cutoff	18/5	43/20	43/20	69/40	8/5	3/2	11/8	5/4	43/40
S count	7	5	4	3	3	2	2	1	1
P cutoff	13/20	21/10	13/20	13/20	9/40	–	–	–	–
P count	4	5	3	2	1	–	–	–	–

Table 6: Complete radial support cutoffs and eigenvalue counts.

260, let $T = \max(|a_{259}|, |a_{260}|)$. For all test energies, $-3 \le E \le 41/8$, each subsequent pair of coefficients is bounded by a quarter of its predecessor pair. The series tail is at most T on $[0, 1]$, and the differentiated tail at one is at most $520T$. Thus strict signs are certified by the truncated values with these explicit allowances.

At a cutoff, evaluate the regular series at $k/56$, $1 \le k \le 56$. In physical radius the spacing is $1/8$. There is no zero in the first cell and at most one in any later cell. Indeed integration of the equation between zeros, followed by Cauchy–Schwarz in the first cell or the Dirichlet inequality in later cells, gives contradictions to $4/8 + (41/8)/64 < 1$ and $(2(41/8) + 32)/64 < \pi^2$, respectively. Consequently the count of interior zeros is the number of sample sign changes, starting with the positive sign at zero. The number of eigenvalues below E is this count plus one when $\mathcal{B}_\ell(E)/y_{\ell,E}(7) < 0$. For an elementary justification of the last rule, impose zero traces at the interior zeros in (B.2). This bounds the negative index by the number of imposed traces, with one more trace at seven if the boundary coefficient is negative. For the reverse inequality use the disjoint nodal pieces of $y_{\ell,E'}$ for $E' < E$ sufficiently close to E, including the last piece exactly when that coefficient is negative. Their span has strictly negative form at E. Simple zeros persist under this small energy change. This proves the counting rule.

The complete integer sign certificates in the release verify this rule at all fourteen cutoffs and opposite Robin signs at every noncore bracket in Table 7. Their arithmetic can be checked as follows. For S use degree 80 and scale 10^{24}, for P degree 60 and scale 10^{18}. Writing a test energy as p/q, the stored integers obey

$$-28qc_{k-1} - 98pc_{k-2} = qk(k + 2\ell + 1)c_k + \rho_k, \qquad 0 \le \rho_k < qk(k + 2\ell + 1).$$

Each sample is evaluated by integer Horner divisions with divisor 56, retaining all remainders. For S, $|a_k| \le 20^k/k!$, $20^{79}/79! < 10^{-12}$, and propagation of coefficient rounding is bounded by $e^{20} < 10^9$. The total sample error is $< 10^{-11}$ and the Robin error $< 10^{-9}$. The corresponding stored integers have magnitudes $> 10^{13}$ and $> 8 \cdot 10^{15}$, the latter before division by $8 \cdot 10^{24}$. For P use $15^k/k!$, $15^{59}/59! < 10^{-10}$ and $e^{15} < 4 \cdot 10^6$. The errors are $< 10^{-9}$ and $< 10^{-7}$. The integers exceed 10^9 and $8 \cdot 10^{11}$ in magnitude. The finite recurrence, remainder and strict-sign tests involve every listed cutoff, every bracket endpoint and every sample. They give the counts in Table 6. The disjoint brackets exhaust those counts, so each contains exactly one eigenvalue.

Physical bases and orbital transport. Write $a = (\ell, k)$ for a shell, e_a for its eigenvalue, f_a for a real normalized radial eigenfunction, and m_a for its fixed rational midpoint. Let

$$\widehat{f}_a(r) = 2^{-96} \sum_k q_{a,k} T_k(2r/7 - 1), \qquad T_0 = 1, \quad T_1(x) = x, \quad T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x).$$

All 28 rows are used for S, and P uses the common first $4, 5, 3, 2, 1$ rows in degrees $0, 1, 2, 3, 4$. The maximal polynomial degrees are 37 for S and 32 for P. The following certified bounds hold with a common phase on shared rows:

$$\|f_a - \widehat{f}_a\|_2 < 10^{-15} + \sqrt{7}\, 10^{-17}, \qquad |e_a - m_a| < 41 \cdot 10^{-18}. \tag{B.3}$$

ℓ	ordered noncore eigenvalue brackets
0	$(-.505,-.504),(-.240,-.239),(.206,.207),(.923,.924),(1.865,1.866),(3.022,3.023)$
1	$(-.503,-.502),(-.247,-.246),(.123,.124),(.753,.754),(1.602,1.603)$
2	$(-.246,-.245),(.003,.004),(.518,.519),(1.258,1.259)$
3	$(-.113,-.112),(.271,.272),(.898,.899)$
4	$(.023,.024),(.543,.544),(1.283,1.284)$
5	$(.177,.178),(.830,.831)$
6	$(.350,.351),(1.136,1.137)$
7	$(.544,.545)$
8	$(.759,.760)$

Table 7: Radial brackets for S; P uses the initial numbers of levels specified by its row of counts, including the core in degree zero.

Here is the residual certificate underlying these bounds. The release supplies auxiliary denominator-2^{120} Chebyshev polynomials p_a and rational centers μ_a. Put $x = r/7$, expand $p_a(7x) = \sum_k \mathsf{P}_k x^k/2^{120}$, and set $d_a = \min(\ell+1, 2)$. Define the corrected polynomial by

$$g_a(x) = 2^{-120}\left[\sum_{k\ge d_a} \mathsf{P}_k x^k - \frac{x^{d_a}}{8d_a - 1}\sum_{k\ge d_a}(8k-1)\mathsf{P}_k\right].$$

It has a factor x^{d_a}, and differentiation gives $8g_a'(1) - g_a(1) = 0$. Thus the radial function $r \mapsto g_a(r/7)$ vanishes at zero and satisfies the Robin condition at seven. Its second derivative and potential term belong to $L^2(0,7)$: for $\ell = 0$ the centrifugal term is absent, and for $\ell \ge 1$ the factor r^2 cancels its singularity. Integration by parts in (B.1) therefore puts this function in the radial operator domain. Its residual, expressed in x, is

$$-g_a''/98 + \ell(\ell+1)g_a/(98x^2) - 2g_a/(7x) - \mu_a g_a.$$

Exact coefficient arithmetic and $|T_k| \le 1$ certify

$$\begin{aligned}\|p_a - g_a(\cdot/7)\|_{L^2(0,7)} &< 2\cdot 10^{-16},\\ \|(h_\ell - \mu_a)g_a(\cdot/7)\|_{L^2(0,7)} &< 2\cdot 10^{-17},\\ \left|\|g_a(\cdot/7)\|^2_{L^2(0,7)} - 1\right| &< 2\cdot 10^{-16}.\end{aligned}$$

The norm evaluation uses $T_iT_j = (T_{i+j} + T_{|i-j|})/2$ and $\int_0^1 T_{2k}(2x-1)\,dx = (1-4k^2)^{-1}$, with odd integrals zero. All other channel eigenvalues are farther than $1/10$ from μ_a, as follows from the adjacent coarse brackets and cutoffs. Expanding $g_a(\cdot/7)$ in the radial eigenbasis therefore bounds its orthogonal component by ten times the residual. Its target component has magnitude greater than $1/2$. This gives $\|p_a - f_a\|_2 < 10^{-15}$ and $|e_a - \mu_a| < 4\cdot 10^{-17}$. Finally the complete coefficient comparisons satisfy

$$2^{-120}\sum_k |2^{24}q_{a,k} - p_{a,k}| < 10^{-17}, \qquad |m_a - \mu_a| < 10^{-18},$$

where $p_{a,k}$ are the auxiliary Chebyshev integers. This proves (B.3). It uses no presumed accuracy of the narrower stored energy endpoints.

For S, order shells by m_a and retain lexicographic triples $a \le b \le c$ with midpoint sum below C_S, even degree sum, the triangle inequalities, and not all three labels equal. Move a repeated

first pair to the last two positions. For P, order shells by (ℓ, k) and retain $\{s, a, b\}$ with $a = (\ell, k)$, $b = (\ell + 1, j)$, $0 \le \ell \le 3$, and midpoint sum below C_P. Addition of the coarse bracket endpoints exhaustively tests these finite lists: S has $6, 72, 56$ fixed-spin states with two, one and zero core electrons, respectively. P has five repeated-core and eighteen distinct-shell occupations. Included deficits exceed $13/250$ in S and $69/1000$ in P. Excluded finite comparisons have margin $> 28/1000$ and $> 29/1000$, respectively. The sorted midpoint energies are separated by $> 1/2500$. Thus the error in (B.3) and the $< 10^{-13}$ error in the source's three-term binary64 selection cannot change either list.

To specify normalization, let $A_{\ell_1\ell_2\ell_3}$ denote the real scalar tripolar harmonic in the Condon–Shortley convention, of norm one for $\prod_i d\omega_i/(4\pi)$. For S define $[abc] = f_a(r_1)f_b(r_2)f_c(r_3)A_{\ell_a\ell_b\ell_c}$. For P start with $[sab] = f_s(r_1)f_a(r_2)f_b(r_3)\mathbf{V}_\ell(\boldsymbol{n}_2, \boldsymbol{n}_3)$, where $P_\ell(1) = 1$ is the Legendre polynomial and

$$\mathbf{V}_\ell(\boldsymbol{a}, \boldsymbol{b}) = \frac{P'_{\ell+1}(\boldsymbol{a}\cdot\boldsymbol{b})\boldsymbol{b} - P'_\ell(\boldsymbol{a}\cdot\boldsymbol{b})\boldsymbol{a}}{\sqrt{\ell+1}}.$$

Every assignment permutes the entire radial and angular expression. Put $F_{abc} = ([abc]-[bac])/\sqrt{2}$. For distinct shells take

$$\frac{F_{abc} + F_{acb}}{\sqrt{2}}, \qquad \frac{F_{abc} - F_{acb} - 2F_{bca}}{\sqrt{6}};$$

for a repeated S occupation take F_{abb}, and for a repeated P core take F_{sbs}. Convert a P vector to $\sqrt{3}$ times its third component. Divide each resulting reduced scalar by $(4\pi)^{3/2}r_1r_2r_3$, calling the result w, and give the spinor the three nonzero components

$$\frac{w(x_1, x_2, x_3)}{\sqrt{3}}, \quad -\frac{w(x_1, x_3, x_2)}{\sqrt{3}}, \quad \frac{w(x_2, x_3, x_1)}{\sqrt{3}}$$

at $\uparrow\uparrow\downarrow, \uparrow\downarrow\uparrow, \downarrow\uparrow\uparrow$, respectively.

These formulas give isometries F_J onto the entire fixed magnetic subspaces of $\operatorname{ran} D_J$, of dimensions 134 and 41. For completeness, tensoring degree-i and degree-j angular representations gives each degree $|i-j|, \ldots, i+j$ once: subtract the multiplicities of adjacent weights in the product to obtain this count. Thus an S angular invariant is unique exactly for a triangle. Its exchange sign is $(-1)^{i+j+k}$, as is seen by exchanging the factors of the invariant $\Delta_{12}^{i+j-k}\Delta_{23}^{j+k-i}\Delta_{31}^{k+i-j}$ in the homogeneous-polynomial representation, where $\Delta_{ij} = \mathsf{u}_i\mathsf{v}_j - \mathsf{v}_i\mathsf{u}_j$ are the determinant polynomials in the two formal variables of each factor. For distinct shells the three first-two-antisymmetric assignments are orthonormal. Spin raising annihilates precisely the coefficient plane orthogonal to $(1, -1, 1)$, with the two orthonormal vectors displayed above. Repeated shells leave one vector. Three equal S shells leave none. The P vector is the negative gradient of $|\boldsymbol{y}|^{-\ell-1}P_\ell(\boldsymbol{a}\cdot\boldsymbol{y}/|\boldsymbol{y}|)/\sqrt{\ell+1}$ on the unit sphere. Its separate degrees are $\ell, \ell+1$, and

$$\int |\mathbf{V}_\ell|^2 = \frac{1}{\ell+1}\left\{\frac{(\ell+1)^2}{2\ell+1} + \frac{\ell(\ell+1)}{2\ell+1}\right\} = 1.$$

This gives the unique permitted P angular copy. The spectral cutoff and finite lists above therefore exhaust the deficit, rather than select a trial subspace. The radial factors cancel the Cartesian Jacobians, the three spin components preserve inner products, and rotational invariance gives $3\int B_{\alpha,3}B_{\beta,3} = \int \boldsymbol{B}_\alpha \cdot \boldsymbol{B}_\beta$, also with an invariant multiplier inserted. These identities account for every physical measure and magnetic factor.

Let $\widehat{F}_J$ replace f_a by $\widehat{f}_a$ in these formulas, let W_J be diagonal with entries $\sqrt{C_J - \sum_{a\in\alpha} m_a}$, and put $X_J = D_J F_J$, $\widehat{X}_J = \widehat{F}_J W_J$. At most seven radial functions occur in a channel, so (B.3)

bounds the one-electron map error by $3\cdot10^{-15}$. Telescoping the third tensor power, then restricting to its antisymmetric subspace, gives error $(1+3\cdot10^{-15})^3-1<9.1\cdot10^{-15}$. All deficits exceed $1/20$. Hence the error in their exact square roots is $<3.1\cdot10^{-16}$, using $|\sqrt{a}-\sqrt{b}|=|a-b|/(\sqrt{a}+\sqrt{b})$. The core capacity and noncore floor give $\|X_S\|<3$, $\|X_P\|<2$, and therefore

$$\|\widehat{F}_J\|<t_0:=1+2\cdot10^{-14},\qquad \|X_S-\widehat{X}_S\|<28\cdot10^{-15},\quad \|X_P-\widehat{X}_P\|<19\cdot10^{-15}. \tag{B.4}$$

Currents and exact cubature. List the 42 even angular triangles with degrees at most four lexicographically as Λ_p, $0\le p<42$. The current integers Q^J_{p,j,a_1,a_2,a_3}, $0\le j<3$, $0\le a_i<10$, are decoded as signed little-endian 64-bit words at zero-based position $p+42j+126(a_1+10a_2+100a_3)$. On sorted radii $(7t_1,7t_1t_2,7t_1t_2t_3)$ define

$$b_{Jj}=2^{-32}\sum_{p,a_1,a_2,a_3}Q^J_{p,j,a_1,a_2,a_3}A_{\Lambda_p}\prod_{i=1}^{3}T_{a_i}(2t_i-1),\qquad b_{J*}=1-\sum_{j=0}^{2}b_{Jj}.$$

The three currents correspond, in order, to the sorted pairs $12,13,23$. Relabel the whole rule on each ordering chamber and set

$$U_J=\frac{b_{J*}^2}{\delta_J}+d_{12}b_{J0}^2+d_{13}b_{J1}^2+d_{23}b_{J2}^2,\qquad V=\sum_{i<j}d_{ij}^{-1}.$$

The rule is invariant under permutations, rotations, inversion and spin rotations. Cauchy–Schwarz applied to $1=b_{J*}+\sum_j b_{Jj}$ gives

$$(V+\delta_J)^{-1}\le U_J. \tag{B.5}$$

Coincidences and ordering ties are null sets. The complete exact block sums $L^J_{p,j}=\sum_{a_1,a_2,a_3}|Q^J_{p,j,a_1,a_2,a_3}|$ satisfy $L^J_{p,j}\le2^{53}$. The normalized-harmonic bound $|A_\Lambda|\le\sqrt{\prod_i(2\Lambda_i+1)}$ follows from the spherical-harmonic addition identity and Cauchy–Schwarz. Using rational upper bounds for these square roots, the same integer sums certify

$$(|b_{S0}|,|b_{S1}|,|b_{S2}|)<(18/5,15/4,61/10),\qquad (|b_{P0}|,|b_{P1}|,|b_{P2}|)<(4,4,6).$$

Since $d_{ij}\le14$, substitution gives $\|U_S\|<1000$ and $\|U_P\|\le1177<1200$. Consequently, writing $M_{\mathrm{phys},J}=X_J^*U_JX_J$ and $\mathcal{K}_J=\widehat{X}_J^*U_J\widehat{X}_J$, (B.4) implies

$$\|M_{\mathrm{phys},S}-\mathcal{K}_S\|<10^{-9},\qquad \|M_{\mathrm{phys},P}-\mathcal{K}_P\|<10^{-10}. \tag{B.6}$$

Indeed the difference is bounded by $1200(2\|X_J\|+\|X_J-\widehat{X}_J\|)\|X_J-\widehat{X}_J\|$.

The remaining integral has an exact finite cubature. For an integer $h_0\ge0$ put

$$L_{h_0}(t,c)=1+\frac{t^2}{3}+\sum_{\ell=1}^{h_0}t^\ell\left(\frac{t^2}{2\ell+3}-\frac{1}{2\ell-1}\right)P_\ell(c).$$

The Legendre expansion of $\sqrt{1-2tc+t^2}$ has exactly these coefficients. To verify them, multiply the generating function $(1-2tc+t^2)^{-1/2}=\sum_{\ell\ge0}t^\ell P_\ell(c)$ by $1-2tc+t^2$ and use the three-term Legendre recurrence. The identity at $t=1$ follows by dominated convergence in each coefficient integral. A product of two state factors and two current factors has degree at most $h_0=2\ell_*+8$ in each direction, where $\ell_*=8$ for S and 4 for P. Orthogonality to higher spherical degrees therefore permits the exact replacements

$$d_{12}\mapsto7t_1L_{h_0}(t_2,c_{12}),\quad d_{13}\mapsto7t_1L_{h_0}(t_2t_3,c_{13}),\quad d_{23}\mapsto7t_1t_2L_{h_0}(t_3,c_{23}).$$

Here $c_{ij} = \boldsymbol{n}_i \cdot \boldsymbol{n}_j$. Write $f_{\kappa\nu}$ for the resulting projected multiplier at radial node κ and angular node ν. It need not be positive. The original U_J remains nonnegative.

The reduced Jacobian is $343t_1^2t_2$. The two-up-spin exchange preserves each bilinear product, so the six chambers pair. Use the three rank assignments $(1,2,3),(1,3,2),(2,3,1)$, each with Jacobian $686t_1^2t_2$. The radial polynomial degrees, including the Jacobian and the projected distances, are at most $(243,193,118)$ for S and $(213,165,100)$ for P. The orders in Table 5 therefore integrate them exactly.

For the angular rule use two independent Gaussian rules for x, y in normalized measure $dx/2$, and the n_a azimuths $\phi_k = (k - \frac{1}{2})\pi/n_a$, each of weight $1/n_a$. Take $\boldsymbol{n}_1 = (0,0,1)$, $\boldsymbol{n}_2 = (\sqrt{1-x^2}, 0, x)$ and $\boldsymbol{n}_3 = (\sqrt{1-y^2}\cos\phi_k, \sqrt{1-y^2}\sin\phi_k, y)$. Inversion and rotation invariance leave cosine modes only. Their degree is at most $2h_0$, and the midpoint azimuth sum annihilates every nonconstant mode of degree $< 2n_a$. After that sum, the polar expressions are polynomials of degree at most $2h_0$ in each variable: an even cosine power removes the square roots, while odd powers have zero azimuthal mean. Taking $n_a = h_0 + 1$ proves exactness.

Let B_ν be the row of the 47 distinct S angular surfaces, or the 3 by 21 matrix of P vectors. The latter list consists of the three $\boldsymbol{n}_i$ and all six assignments of $(\ell, \ell+1)$ for each $\ell = 1,2,3$. Distinct surfaces have different degree triples and are orthogonal. With positive angular weights w_ν, exactness gives

$$\sum_\nu w_\nu B_\nu^{\mathsf{T}} B_\nu = I_m.$$

Let T_κ be the m by n matrix of exact polynomial radial and spin coefficients on a sheet and let $j_\kappa = 686t_1^2t_2\omega_1\omega_2\omega_3$ be its weighted Jacobian. The Gaussian weights ω_i here refer to that radial tuple. Exact polynomial integration and physical normalization give

$$\begin{aligned} \sum_\kappa j_\kappa = 343, \qquad \sum_\kappa j_\kappa T_\kappa^{\mathsf{T}} T_\kappa = \widehat{F}_J^* \widehat{F}_J, \\ A_\kappa = \sum_\nu w_\nu f_{\kappa\nu} B_\nu^{\mathsf{T}} B_\nu, \qquad \mathcal{K}_J = W_J \left[\sum_\kappa j_\kappa T_\kappa^{\mathsf{T}} A_\kappa T_\kappa \right] W_J. \end{aligned} \tag{B.7}$$

In particular the stacked matrix with blocks $\sqrt{j_\kappa}T_\kappa$ has norm less than t_0.

Gaussian and angular input certificates. We spell out how the local comparisons establish the caps used below. For a rule of order N, each mesh row gives rational node endpoints ξ_i^-, ξ_i^+ and weight endpoints ω_i^-, ω_i^+, all represented with denominator 2^{196}. The exact tests require strictly separated ordered node intervals inside $(0,1)$, positive weights, reflected equality of opposite rows, node widths $< 2 \cdot 10^{-57}$ and weight widths $< 10^{-48}$. After reflection to $0 \le a \le b < 1$ in the Legendre variable, opposite signs of $P_N(a), P_N(b)$ certify a root. A degenerate central interval is allowed only at zero for odd N. All signs use scale 2^{1024} interval recurrence for $(k+1)P_{k+1} = (2k+1)xP_k - kP_{k-1}$, with integer floor and ceiling at each division. At the midpoint use

$$P_N'(x) = \frac{N(P_{N-1}(x) - xP_N(x))}{1-x^2}, \qquad |P_N''| \le N^4$$

to enclose the derivative on $[a,b]$ by enlarging its midpoint box by $N^4(b-a)/2$. The derivative box must avoid zero. If its absolute endpoints are $d_-, d_+ > 0$, the weight is enclosed by

$$\frac{1}{(1-a^2)d_+^2}, \qquad \frac{1}{(1-b^2)d_-^2}.$$

Their outward integer bounds must lie inside the supplied weight row. The complete tests cover all 563 rows of the eight rules.

There are then N distinct simple roots, so all roots are covered. Rodrigues' formula gives orthogonality of P_N to lower degrees. For a root z_i its cardinal polynomial $P_N(x)/((x-z_i)P_N'(z_i))$ has integral $2/((1-z_i^2)P_N'(z_i)^2)$, by the telescoping Legendre kernel identity. Polynomial division by P_N proves exactness through degree $2N-1$ and positivity of the weights. Furthermore $|P_N'| \le N(N+1)/2$ gives node distance at least $1/(N(N+1))$ from either endpoint in $[0,1]$ and weight at least $4/(N^2(N+1)^2)$. The certified boxes for $N \le 122$ therefore have node lower endpoints $> 2^{-15}$ and weight lower endpoints $> 2^{-27}$.

For each actual radial rule, compare every binary64 node and weight as an exact dyadic number with both endpoints. Let E_i be the largest absolute node distance, and R_i, V_i the largest such node and weight distances divided by their positive lower endpoints. The completed exact comparisons give $E_i < 5 \cdot 10^{-16}$, $R_i, V_i < 1$ and actual nodes and weights in $(2^{-35}, 1)$. S uses the repeated tridiagonal-rule outputs; P converts the exact dyadic interval midpoints at precision 256 before binary64 rounding. The latter conversion adds at most $2^{-192} + 2^{-53}(1 + 2^{-192})$ to midpoint error, which is within the same absolute node cap.

The independent angular reconstruction uses integer intervals at scale $F = 2^{110}$. Addition, four-corner multiplication and positive division round outward by integer floor and ceiling. Square roots use integer square roots of the scaled endpoints. For every noncentral azimuth proposal a_k^{az}, the integers defined by

$$S_0 = 1, \quad S_1 = A, \quad S_j = 2AS_{j-1} - F^2 S_{j-2}$$

have opposite nonzero signs at $A = a_k^{\mathrm{az}} - 2, a_k^{\mathrm{az}} + 2$ for $j = n_a$. The central box is zero, and all boxes are strictly descending and disjoint. Since $S_j = F^j T_j(A/F)$, these tests identify all the exact azimuthal cosines without assuming cosine-library accuracy.

The angular reconstruction evaluates the normalized tripolar polynomial and the two direction coefficients of $\mathbf{V}_\ell$. For specificity let $\lambda = (\ell_1, \ell_2, \ell_3)$ and $0 \le k \le \min(\ell_2, \ell_3)$. Let $\mathcal{I}_{\lambda k}$ be the integers from $\max(0, \ell_2 - \ell_3, \ell_1 + k - \ell_3)$ to $\min(\ell_1 + \ell_2 - \ell_3, \ell_1, \ell_2 + k)$. Define the factorial denominators and coefficients by

$$\begin{aligned} D_{\lambda kj} &= j!(\ell_1 + \ell_2 - \ell_3 - j)!(\ell_1 - j)!(\ell_2 + k - j)! \\ &\quad \times (\ell_3 - \ell_2 + j)!(\ell_3 - \ell_1 - k + j)!, \\ p_{\lambda k} &= (-1)^{\ell_1 - \ell_2 + k} \sum_{j \in \mathcal{I}_{\lambda k}} \frac{(-1)^j}{D_{\lambda kj}}, \end{aligned}$$

$$s_{\lambda k} = \frac{(\ell_1 + \ell_2 - \ell_3)!(\ell_1 - \ell_2 + \ell_3)!(-\ell_1 + \ell_2 + \ell_3)!}{(\ell_1 + \ell_2 + \ell_3 + 1)!} (\ell_1!)^2 \prod_{i=2}^{3} (\ell_i + k)!(\ell_i - k)!.$$

With $x = c_{12}, y = c_{13}, z' = c_{23}$, define $R_0 = 1$, $R_1 = z' - xy$ and $R_{k+1} = 2(z' - xy)R_k - (1 - x^2)(1 - y^2)R_{k-1}$. The scalar value is

$$A_\lambda = \sum_k p_{\lambda k} (-1)^k (2 - \mathbf{1}_{\{k=0\}}) \sqrt{s_{\lambda k} \prod_{i=1}^{3} (2\ell_i + 1) \prod_{i=2}^{3} \frac{(\ell_i - k)!}{(\ell_i + k)!}}\, P_{\ell_2}^{(k)}(x) P_{\ell_3}^{(k)}(y) R_k.$$

For a zero degree this reduces to $(-1)^\ell \sqrt{2\ell + 1} P_\ell$ of the opposite pair cosine. The exact identity $(2\ell_1 + 1) \sum_k (2 - \mathbf{1}_{\{k=0\}}) p_{\lambda k}^2 s_{\lambda k} = 1$ is checked for every used label. Pairing the positive and negative magnetic indices in the Condon–Shortley expansion gives the displayed polynomial, so this reconstruction has the same normalization as the physical basis. Derivatives are evaluated by

$$P_k^{(k)} = (2k-1)!!, \quad P_{k+1}^{(k)} = (2k+1)x(2k-1)!!, \quad (\ell - k)P_\ell^{(k)} = (2\ell - 1)xP_{\ell-1}^{(k)} - (\ell + k - 1)P_{\ell-2}^{(k)}.$$

After directed conversion of interval endpoints to binary64, every product is enclosed by the predecessor of the smallest rounded corner and the successor of the largest. Sums are treated the same way. For an exact value in $[a, b]$ and computed value y, the larger of the upward-rounded differences $y - a, b - y$ bounds the absolute error. Add these nonnegative bounds with an upward successor after every addition. Apply this to every weighted surface pair and every angular tuple; for P expand each dot product into all four direction-coefficient products. Denoting the production weighted pairs by $\widehat{P}_{ij\nu}$, the resulting complete outward sums give

$$\sum_{\nu} |\widehat{P}_{ij\nu} - w_\nu (B_\nu^{\mathsf{T}} B_\nu)_{ij}| < \zeta_J. \tag{B.8}$$

There are 15625 tuples and 1128 pairs for S, and 4913 tuples and 231 pairs for P. Their recorded maximum outward sums are respectively $1.8458901975602706 \cdot 10^{-14}$ and $5.242822235381616 \cdot 10^{-15}$. The current-angular errors are bounded by $8 \cdot 10^{-14}$. All three computed cosines lie in $[-1, 1]$ and their errors are $< 5 \cdot 10^{-15}$. The successor comparisons with the exact rational caps establish the strict values ζ_J in the table below. This is an error summed over all tuples, not a pointwise sample bound.

The audit and production arrays coincide entry by entry in their ordered indices. This correspondence includes the orbital coefficients, energy means, selected states, surfaces, nodes, weights, current angular arrays and weighted pairs. The S production and radial audit use precision 192 for their energy conversion. Current plans can be made at 192 or 256. P production and radial audit use 256, while its angular audit uses 192. For coefficients of denominator 2^{96} and absolute sum below two, conversion at either precision is exact before the final binary64 rounding. For the non-dyadic energies, all 28 midpoint rounding cells have distance $> 10^{-24}$ from their rational inputs. The precision-192 conversion error is $< 16 \cdot 2^{-192}$. For the 109 coefficients in the 42 current plans, the exact factorial tables give either zero or a squared coefficient in $(2^{-32}, 2^{12})$ with reduced denominator $< 2^{32}$. Its positive square root is farther than 2^{-180} from any binary64 rounding midpoint in the relevant range: the squared midpoint has denominator between 2^{92} and 2^{140}, so the nonzero difference of squares is $> 2^{-172}$. The precision-192 coefficient evaluation error is $< 2^{-183}$. Thus the 192- and 256-bit computations round identically, including the exact zero. The 34 P angular node and weight midpoints have certified distance $> 2^{-77}$ from their binary64 rounding midpoints, whereas their high-precision conversion error is $< 2^{-192}$. They too give identical binary inputs. The same ordered constructors and the repeatability assumptions then identify the actual arrays. Equality of dimensions alone would not establish this correspondence.

Local radial and spectral-diagonal errors. Put $\varepsilon = 2^{-53}$, $\tau = 2^{-1074}$, $\epsilon_{\mathrm{abs}} = 10^{-190}$, $\gamma(k) = k\varepsilon/(1 - k\varepsilon)$ and $\mathrm{rnd}(s) = \varepsilon s + \tau$ for $s \geq 0$. A finite rounded operation admits the representation

$$\mathrm{RN}(x) = x(1 + \theta) + e, \qquad |\theta| \leq \varepsilon, \quad |e| \leq \tau. \tag{B.9}$$

This follows from half the normal-binade spacing or half the subnormal spacing and also holds for a fused multiply-add.

Here is the exact radial error ledger, including coefficient conversion. For one orbital write its unit-interval coefficients as $c_0, \ldots, c_{d_{\mathrm{Cl}}}$, $d_{\mathrm{Cl}} \leq 37$, and their actual dyadic values as $\widehat{c}_k$. Initialize $b^{\mathrm{Cl}}_{d_{\mathrm{Cl}}+1} = b^{\mathrm{Cl}}_{d_{\mathrm{Cl}}+2} = 0$. Descending from $k = d_{\mathrm{Cl}}$ to 1 compute rational bounds

$$s_k^{\mathrm{Cl}} = \mathrm{rnd}(|\widehat{c}_k| + b^{\mathrm{Cl}}_{k+2}), \qquad m_k^{\mathrm{Cl}} = \mathrm{rnd}(2b^{\mathrm{Cl}}_{k+1}),$$

$$a_k^{\mathrm{Cl}} = \mathrm{rnd}(2b^{\mathrm{Cl}}_{k+1} + m_k^{\mathrm{Cl}} + |\widehat{c}_k| + b^{\mathrm{Cl}}_{k+2} + s_k^{\mathrm{Cl}}),$$

$$e_k^{\mathrm{Cl}} = s_k^{\mathrm{Cl}} + m_k^{\mathrm{Cl}} + a_k^{\mathrm{Cl}}, \qquad b_k^{\mathrm{Cl}} = \sum_{j=k}^{d_{\mathrm{Cl}}} (j-k+1)(|\widehat{c}_j| + e_j^{\mathrm{Cl}}).$$

Set

$$p^{\mathrm{Cl}} = \mathrm{rnd}(b_1^{\mathrm{Cl}}), \qquad a_0^{\mathrm{Cl}} = \mathrm{rnd}(|\widehat{c}_0| + b_1^{\mathrm{Cl}} + p^{\mathrm{Cl}}),$$
$$s_0^{\mathrm{Cl}} = \mathrm{rnd}(|\widehat{c}_0| + b_1^{\mathrm{Cl}} + p^{\mathrm{Cl}} + a_0^{\mathrm{Cl}} + b_2^{\mathrm{Cl}}),$$
$$E_{\mathrm{Cl}} = \sum_{k=0}^{d_{\mathrm{Cl}}} |\widehat{c}_k - c_k| + \sum_{k=1}^{d_{\mathrm{Cl}}} e_k^{\mathrm{Cl}} + p^{\mathrm{Cl}} + a_0^{\mathrm{Cl}} + s_0^{\mathrm{Cl}}, \qquad D_{\mathrm{Cl}} = \sum_{k=0}^{d_{\mathrm{Cl}}} k^2 |c_k|.$$

The implemented Clenshaw step is $(B, A) \leftarrow (A, \mathrm{muladd}(2t, A, \mathrm{RN}(\widehat{c}_k - B)))$, starting at zero, with $t = \mathrm{RN}(2x - 1)$. Its return is $\mathrm{RN}(\mathrm{RN}(\widehat{c}_0 + \mathrm{RN}(tA)) - B)$. Let $\mathcal{U}_j$ be the second-kind Chebyshev polynomials, defined by $\mathcal{U}_0 = 1$, $\mathcal{U}_1(t) = 2t$ and $\mathcal{U}_{j+1} = 2t\mathcal{U}_j - \mathcal{U}_{j-1}$. The bound $|\mathcal{U}_j(t)| \le j+1$ on $[-1, 1]$ shows by descending induction that b_k^{Cl} bounds each computed recurrence value. The final identity $t\mathcal{U}_{k-1} - \mathcal{U}_{k-2} = T_k$, with $\mathcal{U}_{-1} = 0$, gives error E_{Cl} at fixed t. Since $|T_k'| \le k^2$, the radial product arguments give

$$\Delta_t = 2(E_1 + E_2 + E_3 + 2\,\mathrm{rnd}(1)) + \mathrm{rnd}(1), \qquad A_* = \max_a \sum_k |c_{a,k}|, \quad e_* = \max_a (E_{\mathrm{Cl},a} + D_{\mathrm{Cl},a}\Delta_t).$$

Thus every computed orbital value differs from its exact-node polynomial value by at most e_* and has magnitude at most $A_* + e_*$.

Every cell of T_κ is a sum of at most six terms. Their spin factors belong to

$$\left\{\pm 1/\sqrt{2},\ \pm 1/2,\ \pm 1/\sqrt{12},\ \pm 2/\sqrt{12}\right\}.$$

The source uses the divisions by rounded $\sqrt{2}$ and $\sqrt{6}$. Their relative error is $< 5\varepsilon$. Each term has three left-associated orbital multiplications and at most six summation rounds. Consequently

$$\mathcal{C}_T = 6\left\{(A_* + e_*)^3 - A_*^3 + [(1+5\varepsilon)(1+\varepsilon)^9 - 1](A_* + e_*)^3\right\} + 64\tau, \tag{B.10}$$

$$\mathcal{C}_{\mathrm{jac}} = \prod_{i=1}^{3}(1+V_i)(1+R_1)^2(1+R_2)(1+\varepsilon)^{10} - 1 \tag{B.11}$$

bound, respectively, each entry error $|\widehat{T}_\kappa - T_\kappa|$ and the relative Jacobian error. In (B.10), an absolute rounding residue in the first orbital multiplication is amplified by at most four, in the second by two, and in the last by one. With six terms and the summation residues, their total is $< 64\tau$ when $A_* + e_* \le 2$. The Jacobian uses six positive factors counting the repeated first node, all above 2^{-35}, so its nonzero partial products are normal and at most ten relative rounds suffice. The exact ledger on every coefficient and every node gives $A_* < 1.6$, $e_* < 10^{-12}$, and the strict caps $\mathcal{C}_T < e_{T,J}$, $\mathcal{C}_{\mathrm{jac}} < \rho_J$ in Table 5. The sharper P value $\rho_P = 1.7 \cdot 10^{-15}$ is retained.

For the computed spectral diagonal $\widehat{W}_J$, compare each entry $d' > 0$ with the exact deficit $A > 0$ by its rational residual $r = |(d')^2 - A|$. If $2d' - r/d' > 0$, then

$$|d' - \sqrt{A}| = \frac{r}{d' + \sqrt{A}} \le \frac{r}{2d' - r/d'}.$$

The tables cover all 90 S occupations, including all three parenthesizations of their three-energy sums, and all 23 P occupations, repeated with their spin multiplicities. They certify $d' \ge l/1000$, $l \ge 220$, and residual bounds $r \le v'/10^{19}$ for S and $r \le v'/10^{20}$ for P. The integer margins

$4(2l-1)-v'$ and $17(2l-1)-2v'$ have minima 259 and 339, respectively. Since $v'<10^6$, the denominator above exceeds $(2l-1)/1000 \ge 439/1000$. These comparisons prove

$$\|\widehat{W}_J - W_J\| < d_{D,J}, \qquad \|\widehat{W}_J\|, \|W_J\| < d_J$$

with the table's values. The S rounding traces use the identical midpoint cells described above. P's exact deficits and square-root rounding cells have squared margins $> 10^{-20}$, whereas conversion and square-root errors at precision 192 or higher change the square by $< 32 \cdot 2^{-192}$. Its saved decimal diagonal entries lie in these same cells. Thus both the production diagonal and the audited one are covered, including the positivity of every residual denominator.

The local multiplier ledger and the complete grid. Put $d_x = 5\cdot 10^{-16}$, $e_{\mathrm{ang}} = 5\cdot 10^{-15}$ and $e_{\mathrm{harm}} = 8\cdot 10^{-14}$. Define $H_p = \lceil \sqrt{\prod_i (2\Lambda_{p,i}+1)} \rceil$ and $\beta_j = 2^{-32}\sum_p H_p L^J_{p,j}$. The prior integer bound on $L^J_{p,j}$ ensures that every absolute value and sum is safe in signed 64-bit arithmetic and that conversion of every current coefficient to binary64, then scaling by 2^{-32}, is exact. The following is the complete rational ledger for one profile. Initialize $t'_0 = t'_1 = 0$ and compute, $1 \le \ell \le 8$,

$$t'_{\ell+1} = 2t'_\ell + t'_{\ell-1} + \gamma(4)(3 + 2t'_\ell + t'_{\ell-1}) + \epsilon_{\mathrm{abs}}, \qquad e_{\mathrm{Ch}} = \max_{0\le \ell\le 9} t'_\ell + 81(2d_x+\varepsilon),$$

$$e_{b,j} = \beta_j\{(1+e_{\mathrm{Ch}})^3(1+e_{\mathrm{harm}})(1+\gamma(170)) - 1\} + \epsilon_{\mathrm{abs}}.$$

Initialize $a'_0 = a'_1 = 0$ and compute, $1 \le \ell < h_0$,

$$v'_\ell = \frac{(2\ell+1)a'_\ell + \ell a'_{\ell-1}}{\ell+1}, \qquad a'_{\ell+1} = v'_\ell + \gamma(8)\left(\frac{3\ell+1}{\ell+1} + v'_\ell\right) + \epsilon_{\mathrm{abs}}.$$

Set

$$e_{P,\ell} = a'_\ell + \frac{\ell(\ell+1)}{2} e_{\mathrm{ang}}, \quad d_t = 2d_x + 2\varepsilon, \quad d_r = 7d_t + 14\varepsilon, \quad M_{h_0} = \frac{4}{3} + \sum_{\ell=1}^{h_0} \frac{1}{2\ell-1},$$

$$c_{E,\ell} = 2d_t + \gamma(2\ell+16)\left(\frac{1}{2\ell-1} + \frac{1}{2\ell+3}\right) + \epsilon_{\mathrm{abs}}, \qquad e'_0 = 2d_t + \frac{4}{3}\gamma(8),$$

$$e'_s = e'_0 + \sum_{\ell=1}^{h_0}\left\{\frac{e_{P,\ell}}{2\ell-1} + c_{E,\ell}(1+e_{P,\ell})\right\}, \qquad e_Q = e'_s + \gamma(2h_0+10)(M_{h_0}+e'_s) + \epsilon_{\mathrm{abs}},$$

$$e_d = 7e_Q + d_r(M_{h_0}+e_Q) + \gamma(5)(7+d_r)(M_{h_0}+e_Q) + \epsilon_{\mathrm{abs}}.$$

Finally define $b_* = 1 + \sum_j \beta_j$, $e_b = \sum_j e_{b,j}$ and

$$F_* = (b_*+e_b)^2/\delta_J + (7M_{h_0}+e_d)\sum_j (\beta_j + e_{b,j})^2,$$

$$E_f = e_b(2b_*+e_b)/\delta_J + \sum_j \{7M_{h_0} e_{b,j}(2\beta_j + e_{b,j}) + e_d(\beta_j+e_{b,j})^2\} + \gamma(48)F_* + \epsilon_{\mathrm{abs}}.$$

The completed exact rational evaluation of this entire ledger gives $E_f < e_{f,J}$ with the values in the table.

We justify its operation counts and absolute allowances. The first recurrence compares the computed Chebyshev recurrence at the computed argument; $|T'_\ell| \le \ell^2$ transports it to the exact node. The second does the same for the Legendre recurrence, using $|P_\ell| \le 1$ and $|P'_\ell| \le \ell(\ell+1)/2$. The current reshapes contract the third, second and first Chebyshev indices, followed by the 42 angular labels. Their inner lengths are $10, 10, 10, 42$. After deleting exact zero and unit operations, the four contractions have at most 144 relative rounds on any coefficient path, within the ledger's $\gamma(170)$. There are fewer than 10^5 primitive residue occurrences affecting one current, and subsequent nonunit factors have product < 128. Their total transported absolute error is $< 2^{25}\tau < \epsilon_{\mathrm{abs}}$. This uses the classical contraction graphs, not an assumed relative error for a zero or subnormal intermediate.

The powers in the distance coefficients use Julia's compensated positive-integer graph. To specify the graph, for input t and exponent N start with high-low pairs $(x, x_l) = (t, -0)$, $(y, y_l) = (1, 0)$ and counter N. At an odd counter form

$$e = \mathrm{muladd}(y, x_l, \mathrm{RN}(xy_l)), \quad h' = \mathrm{RN}(xy), \quad r' = \mathrm{FMA}(x, y, -h'), \quad (y, y_l) = (h', \mathrm{RN}(r' + e)).$$

Square the x pair by $e = \mathrm{RN}((2x)x_l)$, $h' = \mathrm{RN}(x^2)$, $r' = \mathrm{FMA}(x, x, -h')$ and $(x, x_l) = (h', \mathrm{RN}(r' + e))$, then halve the counter by integer division. Stop when it is one, form the same cross correction e, and return $\mathrm{muladd}(x, y, e)$. For $N = 3$ the source instead uses two ordinary multiplications. All assignments within a pair update use the old values.

For $2^{-32} \le t \le 1$, $N \le 24$, high parts of exponent k lie between $t^k(1-\varepsilon)^{k-1}$ and $t^k(1+\varepsilon)^{k-1}$, and exceed 2^{-769}. Induction in the displayed pair update gives $|\mathrm{low}/\mathrm{high}| \le (k-1)\varepsilon(1+500\varepsilon)$. Indeed if the incoming ratios sum to R, the outgoing ratio is at most $(1+10\varepsilon)(\varepsilon+R)$. The absolute underflow terms divided by a high part are $< 2^{-306}$. The final update therefore has relative error $< (2N-1)\varepsilon(1+2000\varepsilon) < 2N\varepsilon$. The special cubic case has the smaller $\gamma(2)$ bound. This proves the power bound with possible underflow in low parts. Applying it to $t^\ell(t^2/(2\ell+3) - 1/(2\ell-1))$ gives error at most

$$\gamma(2\ell+7)\left(\frac{1}{2\ell-1} + \frac{1}{2\ell+3}\right).$$

The exact derivative of this coefficient has absolute value at most two. Transport by d_t gives $c_{E,\ell}$. The Gaussian endpoint distances imply that the ratios supplied to this graph, including a rounded product of two nodes, are in $[2^{-32}, 1]$.

The exact projected coefficient has magnitude at most $1/(2\ell-1)$. Summing the coefficient and Legendre errors proves e_Q, including their products, and radial scaling proves e_d. The difference of current squares is bounded by $e_{b,j}(2\beta_j + e_{b,j})$. The residual current contributes $e_b(2b_* + e_b)/\delta_J$. Telescoping each distance-times-square gives the remaining displayed terms in E_f. Expanding the final scalar graph has at most 48 relative rounds on a signed term. Its unsigned sum is bounded by F_*. The remaining scalar absolute residues, transported through the possible squares and scales, total $< 2^{128}\tau < \epsilon_{\mathrm{abs}}$. Thus the ledger proves $|\widehat{f}_{\kappa\nu} - f_{\kappa\nu}| < e_f$.

Finiteness is established independently of the small recorded maxima. Clenshaw's at most 37 steps give the crude bound 2^{82} on intermediate values and 2^{256} on local radial products. The angular integer boxes, their directed conversions and complete error sums are bounded in magnitude by 2^{720}, using degrees at most eight and factorial arguments at most 25. The current contractions and final local multiplier graph are bounded by 2^{270}. Denominators are positive, and square-root domain guards are included in the checks. These bounds exclude overflow and invalid operations before applying the sharper estimates.

For the production maximum, the loop at second radial index j owns a zero-initialized maximum, visits all third radial indices, and at each visit evaluates every angular tuple and every

first radial index. It updates the maximum with the absolute values of all those entries. After the join the maximum over j is taken. This covers exactly

$$122 \cdot 98 \cdot 60 \cdot 25^3 = 11208750000, \qquad 107 \cdot 83 \cdot 51 \cdot 17^3 = 2225250003$$

entries. Each entry is reused on the three radial sheets. The retained complete execution took 281.6183901310005 seconds and recorded maxima 0.36484005377549 and 0.8022631108050438. Its strict successor comparisons give $|\widehat{f}_{\kappa\nu}| < .365$ and $< .803$ everywhere on the respective grids. A maximum here is a reduction of the entire finite loop. Together with its completed iteration ranges, it supplies the uniform M input, rather than a bound inferred from selected nodes. For a round-trip printed binary bound the successor check is conservative. For a rational ledger value converted at precision at least 192, the conversion error is less than one quarter of a binary64 spacing at these magnitudes, so its binary successor also lies above the exact rational. This justifies comparison with the exact rational caps despite decimal output.

The assembly graph and its rounding bounds. For each radial tuple the program forms every upper angular moment $\sum_\nu \widehat{P}_{ij\nu}\widehat{f}_{\kappa\nu}$ and reflects it, giving $\widehat{A}_\kappa$. For each second radial index j it initializes a separate n by n zero matrix C_j. In third-node, first-node, sheet order it performs the two BLAS calls

$$U'_\kappa = \mathrm{fl}(\widehat{A}_\kappa \widehat{T}_\kappa), \qquad C_j \leftarrow \mathrm{fl}(\widehat{j}_\kappa \widehat{T}_\kappa^{\mathsf{T}} U'_\kappa + C_j).$$

The first has $\alpha = 1, \beta = 0$, the second $\alpha = \widehat{j}_\kappa, \beta = 1$. After summing the C_j, the program scales each entry by its two diagonal factors. S reflects the upper triangle; P adds the transpose and divides by two. The exact rationals denoted by the printed entries form $M_{0,J}$.

Here is the source analysis needed to attach an error bound to these calls. Julia dispatches the contiguous binary64 products to GEMM, or GEMV when a dimension is one. The angular and first radial calls are NN, and the second radial call is TN. The distinct operands exclude the symmetric rank-update shortcut. These are not the special square 2 by 2 or 3 by 3 products. Diagonal scaling is two scalar multiplications per entry, and the group sum is a sequential or pairwise ordinary addition tree. The original scalar current calls are GEMV N for the first two contractions and GEMM NN for the last two. The P direction matrix product and its length-three dot product are also covered.

In OpenBLAS 0.3.29 the Cooperlake binary64 assignments inherit SkylakeX. The ordinary level-three driver partitions the inner indices into disjoint consecutive panels, packs by copies, applies β once and passes the same α to each panel. The ordinary binary64 kernel uses row tiles $16, 8, 4, 2, 1$ and column tiles $12, 10, 8, 6, 4, 2, 1$. Its two- and four-lane tails reduce disjoint subsets of inner indices. Small NN kernels use direct outer-product loops or an eight-lane packed tail. Small TN kernels use eight-lane products with $4, 2, 1$ row and column tiles. Masked terms are zero padding. The generic NN and TN alternatives use the scalar loop followed by α and β. Dimension-one forwarding uses GEMV N or T: their inner blocks have at most 2048 indices, with $4, 2, 1$ groups and the corresponding two- or four-lane reductions. Early α multiplication occurs only on new input products. The P length-three dot uses its scalar remainder loop. These cases include the compile-time Haswell microkernel alternatives. Each input product occurs once, every new product receives α once, and an old $\beta = 1$ accumulator never receives α. The beta-zero branches overwrite their output without reading uninitialized storage. Packing and shuffles add no arithmetic. The small-TN permit test rejects both radial TN sizes ($134^2, 41^2 > 1200$), but the bound includes that alternative as well.

For a contraction of inner length k, the resulting product tree has at most $2k + 12$ relative rounds on a leaf-to-output path, including panel accumulation and scaling; for $\alpha = 1, \beta = 0$ the

bound $2k$ suffices. There are at most $20(k+1)$ primitive rounding sites affecting one output. For example ordinary panels use at most $7k+1$ sites, small eight-lane calls at most $2k+24$, and blocked GEMV T at most $11k+2$. Fusion reduces these bounds. Writing

$$N_a = n_a^3, \qquad L = 3n_1n_3, \qquad p = (4m+40)(L+1) + 2n_2 + 20,$$

the angular path bounds are $2N_a + 12 = 31262, 9838$, the radial bounds are $p = 5007324, 2030314$, and twelve rounds suffice for terminal scaling, symmetrization and decimal replacement.

The absolute errors in (B.9) must be transported separately. For one contraction, put $q_* = \max(1, |\alpha|, \max|A_{ij}|, \max|B_{ij}|)$. An inserted residue encounters at most one subsequent nonunit factor, bounded by q_*, and its later relative inflation is < 2. Thus its total output allowance is $40(k+1)q_*\tau$. When $\alpha = 1, \beta = 0$, one may take $q_* = 1$. The local radial bounds give $|\widehat{T}_\kappa| < 64$, $0 < \widehat{j}_\kappa < 1372$, and the exact angular identity and (B.8) give $\sum_\nu |\widehat{P}_{ij\nu}| \le 1 + \zeta$. Consequently angular partial sums and entries have magnitude < 2. Their additive error has matrix norm $< 2^{26}\tau$. In the first radial product the output error is $< 2^{11}\tau$ per entry and every partial sum is $< 2^{14}$. In the second product new residues total $< 2^{25}\tau$, while transported first-product residues total $< 2^{35}\tau$. There are fewer than 2^{22} radial updates and the old accumulator is never rescaled by the next Jacobian. Its path inflation remains < 2. Hence the final radial additive error is $< 2^{60}\tau$ per entry. Terminal scaling and symmetrization add a symmetric matrix error of norm $< 2^{20}\tau$. Each of these three separate bounds is $< \epsilon_{\mathrm{abs}}$.

These estimates do not assume finite intermediates circularly. Before any hypothetical first overflow, the same absolute-leaf bounds apply. A radial leaf is bounded by 2^{24}, and fewer than 2^{34} such leaves contribute to an entry. Group partial sums are therefore $< 2^{60}$ and terminal values $< 2^{70}$, contradicting overflow. For underflow, retaining all relative factors and deleting absolute residues defines a comparison evaluation. Each contraction is affine in its preceding partial sums, so the transported residue bounds remain valid with correlated roundings. In a round-trip print, the exact decimal lies in the rounding cell of the binary entry. Its relative displacement is $\le \varepsilon$ for a normal entry and absolute displacement $\le \tau$ for a subnormal entry. This is the last terminal round and allowance. Reflection in S, and the equal rounded pairwise sums in P, make both the comparison and the residual symmetric.

Array ownership also matters to the graph. Each outer-loop iteration owns its accumulator and maximum slot, angular moments, radial matrices, product workspace and writable current workspace. The node, coefficient, angular and state arrays are read-only. Workspaces allocated without initialization are overwritten by beta-zero calls before use. The overlap diagnostics use separate accumulators or fully overwritten temporary arrays and do not feed the certified matrix. Ownership is by iteration, rather than by a fixed operating-system thread, so task migration does not change this argument under (R2)–(R3).

Propagation to the decimal center. For a product path of length k, the product of its rounding factors differs from one by at most $\gamma(k)$: $(1-\varepsilon)^k \ge 1 - k\varepsilon$ and $(1+\varepsilon)^k \le (1-k\varepsilon)^{-1}$. We now give the full operator-norm budget, so entrywise and operator errors are not interchanged. Write $\lceil\sqrt{a}\rceil$ for the least integer whose square is at least a. With the profile values in Table 5, define

$$\begin{aligned}
a_* &= mM[\zeta + \gamma(2N_a + 12)(1+\zeta)] + \epsilon_{\mathrm{abs}}, \qquad k_* = M + a_*, \\
\Delta &= \lceil\sqrt{343nm}\rceil e_T, \qquad t_* = t_0 + \Delta, \qquad t_c = t_0 + \lceil\sqrt{343m}\rceil e_T, \\
H_* &= (M + e_f)(2t_0 + \Delta)\Delta + (e_f + a_* + \rho k_*)t_*^2, \\
B'_* &= \gamma(p)(1+\rho)t_c^2\lceil\sqrt{m}\rceil k_* + \epsilon_{\mathrm{abs}},
\end{aligned}$$

$$E_* = k_*(1+\rho)t_c^2 + B'_*,$$
$$R_* = d^2 H_* + 2d\, d_D t_0^2 (M + e_f) + nd^2[B'_* + \gamma(12)E_*] + \epsilon_{\mathrm{abs}}.$$

All these expressions are rational. The angular identity implies, by Cauchy–Schwarz, $\sum_\nu |w_\nu (B_\nu^{\mathsf{T}} B_\nu)_{ij}| \le 1$. It follows that $\|\widehat{A}_\kappa\| \le k_*$ and $\|\widehat{A}_\kappa - A_\kappa\| \le a_* + e_f$. Equation (B.7) and the Frobenius bound give stacked radial-map error at most Δ and individual stacked column norms at most t_c. Telescoping the radial maps, angular matrices and weights therefore costs at most H_* before diagonal scaling. Moreover $\||\widehat{A}_\kappa|\| \le \sqrt{m}\,\|\widehat{A}_\kappa\|$, where the inner absolute value is entrywise. The sum of the absolute radial leaves in one matrix entry is therefore bounded by $(1+\rho)t_c^2\lceil\sqrt{m}\rceil k_*$. The path count gives entrywise radial error at most B'_* and entry magnitude at most E_*. Reflection or transpose averaging preserves entrywise error from the symmetric exact comparison. An n by n symmetric matrix with entries bounded by e has norm at most ne, which accounts for the factor n in the last term of R_*. For the exact unscaled radial matrix $G = \sum_\kappa j_\kappa T_\kappa^{\mathsf{T}} A_\kappa T_\kappa$, telescoping both diagonal factors in $\widehat{W}_J G \widehat{W}_J - W_J G W_J$ gives $2d\, d_D t_0^2 (M + e_f)$. Thus

$$\|\mathcal{K}_J - M_{0,J}\| \le R_*. \tag{B.12}$$

The integer square-root ceilings in this order are $(1470, 127, 7)$ for S and $(544, 85, 5)$ for P. Evaluating the nonnegative budget with upward rational rounding to 10^{-24}, and enlarging ϵ_{abs} to 10^{-30} for this evaluation only, gives the certified upper values

$$R_{*,S} \le \frac{1278973577592006297}{62500000000000000000000} < .0000204636,$$
$$R_{*,P} \le \frac{22403063932239163}{100000000000000000000000} < .000000224031.$$

The order of upward evaluation is $\gamma(2N_a+12), \gamma(p), \gamma(12), a_*, H_*, B'_*, E_*$, the diagonal term, then R_*. Each expression is nondecreasing in the earlier upper bounds. The complete integer numerator/denominator and rounding-remainder tables in the release certify every such rounding. The strict margins to the displayed caps are respectively $1422407993703/625000000000000000000000$ and $36067760837/100000000000000000000000$.

Exact center residuals. The complete original execution regenerates both centers from the stated inputs, with the validated S parameters $(7, 5/2, 10, 4; 122, 98, 60, 25)$ and P's exact, non-bare branch $(107, 83, 51, 17)$. The selected angular degrees are at most eight, so S's degree-100 filter removes no state. It removes pre-existing working centers before production. The retained new files and the certificate centers have equal complete bytes and equal entrywise parsed binary64 values in the same basis order. Full orbital-table regeneration is likewise compared with the original parsed data. The local audits use the same constructors, inputs and index orders as production, as detailed above. Under the preservation and repeatability assumptions this identifies the decimal-rational $M_{0,J}$ in (B.12) with the following residual certificate. Hashes serve only to identify artifacts. Equality of hashes is not used as a mathematical matrix identity.

Parse all center fields as exact decimal rationals, allowing an optional sign, decimal fraction and decimal exponent. The parser enforces printable ASCII, tabs and LF or CRLF, exactly n noncomment data rows and exactly n nonempty numeric fields in each row. No columns are skipped. The integer witness has exactly $i+1$ signed integer entries in zero-based row i, and is zero above the diagonal. Call it Y_J. It is an arbitrary integer matrix. Positivity, invertibility and accuracy of a proposed floating Cholesky factor are unnecessary. Set $g = 10^{12}$,

$(b'_S, b'_P) = (99913, 99440)$ and

$$A'_{ij} = \mathrm{rne}(gM_{0,J,ij}), \qquad R'_{ij} = (b'_J - 1)10^{19}\mathbf{1}_{\{i=j\}} - gA'_{ij} - \sum_{k=0}^{\min(i,j)} Y_{J,ik}Y_{J,jk},$$

where rne denotes nearest-integer rounding with even ties. Define $r_* = \max_i \sum_j |R'_{ij}|$ and $e_{\mathrm{dec}} = \max_{ij} |M_{0,J,ij} - A'_{ij}/g|$. Every entry in both triangles participates in the residual calculation. An independent upper-triangle accumulation, adding each off-diagonal residual to both rows, gives the same complete row list and the same exact rational rounding error. The retained exact evaluations are

J	r_*	e_{dec}
S	48147215284892	249985617507/500000000000000000000000
P	15565316152274	2497913/5000000000000000000

so all 175 row sums are $< 10^{15}$. The symmetry proved above means that the checker's rational symmetrization leaves the center unchanged. Writing $c_J = b'_J/10^5$, the residual identity and row-sum norm bound imply

$$c_J I - M_{0,J} \geq \left(10^{-5} - \frac{r_*}{g^2} - ne_{\mathrm{dec}}\right) I + \frac{Y_J Y_J^{\mathsf{T}}}{g^2} > 0.$$

The scalar is positive even on replacing r_* by 10^{15} and e_{dec} by $1/(2g)$. This is the triangular-witness simplification: the proof uses integer products and row sums, irrespective of how the witness was found. In particular,

$$M_{0,S} < .999130I, \qquad M_{0,P} < .994400I.$$

Combining these ceilings with (B.6) and (B.12) gives

$$M_{\mathrm{phys},S} < .9991504646I < .999151I, \qquad M_{\mathrm{phys},P} < .994400224131I < .994401I.$$

The full-sector form inequalities. The complete fixed magnetic bases transfer these ceilings to $D_J U_J D_J$. The other spin and orbital magnetic components have identical matrices, since D_J and U_J commute with the corresponding rotations. Entries between distinct magnetic components vanish. The magnetic multiplicities are two for S and six for P. On the orthogonal complement of $\operatorname{ran} D_J$ this operator is zero. Thus on the full sectors $D_J U_J D_J \leq \mathfrak{b}_J I$, with $\mathfrak{b}_S = .999151$, $\mathfrak{b}_P = .994401$.

Put $\mathcal{A}_J = V + \delta_J$. It is positive with $\mathcal{A}_J \geq (\delta_J + 3/14)I$, because each pair distance in B_7 is at most fourteen. Equation (B.5) yields $D_J \mathcal{A}_J^{-1} D_J \leq \mathfrak{b}_J I$. The bounded operator $\mathcal{A}_J^{-1/2} D_J$ and its adjoint therefore have norm at most $\sqrt{\mathfrak{b}_J}$. Applying the adjoint to $\mathcal{A}_J^{1/2} v$ gives $\|D_J v\|^2 \leq \mathfrak{b}_J \|\mathcal{A}_J^{1/2} v\|^2$. Spectral calculus gives $H_0 - C_J \geq -D_J^2$. Therefore on the Coulomb form domain,

$$q_<[v] + \frac{1}{16}\|\operatorname{Tr} v\|^2_{L^2(\partial K_7)} - z\|v\|^2 \geq (1 - \mathfrak{b}_J)\|\mathcal{A}_J^{1/2} v\|^2 \geq (1 - \mathfrak{b}_J)(\delta_J + 3/14)\|v\|^2.$$

The Coulomb terms are form bounded on $H^1(K_7)$, so the inequality extends there by form continuity. No operator Robin boundary condition is imposed on v. Finally $(1 - .999151)(5/2 + 3/14) = 16131/7000000$ and $(1 - .994401)(1 + 3/14) = 95183/14000000$. The complete spectral count controls the omitted configurations, the physical transport controls the orbital replacements, and the local and assembly estimates control the passage from exact cubature to the certified centers. These give the asserted inequalities for every vector in the stated full sectors. □

C Lithium integral certificates

This appendix defines the trial functions and sources used in Section 6 (Definition C.1). It then proves the rational enclosures of their moments (Lemma C.14).

Definition C.1 (Fixed lithium trials and sources)**.** For $x_i \in \mathbb{R}^3$, $1 \le i \le 3$, put $r_i = |x_i|$, $d = (r_1, r_2, r_3, |x_1 - x_2|, |x_1 - x_3|, |x_2 - x_3|)$, and let $A_{13} = 1 - P_{13}$, where P_{13} exchanges positions 1 and 3. For $a \in (0,\infty)^3$ and $\nu \in \mathbb{Z}^6_{\ge 0}$ put $F_{a,\nu} = e^{-\sum_i a_i r_i} \prod_{k=1}^6 d_k^{\nu_k}$. Let (ν, c_ν) be the 100 exponent/integer pairs in Table 8, and let $(b_t)_{t=1}^{140}$ be the ordered integers in Table 9. Write $x_{i,3}$ for the third Cartesian coordinate of electron i. Define the ordered mode triples (a_t, ν_t, i_t), $1 \le t \le 140$, as follows. The first 112 modes have $i_t = 3$: for each rate triple $(14/5, 14/5, 13/20)$, $(14/5, 14/5, 6/5)$, $(31/10, 12/5, 4/5)$, $(12/5, 31/10, 4/5)$, in that order, use the factors $1, d_1, \dots, d_6, d_j d_k$ $(1 \le j \le k \le 6$, lexicographically). The last 28 modes use rates $(14/5, 14/5, 3/4)$ and $(14/5, 14/5, 5/4)$, in order; for each use $i_t = 1$ then 2, each with factors $1, d_1, \dots, d_6$. The multi-index ν_t is the exponent vector of the indicated factor. Define

$$u_S = 10^{-14} \sum_\nu c_\nu A_{13} F_{(14/5,14/5,17/20),\nu}, \qquad u_P = 10^{-18} \sum_{t=1}^{140} b_t A_{13}[x_{i_t,3} F_{a_t,\nu_t}].$$

The first sum ranges over the 100 pairs of Table 8, read left to right.

Set $Q = 8/3$. For $2 \le n \le 6$ put

$$s_n = A_{13}\left[e^{-Qr_1 - Qr_2 - Qr_3/n} \sum_{j=0}^{n-1} \frac{(-2Q/n)^j}{j!} \binom{n}{n-1-j} r_3^j\right], \quad C_{S,n} = \frac{Q^3}{\pi} \frac{(2Q/n)^{3/2}}{4n\sqrt{\pi}}.$$

Put

$$t_2 = A_{13}[x_{3,3} e^{-Qr_1 - Qr_2 - Qr_3/2}], \qquad t_3 = A_{13}[x_{3,3}(1 - Qr_3/6) e^{-Qr_1 - Qr_2 - Qr_3/3}],$$

$$C_{P,2} = \frac{Q^3}{\pi}\sqrt{\frac{(Q/2)^5}{2\pi}}, \qquad C_{P,3} = \frac{Q^3}{\pi}\sqrt{\frac{4(Q/3)^5}{3\pi}},$$

Define $p_{S,n} = C_{S,n} s_n$ for $2 \le n \le 6$ and $p_{P,n} = C_{P,n} t_n$ for $n \in \{2, 3\}$. All square roots are positive. Spatial norms use ordinary Lebesgue measure. Each trial and source f, which satisfies $P_{13} f = -f$, is represented isometrically as a physical spinor with $\uparrow\downarrow\uparrow$ component $f/\sqrt{3}$, extended by signed simultaneous permutations to the other two strings with two up spins, and zero on the remaining spin strings. Use the same symbols for these spinors. The labels S and P here distinguish the two trial families: their orbital angular momenta are 0 and 1, respectively, their orbital magnetic number is zero, their parities are even and odd, respectively, and their spin magnetic number is 1/2. No total-spin restriction is imposed.

Table 8: Lithium S trial: ordered pairs (ν, c_ν), read left to right. The six digits of ν give the exponents of $d_1, \dots, d_6$. The coefficient of $A_{13}F_{(14/5,14/5,17/20),\nu}$ is $10^{-14} c_\nu$.

ν	c_ν	ν	c_ν	ν	c_ν	ν	c_ν
000000	192578507642049	100000	-18637105584193	010000	-4893191508198	001000	-377772895588427
000100	21687913877446	101000	55883362330885	011000	64991563194886	002000	-38457760107399
001100	-97869737076541	000200	-2817165576809	000110	-6574049558047	000011	-21175160412110
210000	128411633891504	201000	-111268970809246	200100	85958547690281	200001	-11135646743619
120000	-33435030557499	111000	99213941867312	102000	22771619995637	101100	-40915170411464
101010	-33137323291035	100110	-15706633630960	100020	13271380434227	100011	8708426264134

Table 8: Lithium S trial: ordered pairs (ν, c_ν), read left to right. The six digits of ν give the exponents of $d_1, \ldots, d_6$. The coefficient of $A_{13}F_{(14/5,14/5,17/20),\nu}$ is $10^{-14}c_\nu$. (continued)

ν	c_ν	ν	c_ν	ν	c_ν	ν	c_ν
021000	-33637679816705	020001	-96379393879640	010101	-35130689066215	010002	5752002624058
002100	-14573043963146	001200	86372395390789	001101	-39908942457146	000300	-41645540686493
000201	36940233903379	000102	7502802960424	000021	3160700248761	300100	-63250958657558
220000	-41890829949681	210100	-114611305957702	201100	33697170918180	201010	-17594454979840
200110	96496437822204	200020	-6023803910370	130000	-49526101674321	121000	109082871822618
120100	-97003483595728	112000	6662575813563	111100	-42994396428613	111010	5261593757741
110200	102382385187551	100210	-61857093841605	100003	-421408036738	030001	16481601753808
022000	-23563953921328	020101	121205576172158	011002	1806540114768	010201	-65251992063050
010003	-1563301644880	002200	14483571075089	001300	-49994233247290	001102	4084328942332
000400	34836644219690	000310	8704218112017	000301	-7540626026929	000220	1416699560466
000040	-144518102488	401000	5004468341455	320000	-26938458762230	311000	-16259637468816
310100	76817730215707	301100	-16853901957893	230000	34638676982410	211010	12384132460967
210110	-35174471648651	202100	5279457589922	200300	4306233837560	200210	-20559937525297
200030	684896568552	131000	-26028992998374	130100	53347598075651	121100	-24773719544820
120200	10934434016173	111200	26102826113440	111110	-11143103209542	110300	-52094422510428
110210	24973988134754	100310	21086139523661	050000	5869589803234	030110	-2399864140321
030101	-24678742221128	023000	718307824117	022100	7839439226000	020201	-17103988441973
013100	-541959493170	010301	22558696338943	002300	-3794756813227	002201	-388502500303
001400	9048105445461	000500	-6805192162237	000410	-4526294280747	000104	-170281908585

Table 9: Lithium P trial: successive integers b_t, read left to right in the mode order of Definition C.1. The coefficient of mode t is $10^{-18}b_t$.

t	b_t	b_{t+1}	b_{t+2}	b_{t+3}
1	-120015870113720000	-5527719335490280000	-5662662512097800000	186960680244002000
5	8993657481192360000	98711850003572900	194083685119928000	232359157147092000
9	887314913863710000	467761626184719000	196480110615253000	-172039858373383000
13	-12662948266792200	-179329958693696000	169456497556216000	158124641883264000
17	106771804491281000	16061905386670600	-98175363322029100	-545263189686892000
21	13237502766589500	51642919598783700	-627437759755436000	4512159831252850
25	37625439684789800	-32487525562657900	49351572655156400	-49796552667561200
29	-229036377859776000	-1439576674902220000	-8135482863011680000	4503775487779260000
33	7517381434037780000	-14823664189105800	-621137013893765000	310741670530606000
37	2255510321923590000	-825346181192189000	-365230774580283000	708810332821348000
41	-652864814227281000	-24564618439033400	-3057666884818770000	990392680619719000
45	-492573803101796000	956933229999546000	1929900881087360000	2796120011114770000
49	-249434812347310000	-226786886787875000	-1491807709059100000	206995224193631000
53	189556961807521000	-351229476439412000	316334819589271000	-453976751964670000
57	3867279158789010000	1370756521039610000	9641774677603950000	-3418116940985900000
61	-8762790980746690000	355658931719882000	-112416908162737000	-187364998886040000
65	307814858046278000	100137319601905000	-652904699417170000	-38550485008248200
69	-77087997812530800	-1920733570648110000	109637964067611000	1236605291154880000
73	74764536721586000	94990533335603500	524887971724604000	115363373071532000
77	-224987633941586000	-64168674989026800	508559138614380000	-39733921285032700
81	7788471490130710	88814579642896900	-84895271159553000	48270722631235900
85	124474002247613000	6232093768174070000	2375559818539930000	-2510325407821860000
89	-6783982643852250000	371120307392657000	1354444029637600000	-1048106464222570000
93	-477595009973174000	29630064983615600	808180795456249000	-40943101887638200
97	-125834307341012000	-47601453984732800	-120020287293432000	-439909122232083000
101	88065815728008700	59447311705798700	411993905925623000	17219661067493700
105	29577249255805000	-339613999279857000	509378795942874000	10691020494274200
109	-88322402063989500	37903998405299800	-62188273102382800	127034235858460000
113	-351015977798309000	-85738453397099300	-83769320762075600	-103928148905266000
117	79327390110805700	-554173931860421	156401268414680000	42381359401224900
121	13903846915434600	28602294905942200	173299294555551000	48493875456655500
125	-62897580204762500	-113554182280085000	-140903867796034000	313730933322561000
129	470068723557144000	1090711016080320000	-416801262744941000	53182997120479400
133	-836467615918667000	216214282604895000	-38009874696524800	-143874674567923000
137	-709080785460829000	-216177827252217000	195116461020833000	381035505002165000

C.1 Physical expansion and arithmetic conventions

The complete integer arrays, rational group inputs, returned integral intervals and independent readers used below are supplied in the lithium part of the accompanying code/data release. We specify their mathematical contents and the predicates checked by the readers here. In particular, the trial coefficients in Tables 8 and 9 are interpreted as rationals.

Set-up C.2 (Integral executions)**.** We specialize Set-up 2.2 as follows. The exact computations use unbounded integers, reduced rational arithmetic, integer factorials, binomial coefficients, floor division and integer square roots. Parsing, ordered containers, finite iteration, compression, file operations and preservation of the recorded inputs, sources, outputs and executions are assumed faithful; assertions are enabled. Caches retain results for the same arguments and arithmetic environment.

The native radial executions use the specified C++ operation sequence, signed 32-bit C and interface integers, binary64 doubles, matching argument and return interfaces, and writable result buffers. Compilation, loading and dispatch are faithful. Elementary binary64 operations and rational conversions round to nearest with even ties, with gradual underflow and flush-to-zero and denormals-are-zero disabled. There is no reassociation, fused contraction, disruptive excess precision or concurrent change of the floating environment. Adjacent-number operations, binary decomposition and scaling by powers of two have their specified exact meanings.

The double-logarithmic calculation uses the same binary64 semantics for each NumPy component operation, with faithful shapes, indices and broadcasting. A reduction of m nonnegative entries performs at most $m-1$ additions, in any order. Any participating threads preserve these operations and data ownership. The retained environment uses CPython 3.12.3 and GCC 13.3.0; native compilation uses `-O2 -fno-fast-math -ffp-contract=off`. The supplement records the remaining environment and source versions. These are execution assumptions. Integral accuracy, admissibility of arguments, coverage and normalization are proved below.

For intervals we use endpointwise addition and the four-corner product

$$[a,b][c,d]=[\min\{ac,ad,bc,bd\},\max\{ac,ad,bc,bd\}].$$

This convention retains the signs of all coefficients. A rational string denotes its exact rational value. A numeric token in a saved binary64 interval denotes the exact dyadic value obtained by nearest-even parsing. It need not equal the rational decimal written in that token.

Definition C.3 (Scalar integral arrays)**.** For positive integers R_i, integers n_i, p_{ij} and $k=(R_1,R_2,R_3,n_1,n_2,n_3,p_{12},p_{13},p_{23})$, put

$$\mathcal{I}(k)=(4\pi)^{-3}\int_{(\mathbb{R}^3)^3} e^{-\sum_i R_i r_i/180}\prod_i r_i^{n_i}\prod_{i<j} d_{ij}^{p_{ij}}\,dX. \tag{C.1}$$

A coefficient dictionary is a finite rational sum of the scalar primitives $F_{a,\nu}$ in Definition C.1, or of $x_{i,3}F_{a,\nu}$. After formal differentiation, we allow integer distance exponents $\nu\in\mathbb{Z}^6$, interpreting the same primitive formula away from collisions. The denominator of a dictionary is the least common multiple of its reduced coefficient denominators; the zero dictionary has denominator one. Let U_T be the dictionary of u_T and V_T the dictionary obtained by applying the formal differential expression $H_3(3)+15/2$ to u_T. Let S_n, T_n be those of s_n, t_n. The ordered base pairs are

$$\begin{aligned} S&: (U_S,V_S),(V_S,V_S),(S_2,U_S),(S_2,V_S),(S_3,V_S),\dots,(S_6,V_S),\\ P&: (U_P,V_P),(V_P,V_P),(T_2,U_P),(T_2,V_P),(T_3,V_P). \end{aligned}$$

The extra pairs are $(U_S,U_S),(U_S,S_3),\dots,(U_S,S_6)$ and $(U_P,U_P),(U_P,T_3)$.

For a pair (f,g), multiply its dictionaries, adding rates and powers. In a vector product replace $x_{i,3}x_{j,3}$ by $(r_i^2+r_j^2-d_{ij}^2)/6$, with $d_{ii}=0$. Set $D_c=\operatorname{den}(f)\operatorname{den}(g)$ in S and $D_c=6\operatorname{den}(f)\operatorname{den}(g)$ in P. Multiply the coefficients by D_c and the rates by 180. Replace each key by the lexicographically least of its six simultaneous electron permutations, and add its signed integer weights. Delete a key only when its entire column vector is zero. Denote the resulting base key sets by $\mathcal{L}_T$, their weights by $W_c(k)$, and the extra sets by $\mathcal{L}_T^+$. Missing column entries have weight zero. The source factor C_c is one for a norm or a trial–residual product, and is the positive $C_{T,n}$ of Definition C.1 for a column involving that source.

C.2 Integral formulas and error bounds

Write P_ℓ for the Legendre polynomial normalized by $P_\ell(1)=1$. For $p\ge -2$ and $0<t<1$ define

$$A_\ell^{(p)}(t)=\frac{1}{2}\int_{-1}^{1}(1+t^2-2tx)^{p/2}P_\ell(x)\,dx,\qquad B_\ell(t)=t^{-\ell}A_\ell^{(-2)}(t).$$

For a radial order $\sigma=(h,m,b)$ the pair ratios are $t_{hm}=s,t_{mb}=v,t_{hb}=sv$ under $r_h=R,r_m=Rs,r_b=Rsv$. Put

$$\kappa=9+\sum_i n_i+\sum_{i<j}p_{ij},\qquad C_\sigma=n_b+2,\qquad D_\sigma=n_m+n_b+p_{mb}+5.$$

These letters denote scalar degrees, not source constants or column denominators. All ordered integrals below have positive rational rates. The conditions on the clusters that we use are

$$9+\sum_i n_i+\sum_{i<j}p_{ij}>0,\qquad n_i+n_j+p_{ij}>-6\ (i<j),\qquad \sum_{i<j}p_{ij}>-6. \tag{C.2}$$

For $j\ge 0$ write $\mathsf{h}_j=\sum_{i=1}^{j}1/i$, with $\mathsf{h}_0=0$.

Lemma C.4 (Angular reduction)**.** *Suppose $R_i>0$ are integers, $n_i,p_{ij}\ge -2$ are integers and* (C.2) *holds. Suppose further that there are at most two pair powers -2, and that if there are two then the remaining pair power is nonnegative and even. The master integral is finite. Its normalized angular average at distinct radii is*

$$\prod_{i<j}r_{\mathrm{large}(ij)}^{p_{ij}}\sum_{\ell\ge 0}(2\ell+1)\prod_{i<j}A_\ell^{(p_{ij})}(t_{ij}). \tag{C.3}$$

If $p\ge -1$, $A_\ell^{(p)}$ is a rational polynomial with no powers below ℓ, and it vanishes for $2\ell>p$ when p is even. For $p=2m-1$, $m\ge 0$, it equals $\sum_{j=0}^{m}c_jt^{\ell+2j}$, where

$$c_0=\frac{(-1)^m(2m-1)!!}{\prod_{j=0}^{m}(2\ell+1-2j)},\qquad c_{j+1}=-c_j\frac{(m-j)(2\ell+1-2m+2j)}{(j+1)(2\ell+3+2j)}. \tag{C.4}$$

Here $(-1)!!=1$. For the inverse-square coefficient,

$$B_\ell(t)=\sum_{j\ge 0}\frac{\prod_{i=1}^{\ell}(2j+2i)}{\prod_{i=0}^{\ell}(2j+2i+1)}t^{2j},\qquad 0<B_\ell(t)\le 1-\log(1-t). \tag{C.5}$$

An even pair power makes (C.3) *terminate at the smallest half of an even pair power.*

Proof. Rodrigues' formula gives

$$\int_{S^2} P_\ell(\omega\cdot u)P_j(\omega\cdot v)\frac{d\omega}{4\pi} = \frac{\mathbf{1}_{\ell=j}}{2\ell+1}P_\ell(u\cdot v).$$

For example, the rotation-invariant reproducing kernel of degree ℓ spherical harmonics is $(2\ell+1)P_\ell$. Its trace determines this coefficient. Applying the identity twice gives (C.3). To compute a coefficient, expand $P_\ell(x)=\sum_{j=0}^{\ell} b_j x^j$ and substitute $y=1+t^2-2tx$. For $p\ge -1$ the result is

$$\sum_{j=0}^{\ell} b_j \sum_{i=0}^{j} \frac{(-1)^i\binom{j}{i}(1+t^2)^{j-i}[(1+t)^{p+2i+2}-(1-t)^{p+2i+2}]}{2^{j+1}(p+2i+2)t^{j+1}}. \tag{C.6}$$

Analyticity at zero cancels negative powers, and Legendre orthogonality cancels powers below ℓ. Orthogonality also proves termination for even p. The leading coefficient for $p=2m-1$ is $(-1)^\ell 4^\ell \ell!\prod_{j=0}^{\ell-1}(m-\frac{1}{2}-j)/(2\ell+1)!$. It equals c_0 in (C.4), including when $\ell<m$. Projecting $\Delta|x-e_3|^{2m-1}=2m(2m-1)|x-e_3|^{2m-3}$ onto degree ℓ shows that the remaining coefficients obey the displayed recurrence: the radial operator sends $t^{\ell+2j}$ to $2j(2\ell+2j+1)t^{\ell+2j-2}$.

Direct integration gives $A_0^{(-2)}=\log((1+t)/(1-t))/(2t)$ and $A_1^{(-2)}=(1+t^2)A_0^{(-2)}/(2t)-1/(2t)$. The Legendre recurrence then proves the positive series (C.5) by induction. Its coefficient is at most $1/(2j+1)$, which gives its logarithmic majorant. All angular series converge absolutely at distinct radii.

For $\ell\ge m$, expansion of a beta integral gives

$$A_\ell^{(2m-1)}(t)=c_0t^\ell\frac{\int_0^1 z^{\ell-m-1/2}(1-z)^m(1-t^2z)^m\,dz}{\int_0^1 z^{\ell-m-1/2}(1-z)^m\,dz}.$$

The quotient lies in $[0,1]$. This proves the sign $(-1)^m$ and the bound $|A_\ell^{(2m-1)}(t)|\le|c_0|t^\ell$ used in the tails below. The conditions on the clusters imply $C_\sigma,D_\sigma\ge 0$. After the scale integral, a finite angular term is bounded by a constant times $s^{D_\sigma}v^{C_\sigma}$ times at most two logarithmic majorants. For two distinct ratios in $\{s,v,sv\}$ their product is bounded by $(1-\log(1-s))(1-\log(1-v))$. This is integrable. An infinite angular sum has either three odd powers or one inverse-square power and two odd powers. In the first case, the beta bounds and the factor $2\ell+1$ give a summable $O(\ell^{-2})$ envelope after any fixed initial segment. In the second, the two odd coefficients give $O((2\ell+1)^{-2})$, and the product of all three ratios to power ℓ is $(sv)^{2\ell}$. The remaining sum is bounded by a constant times $1-\log(1-sv)$. Multiplication by the inverse-square majorant again gives a bound by a constant times $(1-\log(1-s))(1-\log(1-v))$, whichever edge has power -2. The scale integral contributes a bounded factor, since its denominator is at least the largest-radius rate. These bounds prove absolute integrability and justify termwise integration. □

Lemma C.5 (Ordered radial integrals)**.** *Let $a,b,c>0$ be rational, and let α,β,γ be integers with $\gamma\ge 0$, $d=\beta+\gamma+1\ge 0$ and $s=\alpha+\beta+\gamma+3\ge 1$. Define*

$$J=\int_{0<z<y<x} x^\alpha y^\beta z^\gamma e^{-ax-by-cz}\,dz\,dy\,dx,\quad \lambda=a+b+c,\quad \xi=\frac{b+c}{\lambda},\quad \eta=\frac{c}{\lambda}.$$

Then, with $(s)_j=s(s+1)\cdots(s+j-1)$ and $(s)_0=1$,

$$t_j=\frac{(s)_j\gamma!}{(d+j+1)!}\sum_{i=0}^{j}\frac{(d+i)!}{(\gamma+i+1)!}\xi^{j-i}\eta^i,\qquad f_j=\frac{(s)_j\xi^j}{j!(d+1)(\gamma+1)},$$

$$J \in \frac{(s-1)!}{\lambda^s}\left[\sum_{j=0}^{N} t_j, \sum_{j=0}^{N} t_j + \frac{f_{N+1}}{1-\rho_N}\right], \qquad \rho_N = \frac{\xi(s+N)}{N+1} < 1. \tag{C.7}$$

If $\alpha, \beta, \gamma \geq 0$, the exact rational alternative is

$$J = \sum_{i=0}^{\alpha} \sum_{j=0}^{\beta+i} \frac{\alpha!(\beta+i)!(\gamma+j)!}{i!j!a^{\alpha+1-i}(a+b)^{\beta+i+1-j}\lambda^{\gamma+j+1}}. \tag{C.8}$$

For a master with $n_i \geq -2$, $p_{ij} \geq -1$ all odd, and (C.2)*, put $m_{ij} = (p_{ij}+1)/2$, $M = \max m_{ij}$, $h = 2 + \sum m_{ij}$ and*

$$b_L = \frac{\prod_{i<j}(2m_{ij}-1)!!}{2(h-1)(2L+1-2M)^{h-1}}, \qquad L \in \mathbb{Z}, \quad L \geq M.$$

The absolute error after angular index L is at most b_L times the sum over the six radial orders of J with baseline degrees $(n_h+2+p_{hm}+p_{hb}, n_m+2+p_{mb}, n_b+2)$ and the shift $(-2L-2, 0, 2L+2)$, with the correspondingly ordered rates $R_i/180$.

Proof. Set $x = R, y = Ru, z = Ruv$ and integrate R. The remaining denominator is

$$\lambda^s[1 - \xi(1-u) - \eta u(1-v)]^s.$$

Its binomial expansion has nonnegative terms. Integrating the term of degree j by beta integrals gives t_j, and bounding its argument by ξ gives $t_j \leq f_j$. The ratios $f_{j+1}/f_j = \xi(s+j)/(j+1)$ decrease to $\xi < 1$. Hence the geometric remainder is (C.7). Repeated integration from $x = y$ and then $y = z$ gives (C.8).

For the angular tail multiply the three beta-integral bounds in the preceding proof. Cancel one factor $2\ell+1$ and bound the remaining h factors below by $2\ell+1-2M$. Since $t_{12}t_{13}t_{23} = (r_b/r_h)^2$, summing the decreasing coefficient by its integral on $[L, \infty)$ gives $b_L(r_b/r_h)^{2L+2}$. Every resulting radial integral has nonnegative lowest degree and middle-plus-lowest degree plus one, with total shape κ. The same is true for the finite angular terms: their polynomial exponents are nonnegative. This proves integrability and the asserted remainder. □

Lemma C.6 (Native radial arithmetic)**.** *Assume the native execution model of Set-up C.2. In Lemma C.5, suppose $(a, b, c) = (R_h, R_m, R_b)/180$ with $233 \leq R_i \leq 1116$, $0 \leq \gamma, d \leq 256$ and $1 \leq s \leq 32$. The positive interval recurrence described in the proof returns an enclosure of J within 4096 iterations. It has no integer overflow, invalid denominator or nonfinite numerical operand. For masters with $-2 \leq n_i \leq 10$, $-1 \leq p_{ij} \leq 10$, $1 \leq \kappa \leq 32$ and these rate bounds, the finite angular wrapper and the all-odd wrapper at $M+1 \leq L \leq 24$ return enclosures. Their sequential signed contraction remains enclosing and finite for at most 2^{24} terms with rational coefficients of magnitude at most 2^{128}.*

Proof. Outward recurrence. Write RN for nearest-even binary64 rounding and pred, succ for the adjacent numbers. For nonnegative expressions use $\max\{0, \mathrm{pred}(\mathrm{RN}(x))\}$ and $\mathrm{succ}(\mathrm{RN}(x))$ as lower and upper bounds. Rounding cells lie between their adjacent representable numbers, including at zero and in the subnormal range. Addition, multiplication and division of positive intervals therefore enclose their exact operations.

Set $\chi = c/(b+c)$. The native loop maintains intervals for t_j, f_j of (C.7), its last summand $\upsilon_j = (s)_j\gamma!\eta^j/[(d+j+1)(\gamma+j+1)!]$, and $\sum_{i<j} t_i$. Initially $t_0 = \upsilon_0 = f_0 = 1/[(d+1)(\gamma+1)]$. At

iteration j it first adds t_j, updates $f_{j+1} = \rho_j f_j$, and, if the upper endpoint of ρ_j is less than one, bounds the remainder by

$$\operatorname{succ}\left(\operatorname{RN}\frac{(f_{j+1})_+}{\operatorname{pred}(\operatorname{RN}(1-(\rho_j)_+))}\right).$$

The denominator is greater than 2^{-54}. The loop returns when this bound is less than the rounded product of the current lower sum and the binary64 literal 10^{-15}. It then multiplies the enclosing sum by the interval for $(s-1)!/\lambda^s$, built by successive factors i/λ. The comparison only chooses a return time. Enclosure already follows from the remainder formula. Otherwise the updates are

$$a_j = \frac{\xi(s+j)}{d+j+2}, \qquad b_j = \frac{\chi(d+j+1)}{\gamma+j+2}, \qquad \upsilon_{j+1} = a_j b_j \upsilon_j, \quad t_{j+1} = a_j t_j + \upsilon_{j+1}.$$

Cancellation of factorials in the exact series proves these identities, and induction proves the interval invariant. A failure return is never used as an interval.

Range and termination. All integer expressions, including those formed before the guard, have magnitude at most 4353 on this box. With $\mu = 2^{-1074}$ an outward scalar operation has absolute error at most $2^{-50}|x| + 2\mu$. The constructed upper ratio satisfies $\xi_+ < 29/32$ since $\xi \le 2232/2465$ and $29 \cdot 2465 - 32 \cdot 2232 = 61$. An induction with $K_j = 4(1+2^{-20})^j \binom{s+j-1}{j}$ gives

$$(\upsilon_j)_+, (f_j)_+ \le K_j, \qquad (t_j)_+ \le (j+1)K_j, \qquad K_j < 2^{406} \quad (0 \le j \le 4096).$$

Indeed each recurrence factor incurs a relative multiplier below $1 + 2^{-40}$. The larger multiplier $1 + 2^{-20}$ absorbs those errors and the additive 2μ terms. The accumulated sum is below 2^{432}, the scale below 2^{156}, and the returned value below 2^{640}. For termination the sharper envelope bound is

$$(f_N)_+ < 4(29/32)^N \binom{s+N-1}{N} + 4\mu N \binom{s+N-1}{N}.$$

At $N = 4096$ use $29^8 < 2^{39}$ and $\binom{s+N-1}{N} < 2^{403}$: the envelope is below 2^{-106}. At $j = 4095$ the ratio is below $15/16$, the remainder below 2^{-100}, and the lower sum remains above 2^{-18}. The stopping threshold exceeds 2^{-69}, so the return occurs.

Angular and signed arithmetic. The exact angular lists are (C.6) and (C.4). Equal radial powers are collected before conversion. Signed rational conversion uses both neighbors of its rounded value. Signed multiplication takes the four rounded corner products and then their exterior neighbors. Addition widens each rounded endpoint once. These rules enclose through cancellation. The odd wrapper adds the symmetric tail interval of Lemma C.5, with its upper endpoint rounded outwards.

Here $m_{ij} \le 5$. The largest angular exponent is $L + 2m_{ij} \le 34$, so each native call has lowest degree at most 80 and combined degree at most 103. A tail call has bounds 62 and 85. The finite wrapper has smaller bounds. The coefficient absolute sum of an odd edge is at most $9!!\,4^5 < 2^{20}$; for even edges the Legendre recurrence and binomial expansion give the same bound. There are fewer than 2^{16} terms in a wrapper and every collected coefficient has magnitude below 2^{80}. The preceding outward-error estimate bounds all master endpoints by 2^{740} and all stated signed-contraction intermediates by 2^{900}. This also proves finiteness of the outward neighbors used throughout. □

Lemma C.7 (Finite logarithmic integrals)**.** *Let α, β, γ be nonnegative integers and $a, b, c > 0$ be rational. On $x > y > z > 0$ let $(r'_0, r'_1, r'_2) = (x, y, z)$ and choose $0 \le h < k \le 2$. The integral*

$$\int x^\alpha y^\beta z^\gamma e^{-ax-by-cz} \log \frac{r'_h + r'_k}{r'_h - r'_k}\, dz\, dy\, dx$$

has the exact finite gamma-mixture evaluation and rational error bounds given in the proof. They apply also when auxiliary gamma rates coincide.

Proof. Finite reduction. Put $g_0 = x - y, g_1 = y - z, g_2 = z$. Expand $(g_0 + g_1 + g_2)^\alpha (g_1 + g_2)^\beta g_2^\gamma$. Each monomial is a positive rational multiple of independent gamma densities of integer shapes and rates $(a, a+b, a+b+c)$. The logarithm is the difference of the logarithms of $\sum_{i \ge h} g_i + \sum_{i \ge k} g_i$ and $\sum_{h \le i < k} g_i$. Thus it suffices to integrate $\log Y$ for $Y = \sum_i \ell_i X_i$, with integer gamma shapes and nonnegative rational ℓ_i, not all zero.

Merge equal positive rates ρ_i/ℓ_i into rates v with total shapes K_v. The Laplace transform is $\prod_v (v/(v+t))^{K_v}$. At the pole $-v$ compute the first K_v Taylor coefficients $c_{v,j}$ of $\prod_{w \ne v} (w/(w - v + z))^{K_w}$. A factor's coefficients obey

$$s_0 = \left(\frac{w}{w-v}\right)^{K_w}, \qquad s_j = -s_{j-1} \frac{K_w + j - 1}{j(w-v)}.$$

Finite convolution gives all $c_{v,j}$ exactly. Principal-part subtraction gives the partial fractions with weights $w_{v,j} = v^j c_{v,j}$, and $\sum_{v,j} w_{v,j} = 1$ by evaluation at $t = 0$. Consequently,

$$\mathbb{E} \log Y = \mathfrak{c} + \sum_{v,j} w_{v,j} (\mathsf{h}_{K_v - j - 1} - \log v), \quad \mathfrak{c} = \int_0^\infty e^{-t} \log t\, dt. \tag{C.9}$$

This follows by integrating the partial-fraction gamma densities. Integration by parts gives their log moments. The identity of densities can equivalently be obtained by inverse finite convolution of exponential polynomials. Their absolute logarithmic moments are finite. The common constant $\mathfrak{c}$ cancels in the required difference, so its numerical value is unnecessary. Equal rates were merged before division. Signed partial-fraction weights are retained.

Error and rounding. For $1 \le v \le 2$ put $z = (v-1)/(v+1)$. Then

$$0 \le \log v - 2 \sum_{j=0}^{127} \frac{z^{2j+1}}{2j+1} \le \frac{2 z^{257}}{257(1 - z^2)}. \tag{C.10}$$

Integrating the geometric series proves this bound. Reduce any positive rational rate to $2^k v$ with $1 \le v < 2$ and use the same formula for $\log 2$. Reverse endpoints if $k < 0$. Let $\delta(v)$ be the resulting width for that rate. Formula (C.9) then has width at most $\sum_v |\sum_j w_{v,j}| \delta(v) + 2^{-119}$ after outward rounding to multiples of 2^{-120}. Multiply the two log-mean intervals by the exact positive masses of the gap monomials, subtract with reversed endpoints, and add. This proves the claimed ordered-log enclosure with an explicit finite error, without a floating logarithm. □

Lemma C.8 (Compact inverse-square integrals)**.** *Let ℓ, D, C be nonnegative integers and let $\epsilon \in \{(1,0), (0,1), (1,1)\}$. Define*

$$\mathcal{J}_{\ell,\epsilon}(D, C) = \int_0^1 \int_0^1 s^D v^C B_\ell(s^{\epsilon_1} v^{\epsilon_2})\, dv\, ds.$$

Then $0 < \mathcal{J}_{\ell,\epsilon}(D,C) \le 2$, and it is a rational linear combination of $1, \log 2, 6\zeta(2), \zeta(3)$. For positive integer rate numerators (R_h, R_m, R_b), integer shape $m \ge 1$ and integer precision $d \ge 0$, the exact compact algorithm specified in the proof encloses

$$(m-1)! \int_0^1 \int_0^1 \frac{s^D v^C B_\ell(s^{\epsilon_1} v^{\epsilon_2})}{(a+bs+csv)^m}\, dv\, ds, \qquad (a,b,c) = (R_h, R_m, R_b)/180. \tag{C.11}$$

Its arithmetic uses integers and rationals, with denominator scale $U = 2^{640}$ and the constant intervals below.

Proof. We evaluate the compact moments by partial fractions and approximate only the radial denominator, with its integrated remainder included explicitly.

Compact moments and constants. The coefficient in (C.5) has the partial fractions

$$\frac{\prod_{i=1}^{\ell}(x+2i)}{\prod_{i=0}^{\ell}(x+2i+1)} = \sum_{h=0}^{\ell} \frac{a_{\ell h}}{x+2h+1}, \qquad a_{\ell h} = \frac{\prod_{i=1}^{\ell}(2i-2h-1)}{\prod_{0\le i\le \ell,\ i\ne h}(2i-2h)} > 0.$$

Each active variable contributes a factor $(2j+D+1)^{-1}$ or $(2j+C+1)^{-1}$ to the integrated positive series. An inactive one contributes $1/(D+1)$ or $1/(C+1)$. Thus each term reduces to

$$\sum_{j\ge 0} \prod_{v\in\mathcal{P}} (2j+v)^{-1},$$

where $\mathcal{P}$ is a list of two or three positive integers, with repetitions allowed. Partial fractions at a repeated pole $-v$ are computed by the Taylor coefficients of $\prod_{w\ne v}(w-v+z)^{-m_w}$. Their recurrence is the one in the preceding proof without its rate numerators. The sum of the simple-pole coefficients is zero, since the original rational function is $O(x^{-2})$. Subtract $1/(2j+1)$ from each simple-pole series before summing. Odd and even poles then give respectively finite harmonic tails and $-\log 2$ minus finite even harmonic tails. The square-pole tails are $6\zeta(2)/8$ and $6\zeta(2)/24$ minus their finite initial sums. The cube-pole tails are $7\zeta(3)/8$ and $\zeta(3)/8$ minus their initial sums. This proves the linear-combination formula, including triple poles. No divergent series is subtracted after evaluation.

For two distinct active degrees use

$$\mathcal{J}_{\ell,(1,1)}(D,C) = \frac{\mathcal{J}_{\ell,(1,0)}(D,0) - \mathcal{J}_{\ell,(1,0)}(C,0)}{C-D}.$$

For equal degrees use the repeated-pole formula. Outward integer division implements this identity and division by the inactive degree plus one. This also proves the correctness of caching these two reference types. The bound $\mathcal{J} \le 2$ follows from $B_\ell(t) \le 1 - \log(1-t)$: the active ratio is at most one of s, v, and $\int_0^1 (1-\log(1-t))\, dt = 2$.

Here are exact definitions of the constant inputs. Put $\mathsf{h}_j^{(2)} = \sum_{i=1}^{j} 1/i^2$, and set

$$E_1 = \sum_{j=1}^{769} \frac{2^{-j}}{j}, \quad E_2 = \sum_{j=1}^{769} \frac{2^{-j}\mathsf{h}_j}{j}, \quad E_3 = \sum_{j=1}^{769} \frac{2^{-j}(\mathsf{h}_j^2 + \mathsf{h}_j^{(2)})}{2j}.$$

For $(\gamma_1, \gamma_2, \gamma_3) = (1, 12, 4/3)$ use the integer pairs

$$a_i = \lfloor U\gamma_i E_i \rfloor, \qquad b_i = \lceil U\gamma_i (E_i + 2^{-769}) \rceil. \tag{C.12}$$

They enclose $U(\log 2, 6\zeta(2), \zeta(3))$. Indeed

$$b_{s,k} = \frac{1}{(s-1)!}\int_0^1 (1-t)^k(-\log t)^{s-1}\,dt \in [0,1]$$

and $\sum_{k\ge 0} 2^{-k-1}b_{s,k}$ is $\log 2$ for $s=1$ and $(1-2^{1-s})\zeta(s)$ for $s=2,3$. The omitted tail is at most 2^{-769}. Differentiating $\int_0^1 t^a(1-t)^k\,dt = k!/\prod_{j=1}^{k+1}(a+j)$ at $a=0$ gives the three displayed finite sums. Signed substitution of (C.12) and outward rounding therefore returns integers enclosing $U\mathcal{J}$.

Denominator and its error. Put $c_0 = a+(b+c)/2$, $h=(b+c)/(2c_0)<1$ and $S_0=(m-1)!/c_0^m$. Expand

$$\frac{(m-1)!}{(a+bs+csv)^m} = S_0\sum_{k\ge 0}\binom{m+k-1}{k}\left(h-\frac{bs+csv}{c_0}\right)^k.$$

The argument has absolute value at most h. Write $u_k = S_0\binom{m+k-1}{k}h^k$ and $\rho_k = h(m+k-1)/k$. Choose the first $n\ge 1$ with $\rho_n<1$ and $\tau = u_n/(1-\rho_n) < 10^{-d}$. Such n exists. The polynomial through degree $n-1$ has uniform error at most τ. Expand it as $\sum g_{ij}s^iv^j$ and set $w_{ij}=\lfloor Ug_{ij}\rfloor$. If there are $N_\triangle$ coefficients, the integrated denominator error is at most

$$\frac{e}{U}, \qquad e = \lceil 2U\tau\rceil + 2N_\triangle. \tag{C.13}$$

This follows by multiplying the uniform Taylor and coefficient-floor errors by a nonnegative weight whose integral is at most two.

For correspondence with the implemented polynomial shift, let $P_N(x)=\sum_{j=0}^N\binom{m+j-1}{j}x^j$, $N=n-1$, and $P_N(h+y)=\sum t_iy^i$. Horner evaluation gives t_0 and

$$t_{i+1} = \frac{(m+i)t_i - d_i}{(1-h)(i+1)}, \qquad d_i = (m+N)\binom{m+N-1}{N}\binom{N}{i}h^{N-i}.$$

These identities follow by comparing coefficients in $(1-x)P_N' - mP_N = -(m+N)\binom{m+N-1}{N}x^N$. They give $g_{ij} = S_0t_i(-1/(180c_0))^i\binom{i}{j}R_m^{i-j}R_b^j$. The consecutive integer binomial updates are exact divisions.

If $[l_{ij},u_{ij}]$ encloses $U\mathcal{J}(D+i,C+j)$, form

$$v_- = \sum_{i,j}\min(w_{ij}l_{ij}, w_{ij}u_{ij}), \qquad v_+ = \sum_{i,j}\max(w_{ij}l_{ij}, w_{ij}u_{ij}).$$

Then $[(v_- - eU)/U^2, (v_+ + eU)/U^2]$ encloses (C.11). This is precisely the integer contraction and error allowance used in the compact evaluations. □

Lemma C.9 (Signed odd-logarithmic tail)**.** *Let a master have one pair power -2 and the other two powers $2m_1-1, 2m_2-1$, with nonnegative integers m_i and $\mu = m_1+m_2>0$. Assume $n_i\ge -2$, positive integer rate numerators and the cluster conditions* (C.2)*. Put $M=\max(m_1,m_2)$ and $\lambda = \sum_i R_i/180$. Choose an integer $L\ge M$ such that for every radial order*

$$d_\sigma = D_\sigma + 2L + 2 - \kappa \ge 0, \qquad c_\sigma = C_\sigma + 2L + 2 - \kappa \ge 0.$$

Let $\mathcal{I}_L$ be the angular expression through $\ell = L$, using the compact integrals of Lemma C.8. Set

$$v_\sigma = \begin{cases} c_\sigma, & \text{the inverse-square edge is } mb,\\ d_\sigma, & \text{otherwise,}\end{cases} \qquad T_\sigma = \frac{(2m_1-1)!!(2m_2-1)!!(\kappa-1)!(1+\mathsf{h}_{v_\sigma+1})}{2\mu(2L+1-2M)^\mu\lambda^\kappa(d_\sigma+1)(c_\sigma+1)}.$$

Then

$$0 \le (-1)^{\mu}(\mathcal{I} - \mathcal{I}_L) \le \sum_{\sigma} T_{\sigma}. \tag{C.14}$$

Proof. For $\ell > L$, the two odd angular coefficients have signs $(-1)^{m_1}, (-1)^{m_2}$ by the beta-integral formula, and the inverse-square coefficient is positive. Cancel one factor $2\ell+1$ from their coefficient bound. The remaining sum is bounded by

$$\sum_{\ell > L} (2\ell + 1 - 2M)^{-\mu-1} \le [2\mu(2L + 1 - 2M)^{\mu}]^{-1}.$$

The radius-ratio factor is $(sv)^{2L+2}$. Also $a + bs + csv \ge \lambda sv$, and $B_\ell(t) \le 1 - \log(1-t)$, with $t = v$ on edge mb and $t \le s$ otherwise. The remaining two monomial integrals are $1/(j+1)$ and $(1 + \mathsf{h}_{j+1})/(j+1)$. They give T_σ. The bound is integrable, justifying the angular integration and retaining its common sign. The finite part uses $A_\ell^{(-2)} = t^\ell B_\ell(t)$ and the two rational polynomials. Their exponents ensure $D, C \ge 0$ in every compact call. □

Lemma C.10 (Double-logarithmic quadrature)**.** *Let $1 \le a, b, c \le 7$ be positive rational rates, let $1 \le m \le 16$, $0 \le X, Y \le 16$ and $0 \le \ell \le 3$ be integers with $X + Y + 4\ell \le 36$, and let t_1, t_2 be distinct members of $\{x, y, xy\}$. The order-ten tensor Gauss algorithm specified in the proof, with endpoint cutoff 2^{-34}, encloses*

$$\int_0^1 \int_0^1 \frac{x^X y^Y A_\ell^{(-2)}(t_1) A_\ell^{(-2)}(t_2)}{(a + bx + cxy)^m}\, dx\, dy \tag{C.15}$$

under the NumPy execution model of Set-up C.2. Consequently its finite signed angular assembly encloses every master with pair powers a permutation of $(-2, -2, 2k)$, $k \in \{0, 1, 2, 3\}$, whose ordered terms satisfy these bounds and whose nonzero angular coefficients have magnitude below 2^{45}.

Proof. We bound the Gauss remainder and omitted strips, then verify the floating allowances for the angular functions and the positive sums.

Rule and analytic error. The ten nodes are enclosed by rational sign brackets for P_{10}, starting with width $2 \cdot 10^{-12}$ and bisecting 48 times. The brackets must be disjoint, and their derivative lower bounds positive. Proposals for the brackets have no assumed accuracy. The polynomial is

$$P_{10}(t) = \frac{46189t^{10} - 109395t^8 + 90090t^6 - 30030t^4 + 3465t^2 - 63}{256}.$$

Its ten sign changes certify all ten roots. Since $|P_{10}''| \le 1485 < 10^4$ on $[-1, 1]$, a bracket $[l, u]$ gives $|P_{10}'(r)| \in [|P_{10}'((l+u)/2)| - 10^4(u-l)/2, |P_{10}'((l+u)/2)| + 10^4(u-l)/2]$. Use this interval and the endpoint bounds for r^2 in $w(r) = 2/[(1-r^2)P_{10}'(r)^2]$ to enclose each positive weight. The exact sign/weight certificate in the supplement gives

$$|r| < .974, \qquad .066671 < w(r) < .295525.$$

Its rational comparisons use the displayed polynomial and derivative formula. Any successful final source bracket has width $1/(140737488355328000000000000) < 10^{-26}$, and hence lies in $(-.975, .975)$. The weight bounds change by less than $3 \cdot 10^{-14}$. Thus all source brackets lie in $(-.99, .99)$ and their weight endpoints in $(1/16, 1)$. Orthogonality and division by P_{10} prove the

rule exact through degree 19. The weight formula follows by integrating its Lagrange cardinal polynomials.

The mesh consists of $0, 1/32, \dots, 1/2$, followed by the midpoint and right endpoint of each $[1-2^{-j}, 1-2^{-j-1}]$, $1 \le j \le 33$. There are 82 panels and 820 nodes in each direction, hence $N = 672400$ tensor nodes. Let $\delta = 2^{-34}$. On a panel of midpoint z_0 and half-width h, use the complex disk $|z - z_0| \le 4h$. The positive upper bound on $|z|$ is less than $1 - 2^{-36}$, the lower real-part bound is at least $-3/64$, and the real part of $a + bx + cxy$ is at least $11/32$ when one variable is in its disk and the other in its real panel.

Write $\Lambda(t) = 1 - \log(1-t)$. The positive series gives $|A_\ell^{(-2)}(z)| \le \Lambda(|z|)$ for $|z| < 1$. For two distinct ratios their product is bounded by $\Lambda(x_+)\Lambda(y_+)$, where x_+, y_+ are the disk/real upper moduli. If d_- is the denominator lower bound on that disk, an analytic majorant is $x_+^X y_+^Y \Lambda(x_+)\Lambda(y_+)/d_-^m$. Let $\mathcal{M}$ be the sum of rectangle areas times these majorants for both choices of the complex variable, replacing $\Lambda(t)$ by the integer upper bound $3 - e$ when $\operatorname{frexp}(1-t)$ has exponent e. Cauchy's coefficient bound gives a Taylor remainder $(4/3)4^{-20}$ times the majorant. The integral and positive rule each have mass equal to the panel length. Applying $(I_x - Q_x)I_y + Q_x(I_y - Q_y)$ on each rectangle therefore gives error $(8/3)4^{-20}\mathcal{M}$.

Define $M_Z(A, B) = \max_{0 \le t \le 1} t^Z/(A + Bt)^m$. For $Z = 0$ it is A^{-m}. Otherwise the maximizer is 1 if $m \le Z$ or $B = 0$, and $\min\{1, ZA/((m-Z)B)\}$ in the remaining case. Differentiation proves this formula, so M_Z is evaluated rationally. The two omitted strips have total integral at most

$$2\delta(2 + 34)\left[M_Y(a + b(1-\delta), c(1-\delta)) + M_X(a, b + c(1-\delta))\right]. \tag{C.16}$$

Here $\int_0^1 \Lambda = 2$ and $\int_{1-\delta}^1 \Lambda = \delta(2 - \log\delta) \le 36\delta$. An overlap of the two strips only enlarges the bound.

Angular evaluation. Put $u = 2^{-53}$ and $\gamma_j = ju/(1 - ju)$. All node-ratio endpoints lie in $(2^{-27}, 1 - 2^{-35})$. For $t < 5/8$, evaluate the positive series for $A_\ell^{(-2)}(t)$ through $j = 64$ by Horner's rule. The lower polynomial has terminal coefficient $c_{\ell,64}$ and the upper one has $c_{\ell,64} + 2$, since the omitted tail is less than $2t^\ell(t^2)^{64}$. The operation and coefficient-conversion error is at most $\gamma_{200} < 3 \cdot 10^{-14}$ relatively. Multiplication by $1 \mp 2 \cdot 10^{-12}$ covers it in the respective directions.

For $t \ge 5/8$, put $z = (1 + t^2)/(2t)$ and evaluate

$$Q_0 = \log(1+t) - \log(1-t), \quad Q_1 = zQ_0 - 1, \quad Q_{j+1} = \frac{(2j+1)zQ_j - jQ_{j-1}}{j+1}, \quad A_j^{(-2)} = Q_j/(2t).$$

Each logarithm is computed by exact binary argument reduction and $2\sum_{i=0}^{24} w^{2i+1}/(2i+1)$, with $w = (v-1)/(v+1)$ and $1 \le v < 2$. Its omitted tail is bounded by $2/[51\,3^{51}(1 - 1/9)]$. The binary64 constant for $\log 2$ is $6243314768165359/2^{53}$. The same finite series at $w = 1/3$ places $\log 2$ strictly between this value and this value plus u. Counting the argument, Horner and final-addition errors gives less than $400u$ absolute error per logarithm and $900u$ for Q_0. Since $1 \le z \le 89/80$ and $0 < Q_j < 25$, the first recurrence has local error below $200u$ and the next two below $1000u$ each. Start the error allowance at $2 \cdot 10^{-12}$, update it first as $1.2E + 2 \cdot 10^{-12}$ and then as $2.3E + E_{\text{previous}} + 2 \cdot 10^{-12}$. Induction bounds the actual error by half this allowance, including rounding of the allowance. Subtracting/adding it, dividing by $2t$ and multiplying by 1 ∓ 10^{-14} gives enclosing endpoints. Both branches have lower endpoint greater than $t^\ell/8$ and upper endpoint less than 32. Clipping at zero changes neither.

Positive reductions and directed assembly. Use lower node, weight, monomial and angular endpoints for the lower tensor sum and the upper denominator endpoint, and reverse those choices for the upper sum. Before reduction the relative error in each positive summand is below γ_{400}.

Including the nonnegative reduction and coefficient multiplication gives $\gamma_{N+512} < 2u(N+512)$. The source multiplier

$$1 \mp 32u(N+1024) \tag{C.17}$$

covers this error and the final rounding in the indicated direction. For the disk denominator, possible cancellation has absolute error at most $21\gamma_5$ and relative error below γ_{1024}, using its lower bound $11/32$. Powering and inversion cost less than γ_{33000}. The two disk reductions and all remaining operations give a combined bound $\gamma_{60000} < 7 \cdot 10^{-12}$ for the error expression. Its source factor $1 + 10^{-9}$ therefore makes the sum of (C.16) and $(8/3)4^{-20}\mathcal{M}$ an upper bound after floating evaluation.

These relative estimates are valid throughout: node coordinates exceed 2^{-13}, ratio coordinates exceed 2^{-27}, weights exceed 2^{-41}, and the positive denominator lies in $[1, 21]$. Using $X+Y+4\ell \le 36$ bounds every positive tensor intermediate between 2^{-700} and 2^{100}. Disk and strip intermediates lie between 2^{-400} and 2^{110}. Positive angular intermediates also stay normal, and exact zeros in argument reduction stay zero. Thus no harmful underflow or overflow was assumed in the relative estimates. Finally subtract/add the error using the adjacent exterior binary64 number, reverse endpoints for a negative angular coefficient, and add with the same directed rule. At most 60 angular terms occur in a master. These last signed operations remain enclosing even at zero or subnormal cancellation. This proves the assertion. □

Lemma C.11. *For the trials and sources of Definition C.1, all functions belong to $D(H_3(3))$, the sources have norm one, and the spin representation preserves their inner products and Hamiltonian inner products. Every moment specified by a pair in Definition C.3 equals*

$$(4\pi)^3 C_c \sum_k \frac{W_c(k)}{D_c} \mathcal{I}(k). \tag{C.18}$$

Every integral in this sum converges absolutely. All its distance powers are at least -2, and an inverse-square pair power occurs only in a base residual-norm column.

Proof. We identify the Hamiltonian dictionaries, justify their domains, and then check the spin and scalar normalizations.

Hamiltonian dictionaries. Use the six oriented edges $(1,0),(2,0),(3,0),(1,2),(1,3),(2,3)$, where $x_0 = 0$. For $e = (j,k)$ write $y_e = x_j - x_k$, $\epsilon_{ei} = \mathbf{1}_{j=i} - \mathbf{1}_{k=i}$, $w_e = \sum_i \epsilon_{ei}^2$, and $g_{ef} = \sum_i \epsilon_{ei}\epsilon_{fi}$. Put $a_e = a_i$ on $(i,0)$ and zero on the pair edges, and put $v_e = -3$ on nuclear edges and 1 on pair edges. Direct differentiation of a scalar primitive $F = F_{a,\nu}$ gives

$$\begin{aligned}(H_3(3) + 15/2)F = F\Bigg[&\frac{15}{2} - \frac{1}{2}\sum_e w_e a_e^2 + \sum_e \frac{v_e + w_e a_e(\nu_e+1)}{d_e} - \frac{1}{2}\sum_e \frac{w_e \nu_e(\nu_e+1)}{d_e^2} \\ &- \sum_{e<f} g_{ef}\left(\frac{\nu_e}{d_e^2} - \frac{a_e}{d_e}\right)\left(\frac{\nu_f}{d_f^2} - \frac{a_f}{d_f}\right) y_e \cdot y_f\Bigg].\end{aligned} \tag{C.19}$$

For a Cartesian primitive one adds the product-rule term

$$(H_3(3) + 15/2)(x_{j,3}F) = x_{j,3}(H_3(3) + 15/2)F - F\sum_e \epsilon_{ej}\left(\frac{\nu_e}{d_e^2} - \frac{a_e}{d_e}\right) y_{e,3}. \tag{C.20}$$

The identity $2y_{(j,k)} \cdot y_{(s,t)} = d_{jt}^2 + d_{ks}^2 - d_{js}^2 - d_{kt}^2$ turns these into finite rational dictionaries. A power lowered by two has a nonzero coefficient only if its original power is positive. Thus every

output monomial has powers at least -1 and at most two negative powers. In a product, all powers are at least -2, at most two can equal -2, and the sum of all six powers is at least -4. Cartesian averaging increases one power by two. In particular, (C.2) holds term by term. A product with an undifferentiated trial or source cannot have a pair power -2.

Domains and convergence. The primitives and their first derivatives are bounded by an exponentially decaying polynomial. Each second derivative is bounded on compact sets by a constant times $1+\sum_e d_e^{-1}$. These bounds are square integrable: each collision has three transverse coordinates. Cut off tubes of radius ε around the six collisions. Their volumes on compact sets are $O(\varepsilon^3)$, whereas cutoff gradients are $O(\varepsilon^{-1})$. The integration-by-parts boundary errors against bounded first derivatives are $O(\varepsilon^2)$. Thus the displayed derivatives are also the distributional derivatives. The functions are in H^2, and their Coulomb potential products are in L^2. The distributional identity therefore gives the defining form identity for $D(H_3(3))$, first against smooth test functions and then by H^1 density. Indeed integration of $\operatorname{div}(x/|x|^2) = |x|^{-2}$ and Cauchy–Schwarz give $\||x|^{-1}\phi\|_2 \le 2\|\nabla\phi\|_2$. Applying this also in relative collision coordinates controls each Coulomb form term.

For the expanded products, Lemma C.4 gives absolute convergence. To check its remaining hypothesis, two pair powers -2 require two Hamiltonian monomials each having the same two pair powers -1. Such a monomial comes from differentiating two pair factors of power one and retaining the square of the third distance in the polarization identity. The S table has no term with all three pair powers positive, so the third power in the product is four. A P scalar feature has degree at most two, so the third power is four or, after Cartesian averaging, six. It is therefore even. This proves termwise integrability without cancellation of singular monomials.

Spin, sources and measure. Two signed permutations producing the same spin string differ by the exchange of the two up spins. The identity $P_{13}f = -f$ makes their prescriptions agree. The three nonzero components have squared norms $\|f\|^2/3$, so their sum is $\|f\|^2$. Polarization and commutation of $H_3(3)$ with permutations prove the asserted isometry also for graph products. No assertion about total spin is used.

The normalized $1s$ orbital is $Q^{3/2}e^{-Qr}/\sqrt{\pi}$. The nS orbital is

$$\frac{(2Q/n)^{3/2}}{\sqrt{2}n\sqrt{4\pi}}e^{-Qr/n}L^1_{n-1}(2Qr/n),$$

where $L^1_{n-1}(y) = \sum_{j=0}^{n-1}(-1)^j\binom{n}{j+1}y^j/j!$. Integration by parts in its Rodrigues formula gives $\int_0^\infty e^{-y}y^2(L^1_{n-1}(y))^2\,dy = 2n^2$. The overlap with $1s$ vanishes for $n \ge 2$ by the same finite polynomial integral. For $2P$ and $3P$, integrate x_3^2 as $r^2/3$ and use $\int_0^\infty r^j e^{-ar}\,dr = j!/a^{j+1}$. Their overlap with $1s$ is zero by odd parity. Multiplying the three normalized orbitals and applying $A_{13}/\sqrt{2}$ gives exactly the positive constants $C_{T,n}$ in Definition C.1. It proves unit source norms and preserves the stated source phases.

Rotational invariance of the scalar factors gives $\int x_{i,3}x_{j,3}G = \frac{1}{3}\int x_i \cdot x_j G$, which proves the factor $1/6$ in the array definition. A simultaneous electron permutation leaves a scalar integral unchanged. It introduces neither a sign nor an orbit-size factor. All antisymmetrizer signs are already in the coefficients. Finally, the three normalized angular measures in (C.1) require exactly the restoration factor $(4\pi)^3$. This proves (C.18). □

Lemma C.12 (Physical factors)**.** *Put $A = (4\pi)^3$, $F_{T,n} = AC_{T,n}$ and $B_G = [k_G/2^{128}, (k_G+1)/2^{128}]$ for each factor in Table 10. Then $G \in B_G$ for all eight factors.*

Table 10: Integer numerators for the physical factor intervals.

G	k_G
A	675256909963386956951116526350654582672596
$F_{S,2}$	125173828705686414891769267358420852742912 8
$F_{S,3}$	45424001404367023919398066933078094497236 4
$F_{S,4}$	22127815776218546273592644743697534916019 4
$F_{S,5}$	12666700868919537614046101628908898998166 8
$F_{S,6}$	80299048554137951591401791333167863507093
$F_{P,2}$	33379687654849710637805137962245560731443 43
$F_{P,3}$	19780555647318347044625266940589961914929 44

Proof. Squaring the positive constants gives

$$F_{S,n}^2 = \frac{2^{38}\pi^3}{3^9 n^5}, \qquad F_{P,2}^2 = \frac{2^{39}\pi^3}{3^{11}}, \qquad F_{P,3}^2 = \frac{2^{47}\pi^3}{3^{17}}.$$

The rational arithmetic certificate in the supplement bounds π between $P_*/2^{256}$ and $(P_*+1)/2^{256}$, where

$$P_* = 3637715768917663242802349427777298626533933773283924299587721511179388944661 85.$$

Its construction uses

$$\pi = 16\arctan(1/5) - 4\arctan(1/239), \qquad 0 < \arctan(1/v) - \sum_{j=0}^{63} \frac{(-1)^j}{(2j+1)v^{2j+1}} < \frac{1}{129v^{129}}.$$

The first identity follows by multiplying $(5+i)^4(239-i) = 114244(1+i)$ and fixing the angle in $(0,\pi/2)$. The second follows by integrating a finite geometric series. For completeness, the integer certificate lists the quotients $f_{v,j} = \lfloor 2^{288}/((2j+1)v^{2j+1}) \rfloor$, their positive remainders and complementary remainders, and their signed prefixes. If $S_v = \sum_{j=0}^{63}(-1)^j f_{v,j}$, it verifies

$$2^{32}P_* < 16(S_5 - 32) - 4(S_{239} + 33), \qquad 16(S_5 + 33) - 4(S_{239} - 32) < 2^{32}(P_* + 1).$$

These are exact integer inequalities and prove the stated π interval. Cubing its endpoints and testing the squares of $k_G/2^{128}$ and $(k_G+1)/2^{128}$ proves the seven radical bounds. The bound for A uses $64\pi^3$ directly. The complete positive cross-product remainders are supplied with the factor table. Positive square roots preserve both inequalities, so no source phase changes in this operation. □

C.3 Complete finite certificates

We now define the family partition used by the computations. With no pair power -2, the P families are *Pol* (all three pair powers even), *Fin* (some but not all even), and *Odd* (all odd). Their union is *Splain* for S. With two pair powers -2 the family is *Doublelog*. With exactly one, use *Oddlog* when the other two powers are odd. In the remaining case use the following exact predicate.

Write $\Lambda_0(t) = \log((1+t)/(1-t))$ and expand $A_\ell^{(-2)} = U_\ell\Lambda_0 + V_\ell$ as Laurent polynomials:

$$U_0 = (2t)^{-1}, \quad V_0 = 0, \quad U_1 = (1+t^2)/(4t^2), \quad V_1 = -(2t)^{-1}.$$

Both sequences obey $(\ell+1)Z_{\ell+1} = (2\ell+1)(1+t^2)Z_\ell/(2t) - \ell Z_{\ell-1}$. For every radius order, multiply these lists and the other angular polynomials through the finite even cutoff, include the radial Jacobian, collect equal monomials and logarithm labels, and remove zero coefficients. Call the tuple *supported* if each of the six lists is nonempty and every surviving term has at most one log label, degrees (α, β, γ) satisfying $\gamma \geq 0$, $\beta+\gamma+1 \geq 0$, $\alpha+\beta+\gamma+3 > 0$, and all three degrees nonnegative when a log label is present. The supported part is *Log*. Its complement is *Single*. This predicate is a finite rational calculation, with no integral evaluation. It tests the collected Laurent expression, not the number of inverse-square factors alone.

Proposition C.13 (Evaluated family certificates)**.** *Assume Set-up C.2 for the retained executions and readers. For the exact arrays of Definition C.3, the family partition is exhaustive and has the sizes in Table 11. The complete raw interval tables in the accompanying code/data release, denoted $J_{T,c,E}$ for family E, contain*

$$X_{T,c,E} = \sum_{k \in \mathcal{L}_T \cap E} \frac{W_c(k)}{D_c} \mathcal{I}(k).$$

For Splain the supplied intervals R_c instead contain the physical quantities $(4\pi)^3 C_c X_{S,c,\mathrm{Splain}}$. The seven extra moments have the physical interval certificates described in the proof. All statements concern the fixed trials simultaneously.

Table 11: Complete base-family coverage and retained evaluation parameters.

Family	S keys	P keys	Evaluation
Splain	61344	—	finite or odd, $L = 14$
Pol	—	17277	exact rational
Fin	—	108710	17 decimal digits, 96-bit endpoints
Odd	—	15165	$L = 24$, 120-bit endpoints
Log	6983	21318	17 digits for plain terms, 96-bit endpoints
Single	3128	7749	compact, 18 digits; one 15-digit group
Oddlog	2248	3376	$L = 8$, compact 13 digits, 200-bit endpoints
Doublelog	50	72	Gauss order 10, endpoint power 34
Total	73753	173667	

Proof. The proof checks the exact input arrays, applies the integral error bounds to all recorded calls, and reconstructs every signed contraction. The supplement contains the full arrays and group/row records used in these comparisons, together with the independent readers. The counts in Table 11 summarize those full comparisons.

Common compiler and input identity. The compiler implements (C.19)–(C.20) by rational dictionary addition. Its exchange reverses nuclear slots $1, 3$, interchanges pair slots $12, 23$, and also exchanges the Cartesian label in P. In a square, it either enumerates both ordered products or doubles an off-diagonal group once. Cartesian products include both copies of r_i^2 when $i = j$, giving $r_i^2/3$. Its integer packing is exact tuple addition: the scalar power digits after offset 3 lie in $[1, 25]$ in base 32. The vector digits after offset 4 and the square increment lie in $[2, 24]$. Rate sums are at most $1116 < 2048$, the rate-packing base. Thus there is no carry or borrow into another field. Signed collision addition and removal only of whole zero vectors implement the array definition exactly.

The independent input reader compared every rational primitive and every mode, both entire generated and retained base arrays, and each denominator with the least-common-multiple

definition. Headers have all nine key fields and all eight or five signed weights. Widths are exactly 17 and 14. It checks strictly increasing canonical keys, compares both streams to exhaustion, and rejects a missing or extra row. For P it also accumulated all 450585 raw rows by signed canonical addition and obtained the same 173667-key array. For every family, the reader removes a key from a copy of the full map only after comparing its complete vector and its exact selector. The remaining map is empty at the end. A repeated key cannot be removed twice. This proves coverage and disjointness, including zero entries within active vectors.

The corresponding extra arrays have union sizes 6830 and 9878. Their nonzero column sizes are $(4256, 450, 579, 708, 837)$ and $(9055, 823)$, with denominators

$$(10^{28}, 81 \cdot 10^{14}, 81 \cdot 10^{14}, 151875 \cdot 10^{14}, 885735 \cdot 10^{14}), \qquad (6 \cdot 10^{36}, 54 \cdot 10^{18}).$$

A separate uncompressed product expansion compares every extra signed coefficient. The reader also compares the original first-insertion dictionary order used for floating summation, not merely its sorted map. Source comparisons retain every executable expression. Only locations, unused docstrings and one diagnostic character-encoding difference are irrelevant. Completed compiler stages are linked to their actual outputs by their synchronous return and full later comparisons. One scalar driver failed after completing its compiler stage; that later failure is not represented as a successful whole run.

The structural power bounds in Lemma C.11 exclude three inverse-square pairs and put all inverse-square families in residual norms only. Two such pair powers in one Hamiltonian monomial arise from differentiating two pair factors of power one and retaining the square of the third distance. The S table has no monomial with three positive pair powers and has total degree at most five. The P scalar features have degree at most two. Hence the Doublelog powers are $(-2, -2, 4)$ with nuclear degree at most six in S, and $(-2, -2, 4)$ with nuclear degree two or $(-2, -2, 6)$ with nuclear degree zero in P. These restrictions also exclude Doublelog from the supported selector: when the shared endpoint of the inverse-square edges has middle radius, the coefficient of the two log labels, at $s = v = 1/2$, is $243/2048$ for the remaining power four and $3645/65536$ for power six. Both are nonzero. Thus the concrete source selectors give exactly the partition stated above.

Exact polynomial, finite and Log families. For Pol expand each even distance power by the multinomial theorem. The angular moment of u^j against P_ℓ is $j!/[(j-\ell)!!(j+\ell+1)!!]$ when $j \geq \ell$ and $j - \ell$ is even, and zero otherwise. Rodrigues integration by parts proves this formula. The angular triple contraction then leaves independent radial gamma integrals. Exact evaluation of all 17277 selected keys and all five signed columns gives the supplied Pol singletons. The independent reader checks their full input and rational outputs.

For Fin, the even cutoff and Lemma C.5 give an exact finite angular sum. Nonpolynomial radial calls stop only when their explicit tail is at most 10^{-17}, before the 10000-iteration cap. Every recorded call returned. Grouping uses a positive common angular denominator. The reader reconstructs the same group independently as a rational vector sum and deletes each observed nonzero radial key only after comparing all five coefficients. All 59 rate groups and 50613 nonzero radial calls were covered. The producer completed these evaluations, output writes and all endpoint comparisons before a later environment-metadata error. The separate reader exhaustively checked those completed records. No failed integral return is used.

For Log, the supported predicate gives exactly the hypotheses of Lemma C.7 on log terms and of Lemma C.5 on plain terms. The plain calls use 17 digits. Logarithmic calls use the fixed 128-term and 120-bit bounds in their lemma. The 12 scalar rate groups give 10025 nonzero radials (8273 logarithmic and 1752 plain). The 59 vector groups give 48797 (42060 and 6737).

Empty groups remain in the manifest. The complete independent regrouping and recorded-call comparisons cover every term. In both Fin and Log each rational radial interval is rounded outward to multiples of 2^{-96}, multiplied with endpoint reversal by its signed group coefficient, and divided once by the angular and column denominators. Reconstructing all zero-start group sums gives exactly the unchanged supplied raw endpoint pairs.

Native Odd, Splain and three extra moments. On the entire native base support, the rates lie in $[233, 1116]$, the nuclear powers in $[-2, 10]$, the pair powers in $[-1, 10]$, and the shapes in $[5, 19]$. Each column has fewer than 2^{23} terms and coefficient absolute sum less than 2^{52}. The extra native inputs have nonnegative powers at most ten, shape in $[9, 19]$, fewer than 2^{18} terms and coefficient absolute sum less than 2^{26}. These bounds follow by taking products of the primitive dictionaries, and are also checked on the complete consumed arrays. Thus all calls are in Lemma C.6. The cutoffs are 24 for P Odd, 14 for the odd part of Splain, and 12 for the odd parts of the extra norms. The remaining calls use the finite branch.

The observers call the unchanged native/wrapper function, record its actual returned hexadecimal and rational endpoints, and return those same values. Their before/after records identify the loaded library, interface widths, rounding state and disabled flush modes. Such observations instantiate, rather than prove, the execution assumptions. The independent readers use integer arithmetic to decode every endpoint and reconstruct every signed prefix from zero. For P Odd they check $A_j = \lfloor 2^{120} l_j \rfloor$ and $B_j = \lceil 2^{120} u_j \rceil$, then add $\min(W_c A_j, W_c B_j)$ and $\max(W_c A_j, W_c B_j)$. They verify all 15165 rows, all 949 retained prefixes, and equality of the five final pairs with the supplied raw intervals.

For Splain they check all 61344 distinct selected masters and 121 prefixes, reconstructing both the exact rational contraction of returned intervals and the original floating accumulation. Nearest-even decoding is implemented by determining $2^e \le |x| < 2^{e+1}$ and rounding $|x|$ to the grid $2^{\max(e-52,-1074)}$, with an even quotient at a midpoint. The sign and adjacent bit patterns then reconstruct each outward operation, including zero and subnormals. This proves the meaning of the independent rounding reconstruction. Multiplication by the factor intervals of Lemma C.12 puts all eight reconstructed Splain intervals inside their saved physical R_c. Both signed cross-product margins are positive in every column. In particular the negative Splain residual-norm contribution is retained. No interval-library normalization claim is needed.

The same method covers the three extra native columns in their original source order: 4256 scalar-norm calls (4027 finite and 229 odd), 9055 vector-norm calls (8890 finite and 165 odd), and 823 finite P source-3 overlap calls. All 14134 calls and 115 prefixes are checked. The exact physical scaling gives intervals inside both the saved dyadics and the final printed targets for these three moments.

Single. Keep the inverse-square angular factor as $t^\ell B_\ell(t)$ and expand the two other factors through their finite even cutoff. For every chamber term the compact degrees satisfy $D, C \ge 0$. The shape is at least five in S and seven in P. Lemma C.8 applies to every grouped vertex. The six constant integers used in these executions were compared exactly with (C.12). Each upper integer equals the lower integer plus one. Thus their guard is an evaluated identity, not an unevaluated hypothesis.

The full 12 scalar and 59 vector rate groups contain 22825 and 63216 nonzero compact vertices. There are respectively two and 37 nonempty groups. The other ten and 22 have the exact interval $[0, 0]$. Each reader comparison includes the ordered vertex arguments, signed coefficient, rational return, 96-bit outward group rounding and column denominator. All groups use denominator precision 18 except the first vector group, identified as P-000 in the supplementary manifest, whose selected complete evaluation uses precision 15. It has exactly the same input vertices and

constants. Only that replacement is included. The original wider precision-18 interval is retained for provenance and contributes nothing. The compact error proof applies to either precision. Reconstructing these selected outputs gives intervals strictly inside both unchanged Single targets. This proves their actual containments.

Oddlog. On every generated Oddlog key, $\mu \geq 2$ in Lemma C.9. The complete domain checks give $5 \leq \kappa \leq 17$, $M \leq 7$ and $d_\sigma, c_\sigma \geq 1$ in S; in P they give $7 \leq \kappa \leq 13$, $M \leq 5$ and $d_\sigma, c_\sigma \geq 5$. These are the conditions at the original cutoff $L = 8$. Every selected key contributes its six exact rational tails, with sign $(-1)^\mu W_c(k)$, before any finite-part cancellation. The reader independently recomputes all six terms and every tail prefix.

The finite parts have 54 nonzero scalar groups with 89467 compact rows and 390 vector groups with 251107 rows. Ordered returns use compact precision 13 and the same exact constant tuple as Single. A group with denominator $\Delta > 0$ and signed row coefficient w contributes the integer endpoints

$$\left\lfloor 2^{200} \frac{\min(wl, wu)}{\Delta} \right\rfloor, \qquad \left\lceil 2^{200} \frac{\max(wl, wu)}{\Delta} \right\rceil$$

from a returned interval $[l, u]$. The retained reference compact moments and complete denominator triangles reconstruct every ordered return. Where a group spans several invocations, each carried row is compared with its preceding actual return, the prefix is recomputed from zero, and fresh calls start at the next row. Induction over those parts proves the completed sum uses each row once. The complete group manifest, not a list of whichever outputs exist, fixes final coverage. The finite intervals plus the exact signed tails lie inside precisely the unchanged cutoff-8 Oddlog targets in both sectors. This establishes both actual family containments.

Doublelog. The complete selected lists have 50 scalar and 72 vector keys. The structural forms proved above give the ordered quadrature bounds

	m	X	Y	$X + Y + 4\ell$
S	9–15	0–15	0–12	≤ 33
P	11	0–11	0–8	≤ 28

with $\ell \leq 2$ and $\ell \leq 3$, respectively. For example, if the even edge is mb, its polynomial power j gives $X = n_m + n_b + 5 + 2k$, $Y = n_b + 2 + j$. The other two placements give $X = n_m + n_b + 3 + j$ and $Y = n_b + 2$ or $n_b + 2 + j$. Expanding $(1 + t^2 - 2tx)^k$ for $k = 2, 3$ verifies these bounds for every angular term. The rates lie in $[234, 1116]/180$. Thus Lemma C.10 applies to every recorded order-ten, endpoint-power-34 call. All 122 complete input/return records are compared independently. Their exact signed rational contractions equal the unchanged two Doublelog endpoint pairs. All other columns are zero.

Four extra scalar overlaps. Every row of Table 8 has a zero pair power. Multiplication by s_n, $3 \leq n \leq 6$, preserves this property, so its angular cutoff is zero. For a pair with radii $R > r$, its average is

$$\sum_{j=0}^{\lfloor (p+1)/2 \rfloor} \frac{\binom{p+2}{2j+1}}{p+2} R^{p-2j} r^{2j}.$$

Each edge lowers its larger-radius exponent by at most one. The radial Jacobian starts it at at least two. All ordered degrees are therefore nonnegative. An independent gap-coordinate expansion $x = g_0 + g_1 + g_2$, $y = g_1 + g_2$, $z = g_2$ evaluates these integrals as finite gamma products, independently of the original evaluator. Writing $u_S = A_{13} f$ and $s_n = A_{13} g_n$ gives

$$\langle p_{S,n}, u_S \rangle = 2C_{S,n}(\langle g_n, f \rangle - \langle P_{13} g_n, f \rangle).$$

All $4 \cdot 2 \cdot 100 = 800$ signed primitive contributions, their 80 block sums and prefixes, and the direct-minus-exchange totals were evaluated and compared as exact rationals. Applying Lemma C.12, with reversed endpoints for the negative totals, gives the four printed physical targets. This argument establishes those targets directly. It does not claim containment in narrower saved scalar-overlap dyadics.

The common array identity identifies the physical meaning of every sum. The kernel lemmas prove the enclosures of every used return, and the exhaustive independent signed contractions prove the stated family and extra-moment containments. □

Lemma C.14 (Physical lithium moments)**.** *Assume Set-up 2.2 for the specified integral and endpoint computations. In the fixed-nucleus spin-*$1/2$ *Hartree model let* $H = H_3(3)$ *and use the trials and sources of Definition C.1. Put* $h_T = (H + 15/2)u_T$ *for* $T \in \{S, P\}$*. Then the trials and sources belong to* $D(H)$*, the sources have norm one, and the following twenty intervals contain the indicated physical moments simultaneously. Every displayed decimal endpoint is an exact rational.*

moment for trial T	S	P
$\langle u_T, h_T\rangle$	$[.633872331183, .633872821461]$	$[1.058162598846, 1.058162654330]$
$\|h_T\|^2$	$[.100526504813, .107640835047]$	$[.381799258126, .383836614894]$
$\|u_T\|^2$	$[25.861096622130, 25.861096625746]$	$[8.460567526663, 8.460567530500]$
$\langle p_{T,2}, u_T\rangle$	$[4.369279500354, 4.369279500364]$	$[2.498720734985, 2.498720734986]$
$\langle p_{T,2}, h_T\rangle$	$[.162740889161, .162740939941]$	$[.467043822051, .467043822207]$
$\langle p_{T,3}, u_T\rangle$	$[-2.519811045442, -2.519811045409]$	$[-1.451977551312, -1.451977551218]$
$\langle p_{T,3}, h_T\rangle$	$[.035012429476, .035012489149]$	$[.074296072339, .074296072543]$
$\langle p_{S,4}, u_S\rangle$	$[-.351885973731, -.351885973646]$	$--$
$\langle p_{S,4}, h_S\rangle$	$[-.018396812622, -.018396752955]$	$--$
$\langle p_{S,5}, u_S\rangle$	$[-.194319038379, -.194319038203]$	$--$
$\langle p_{S,5}, h_S\rangle$	$[-.009880462815, -.009880405542]$	$--$
$\langle p_{S,6}, u_S\rangle$	$[-.129253886225, -.129253885908]$	$--$
$\langle p_{S,6}, h_S\rangle$	$[-.006454330094, -.006454274838]$	$--$

Proof. Lemma C.11 proves the domain, source-norm and spin assertions and identifies the physical moments with the signed scalar sums. We assemble the thirteen base columns, then use the seven extra-moment certificates.

Base columns. Use the raw family intervals $J_{T,c,E}$ and physical Splain intervals R_c of Proposition C.13. Let $G_{T,c} = A$ for the first two base columns and $G_{T,c} = F_{T,n}$ for a column involving source n. The physical base moments are enclosed by

$$Y_{P,c} = B_{G_{P,c}}(J_{P,c,\mathrm{Pol}} + J_{P,c,\mathrm{Fin}} + J_{P,c,\mathrm{Odd}} + J_{P,c,\mathrm{Log}} + J_{P,c,\mathrm{Single}} + J_{P,c,\mathrm{Oddlog}} + J_{P,c,\mathrm{Doublelog}}),$$
$$Y_{S,c} = R_c + B_{G_{S,c}}(J_{S,c,\mathrm{Log}} + J_{S,c,\mathrm{Single}} + J_{S,c,\mathrm{Oddlog}} + J_{S,c,\mathrm{Doublelog}}).$$

Here B_G is the factor interval of Lemma C.12, and products use all four corners. Each raw family already includes its column denominator. The factor $(4\pi)^3 C_c$ enters once. In particular, R_c is added in physical units, with its sign retained.

The independent endpoint reader consumes every column of these complete family tables. It checks that every inverse-square family is zero outside the residual-norm column, that the Oddlog cutoff is 8, and that the headers and family sizes agree with the complete arrays. It decodes numeric endpoints as exact nearest-even dyadics: for a positive rational token x, choose the integer e with $2^e \le x < 2^{e+1}$ and round $x/2^{\max(e-52,-1074)}$ to the nearest integer, taking the even integer at a tie. Negative tokens are decoded by symmetry. Rational strings remain rational. Thus no decimal-to-binary uncertainty is omitted.

The retained exact calculation forms all thirteen $Y_{T,c}$ and compares their endpoints by integer cross multiplication. For $a/b \geq c/d$, with $b, d > 0$, the tested integer is $ad - bc$. It also reproduces exactly all thirteen final endpoint pairs of the original collector, using that collector's rational factor intervals. The tighter factor intervals used here give the first thirteen outer boxes in Table 12. Each box is formed as $[\lfloor 10^{14} \inf Y_{T,c} \rfloor, \lceil 10^{14} \sup Y_{T,c} \rceil]/10^{14}$. The complete exact endpoint and cross-product data are in the accompanying supplement. Every displayed outer box is contained in its claimed interval.

Table 12: Exact outer numerators for the final endpoint comparisons; both columns are divided by 10^{14}.

Moment	Lower numerator	Upper numerator
$\langle u_S, h_S \rangle$	63387233118325	63387282146003
$\|h_S\|^2$	10052650481383	10764083504630
$\langle p_{S,2}, u_S \rangle$	436927950035475	436927950036339
$\langle p_{S,2}, h_S \rangle$	16274088916118	16274093994007
$\langle p_{S,3}, h_S \rangle$	3501242947645	3501248914850
$\langle p_{S,4}, h_S \rangle$	-1839681262135	-1839675295536
$\langle p_{S,5}, h_S \rangle$	-988046281448	-988040554218
$\langle p_{S,6}, h_S \rangle$	-645433009391	-645427483813
$\langle u_P, h_P \rangle$	105816259884616	105816265432999
$\|h_P\|^2$	38179925812656	38383661489309
$\langle p_{P,2}, u_P \rangle$	249872073498570	249872073498571
$\langle p_{P,2}, h_P \rangle$	46704382205165	46704382220679
$\langle p_{P,3}, h_P \rangle$	7429607233961	7429607254257
$\|u_S\|^2$	2586109662213062	2586109662574588
$\|u_P\|^2$	846056752666313	846056753049941
$\langle p_{P,3}, u_P \rangle$	-145197755131125	-145197755121823

Extra columns. The three native extra moments are contained in their saved physical intervals by Proposition C.13. The endpoint reader encloses those dyadics by the last three rows of Table 12 and checks their containment in the printed targets by the same cross products. The four remaining scalar overlaps, with $3 \leq n \leq 6$, are enclosed directly in their printed targets by the exact gap-coordinate calculation in that proposition. This uses no stronger claim about the saved overlap dyadics. The thirteen base enclosures, the three native extra enclosures and the four exact overlap enclosures therefore give all twenty physical moments of the same fixed trials and sources. □

D Helium quadratic-weight certificates

This appendix proves the two computer-assisted inputs of Section 4. The first is the pointwise lower bound for the weighted repulsion (Lemma D.2). The second is the pair of eigenvalue counts for the one-electron operator (Lemma D.4). The conventions are those of Appendix A. Every accepted inequality is evaluated in exact rational arithmetic. Floating-point arithmetic is used only to propose auxiliary vectors and knot values. In this appendix, Set-up 2.2 means faithful Python integer and rational operations, file operations and execution records, with assertions enabled. The accompanying code/data release contains the saved certificates, their exact readers and the completed execution records.

Definition D.1 (Helium quadratic-weight data)**.** Let g be the continuous function on $[0,\infty)$ that is affine between the knots

r	$1/10$	$2/5$	$3/2$	5	20
$g(r)$	$41/10$	$33/10$	$1/2$	$-1/10$	3

and constant on $[0,1/10]$ and on $[20,\infty)$, and put $f(r)=2r+g(r)$. With (b_a,δ_a) from (4.1), $\lambda_1=22/25$, $\lambda_2=19/100$, and $B_a(s)=(s-b_a)_+^2-\min\{s/b_a,1\}/(2\delta_a)$ as in Proposition 3.4, define for $x=(x_1,\dots,x_4)\in(\mathbb{R}^3)^4$ with pairwise distinct positions

$$D(x)=\sum_{i=1}^{4} f(r_i)-\sum_{i<j}\frac{r_i^2+r_j^2+2}{d_{ij}}-\lambda_1 B_1(q_1)-\lambda_2 B_2(q_2),$$

where $q_1\le q_2$ are the two smallest radii.

D.1 The four-electron quadratic screen

Lemma D.2 (Four-electron quadratic screen)**.** *Assume Set-up 2.2 for the specified He4 quadratic certificate execution. Then $D(x)\le 1$ for every $x\in(\mathbb{R}^3)^4$ with pairwise distinct positions.*

The floating-point supremum of D is about 0.786, attained near the radii $(2.70, 5.43, 7.66, 7.66)$ with the two largest electrons antipodal. The certification uses the slack 0.21 between this value and the bound. The constant 1 enters the proof of Theorem 4.4 as the term $-\|u\|^2$.

Proof. D is invariant under permutations of the electrons, so it suffices to consider ordered radii $r_1\le r_2\le r_3\le r_4$, where $q_a=r_a$. The certificate covers the ordered radius space $\{0\le r_1\le\cdots\le r_4\}$ by boxes $\prod_i[x_i,y_i]$, with $x_i\le y_i$ nondecreasing in i and $y_i=\infty$ permitted, and proves $D\le 1$ on each box by an explicit upper bound $\mathcal{U}(\text{box})$ computed in rational arithmetic. A box with $\mathcal{U}>1$ is bisected by a fixed deterministic rule. Normally the box is cut at the midpoint of the bounded coordinate i maximizing the relative width $(y_i-x_i)/(x_i+\frac{3}{10})$. When every bounded relative width is below $\frac{1}{20}$, its first unbounded coordinate is cut instead, at $\max\{2x_i,x_i+1\}$. The children are intersected with the ordered cone. This continues until every leaf is accepted. The root boxes are the 4845 nondecreasing index tuples of the radial partition $0,\frac{1}{10},\frac{2}{5},1,\frac{3}{2},2,3,4,5,8,12,20,40,80,160,320,640,\infty$. Hence no coordinate interval of any box contains a knot of g or one of b_1,b_2 in its interior. Consequently f is affine and B_a is quadratic on each coordinate interval.

Bounded boxes. Four elementary estimates give $\mathcal{U}$.

1. *Angle elimination.* For $b,K>0$ and $d>0$, $b/d\ge\frac{3}{2}b^{2/3}K^{1/3}-\frac{1}{2}Kd^2$ (the arithmetic–geometric mean inequality for $b/(2d), b/(2d), Kd^2/2$). For a positive semidefinite 4×4 matrix K with nonnegative entries, $\sum_{i<j}K_{ij}d_{ij}^2\le\sum_i r_i^2(K\mathbf{1})_i$, because the difference equals $-\sum_{i,j}K_{ij}\,x_i\cdot x_j\le 0$. The certificate uses $K=vv^{\mathsf T}+uu^{\mathsf T}$ with $v,u\in\mathbb{Q}_+^4$ proposed by a floating-point optimizer and recorded, on a recorded subset S of the bounded coordinates. The choice affects the tightness of $\mathcal{U}$ and not its validity. Hence, on the box and for pairs in S,

$$\sum_{i<j}\frac{r_i^2+r_j^2+2}{d_{ij}}\ge\sum_{i<j}\tfrac{3}{2}\,\psi(r_i,r_j)\,K_{ij}^{1/3}-\tfrac{1}{2}\sum_i r_i^2(K\mathbf{1})_i,\qquad \psi(r_i,r_j)=(r_i^2+r_j^2+2)^{2/3}.$$

2. *Convexity and roots.* The function ψ is jointly convex, because its Hessian is $\frac{4}{3}(2+s)^{-4/3}[(2+s)I - \frac{2}{3}\,rr^{\mathsf{T}}] \succeq 0$ with $s = r_i^2 + r_j^2$. Hence on the box ψ is bounded below by its tangent plane at the box centre. The value and gradient of this plane are enclosed by rational bounds. Every cube root is replaced by a rational bound of the correct direction, certified by an integer power comparison.

3. *Moments.* B_a is convex, so it is bounded below by its tangent at the box centre, and $-\lambda_a B_a(r_a)$ by an affine function of r_a.

4. *Vertex maximization.* After 1–3, D is bounded on the box by a sum of affine functions of the r_i and the convex term $\frac{1}{2}\sum_i r_i^2 (K\mathbf{1})_i$. The maximum of this bound over the box is attained at one of the sixteen vertices, where it is evaluated exactly.

Unbounded boxes. For a pair with an unbounded radius the pair term is bounded instead by the elementary inequalities $(r_i^2 + r_j^2)/d_{ij} \geq \max\{|r_i - r_j|, (r_i + r_j)/2\}$, which follow from $d_{ij} \leq r_i + r_j$ and $r_i^2 + r_j^2 \geq |r_i^2 - r_j^2|$, together with $2/d_{ij} \geq 2/(y_i + y_j)$ on bounded pairs and 0 otherwise. These make $\mathcal{U}$ an affine function of each unbounded radius. Its slope is nonpositive in r_3 and r_4, because each such electron receives at least $\frac{3}{2}r_i$ from its pairs against $2r_i$ from f only when all four radii are large, and that configuration is where the moment terms act. For r_1 and r_2 the remaining positive slope is absorbed by the concave quadratic $-\lambda_a(r_a - b_a)^2$, whose maximum over the ray is explicit. The same elementary bounds are used for bounded pairs not contained in S, where $|r_j - r_i|$ is taken when the centre radii satisfy $r_j \geq 3r_i$ and $(r_i + r_j)/2$ otherwise, together with $2/d_{ij} \geq 2/(y_i + y_j)$. The certificate records S for each accepted box.

Coverage and execution. The children of a box are two boxes whose union is the box intersected with the ordered cone, so the accepted leaves cover the ordered radius space. Since D is symmetric, they cover $(\mathbb{R}^3)^4$ minus the collision sets. The execution (`certify_screen_dump.py` with the data of Definition D.1 and target 1) terminated after evaluating 69,119 boxes, of which 36,982 were accepted and the rest bisected. The maximal depth was 15 and the smallest accepted slack was $1 - \mathcal{U} = 1.483 \cdot 10^{-4}$. The run took 4.0 hours on one core, and no box failed. The log of evaluated boxes, with the recorded S and (v, u) of each accepted box, is re-read by the exact reader (`replay_screen.py`). The reader rebuilds the bisection tree from the root boxes with the rule above, recomputes every $\mathcal{U}$ in rational arithmetic and confirms that every leaf is accepted. It uses no optimizer. □

Remark D.3 (Controls). Two checks were run that are not part of the proof. (a) Asked to certify the target $\frac{7}{10}$, which lies below the numerical supremum 0.786, the same program fails, reporting the box $(2.8139, 5.7598, 8.8755, 9.0018)^{\pm 10^{-4}}$ with $\mathcal{U} = 0.70007$, next to the true maximizer. (b) A randomized test compared $\mathcal{U}$ with angle-optimized sampled values of D on 300 random ordered boxes and found no violation.

D.2 The helium radial indices

Lemma D.4 (Helium radial indices)**.** *Let h be the operator of* (4.3)*. With spin excluded from the strictly negative form index,*

$$n_-\Big(h + \frac{197}{100}\Big) = 0, \qquad n_-\Big(h + \frac{3}{25}\Big) \leq 1.$$

(Floating-point values, not used in the proof: the two lowest s-levels of h are -1.948 and -0.095, and the lowest p-level is 0.451.)

Proof. Reduction to radial forms. Put $a(r) = 2 + r^2$ and, for a real level τ,

$$V_\tau(r) = -\frac{2}{r} + \frac{2r + g(r) - \tau}{2 + r^2} - \frac{r^2}{2(2 + r^2)^2}.$$

For φ in the form domain of h, the function $\psi = a^{1/2}\varphi$ lies in $H^1(\mathbb{R}^3)$, since $|\nabla a^{1/2}|^2 = r^2/(2 + r^2) \le 1$, and integration by parts on compactly supported functions followed by density gives

$$q_h[\varphi] - \tau\|\varphi\|^2 = \int_{\mathbb{R}^3} \Big(\frac{1}{2}|\nabla\psi|^2 + V_\tau|\psi|^2\Big)dx,$$

the term $-\frac{3}{2}$ of h being exactly the term $-\frac{1}{2}a^{1/2}\Delta a^{1/2} + \frac{1}{2}|\nabla a^{1/2}|^2 = -\frac{3}{2} + \frac{r^2}{2(2+r^2)}$ produced by the substitution, up to the displayed last term of V_τ. The map $\varphi \mapsto a^{1/2}\varphi$ is injective, so $n_-(h - \tau) \le n_-(-\frac{1}{2}\Delta + V_\tau) = \sum_{\ell\ge 0}(2\ell + 1)\, n_-(q_{\ell,\tau})$, where

$$q_{\ell,\tau}[u] = \int_0^\infty \Big(\frac{1}{2}|u'|^2 + \Big(V_\tau + \frac{\ell(\ell + 1)}{2r^2}\Big)|u|^2\Big)dr$$

on $H^1_0((0,\infty))$. Since $q_{\ell,\tau}$ increases with ℓ and with $-\tau$, it suffices to prove

$$n_-(q_{1,\tau_1}) = 0, \qquad n_-(q_{0,\tau_1}) \le 1, \qquad n_-(q_{0,\tau_0}) = 0, \qquad \tau_0 = -\frac{197}{100},\ \tau_1 = -\frac{3}{25}.$$

Supersolution criterion. Let $W = V_\tau + \ell(\ell + 1)/(2r^2)$ and let y be locally Lipschitz on an open interval $J \subset (0,\infty)$ with

$$y' + y^2 \le 2W \quad \text{on } J. \tag{D.1}$$

For $u \in C_c^\infty(J)$, integrating $-\operatorname{Re}(\bar u' u)\, y = -\frac{1}{2}(|u|^2)'y$ by parts gives

$$\int_J \Big(\frac{1}{2}|u'|^2 + W|u|^2\Big) = \int_J \frac{1}{2}|u' - yu|^2 + \int_J \Big(W - \frac{1}{2}(y' + y^2)\Big)|u|^2 \ge 0,$$

and by density $q_{\ell,\tau} \ge 0$ on all form-domain functions vanishing at the finite endpoints of J. With $J = (0,\infty)$ the index is 0. With $J = (0, c)$ and $J = (c,\infty)$ it is at most 1, because one Dirichlet condition has been imposed.

The certificates. Take

$$y = \frac{\ell + 1}{r} + \frac{k}{r - c} + z(r), \qquad k \in \{0, 1\},$$

with z piecewise affine with rational knots $0 = r_0 < \cdots < r_N = 40$ and $z = \alpha/r$ on $[40,\infty)$, $\alpha \in \mathbb{Q}$. The values $z(0) = -2/(\ell + 1)$ for $k = 0$, $z(0) = 1/c - 2$ for $k = 1$, and $z(c) = -1/c$ cancel the Coulomb pole at the origin and the pole at the cut identically. The knots of g are among the r_j, so g is affine on each knot interval. The expression $y' + y^2 - \ell(\ell + 1)/r^2$ equals $z' + 2(\ell+1)z/r + z^2$ for $k = 0$ and $z' + z^2 + 2z/r + 2(1+rz)/(r(r-c))$ for $k = 1$, $\ell = 0$. Multiplying (D.1) by $r(2 + r^2)^2|r - c|^k$ therefore turns it, on each knot interval, into a polynomial inequality $Q(r) \ge 0$ of degree at most eight with rational coefficients. Each is certified by nonnegativity of its Bernstein coefficients after bisection. The same method is used on $[40, 400]$. On $[400,\infty)$ the inequality is certified by nonnegativity of all Taylor coefficients at 400. The three certificates are:

(A) $\ell = 1$, $\tau = \tau_1$, $k = 0$, $\alpha = 1$: 76 pieces; gives $n_-(q_{\ell,\tau_1}) = 0$ for all $\ell \ge 1$.

(B) $\ell = 0$, $\tau = \tau_1$, $k = 1$, $c = 75450851/50000000$, $\alpha = 23/100$: 502 pieces; gives $n_-(q_{0,\tau_1}) \le 1$.

(C) $\ell = 0$, $\tau = \tau_0$, $k = 0$, $\alpha = 2$: 617 pieces; gives $n_-(q_{\ell,\tau_0}) = 0$ for all $\ell \geq 0$.

The knot values $z(r_j)$ were proposed by a floating-point integration of the regular solution of h at the raised levels $\tau + \varepsilon$ ($\varepsilon = 0.15, 0.012, 0.011$), and were rounded to multiples of 10^{-9}. The Riccati residual $2\varepsilon/(2 + r^2)$ of this solution is the slack that the piecewise affine interpolation uses. The proposal is not part of the proof. The certificate is the list of knots and values (`levels_super_certificate.json`, 1195 polynomial inequalities). It is generated by `certify_levels_super.py` and re-checked in exact arithmetic by `replay_levels_super.py` in a few seconds. The reader rejects the certificate when a single knot value of (B) is raised by $1/50$. □

Remark D.5 (Cross-check). The same four index counts $(0, 0, 1, 0)$, for (ℓ, τ) equal to $(0, \tau_0)$, $(1, \tau_0)$, $(0, \tau_1)$ and $(1, \tau_1)$, were first obtained by the cell lower-form method of Appendix A (`certify_levels.py`). That computation uses 24,005 cells from $r_0 = 1/256$ to 40, cellwise constant lower bounds on V_τ, the Dirichlet–Poincaré constant $4.9 < \pi^2/2$, and exact pivot counting of the assembled tridiagonal matrix in outward-rounded interval arithmetic. The two methods agree. The levels τ_0, τ_1 leave room: the floating-point ground level of h is 0.022 above τ_0, and its first excited s-level is 0.025 above τ_1.

E Proofs deferred from the main text

This appendix contains the proofs deferred from Sections 3, 5 and 6. Each proof uses the notation of the section in which its statement appears.

E.1 The regional lower bound

Proof of Lemma 3.3. Angular repulsion. For positive radii and directions $n_i, n_k \in S^2$, maximizing $1 + \tau^2 - 2\tau z$ over $0 \leq \tau \leq 1$ gives

$$\frac{1}{|r_i n_i - r_k n_k|} \geq \min\{r_i^{-1}, r_k^{-1}\}\, c(n_i \cdot n_k).$$

Let $2 \leq h \leq N$ be an integer and let $n_1, \dots, n_h$ be directions. Consider the tangent to the convex function $[2(1 - z)]^{-1/2}$ at $z = -1/(h - 1)$. By convexity, this tangent lies below the untruncated function. Its maximum on $[-1, 1]$ is $\frac{3}{2}\sqrt{(h - 1)/(2h)}$, which is at most 1 exactly when $h \leq 9$. Hence the tangent lies below c. Since $0 \leq |\sum_i n_i|^2 = h + 2\sum_{i<k} n_i \cdot n_k$, summing these tangents yields

$$\sum_{1 \leq i < k \leq h} c(n_i \cdot n_k) \geq \binom{h}{2} \sqrt{\frac{h - 1}{2h}} \geq D_h.$$

For $h \leq 1$ the empty sum equals $D_h = 0$.

Exterior radial bound. For a reduced radial Dirichlet test $g \in C_c^\infty((R, \infty))$, expanding the nonnegative integral $\frac{1}{2}\int_R^\infty F^2 |(g/F)'|^2$ with $F(r) = (r - R)e^{-\lambda(r-R)}$ gives

$$\int_R^\infty \left(\frac{1}{2}|g'|^2 - \frac{\kappa}{r}|g|^2\right) dr \geq \int_R^\infty \left(-\frac{\lambda^2}{2} + \frac{\lambda}{r - R} - \frac{\kappa}{r}\right) |g|^2 dr \geq -C\|g\|^2.$$

The second inequality is the identity, for $t > 0$,

$$\frac{1}{t} - \frac{\sigma^2}{t + R} + \frac{(\sigma - 1)^2}{R} = \frac{((\sigma - 1)t - R)^2}{Rt(t + R)} \geq 0.$$

For a three-dimensional function w vanishing on $\{|x| \le R\}$, apply this inequality to its reduced radial slices rw and discard the nonnegative angular kinetic energy. Dirichlet form density extends the bound to all such H^1 functions, componentwise and on almost every slice in the other variables.

Assembly. Recall that the j electrons with radii below b are the core electrons and the other $N-j$ are the outer electrons. By Theorem 3.2, the kinetic and nuclear terms of each core electron contribute at least $-Z^2/2$. We drop the repulsion among core electrons. Each pair of one core electron and one outer electron satisfies

$$\frac{1}{|x_i - x_{\mathrm{core}}|} \ge \frac{1}{r_i + b} \ge \frac{R}{(R+b)r_i}.$$

Apply the radial bound with the charge κ to each outer electron. This leaves the potential $-(Z-\kappa)/r_i$. Write $t_i = R/r_i \in (0,1]$ for the inverse scaled radius of the electron. The remaining potential of the outer electrons is bounded below by

$$\frac{1}{R}\left[\sum_{i<k} c(n_i \cdot n_k)\min(t_i, t_k) - A_j \sum_i t_i\right],$$

where both sums range over the outer electrons. For fixed directions the bracket is concave on $[0,1]^{N-j}$, so its minimum is attained at a vertex. A vertex with h coordinates equal to one has value at least $D_h - A_j h$ by the angular bound. Collecting the three contributions gives the assertion. □

E.2 The ground state of neutral helium

Proof of Lemma 5.3. The trial function and its error. Put $s = r_1 + r_2$, $\xi = r_1 - r_2$, $d = d_{12}$, $\alpha = 13/4$, and $g = 2\alpha$. Let $C(s, \xi, d)$ be the integer polynomial specified by the 372 coefficients of the fixed neutral trial in the accompanying code/data release. Its degree is fourteen and all powers of ξ are even. The source polynomial is $10^{-25}C$. Set $D = d(s^2 - \xi^2)$, and let χ be the normalized spin singlet. On the domain $s \ge 0$, $0 \le d \le s$, $-d \le \xi \le d$, define

$$\mathcal{J}(B) = \int e^{-gs} B(s,\xi,d)\, ds\, d\xi\, dd, \qquad \mathcal{K}(B) = \int e^{-gs}\frac{B(s,\xi,d)}{D}\, ds\, d\xi\, dd.$$

The physical volume element is $\pi^2 D\, ds\, d\xi\, dd$. Thus, with $\mathcal{N} = \mathcal{J}(DC^2) > 0$, the trial function is $\psi = e^{-\alpha s} C\chi/(\pi\sqrt{\mathcal{N}})$. Its second weak derivatives and its Coulomb potential times ψ are bounded by a polynomial times $e^{-\alpha s}(1 + r_1^{-1} + r_2^{-1} + d^{-1})$, which is square integrable. Hence ψ belongs to $D(H_2(2))$. Its spatial factor is symmetric and rotationally invariant.

We now list the integrals and error bounds used in this calculation. For nonnegative integers p, j, k, put $m = p + j + k$. Odd j gives zero. For even j,

$$\mathcal{J}(s^p \xi^j d^k) = \frac{2(m+2)!}{(j+1)(j+k+2)g^{m+3}}, \qquad \mathcal{K}(s^p \xi^j d^k) = \frac{(m-1)!}{g^m} 2\int_0^1 \int_x^1 \frac{x^j y^{k-1}}{1-x^2}\, dy\, dx.$$

The second formula is used only for $m > 0$. For $k > 0$, integration in y and finite geometric sums reduce its angular integral to rational numbers and $\log 2$. For $k = 0$ that integral is $\pi^2/4 - 2\sum_{h=0}^{j/2-1}(2h+1)^{-2}$, with an empty sum when $j = 0$. For $\tau = -2903724/10^6$, the polynomial obtained by clearing the denominator in the residual is

$$\mathcal{R} = D[-C_{ss} - C_{\xi\xi} - C_{dd} + 2\alpha C_s - (\alpha^2 + \tau)C] - 4sdC_s + 4(\alpha - 2)sdC + 4\xi d C_\xi$$

$$-2(s^2-\xi^2)C_d-2s(d^2-\xi^2)C_{sd}+2\alpha s(d^2-\xi^2)C_d-2\xi(s^2-d^2)C_{\xi d}+(s^2-\xi^2)C.$$

The Cartesian chain rule gives $(H_2(2)-\tau)(e^{-\alpha s}C\chi)=e^{-\alpha s}\mathcal{R}\chi/D$. Put $\mu=\langle\psi,H_2(2)\psi\rangle$, $v=\|(H_2(2)-\mu)\psi\|^2$, and $m_j=\|r_1^{j/2}\psi\|^2$ for $0\le j\le 16$. Consequently

$$\mu=\tau+\frac{\mathcal{J}(C\mathcal{R})}{\mathcal{N}},\qquad v=\frac{\mathcal{K}(\mathcal{R}^2)}{\mathcal{N}}-(\mu-\tau)^2,\qquad m_j=\frac{\mathcal{J}(DC^2((s+\xi)/2)^j)}{\mathcal{N}}.$$

All these expressions are finite. Polynomial multiplication and the displayed monomial integrals were evaluated exactly. To enclose the two constants in v, the calculation used

$$\ell=2\sum_{b=0}^{31}\frac{1}{(2b+1)3^{2b+1}},\qquad A(x)=\sum_{b=0}^{31}\frac{(-1)^b x^{2b+1}}{2b+1},$$

$$\ell<\log 2<\ell+\frac{2}{65\,3^{65}(1-1/9)},\qquad A(x)\le\arctan x\le A(x)+\frac{x^{65}}{65},\quad x\in\{1/5,1/239\},$$

and $\pi=16\arctan(1/5)-4\arctan(1/239)$. Signed rational substitution gives an upper bound $\bar v\ge v$ with the following recorded enclosures:

$$-\frac{29037243720149832}{10^{16}}\le\mu<-\frac{29037243720149831}{10^{16}},$$
$$0\le v\le\bar v<\frac{12177071684819}{10^{20}},$$
$$-\frac{29037246736334271}{10^{16}}\le\mu-\frac{\bar v}{-5/2-\mu}<-\frac{29037246736334270}{10^{16}}.$$

The neutral level and its gap. Write $h=-\Delta/2-2/r$, including the two spin copies. By Theorem 3.2, $h_1+h_2\ge -5/2$ on the complement of the doubly occupied $1s$ determinant. Nonnegative repulsion and the min–max principle therefore leave at most one spectral dimension of $H_2(2)$ below $-5/2$. The trial function just computed supplies that dimension. Hence E is simple and the rest of the spectrum lies above $-5/2$. Theorem 5.1 gives the asserted energy interval. The spectral projection of ψ onto this level is nonzero. The symmetries of ψ give the stated choice of Φ.

For the sharper gap, let P_{00} project onto that $1s^2$ determinant and P_{12} onto the configurations with one $1s$ and one $n=2$ electron. The normalized $1s$, $2s$, and $2p$ radial factors are proportional to e^{-2r}, $(1-r)e^{-r}$, and re^{-r}. The identity $\int_0^\infty r^j e^{-br}\,dr=j!/b^{j+1}$ gives their mean radii $3/4, 3, 5/2$. Thus $P_{12}d_{12}P_{12}\le(15/4)P_{12}$. Weighted Cauchy–Schwarz, followed by the supremum over unit vectors in $\operatorname{ran}P_{12}$, gives $d_{12}^{-1}\ge(4/15)P_{12}$ on the full space. On $P_{00}^{\perp}$ the nuclear energy is $-5/2$ on P_{12} and at least $-20/9$ on its complement. Thus every form-domain vector $\zeta\perp\operatorname{ran}P_{00}$ satisfies

$$\mathfrak{q}_{2,2}[\zeta]\ge\min\{-5/2+4/15,-20/9\}\|\zeta\|^2=-\frac{67}{30}\|\zeta\|^2.$$

The rank-one min–max comparison now gives $H_2(2)|_{\Phi^\perp}\ge -67/30$. Since $-67/30-\mu>67039/100000$, this proves the required gap.

Moments and tails of the exact state. Put $\beta=-5/2$, $L_0=\mu-\bar v/(\beta-\mu)$, and $\epsilon=(\mu-L_0)/(\beta-L_0)$. The spectral gap at β gives, after choosing the phase of Φ,

$$\|\psi-\Phi\|^2\le 2-2\sqrt{1-\epsilon}\le d_*^2,\qquad d_*=\frac{86434345026}{10^{14}}.$$

The last comparison was made rationally as $d_*^2 - d_*^4/4 \geq \epsilon$, with $d_* < 1$. Let $\eta = -2 - \mu > 0$ and $c_j = (1 + \sqrt{1 + \eta j^2/2})/\eta$ for $1 \leq j \leq 8$. Testing the eigenfunction equation with $\min(r_1, T)^{2j}\Phi$ gives, for $X_T = \|\min(r_1, T)^j \Phi\|$,

$$\eta X_T^2 \leq 2X_T \|r_1^{j-1}\Phi\| + \frac{j^2}{2}\|r_1^{j-1}\Phi\|^2.$$

Here the other electron's one-body energy is at least -2 and the repulsion is nonnegative. Induction and monotone convergence give $\|r_1^j\Phi\| \leq c_j\|r_1^{j-1}\Phi\|$ through $j = 8$. For $1 \leq k \leq 4$, set

$$a_k = m_{2k} + d_*\sqrt{m_{4k}}, \qquad b_k = d_* \prod_{j=k+1}^{2k} c_j.$$

Cauchy–Schwarz applied to the difference of the two moments gives $\|r_1^k\Phi\|^2 \leq a_k + b_k\|r_1^k\Phi\|$. All radicals were enclosed by

$$\frac{\mathrm{isqrt}(\lfloor 10^{28}x \rfloor)}{10^{14}} \leq \sqrt{x} < \frac{\mathrm{isqrt}(\lfloor 10^{28}x \rfloor) + 1}{10^{14}} \quad (x \geq 0),$$

where $\mathrm{isqrt}(n) = \lfloor \sqrt{n} \rfloor$ for integers $n \geq 0$. Using upper enclosures in a_k, b_k, the four positive lower bounds for $M_k^2 - a_k - b_k M_k$ were, respectively,

$$\frac{50747334}{10^{14}}, \quad \frac{106072203}{10^{14}}, \quad \frac{101118508}{10^{14}}, \quad \frac{2413688788}{10^{14}}.$$

Also $M_k > b_k/2$ in every case, proving the moment bounds.

For completeness, the 121 trial-tail calculations used the same polynomial. Integrating d first and splitting at $r_1 = r_2$ gives its normalized radial density as $f(r)e^{-gr} + \widetilde{f}(r)e^{-2gr}$ with rational polynomials $f, \widetilde{f}$. Each tail integral is evaluated termwise using

$$\int_t^\infty r^j e^{-br}\, dr = \frac{j!}{b^{j+1}} e^{-bt} \sum_{h=0}^{j} \frac{(bt)^h}{h!}.$$

To enclose e^{-x}, scale x by a power of two into $[0, 1]$, use the alternating Taylor polynomial of degree 80 with remainder bounded by $x^{81}/81!$, and square back with outward rounding to multiples of 10^{-100}. Signed substitution in the two polynomials produced rational upper bounds Q_j for the trial tails at $j/8$. Every row, $8 \leq j \leq 128$, satisfies

$$\|\mathbf{1}_{\{r_1 \geq j/8\}}\psi\|^2 \leq Q_j, \qquad (\sqrt{Q_j} + d_*)^2 \leq P_j, \qquad 0 \leq P_j \leq 1,$$

and all 120 consecutive comparisons give $P_{j+1} \leq P_j$. The root comparisons are integer square comparisons at scale 10^{14}. The full rational polynomials and endpoint tables are included with the trial function. The triangle inequality transfers these bounds to Φ. Monotonicity of tail probabilities gives the claimed step function for every $t \geq 0$, and exchange symmetry gives the assertions for electron two. □

E.3 The complementary sectors

Proof of Lemma 5.4. We first remove the sectors without a doubly occupied $1s$ shell. Pair excitation bounds then control every remaining angular pattern with $L \geq 2$.

An unfilled $1s$ *shell.* Let $h = -\Delta/2 - 2/r$, with both spin copies, and let D_2 project onto the configurations with exactly two $1s$ electrons. Shell n contains the angular momenta $\ell = 0, \dots, n-1$. Indeed, the radial factors $r^\ell e^{-2r/n} L^{2\ell+1}_{n-\ell-1}(4r/n)$, with the associated Laguerre polynomials, satisfy the radial eigen-equation and give $\sum_{\ell=0}^{n-1}(2\ell+1) = n^2$ spatial eigenfunctions. They exhaust the multiplicity in Theorem 3.2. Within $D_2^\perp$ let F project onto the configurations with one $1s$ and two $n = 2$ electrons. By Theorem 3.2, $\sum_i h_i = -3$ on F and $\sum_i h_i \geq -49/18$ on $D_2^\perp \cap F^\perp$. For $V = \sum_{i<j} d_{ij}^{-1}$,

$$V^{-1} \leq \frac{\sum_{i<j} d_{ij}}{9} \leq \frac{2}{9}\sum_i r_i, \qquad FV^{-1}F \leq \frac{3}{2}F.$$

The last bound uses the mean radii $3/4, 3, 5/2$ of the $1s, 2s, 2p$ orbitals, as computed in Lemma 5.3. Weighted Cauchy–Schwarz gives $V \geq (2/3)F$ on the full space, including its off-diagonal couplings. Thus $D_2 u = 0$ implies the lower bound $-49/18$. The range of D_2 consists of a $1s^2$ spin singlet with an additional electron. It has total spin $1/2$ and parity $(-1)^L$. Hence every sector in the first assertion is annihilated by D_2. Lemma 5.3 gives $-49/18 > E$.

Pair excitation bounds. For the antisymmetric pair j, k, write $H_{jk} = h_j + h_k + d_{jk}^{-1}$ and denote its orbital angular momentum by J_{jk}. On $J_{jk} \neq 0$, only the $1s\,2p$ configurations lie below $-20/9$ for $h_j + h_k$. Their energy is $-5/2$, and their compressed distance is at most $3/4 + 5/2 = 13/4$. The weighted Cauchy–Schwarz argument used above gives a repulsion contribution $4/13 > 5/18$ on this subspace. Therefore

$$H_{jk}\big|_{\{J_{jk}\neq 0\}} \geq -20/9.$$

We also need $H_{jk}|_{\{J_{jk}=2\}} \geq \lambda_2$, where $\lambda_2 = -2056247529/10^9$. The deficit $(\lambda_2 - h_j - h_k)_+$ on this pair sector consists precisely of the $1s\,nd$ configurations for $n = 3, 4, 5$. Indeed their energies are $\epsilon_n = -2(1 + n^{-2})$, whereas the next shell has energy $-37/18 > \lambda_2$.

We now compute the matrix elements of the distance d_{jk} in these configurations, including normalization. At unit charge use the normalized core $2e^{-r}Y_{00}$ and $R_n(r)Y_{20}/\sqrt{S_n}$, with $Y_{00} = (4\pi)^{-1/2}$ and $Y_{20}(\omega) = \sqrt{5/(4\pi)}(3\omega_3^2 - 1)/2$. Write $R_n(r) = e^{-r/n}\sum_a c_{na} r^a$, with

$$\sum_a c_{3a} r^a = r^2, \quad \sum_a c_{4a} r^a = 6r^2 - \frac{r^3}{2}, \quad \sum_a c_{5a} r^a = 21r^2 - \frac{14r^3}{5} + \frac{2r^4}{25}.$$

The factorial integral gives $(S_3, S_4, S_5) = (98415/8, 737280, 123046875/8)$ for $S_n = \int_0^\infty r^2 R_n(r)^2\, dr$. Define the charge-two orbitals $\phi_{1s}(x) = \sqrt{8/\pi}e^{-2|x|}$ and $\phi_{nd,0}(x) = 2^{3/2}R_n(2|x|)Y_{20}(x/|x|)/\sqrt{S_n}$. Their normalization follows from S_n, and substitution gives $h\phi_{nd,0} = -2n^{-2}\phi_{nd,0}$. This unitary dilation divides every distance matrix element by two. For $\sigma \in \{-1, 1\}$ set $\chi_n^\sigma = (\phi_{1s} \otimes \phi_{nd,0} + \sigma\phi_{nd,0} \otimes \phi_{1s})/\sqrt{2}$ and put

$$T_{nm}^\sigma = \frac{\delta_{nm}}{\lambda_2 - \epsilon_n} - \langle \chi_n^\sigma, d_{jk}\chi_m^\sigma\rangle, \qquad 3 \leq n, m \leq 5.$$

Both exchange signs are needed, paired respectively with triplet and singlet spin.

The following formulas specify all six entries for each sign. For nonnegative integers A, B and positive α, β define

$$I_{A,B}(\alpha,\beta) = \sum_{h=0}^{A}\binom{A}{h}\frac{h!(A+B-h)!}{\alpha^{h+1}(\alpha+\beta)^{A+B-h+1}},$$

For $k \in \{2, 4\}$, whenever the following subscripts are nonnegative, set $\mathcal{M}_k(A, B; \alpha, \beta) = I_{A+1-k,B+k}(\alpha,\beta) + I_{B+1-k,A+k}(\beta,\alpha)$. The first expression is the integral of $x^A y^B e^{-\alpha x - \beta y}$ on

$0<y<x$. The second inserts $\min(x,y)^{k}\max(x,y)^{1-k}$ on the whole quadrant. For $q=1/n+1/m$, set

$$\begin{aligned}\mathcal{J}_{nm}&=\sum_{a,b}c_{na}c_{mb}\Big[\frac{(a+b+3)!}{q^{a+b+4}}+\frac{(a+b+1)!}{q^{a+b+2}}\\&\qquad-\frac{(a+b+2)!}{2(q+2)^{a+b+3}}-\frac{(a+b+1)!}{(q+2)^{a+b+2}}\Big],\\\mathcal{K}_{nm}&=\frac{4}{5}\sum_{a,b}c_{na}c_{mb}\Big[-\frac{1}{3}\mathcal{M}_{2}(2+a,2+b;1+1/n,1+1/m)\\&\qquad+\frac{1}{7}\mathcal{M}_{4}(2+a,2+b;1+1/n,1+1/m)\Big].\end{aligned}$$

Then $\langle\chi^{\sigma}_{n},d_{jk}\chi^{\sigma}_{m}\rangle=(\mathcal{J}_{nm}+\sigma\mathcal{K}_{nm})/(2\sqrt{S_nS_m})$. To verify the angular factors, put $P_2(z)=(3z^2-1)/2$. For $t\in[0,1]$ the two required Legendre integrals are

$$\frac{1}{2}\int_{-1}^{1}\sqrt{1-2tz+t^{2}}\,dz=1+\frac{t^{2}}{3},\quad\frac{1}{2}\int_{-1}^{1}\sqrt{1-2tz+t^{2}}P_{2}(z)\,dz=-\frac{t^{2}}{15}+\frac{t^{4}}{35}.$$

The direct term after integration of the core radius is $r+r^{-1}-e^{-2r}(1/2+r^{-1})$. These expressions and the factorial integral give $\mathcal{J}_{nm},\mathcal{K}_{nm}$ above.

To certify positivity explicitly, put

$$\mathcal{R}=\operatorname{diag}(\sqrt{2S_3},\sqrt{2S_4},\sqrt{2S_5}),\quad\mathcal{D}=\operatorname{diag}(1/100,1/1000,1/4000),\quad C^{\sigma}=\mathcal{D}\mathcal{R}T^{\sigma}\mathcal{R}\mathcal{D}.$$

Exact rational evaluation of the displayed finite sums gives $M^{\sigma}_{ab}\le 10^{12}C^{\sigma}_{ab}<M^{\sigma}_{ab}+1$ for all entries, with

$$M^{-}=\begin{pmatrix}1768956319004&3195429484308&1425938046736\\3195429484308&5918065868414&5182703988325\\1425938046736&5182703988325&47739795688034\end{pmatrix},$$

$$M^{+}=\begin{pmatrix}1771465086085&3196795969804&1427082503973\\3196795969804&5918811502224&5183328970125\\1427082503973&5183328970125&47740319728321\end{pmatrix}.$$

Use

$$\mathcal{Q}=\begin{pmatrix}1000000&-1806393&31477566\\0&1000000&-17871894\\0&0&1000000\end{pmatrix},\qquad\mathcal{B}=10^{-6}\mathcal{Q}.$$

Integer multiplication shows that every diagonal-dominance margin of both $\mathcal{Q}^{\mathsf{T}}M^{\sigma}\mathcal{Q}$ exceeds 10^{20}. The smallest is 116876133928111213080. Each absolute column sum of $\mathcal{B}$ is less than 51, so the entrywise enclosure error contributes operator norm less than $3\cdot51^{2}\,10^{-12}$. It follows that

$$\mathcal{B}^{\mathsf{T}}C^{\sigma}\mathcal{B}\ge(10^{-4}-7803\cdot10^{-12})I=\frac{99992197}{10^{12}}I>0.$$

All congruences are invertible. Thus $T^{+},T^{-}>0$. Rotational invariance makes these distance matrices identical in all five magnetic components. For $\mathcal{A}=(\lambda_2-h_j-h_k)_{+}$ on $J_{jk}=2$, conjugating by its positive spectral diagonal gives $\mathcal{A}^{1/2}d_{jk}\mathcal{A}^{1/2}\le I$. Weighted Cauchy–Schwarz implies $d_{jk}^{-1}\ge\mathcal{A}$, proving the desired pair bound with all spin and magnetic components.

All angular patterns with $L \geq 2$. Set $U = -2903651/10^6$, $g_1 = -20/9 - U$, and $g_2 = \lambda_2 - U$. Lemma 5.3 gives $E < U$. If Q_i projects the complementary pair onto $J_{jk} = 0$, the pair bounds imply $H_{jk} \geq E + g_1(1 - Q_i)$, with gain g_2 on a pure $J_{jk} = 2$ subspace. Localize by $\xi_i = r_i/\rho$, so $\sum_i \xi_i^2 = 1$. The localization error is ρ^{-2}. The radial Hardy inequalities for the marked electrons return $3/(8\rho^2)$, and their angular kinetic energy returns $\sum_i \ell_i(\ell_i+1)/(2\rho^2)$ on a block of individual angular momenta (ℓ_1, ℓ_2, ℓ_3). For $w_i = \xi_i^2$, define

$$\overline{d} = \min\{\sqrt{3}, \sqrt{8(1-w_1)}, \sqrt{8(1-w_2)}, \sqrt{8(1-w_3)}\}.$$

The remaining attraction is at worst $-\overline{d}/\rho$. Indeed its dimensionless coefficient is $2\sum_i \xi_i - \rho^{-1}\sum_{i<j}(r_i^2 + r_j^2)/d_{ij}$. The pairwise triangle inequality bounds it by $\sum_i \xi_i \leq \sqrt{3}$. Also $(r_i^2 + r_j^2)/d_{ij} \geq |x_i + x_j|$ and $\sum_{i<j} |x_i + x_j| \geq 2r_i$, giving the other three bounds. We apply the pair inequalities to $\xi_i u$ before resolving individual angular momenta, so antisymmetry of each residual pair is retained. The resulting comparison commutes with the individual angular Casimirs and can then be estimated block by block.

Call i eligible if $\ell_j = \ell_k$ and $\ell_i = L$. Only eligible labels can have $Q_i \neq 0$. There are zero, one, or three eligible labels, because two eligible labels force the third to be eligible. With one eligible label put $b = 1 - w_i$. With three choose a label of maximal w_i and again put $b = 1 - w_i$. In the three-label case $\ell_1 = \ell_2 = \ell_3 = L$. The normalized pair-singlet orbital vectors at fixed total magnetic index $m_0 \in \{-L, \ldots, L\}$ are

$$|L, m_0\rangle_i \otimes \frac{1}{\sqrt{2L+1}} \sum_{m=-L}^{L} (-1)^{L-m} |L, m\rangle_j |L, -m\rangle_k.$$

Their pairwise absolute overlaps are $1/(2L+1) \leq 1/5$. Thus $(1 - Q_i) + (1 - Q_j) \geq (4/5)I$ and, since $w_i \geq b/2$, $\sum_h w_h(1 - Q_h) \geq (2/5)bI$.

The coefficient of ρ^{-2} before absorbing $-\overline{d}/\rho$ is $\frac{1}{2}\sum_i \ell_i(\ell_i + 1) - 5/8$. Completing the square and using $\overline{d}^2 \leq 3$ or $\overline{d}^2 \leq 8b$ gives the exhaustive bounds in Table 13. In the exceptional pattern

Eligible labels and pattern	Coefficient of ρ^{-2}	Exact value
None	$11/8 - 3/(4g_1)$	13461449/49062872
One, other patterns	$35/8 - 2/g_1$	70650065/49062872
One, permutations of $(2, 0, 0)$	$19/8 - 2/g_2$	100665949/6779227768
Three	$67/8 - 5/g_1$	50901553/49062872

Table 13: Lower coefficients after absorbing the remaining attraction, for every angular block with $L \geq 2$.

the other two pairs have pure angular momentum two, which supplies $g_2 b$. Every coefficient exceeds $1/80$. For the smallest one, $80 \cdot 100665949 = 8053275920 > 6779227768$. The case $b = 0$ has $\overline{d} = 0$ and requires no division by b.

These estimates initially hold away from $\rho = 0$. The nine-dimensional Hardy inequality $\int \rho^{-2}|u|^2 \leq (4/49)\int |\nabla u|^2$ justifies removing a cutoff there. Form continuity removes the outer cutoff and the smoothness restriction. Orthogonal summation proves the second assertion on the closed sum of all $L \geq 2$ sectors. □

E.4 The exterior estimate

Proof of Lemma 5.5. We localize according to which electrons have radii comparable to the largest radius. Call these electrons marked. When exactly one electron is marked, the spectral gap of

neutral helium controls the coupling between that electron and the other two. Completing a square in the radial variable of the marked electron then absorbs the localization error and leaves a boundary term. When two or three electrons are marked, the form exceeds E by a positive amount.

Localization and its constants. Use Φ, p_0, M_k from Lemma 5.3, and put

$$R = 7, \quad c = \frac{12}{25}, \quad a = \frac{99}{100}, \quad C = \frac{14629801296936}{10^{12}}, \quad K = \frac{1105489614522}{10^{12}}.$$

Let θ be zero on $[0, c]$, equal to $\pi/2$ on $[a, \infty)$, and affine in $\operatorname{arsinh} t$ between c and a. For $s = \max_i r_i$ and $A \subset \{1, 2, 3\}$ define

$$\chi_A = \prod_{i \in A} \sin\theta(r_i/s) \prod_{i \notin A} \cos\theta(r_i/s).$$

Then $\sum_A \chi_A^2 = 1$, and a maximizing label belongs to every nonzero branch A. In that branch, $r_i \geq cs$ for $i \in A$ and $r_i \leq as$ for $i \notin A$. Differentiating the product partition, including the derivative of s, gives the localization error

$$W = \frac{1}{2} \sum_A |\nabla \chi_A|^2 \leq \frac{C}{s^2}.$$

Indeed $|\nabla(r_i/s)|^2 = (1 + (r_i/s)^2)/s^2$ for each nonmaximizing label, and there are at most two such labels. The finite cutoff calculation uses $h = (a - c)/256$ and

$$t_j = \frac{\operatorname{isqrt}(\lceil 10^{24}(1 + (c + jh)^2)\rceil) + 1}{10^{12}}, \qquad w = h \sum_{j=1}^{256} t_j^{-1}.$$

The right endpoint sum gives $\operatorname{arsinh} a - \operatorname{arsinh} c \geq w$. The exact rational comparisons yield

$$\left(\frac{11}{7w}\right)^2 \leq C, \qquad \sum_{\ell=4}^{320} \frac{a^{2\ell-8}}{2\ell+1} + \frac{a^{634}}{643(1-a^2)} \leq K.$$

The first uses $\pi < 22/7$. The second bounds all omitted multipoles by a geometric series. The root inequalities are checked by squaring positive integers, and both sums by clearing positive denominators. On a singleton branch, with marked position y and $r = |y| = s$, the sharper bound is $W \leq C(\mathbf{1}_{\{r_j \geq cr\}} + \mathbf{1}_{\{r_k \geq cr\}})/(2r^2)$. Use the same volume expression for $q_>$ on the localized spinors, which need not be fully antisymmetric. Expanding their gradients gives

$$q_>[u] - E\|u\|^2 = \sum_A \left(q_>[\chi_A u] - E\|\chi_A u\|^2 - \int_{\Omega_7} W |\chi_A u|^2 \right).$$

The neutral core in a singleton branch. At fixed y and spin, the two unmarked electrons remain antisymmetric and their radii are at most ar. On their full space define

$$V_y = \sum_{i=1}^{2} \mathbf{1}_{\{r_i \leq ar\}} (|y - x_i|^{-1} - r^{-1}), \qquad W_y = \frac{C}{2r^2} \sum_{i=1}^{2} \mathbf{1}_{\{r_i \geq cr\}}.$$

The radial one-electron marginal of Φ and the spherical mean of $|y - x|^{-1}$ for $|x| < r$ give $\langle \Phi, V_y \Phi \rangle = 0$. Orthogonality of the Legendre polynomials in the convergent multipole expansion, followed by the moment bounds, gives

$$r^2 \|V_y \Phi\| \leq \mathcal{M}(r) := 2\sqrt{\frac{M_1^2}{3} + \frac{M_2^2}{5r^2} + \frac{M_3^2}{7r^4} + \frac{K M_4^2}{r^6}}.$$

For degrees at least four, use $r_i^{2\ell} \le r_i^8 (ar)^{2\ell-8}$ on the cutoff support. Put

$$p(r) = \min\left\{ p_0(cr), \left(\frac{M_j}{(cr)^j}\right)^2 : 1 \le j \le 4 \right\}, \qquad g(r) = \frac{67039}{100000} - \frac{2a}{(1+a)r} - \frac{C}{r^2}.$$

Then $\langle \Phi, W_y \Phi \rangle \le C p(r)/r^2$ and $\|W_y \Phi\| \le C\sqrt{p(r)}/r^2$. Each summand of V_y is at least $-a/((1+a)r)$, so the restriction of $H_2(2) + V_y - W_y - E$ to $\Phi^\perp$ has lower bound $g(r)$. This is positive for $r \ge 7$, since

$$g(7) = \frac{39993614855531}{174125000000000} > \frac{22968}{100000}.$$

Writing a core vector as $\alpha\Phi + v$, $v \perp \Phi$, and completing the square in $\|v\|$ proves

$$H_2(2) + V_y - W_y - E \ge -\frac{D(r)}{r^2} I, \qquad D(r) = C p(r) + \frac{[\mathcal{M}(r) + C\sqrt{p(r)}]^2}{g(r) r^2}.$$

Both p and $\mathcal{M}$ decrease with r, while $g(r)r^2$ increases. Thus D is nonincreasing on $[7, \infty)$.

The radial table and the boundary term. The exterior table in the code/data release has nodes $\varrho_i = 3584/i$, $1 \le i \le 512$. For each node its row selects a rational candidate $\widetilde{p}_i$ from the five candidates defining $p(\varrho_i)$, hence $\widetilde{p}_i \ge p(\varrho_i)$. It gives rational upper bounds

$$\mathcal{A}_i \ge \mathcal{M}(\varrho_i) + C\sqrt{\widetilde{p}_i}, \qquad \widetilde{D}_i = C\widetilde{p}_i + \frac{\mathcal{A}_i^2}{g(\varrho_i)\varrho_i^2} \ge D(\varrho_i).$$

The two square roots in $\mathcal{A}_i$ are rounded upward at scale 10^{12} by the same integer-square-root rule as above. All 512 rows of the rational sequence $F_0, \dots, F_{512}$ satisfy

$$F_0 = 0, \qquad F_{i-1} < F_i < 1,$$
$$iF_i - (i-1)F_{i-1} - F_i^2 - 2\widetilde{D}_i \ge \frac{2863835767937}{10^{24}} > 0, \qquad F_{512} = \frac{123555069308}{10^{12}}.$$

These are the results of integer comparisons after clearing the positive denominators, including $g(\varrho_i)$. The complete selected candidates, upper roots, and F_i are in the exterior table. They imply a bound on every radius, as follows.

For $0 \le x \le 1$, interpolate $Y(x) = xf(x)$ linearly through $(i/512, iF_i/512)$ and set $f(x) = Y(x)/x$ for $x > 0$. On the ith cell, $0 \le f(x) \le F_i$ and $Y'(x) = iF_i - (i-1)F_{i-1}$. Since $7/x \ge \varrho_i$,

$$Y'(x) - f(x)^2 \ge 2D(7/x).$$

The first cell covers the entire tail $r \ge 3584$. For the vector field $\mathcal{V}(y) = (1 - f(7/|y|))y/|y|^2$, expansion of a square on $\Omega = \{y : |y| > 7\}$, with outward unit normal ν, gives for $\zeta \in H^1(\Omega)$

$$\frac{1}{2}\int_\Omega |\nabla\zeta|^2 \ge \frac{1}{2}\int_\Omega (\operatorname{div}\mathcal{V} - |\mathcal{V}|^2)|\zeta|^2 - \frac{1}{2}\int_{\partial\Omega} \mathcal{V}\cdot\nu\,|\zeta|^2.$$

Apply this to the marked-coordinate slices of the localized spinor. The volume coefficient is $[Y'(x) - f(x)^2]/(2r^2)$, which absorbs the negative term in the lower bound of the preceding step. At $r = 7$ the outward normal of the exterior is $-y/7$. Hence the boundary coefficient is

$$\frac{1 - F_{512}}{14} = \frac{0.876444930692}{14} > \frac{1}{16}.$$

The vector field is continuous across all cell interfaces, so no internal boundary terms occur.

Two or three marked electrons. For $k = |A| \in \{2, 3\}$ use the marked coordinates $X = (x_i)_{i\in A}$ and $T = |X|^2$. At fixed unmarked coordinates apply the square on $\{X : \max_{i\in A} r_i > R\}$ with vector field kX/T. Its volume contribution is $k(k-1)/T \geq (k-1)/s^2$. On an exposed face its boundary contribution is $kR/(2T) \geq 1/(2R) = 1/14$. For $k = 2$ the unmarked electron contributes at least -2 by Theorem 3.2. The triangle bound on each pair distance and minimization over the marked radii give the remaining volume bounds

$$\frac{90372}{100000} - \frac{A_2}{s} - \frac{C-1}{s^2}, \qquad \frac{290372}{100000} - \frac{A_3}{s} - \frac{C-2}{s^2},$$

where

$$A_2 = 2 + \frac{2}{c} - \frac{1}{1+c} - \frac{1}{1+a} - \frac{1}{c+a}, \qquad A_3 = 2 + \frac{4}{c} - \frac{2}{1+c} - \frac{1}{2c}.$$

For example, the two-marked potential is bounded below by $s^{-1}[-2 - 2/t + 1/(1+t) + 1/(1+a) + 1/(t+a)]$, $c \leq t \leq 1$. Its derivative is positive. The three-marked expression increases in each of its two radius ratios by the same derivative comparison. Both displayed volume bounds increase with $s \geq 7$, and at seven their exact values are

$$\frac{9567964312983109}{947065875000000000} > 0, \qquad \frac{1027725017005013}{679875000000000} > 0.$$

Every branch therefore has nonnegative volume contribution and boundary coefficient at least $1/16$. Fixing the unmarked coordinates introduces no extra boundary: a branch vanishes wherever an unmarked label attains the maximum, and its nonzero traces lie on the exposed faces of ∂K_7. Summing the localization identity gives the claim because $\sum_A \chi_A^2 = 1$ also on those faces. The argument first applies to smooth restrictions. The exterior is a Lipschitz domain, including its corners, so extension, smooth approximation, and continuity of the trace give the free-trace H^1 assertion. Coulomb forms pass to this limit by the three-dimensional Hardy inequality in each electron and relative coordinate. No spectral or boundary condition on u is used. □

E.5 The upper bound for the lithium anion

Proof of Proposition 6.1. The trial function and its matrix elements. The trial function is specified by a table of 150 rows of integers in the accompanying code/data release. Its columns are $(c_\alpha, a_{\alpha1}, \dots, a_{\alpha4}, b_{\alpha12}, b_{\alpha13}, b_{\alpha14}, b_{\alpha23}, b_{\alpha24}, b_{\alpha34})$, with $1 \leq \alpha \leq 150$. The coefficients c_α have no additional scale. Put $D = 10^5$. For $x = (x_1, \dots, x_4)$, let $X_\nu = (x_{1\nu}, \dots, x_{4\nu})^T \in \mathbb{R}^4$, $1 \leq \nu \leq 3$, be the column of νth Cartesian coordinates of the electron positions. With e_i the coordinate vectors of $\mathbb{R}^4$, set

$$A_\alpha = \operatorname{diag}(a_{\alpha1}, \dots, a_{\alpha4}) + \sum_{i<j} b_{\alpha ij}(e_i - e_j)(e_i - e_j)^T, \qquad f_A(x) = \exp\left(-D^{-1}\sum_{\nu=1}^{3} X_\nu^T A X_\nu\right).$$

Every row has $a_{\alpha i} > 0$ and $b_{\alpha ij} \geq 0$, so $y^T A_\alpha y = \sum_i a_{\alpha i} y_i^2 + \sum_{i<j} b_{\alpha ij}(y_i - y_j)^2 > 0$ for $y \neq 0$. Let P_{ij} denote the exchange of the positions i, j. Then

$$F = \sum_{\alpha=1}^{150} c_\alpha f_{A_\alpha}, \qquad \Phi = (1 - P_{12})(1 - P_{34})F$$

are Schwartz functions. Assign $\Phi/\sqrt{6}$ to the spin component $\uparrow\uparrow\downarrow\downarrow$ and extend by signed simultaneous permutations to the other five components with two up spins. Set all other components to zero. Since Φ changes sign under both within-spin transpositions, this defines a fully antisymmetric spinor Ψ. The extension is isometric and preserves the Coulomb form. Thus Ψ belongs to the form domain in Set-up 2.1. The argument does not require Ψ to be an eigenfunction of the total spin.

For $1 \le \beta \le \alpha \le 150$ and $\sigma \in \{1, (12), (34), (12)(34)\}$, let B be A_β with both indices permuted by σ. The signs of these four permutations are $+, -, -, +$. For each such triple and $v \in \mathbb{R}^4 \setminus \{0\}$, define

$$G = A_\alpha + B, \quad g = \det G, \quad \Gamma = \operatorname{adj} G, \quad \tau = \operatorname{tr}(A_\alpha \Gamma B), \quad n(v) = v^T \Gamma v,$$
$$S = D^6 g^{-3/2}, \qquad T = \frac{3\tau}{Dg}, \qquad J(v) = 2\sqrt{\frac{g}{\pi D n(v)}}, \qquad \omega = c_\alpha c_\beta (2 - \mathbf{1}_{\alpha=\beta}) \operatorname{sgn}(\sigma).$$

Gaussian integration gives $\langle f_{A_\alpha}, f_B \rangle = \pi^6 S$. Under the normalized product density, each column X_ν has covariance $(D/2)G^{-1}$. Differentiating the two Gaussians therefore gives the kinetic quotient $3\operatorname{tr}(A_\alpha G^{-1} B)/D = T$. Radial integration of the Gaussian vector $\sum_i v_i x_i$ gives the Coulomb quotient $J(v)$. Thus, with all sums below over these triples,

$$\mathcal{N} = \sum \omega S, \qquad \mathcal{H} = \sum \omega S \left(T - 3 \sum_i J(e_i) + \sum_{i<j} J(e_i - e_j) \right)$$

satisfy

$$\|\Psi\|^2 = 4\pi^6 \mathcal{N}, \qquad \mathfrak{q}_{4,3}[\Psi] = 4\pi^6 \mathcal{H}. \tag{E.1}$$

Indeed, $\mathcal{A} = (1 - P_{12})(1 - P_{34})$ is self-adjoint, $\mathcal{A}^2 = 4\mathcal{A}$, and it commutes with the form. The matrix after summing the four permutations is symmetric, which justifies the factor two for $\alpha > \beta$. There are exactly $4 \cdot 150 \cdot 151/2 = 45300$ terms. None is discarded according to its sign or magnitude.

Exact kernel enclosures. Put $M = 2^{120}$ and

$$p_0 = \frac{3141592653589793}{10^{15}}, \qquad p_1 = \frac{3141592653589794}{10^{15}}.$$

These enclose π strictly. To verify this in rational arithmetic, put $L_k = \sum_{j=0}^{29} (-1)^j / ((2j+1) k^{2j+1})$ and $\epsilon_k = 1/(61 k^{61})$ for $k = 5, 239$. The tangent addition formula and the alternating-series remainder give

$$p_0 < 16 L_5 - 4(L_{239} + \epsilon_{239}) < \pi < 16(L_5 + \epsilon_5) - 4 L_{239} < p_1.$$

The outer inequalities are finite rational comparisons. For each kernel, the positive definite matrix G gives $g > 0$ and $n(v) > 0$ for the four $v = e_i$ and six $v = e_i - e_j$. Define the integers

$$s_{\mathrm{l}} = \left\lfloor \sqrt{M^2 D^{12}/g^3} \right\rfloor, \qquad s_{\mathrm{u}} = s_{\mathrm{l}} + 1,$$
$$t_{\mathrm{l}} = \lfloor 3\tau M/(Dg) \rfloor, \qquad t_{\mathrm{u}} = t_{\mathrm{l}} + 1,$$
$$j_{\mathrm{l}}(v) = \left\lfloor \sqrt{4M^2 g/(p_1 D n(v))} \right\rfloor, \qquad j_{\mathrm{u}}(v) = \left\lfloor \sqrt{4M^2 g/(p_0 D n(v))} \right\rfloor + 1,$$
$$k_{\mathrm{l}} = t_{\mathrm{l}} - 3\sum_i j_{\mathrm{u}}(e_i) + \sum_{i<j} j_{\mathrm{l}}(e_i - e_j), \qquad k_{\mathrm{u}} = t_{\mathrm{u}} - 3\sum_i j_{\mathrm{l}}(e_i) + \sum_{i<j} j_{\mathrm{u}}(e_i - e_j),$$
$$h_{\mathrm{l}} = \min(s_{\mathrm{l}} k_{\mathrm{l}}, s_{\mathrm{u}} k_{\mathrm{l}}), \qquad h_{\mathrm{u}} = \max(s_{\mathrm{l}} k_{\mathrm{u}}, s_{\mathrm{u}} k_{\mathrm{u}}).$$

For a nonnegative rational a/b, its square-root floor equals the integer square root of $\lfloor a/b \rfloor$: both are the unique $k \geq 0$ with $k^2 \leq a/b < (k+1)^2$. It follows that $s_{\mathrm{l}} \leq MS < s_{\mathrm{u}}$ and that $[h_{\mathrm{l}}, h_{\mathrm{u}}]$ encloses $M^2 S(T - 3\sum_i J(e_i) + \sum_{i<j} J(e_i - e_j))$. The two-corner product bounds remain valid for either sign of the k endpoints because both s endpoints are nonnegative. Accumulate signed intervals by

$$\begin{aligned} N_- &= \sum \min(\omega s_{\mathrm{l}}, \omega s_{\mathrm{u}}), \quad N_+ = \sum \max(\omega s_{\mathrm{l}}, \omega s_{\mathrm{u}}), \\ H_- &= \sum \min(\omega h_{\mathrm{l}}, \omega h_{\mathrm{u}}), \quad H_+ = \sum \max(\omega h_{\mathrm{l}}, \omega h_{\mathrm{u}}). \end{aligned}$$

Then

$$\frac{N_-}{M} \leq \mathcal{N} \leq \frac{N_+}{M}, \qquad \frac{H_-}{M^2} \leq \mathcal{H} \leq \frac{H_+}{M^2}. \tag{E.2}$$

These are complete rounding bounds, including signed cancellation.

Evaluation and strictness. The completed exact evaluation of the specified 150 rows gives

$$\begin{aligned} N_- > 0, \qquad & H_+ < 0, \\ \left\lfloor \frac{10^9 H_-}{M N_-} \right\rfloor = -7497020241, \qquad & \left\lceil \frac{10^9 H_+}{M N_+} \right\rceil = -7497020240. \end{aligned} \tag{E.3}$$

The input, executable checker and complete execution record are supplied with the table in the accompanying code/data release. The checker reads every eleven-integer row, checks the row signs, and visits every lower-triangular pair and all four permutations. Its cofactor expansion computes Γ and g exactly. Its kinetic sum is $3\sum_{i,j,k}(A_\alpha)_{ij}\Gamma_{jk}B_{ki} = 3\tau$. Nuclear and pair cofactor forms are respectively Γ_{ii} and $\Gamma_{ii} + \Gamma_{jj} - 2\Gamma_{ij}$, so its kernel is precisely the one just proved. The execution uses Python integers, rational arithmetic, signed floor division and integer square roots, with assertions enabled. Faithful input reading, execution and output recording have the meaning of Set-up 2.2. No floating-point accuracy assumption enters this evaluation.

Since $N_- > 0$, some $c_\alpha \neq 0$. The identity-permutation diagonal term then has positive weight c_α^2 and strict overlap upper bound $MS < s_{\mathrm{u}}$. Hence $\mathcal{N} < N_+/M$, while $\mathcal{H} \leq H_+/M^2 < 0$. Equations (E.1)–(E.3) therefore give

$$-7.497020241 \leq \frac{H_-}{MN_-} \leq \frac{\mathfrak{q}_{4,3}[\Psi]}{\|\Psi\|^2} < \frac{H_+}{MN_+} \leq -7.497020240.$$

The variational principle proves the proposition. □

Use of generative AI

The supplied helium and lithium arguments and numerical witnesses were drafted with use of `gpt-6-astra` and `fable-5.2`, then audited, simplified, and assembled using Pharos. The project was configured with the `gpt-6-astra` model, with `ultra` reasoning effort for the main agent and seven proof workers: three at `xhigh` and four at `max`. The recorded final lithium verification used the same model at `max`.

Human direction specified verification of the supplied results, reuse of sufficient existing work, a unified concise presentation, and a reproducible code/data supplement. The review procedure required mathematical arguments, correctness of the concrete checkers, complete inputs and execution evidence, with explicit exact and floating-point runtime assumptions. This was automated mathematical review, not proof-assistant verification. The supplied claims and witnesses are attributed separately from their verification and simplification. The computation methods and error bounds are given in Appendices A–D. The helium-dianion proof of Section 4 and Appendix D, together with its certificate generators, exact readers, and the accompanying release module, were prepared with `fable-5.2`.

Data and code availability

An accompanying reproducibility supplement is available on Zenodo at `https://doi.org/10.5281/zenodo.24130570`.

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The supplied arguments were audited and this manuscript was prepared using the Pharos system, an automated mathematical reasoning system built on Rethlas [20]. The details of the use of generative AI are documented in Appendix E.5 for transparency. The authors are fully responsible for the correctness of the paper.

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