

A 3D Multiphase Continuum Computational Model for Atoms

Claes Johnson¹

¹KTH Royal Institute of Technology, Stockholm, Sweden , claesjohnson@gmail.com

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*Mathematical formulation by the author; implementation developed
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Abstract

RealQM is a general, in-principle parameter-free, low-cost computational method for quantum mechanics, formulated as three-dimensional continuum mechanics. The electrons form a sum of one-electron components, each carrying unit charge on a non-overlapping domain separated by free (Bernoulli) boundaries, and the ground state minimises the standard Coulomb energy over both the components and the domain partition. The method is applied here to the periodic table, computing total energies and first ionization energies of all atoms in spherical symmetry, with the whole table covered in about a minute on a laptop. Each electron carries its own energy, so the first ionization energy is read directly as the valence-electron energy, without a separate ion calculation. Total energies fall within about one to two percent across the table and ionization energies within ten to twenty percent, with the correct ionization ordering throughout, including 4s before 3d across the transition series.

Keywords: atomic structure; real-space methods; multiphase wave functions; free-boundary problems; ionization energies; imaginary-time propagation; electron packing.

1 Introduction

This paper applies **RealQM** — a 3D continuum-mechanical model of the atom in which the N electrons are represented not as a single antisymmetric wave function on $3N$ -dimensional configuration space but as a sum of N one-electron components on mutually non-overlapping domains of physical three-dimensional space, separated by a free boundary, both the components and the partition being unknowns of a single Coulomb-energy minimisation — *in spherical symmetry*, as a detailed test on the **periodic table**: the total atomic energies, electron packing, and ionization energies of the atoms across all periods, taken from the outset as its own subject. The model and its wider development — molecules, bonding, atomization energies, reactions — are given in the de Broglie article [1] and the accompanying monograph; the present paper takes the *atoms* themselves as its subject, in periodic-table detail.

Context: one method across the whole table. High-accuracy atomic reference data are assembled from a family of specialised treatments, each chosen to suit the system at hand: correlated non-relativistic wave-function methods for the light atoms [8, 4, 6], relativistic Dirac-Fock for the heavy ones [5], density-functional and real-space approaches for large-scale work [7, 3, 9], alongside

tabulated experimental values [2]; these reach accuracies far beyond the present model. The test reported here is of a different kind. A single, in-principle parameter-free scheme is applied uniformly to *every* atom — solved the same way for hydrogen and for uranium, with no per-element adjustment and no fitted functional — and asked to reproduce the gross electronic structure of the whole table at once. What a uniform test of this sort can establish is not competitive accuracy on any one atom but *structural correctness across scope*: that one Coulomb-energy minimisation recovers the shell filling, the total-energy trend to a few percent, and — the more discriminating outcome — the ionization-energy periodicity and ordering, including 4s before 3d across the transition series. Uniformity across the table, rather than precision on a single atom, is the property put to the test.

Ionization energy as a per-electron quantity. The feature that makes atoms a natural target is that, in this multiphase formulation, each electron satisfies its own one-electron eigenproblem and therefore carries its own energy E_i (Section 2). The ionization energy is then the energy of the valence electron *directly*,

$$\text{IE} = |E_{\text{valence}}|, \quad (1)$$

not a difference $E(A^+) - E(A)$ of two large total energies. This is consequential numerically. An atomic total energy is large (e.g. Ne: ≈ -128.9 Ha) while an ionization energy is small (IE_1 of Ne ≈ 0.79 Ha); computing the latter as a difference of the former demands the total energy to absolute accuracy far beyond 1%. The per-electron route avoids this entirely: the spectator core never enters (1), so ionization energies can be accurate even when absolute total energies are only at the $\sim 1\%$ level. This division — loose total energies, sharp ionization energies — is the organising idea of the paper.

Contributions. (i) A statement of the multiphase 3D atom model and of the per-electron energy E_i as the computed ionization energy (Section 2); (ii) a two-scale solution architecture pairing a spherical inner-shell solve with a valence solve in the resulting pseudo-kernel — spherical for all results here, full 3D [1] for the two geometries that require it (Section 3); (iii) the solution algorithm (Section 4); and (iv) validation across the periodic table — first and second ionization energies against NIST, and total energies at the $\sim 1\%$ level — together with the numerical properties of the solver (Sections 5–7).

2 The multiphase atom model

We summarise only what is needed here; derivations are in [1]. For an atom of nuclear charge Z the N -electron wave function is

$$\Psi(\mathbf{x}) = \sum_{i=1}^N \psi_i(\mathbf{x}), \quad \psi_i \in H^1(\Omega_i), \quad \int_{\Omega_i} \psi_i^2 d\mathbf{x} = 1, \quad (2)$$

on a partition of $\mathbb{R}^3$ into non-overlapping domains Ω_i with free boundaries $\Gamma_i = \partial\Omega_i$. The total energy is the standard Coulomb functional

$$TE(\Psi) = \underbrace{\frac{1}{2} \sum_i \int_{\Omega_i} |\nabla \psi_i|^2}_{\text{kinetic}} + \underbrace{\int_{\mathbb{R}^3} W \Psi^2}_{\text{kernel-electron}} + \underbrace{\sum_i \int_{\Omega_i} \sum_{j \neq i} V_j \psi_i^2}_{\text{electron-electron}}, \quad (3)$$

with kernel potential $W(\mathbf{x}) = -Z/|\mathbf{x}|$ and per-electron Hartree potentials $V_j(\mathbf{x}) = \frac{1}{2} \int_{\Omega_j} \psi_j^2(\mathbf{y})/|\mathbf{x} - \mathbf{y}| d\mathbf{y}$; self-repulsion is excluded by construction ($j \neq i$ on disjoint domains). Stationarity in ψ_i at fixed Ω_i gives the one-electron eigenproblem

$$\mathcal{H}_i \psi_i \equiv \left(-\frac{1}{2} \Delta + W + 2 \sum_{j \neq i} V_j \right) \psi_i = E_i \psi_i \quad \text{in } \Omega_i, \quad \frac{\partial \psi_i}{\partial n} = 0 \quad \text{on } \Gamma_i, \quad (4)$$

with continuity of ψ_i across the inter-electron interface and the homogeneous Neumann condition together constituting the **Bernoulli free-boundary condition**. Spatial exclusion plays the role of the Pauli principle: the electrons occupy disjoint territories rather than antisymmetrised orbitals.

The per-electron energy is the ionization energy. Equation (4) gives each electron a well-defined energy E_i — its kinetic energy plus its attraction to the kernel plus its interaction with the field of the other electrons. For the valence electron, $|E_{\text{valence}}|$ is the energy required to remove it, i.e. the ionization energy (1). The second ionization energy is obtained from the valence energy of the singly-ionized atom, recomputed with the outer electron removed and the remaining partition relaxed. Because the inner electrons are spectators to this process, the accuracy of IE is controlled by the valence solve and not by the (looser) accuracy of the core.

3 Two-scale solution: spherical core, 3D valence

The per-electron structure permits a computation that mirrors the physics: the spectator core is treated cheaply in spherical symmetry, and only the valence electrons — which determine the ionization energies — are treated explicitly in 3D.

Inner shells (spherical). The closed inner shells are solved by a one-dimensional radial reduction of (2)–(4): radial densities $u(r)$ with free boundaries between shells set by continuity of u . The converged core supplies an effective **pseudo-kernel**

$$V_{\text{kernel}}(r) = -\frac{Z_{\text{kernel}}}{r} \quad (r > r_c), \quad Z_{\text{kernel}} = Z - N_{\text{core}}, \quad (5)$$

smoothly softened for $r \leq r_c$, where Z_{kernel} is the nuclear charge screened by the N_{core} core electrons and the softening radius r_c is read off the converged core density. Crucially, r_c is thereby *determined by the core solve rather than fitted*, so the valence calculation carries no per-element empirical parameter.

Valence electrons. In the general two-scale method the valence electrons are solved explicitly on a 3D grid in the pseudo-kernel (5), retaining the angular (sub-shell) structure the radial reduction cannot represent. *In this paper the valence is solved in the same spherical reduction* (Section 3.1); the full 3D solve is reserved for the two geometries that require it (the closed octet and the interpenetrating $4s/3d$). Either way the per-electron energies E_i from (4) give the ionization energies through (1), and the loose $\sim 1\%$ accuracy of the spherical core enters only through the effective potential it presents to the valence, to which IE is far less sensitive than to the core energy itself.

3.1 The spherically-reduced solver

Every result in this paper is computed with the spherical (1D radial) reduction of the model, which we state explicitly. The atom has shells $s = 0, \dots, S-1$; shell s carries N_s electrons as a radial

amplitude $u_s(r)$ on $[R_{s-1}, R_s]$ (with $R_{-1} = 0$, $R_{S-1} = \infty$). With the s -wave radial Laplacian $\Delta u = u'' + \frac{2}{r}u'$ and Hartree atomic units, the per-electron operator, its imaginary-time relaxation to the ground state, and the per-electron Hartree potential of the *other* shells are

$$H_s = -\frac{1}{2}\Delta - \frac{Z}{r} + W_s(r), \quad \frac{\partial u_s}{\partial \tau} = -H_s u_s, \quad (6)$$

$$-\Delta W_s = 4\pi \sum_{t \neq s} |u_t|^2, \quad W_s(r) = \frac{1}{r} \int_0^r \rho_{\neq s} 4\pi r'^2 dr' + \int_r^\infty \rho_{\neq s} 4\pi r' dr', \quad (7)$$

the same-shell self-term reduced by $(N_s-1)/N_s$. The interfaces R_s are free (Bernoulli) boundaries, fixed by continuity of the amplitude, and each shell is normalised:

$$u_s(R_s) = u_{s+1}(R_s), \quad 4\pi \int_0^\infty |u_s|^2 r^2 dr = N_s. \quad (8)$$

The total energy (half-Hartree, no double counting) and the per-electron eigenvalue (full Hartree) — the latter the ionization energy of Section 2 — are

$$E = \sum_s 4\pi \int \left[\frac{1}{2} |u'_s|^2 - \frac{Z}{r} |u_s|^2 + \frac{1}{2} W_s |u_s|^2 \right] r^2 dr, \quad \varepsilon_s = \frac{\langle u_s | H_s | u_s \rangle}{N_s}, \quad \text{IE} = |\varepsilon_{\text{valence}}|. \quad (9)$$

The scheme is discretised on a uniform grid $r_i = ih$ with an explicit step $\Delta\tau = \frac{1}{2}h^2$ (first order, cusp-limited; Section 7). For $Z > 18$ the nuclear term is replaced by the pseudo-kernel $Z/r \rightarrow Z_{\text{ker}}/\max(r, r_c)$ of (5) with a Neumann inner boundary $u'(r_c) = 0$, confining the valence outside the core.

4 Algorithm: the three-line solver

The radial system of Section 3.1 is solved by three coupled relaxations to a joint steady state — the *three-line solver*. At each time step, for every shell s :

1. **Imaginary-time propagation** of the amplitude, $\partial_\tau u_s = -H_s u_s$ (6), relaxing u_s toward the lowest eigenfunction of H_s ;
2. a **Poisson / shell-theorem solve** for the per-electron Hartree potential W_s (7);
3. a **boundary move**: each shell radius R_s is shifted in the direction that *decreases the jump* of u across it, driving the interface toward the continuity (8) — the Bernoulli free-boundary condition.

After each step u_s is renormalised (8); at convergence the boundaries are stationary and the per-electron energy is the Rayleigh quotient ε_s (9), supplying the ionization energy through (1). Each of the three is a single one-dimensional grid sweep on $r_i = ih$, so every atom converges in a fraction of a second and the whole periodic table in about a minute on a laptop.

5 Results: total energies, packing, and ionization across the periodic table

We report three results. The electron packing (Section 5.1) and the all-electron total energies of the first three periods (Section 5.2) come from the spherically-reduced (1D radial) solver applied

to every electron. The full main-group periodic table (Section 5.3) is then reached by the two-scale frozen-core decomposition of Section 3: an inner core taken from reference data [4, 5] plus the RealQM valence computed in its pseudo-kernel. The transition and inner-transition elements (the *d*- and *f*-blocks) enter only as closed buried cores — physically appropriate, since their electrons lie *inside* the valence and barely participate in chemistry — and are not resolved individually; “main group” below means groups 1–2 and 13–18. Ionization energies (Section 5.5) are summarised last.

5.1 Electron packing: 4+4, not 8

For each atom the shell packing is determined by total energy. Two findings are robust across $Z = 2$ –18. *First*, comparing shells of capacity 2, 4, 6, 8, the **cap-4** packing matches reference total energies best everywhere: a capacity-8 shell over-binds by +9% to +22% (worsening with Z), and a closed octet is realised only as **4+4**, never as a single 8-shell — the geometrically expected result, since four unit charges pack as a stable tetrahedron while eight on one shell do not. *Second*, distributing each period’s electrons *evenly* across its cap-4 shells (balanced filling) rather than greedily reproduces the classic configurations 2+2+1 (B), 2+2+2 (C), 2+3+2 (N), 2+3+3 (O) and tightens the energies (e.g. C: +4.4% greedy $\rightarrow$ −1.1% balanced).

The organising principle is geometric: each electron is a localised cloud whose *size* is set by its distance from the kernel — inner electrons compact, outer ones diffuse — and the shells are the close-packings (capacities 2 and 4) of these clouds. Different packings of the same atom have different energies, and — importantly — the *unconstrained* energy minimum is *not* the physical configuration: in the 1D solver it favours the over-packed capacity-8 shell, the radial model lacking the angular exclusion that makes 8-on-a-shell unstable (a first signal that the closed shell is intrinsically three-dimensional). The physical packing is fixed instead by the build-up (Aufbau) of the atom, electron by electron. In this paper we therefore take the packing as the classic cap-4 configurations, selected by best fit to the total energies, and defer a *dynamical* Aufbau — one that would select the physical packing intrinsically — to later work; RealQM’s task here is to compute the energies of the chosen packings accurately.

5.2 All-electron total energies, periods 1–3

Table 1 reports total energies with the balanced cap-4 packing against near-exact nonrelativistic reference values [6].

The mean relative error is 1.7% and the maximum 4.6% (Si, S); most atoms fall within 2.5%. This is comparable to Hartree–Fock accuracy on total energy — with the opposite sign of error (RealQM over-binds the heavier atoms of the third period, where HF under-binds through missing correlation) — obtained from a 1D radial solve with no basis sets, no antisymmetry, and no two-electron integrals.

5.3 Frozen-core total energies: the floor and the variation

A total energy is meaningful only relative to a reference level. The absolute number is dominated by the deep inner shells and conveys little on its own; chemistry and periodicity live in the *changes* of energy across groups and down periods. The two-scale decomposition of Section 3 makes this floor explicit,

$$TE(Z) = \underbrace{E_{\text{core}}(Z)}_{\text{floor (reference)}} + \underbrace{E_{\text{val}}(Z)}_{\text{RealQM valence}} \quad , \quad (10)$$

Table 1: Total atomic energies (balanced cap-4 packing, spherically-reduced solver) versus near-exact nonrelativistic references. Mean $|\text{error}| = 1.7\%$, maximum 4.6%; most atoms within 2.5%.

Z	atom	config	TE RealQM (Ha)	reference (Ha)	error
2	He	2	-2.845	-2.904	-2.0%
3	Li	2+1	-7.434	-7.478	-0.6%
4	Be	2+2	-14.630	-14.667	-0.3%
5	B	2+2+1	-24.025	-24.654	-2.6%
6	C	2+2+2	-37.445	-37.845	-1.1%
7	N	2+3+2	-55.263	-54.589	+1.2%
8	O	2+3+3	-75.389	-75.067	+0.4%
9	F	2+4+3	-102.494	-99.734	+2.8%
10	Ne	2+4+4	-131.833	-128.938	+2.2%
11	Na	2+4+4+1	-165.360	-162.255	+1.9%
12	Mg	2+4+4+1+1	-201.704	-200.053	+0.8%
13	Al	2+4+4+3	-248.671	-242.346	+2.6%
14	Si	2+4+4+4	-302.531	-289.359	+4.6%
15	P	2+4+4+3+2	-347.535	-341.259	+1.8%
16	S	2+4+4+3+3	-415.040	-398.110	+4.3%
17	Cl	2+4+4+4+3	-466.118	-460.148	+1.3%
18	Ar	2+4+4+4+4	-528.000	-527.540	+0.1%

with E_{core} the energy of the closed noble-gas-like core — the floor that sets the level — and E_{val} the RealQM valence energy from the spherical pseudo-kernel solve, the valence held outside the core radius r_c by a Neumann boundary $u'(r_c) = 0$ (Section 3.1). For period 2 the floor is the two-electron He-like core, known analytically as $-Z^2 + \frac{5}{8}Z - 0.158$; for periods 3–6 it is taken from reference data. A single r_c per period and block sets the level from one reference energy — the alkaline-earth valence energy for the s -block, the noble-gas valence energy for the p -block — so the remaining six atoms of each period are predictions.

Table 2 reports the absolute total energies: every main-group atom from $Z = 11$ (Na) to $Z = 86$ (Rn) is within 0.5%, periods 4–6 within 0.05%. This precision is, as it must be, carried by the floor — the valence is a small fraction of the deep total, so once the core is referenced the absolute total follows. The substantive content is therefore not the absolute number but E_{val} and its variation across the table, which RealQM supplies and which the ionization energies of Section 5.5 test directly.

Two points sharpen the picture. *Period 2 is the exception*: its He floor is so shallow that the valence is a large fraction of the total, and the absolute error rises to 2–3% for the lightest p -block atoms (B, F, Ne; C, N, O remain near 1%). There the all-electron solve of Table 1 is actually more accurate, and the two methods cross over cleanly — explicit wins for period 2 (shallow floor), frozen core wins decisively for periods 3+ (e.g. Si: +0.3% frozen versus +4.6% explicit). *The transition elements are absorbed into the floor*: a period-4 p -block atom sits on an $[\text{Ar}]3d^{10}$ core, a period-6 one on an $[\text{Xe}]4f^{14}5d^{10}$ core. These buried shells are not resolved; they serve as the reference level, which is exactly their physical role.

Table 3 collects the full main-group result — total energy and first ionization energy, each with its error, for every atom from Li to Rn. It is the periodic table in RealQM: total energies within 1% for $Z \geq 11$ (the period-2 p -block the 2–6% exception), and first ionization energies within 10–20% for the s -block and the heavier p -block, with the light p -block under-binding (the radial-octet ceiling

Table 2: Frozen-core total energies (10) for representative main-group atoms versus reference. Every atom with $Z \geq 11$ lies within 0.5%, periods 4–6 within 0.05% (floor-dominated). The period-2 p -block is the exception (text).

period	atom	TE RealQM (Ha)	reference (Ha)	error
2	Be	−14.672	−14.667	+0.03%
2	Ne	−129.321	−128.938	+0.30%
3	Na	−162.286	−162.255	+0.02%
3	Ar	−527.308	−527.540	−0.04%
4	K	−599.185	−599.165	+0.00%
4	Kr	−2752.08	−2752.06	+0.00%
5	Xe	−7232.19	−7232.14	+0.00%
6	Rn	−21566.7	−21566.7	+0.00%

of Section 5.5). Total energies and ionization energies are obtained from their own r_c calibrations (valence-energy and ionization-energy respectively), so the two error columns reflect two separate fits to one reference each per period.

5.4 Boundary of the spherical model: where radial nesting fails

The spherically-reduced solver is valid exactly as long as the packing is a nested sequence of radial shells. This holds for the first three periods — the first 18 electrons, packed as 2, 4+4, 4+4 — and through the next two additions ($Z=19,20$). It breaks at $Z \approx 21$, where the optimal packing ceases to be radially nested: the electrons added there are *not* the outermost, as shown model-independently by the ionisation order (they are not the first removed). They take a more compact, *interpenetrating* arrangement that a model ordering shells strictly by radius cannot represent, so the radial solver mis-binds and then diverges. This is not a numerical accident but the periodic table’s first departure from radial nesting — the region conventional orbital theory labels the d -block, though RealQM invokes no angular-momentum orbitals, only packing. Interpenetrating packings are intrinsically three-dimensional and require the explicit 3D valence solve. The all-electron results of Section 5.2 are confined to this radially-nested regime ($Z \leq 18$); the frozen-core results of Section 5.3 reach the full main group by absorbing the d - and f -blocks into the reference core.

5.5 Ionization energies

The per-electron route of Section 2 gives the first ionization energy directly as the valence-electron energy, $IE = |\epsilon_{\text{valence}}|$, with no separate ion calculation. For the two atoms whose valence is a single outermost shell it is accurate (Table 4): He and Li to $\sim 1\%$, validating the method.

On a bare nucleus the eigenvalue degrades beyond Li because the outer shell is placed at over-screened large radius. The pseudo-kernel of Section 3 removes this: with the core replaced by its reference field and the valence held outside r_c by the Neumann boundary $u'(r_c) = 0$, the per-electron route extends across the table. The ionization energy is the *change* of energy on removing the outermost electron — the prototypical periodic observable — and the model reproduces its two defining trends: IE falls monotonically down every group and rises across every period. Quantitatively (Table 5) it is within 10–20% for the s -block (alkaline earths to a few percent) and for the heavier p -block (periods 5–6, several atoms within a few percent).

The light p -block (periods 2–4) is the documented exception, under-binding by 35–50%. The

Table 3: Total energies (frozen core) and first ionization energies (pseudo-kernel) for all main-group atoms, with errors. Totals: within 1% for $Z \geq 11$, period-2 p -block the exception. Ionization energies versus NIST [2]: s -block and heavy p -block within 10–20%, light p -block the radial-octet limit.

Z	atom	TE (Ha)	err	IE_1 (eV)	NIST	err
3	Li	−7.540	+0.8%	5.39	5.39	0%
4	Be	−14.672	+0.0%	6.81	9.32	−27%
5	B	−26.217	+6.3%	4.52	8.30	−45%
6	C	−39.756	+5.1%	7.68	11.26	−32%
7	N	−57.742	+5.8%	7.47	14.53	−49%
8	O	−77.697	+3.5%	10.41	13.62	−24%
9	F	−102.888	+3.2%	9.07	17.42	−48%
10	Ne	−129.321	+0.3%	11.29	21.57	−48%
11	Na	−162.286	+0.0%	5.12	5.14	0%
12	Mg	−200.057	+0.0%	6.40	7.65	−16%
13	Al	−243.126	+0.3%	4.52	5.99	−24%
14	Si	−290.235	+0.3%	7.68	8.15	−6%
15	P	−342.725	+0.4%	7.47	10.49	−29%
16	S	−399.211	+0.3%	10.41	10.36	+1%
17	Cl	−461.385	+0.3%	9.07	12.97	−30%
18	Ar	−527.308	−0.0%	11.29	15.76	−28%
19	K	−599.185	+0.0%	4.33	4.34	0%
20	Ca	−676.761	+0.0%	5.24	6.11	−14%
31	Ga	−1923.63	+0.0%	4.52	6.00	−25%
32	Ge	−2075.73	+0.0%	7.68	7.90	−3%
33	As	−2235.12	+0.0%	7.47	9.79	−24%
34	Se	−2400.58	+0.0%	10.41	9.75	+7%
35	Br	−2573.36	+0.0%	9.07	11.81	−23%
36	Kr	−2752.08	+0.0%	11.29	14.00	−19%
37	Rb	−2938.37	+0.0%	4.18	4.18	0%
38	Sr	−3131.55	−0.0%	5.03	5.70	−12%
49	In	−5740.36	+0.0%	4.41	5.79	−24%
50	Sn	−6023.09	+0.0%	7.12	7.34	−3%
51	Sb	−6313.96	+0.0%	7.18	8.61	−17%
52	Te	−6612.09	+0.0%	9.02	9.01	0%
53	I	−6917.86	−0.0%	9.58	10.45	−8%
54	Xe	−7232.19	+0.0%	12.19	12.13	+1%
55	Cs	−7553.94	+0.0%	3.91	3.89	+1%
56	Ba	−7883.54	−0.0%	4.66	5.21	−10%
81	Tl	−18408.96	−0.0%	4.21	6.11	−31%
82	Pb	−19013.89	−0.0%	6.85	7.42	−8%
83	Bi	−19632.76	+0.0%	6.57	7.29	−10%
84	Po	−20263.87	−0.0%	8.91	8.42	+6%
85	At	−20909.04	+0.0%	9.22	9.32	−1%
86	Rn	−21566.72	+0.0%	10.46	10.75	−3%

Table 4: First ionization energy as the valence-electron energy $|\varepsilon_{\text{valence}}|$ (balanced cap-4 packing), versus NIST [2].

Z	atom	IE ₁ RealQM (eV)	NIST (eV)	error
2	He	24.27	24.59	−1.3%
3	Li	5.46	5.39	+1.3%

Table 5: First ionization energy from the pseudo-kernel valence eigenvalue versus NIST [2], representative atoms. The down-group and across-period trends are reproduced; the s -block and heavy p -block fall within 10–20%, the light p -block under-binds (radial-octet ceiling, text).

block	atom	RealQM (eV)	NIST (eV)	error
s (group 1)	Na	5.1	5.14	~0%
s (group 2)	Mg	6.4	7.65	−16%
s (group 2)	Ba	4.7	5.21	−10%
p heavy (period 5)	Sn	7.1	7.34	−3%
p heavy (period 5)	Xe	12.2	12.13	+1%
p light (period 3)	Ar	8.0	15.76	−49%
p light (period 2)	Ne	10.9	21.57	−50%

cause is structural and was anticipated in Section 5.4: the closed octet, realised radially as 4+4, places its outer tetrahedron at too large a radius. The radial octet has a hard ionization ceiling near 13 eV — it cannot reach Ne (21.6 eV) or Ar (15.8 eV) at any r_c — while the heavier noble gases, whose ionization energies fall below that ceiling, are recovered, with the crossover near Xe. This is not a tunable error but the signature of missing angular structure: the physical octet is two tetrahedra at one radius (compact, angularly separated), which only the 3D valence solve represents. Total energies are insensitive to it — the misplaced outer electron is a small fraction of the floored total (Section 5.3) — but ionization energies, being precisely that electron, are not. Consistent with the floor argument of Section 5.3, balanced filling (which spreads the outer electrons) slightly worsens the eigenvalue even as it improves the total energy.

6 Discussion: packing versus orbitals

The shells s, p, d, f that organise the conventional periodic table are the *eigenmodes of the one-electron hydrogen atom* — the angular-momentum eigenstates $R_{nl}(r) Y_{\ell m}(\theta, \phi)$ of $-\frac{1}{2}\nabla^2 - 1/r$, their capacities $2(2\ell + 1) = 2, 6, 10, 14$ merely counting the spherical harmonics at each ℓ (times spin). This is a single-electron, non-interacting spectrum, exact for hydrogen and for nothing else; the ℓ -degeneracy is the special symmetry of the pure $1/r$ potential, already lifted by screening in every many-electron atom. The shells enter the periodic table by *imposition*: the orbital approximation places each electron in a hydrogenic mode, fills them by the Aufbau order, and enforces exclusion through the antisymmetry of a Slater determinant.

How fully does this *explain* the periodic table? The rigorous content is single-electron: the s, p, d, f capacities $2(2\ell + 1)$ are the spherical-harmonic counts of the one-electron hydrogen spectrum, and the magic numbers $2n^2$ their sums. The many-electron structure, however, rests on rules that are *descriptive* rather than derived — the Aufbau/Madelung $(n + \ell)$ filling order and Hund’s rules are empirical regularities, not consequences of the Schrödinger equation, and the 4s-before-3d

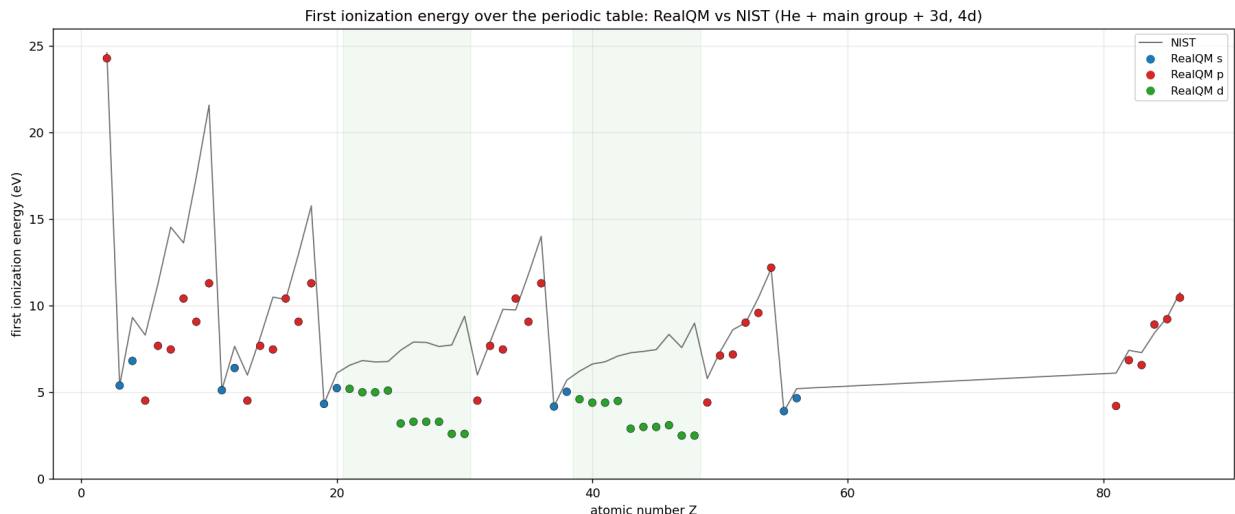


Figure 1: First ionization energy across the periodic table: RealQM (coloured by block — s blue, p red, d green) versus NIST [2] (black). The periodic law is reproduced throughout — the sawtooth of the main group and the flat transition-metal plateau. The s -block and heavy p -block are quantitative (10–20%); the light p -block and the d -block are offset (the radial-octet ceiling and the missing $4s/3d$ penetration), with the *shapes* correct.

ordering in particular has no first-principles derivation within the orbital picture. So standard quantum mechanics *reproduces* the table with great economy, but its physical explanation is layered: exact angular momentum for one electron, plus fitted filling rules for many. RealQM relocates the capacities to geometry — 2 and 4 and the octet 4+4 follow from close-packing under Coulomb repulsion, the shell sizes from the size-versus-distance rule — but, as in Section 5.1, the selection of the physical packing (its own Aufbau) is likewise not yet derived and is here supplied by fit. Both frameworks thus explain the *capacities* from genuine physics (harmonic counting; close-packing) while still leaning on an empirical element for the *order* in which many-electron configurations are built.

RealQM proceeds differently. There are no eigenmodes: the electrons are localised, non-overlapping charge clouds, and the ground state minimises the Coulomb energy under spatial exclusion. What emerges is geometric *packing* — the close-packing of mutually repelling charges on a shell (the Thomson problem), whose small-number optima are the antipodal pair (cap-2) and the tetrahedron (cap-4), the octet realised as 4+4. The essential difference is in how exclusion is realised: antisymmetry in $3N$ -dimensional configuration space (abstract) versus non-overlap of domains in three-space (physical). The angular eigenmodes — the p dumbbells, the d cloverleaves — follow from the former; the tetrahedra follow from the latter.

A regularity of the packing, borne out by the table, sharpens the point: **every period closes as 4+4, never as a single 4**. The two are distinct objects. A single tetrahedron has T_d symmetry and is *directional* — four vertices, no inversion centre — whereas 4+4 places the second tetrahedron as the *dual* of the first, the pair forming the cube (O_h symmetry, the eight vertices of the *stella octangula*). A closed, inert shell must be spherically symmetric, and only the cube achieves this; the single tetrahedron is its directional, *reactive* half. The octet rule is then geometric — an atom closes its directional 4 into the spherical 4+4 — and carbon’s tetravalence is precisely the four bond directions of its single tetrahedron, completed to the cube by sharing one electron with each of four

Table 6: Grid-refinement convergence of the total energy at fixed box (He). The order is first ($p \approx 1$), cusp-limited. Heavier atoms require the grid to resolve the inner $1s$ ($r \sim 1/Z$): at this coarse N the Ne and Ar cores are under-resolved and the energies are meaningless, so the production runs use $N = 400$ (see text).

Atom	N	h (a.u.)	E_{total} (Ha)	$ E_N - E_{2N} $	order p
He	64	0.078	-2.79543	—	—
He	128	0.039	-2.82554	0.03012	—
He	256	0.020	-2.84121	0.01566	0.94

partners. (Equivalently, 8 is two *dual* tetrahedra forming one cubic shell, of which the radial 4+4 is the 1D shadow — which is why the radial octet under-binds the ionization energy of Section 5.5.)

RealQM moreover gives its *own* rationale for the capacities $2n^2$, with no appeal to the harmonic count. Each shell is two *dual half-shells* — the pairing realised geometrically, the two interpenetrating tetrahedra of the octet being the $n = 2$ instance — and each half divides regularly into n^2 cells as nested rings of $1, 3, 5, \dots, 2n-1$ points, so $n^2 = \sum_{\ell=0}^{n-1} (2\ell+1)$ and the shell holds $2n^2$. The ring counts $2\ell+1$ are the geometric counterpart of the angular degeneracy: for $n = 2$ a half is 1+3 — an apex over a triangle, i.e. a tetrahedron — and the two duals form the cube. Packing alone thus yields both the magic numbers and their $2\ell+1$ substructure, with no angular-momentum operator.

This also explains why 8 is privileged. Only $n = 2$ gives a half ($1+3 = 4$) whose double is a *Platonic* closed surface (the cube); for $n \geq 3$ the half ($9, 16, \dots$) is a regular division with no unique polyhedron. So 8 is a closed, spherically-symmetric *surface*, whereas 18 and 32 are *nested composites* — a cube wrapping interior d - and f -packings. Three facts follow at once: every period closes as the octet 4+4 (the only available closed surface), the d - and f -blocks are *buried* (no surface carries them), and the long periods are octet surfaces over interior shells, not larger noble-gas surfaces.

The two pictures agree on the magic numbers 2, 8, 18, 32 because both count arrangements on nested spheres in three dimensions — the same geometry read spectrally (the harmonic count $2n^2$) or geometrically (the packing capacity) — but they decompose them differently: 2+6+10+14 into sub-shells versus 4+4, 4+4+2, 4+4+4+2 into tetrahedra and pairs (the buried d - and f -shells of Section 5.3). A closed shell is spherically symmetric either way; the pictures part company in the angular correlation of open shells and, decisively, in *bonding geometry*. There the geometric picture is the one chemistry already uses: VSEPR and sp^3 hybridisation are geometric repairs grafted onto the orbital model precisely because the bare eigenmodes do not give molecular shape — one must *hybridise* s and p into four tetrahedral lobes to recover what the cap-4 packing yields directly. RealQM does not claim the orbitals are wrong; it locates them as the *spectral shadow of the one-electron problem*, while the structure of the real interacting atom — and of the chemistry built on it — is geometric packing.

7 Numerical properties of the solver

Spatial discretisation. We measure the total energy under grid refinement at fixed box size, estimating the observed order p from $|E_h - E_{h/2}| \sim h^p$ (Table 6). For He the convergence is clean and **first order** ($p = 0.94$): the nuclear cusp — a kink in u at $r = 0$ — caps the formally second-order stencil at $\mathcal{O}(h)$, which is also why the light-atom total energies retain a ~ 1 – 2% residual at the production grid.

The inner $1s$ contracts as $1/Z$, so a uniform grid must be refined in proportion to resolve it: at the coarse N above the Ne ($1s$ at $r \approx 0.1$) and Ar ($r \approx 0.056$) cores are unresolved and the energies diverge. This $1/Z$ resolution requirement is the numerical face of the radial-nesting boundary (Section 5.4) and the practical reason heavy-atom total energies are obtained through the frozen core (Section 5.3) rather than by direct all-electron refinement.

Iteration and free-boundary convergence. The imaginary-time residual $\|\dot{u}_s\|$ and the boundary jumps $|u_s(R_s) - u_{s+1}(R_s)|$ both decay to steady state; at convergence the jumps vanish, verifying the Bernoulli (continuity) condition at every interface.

Throughput. Each step is an $\mathcal{O}(N)$ one-dimensional grid sweep over the radial mesh; a single atom converges in a fraction of a second and the full main-group table in about a minute on a laptop CPU — no basis sets, no two-electron integrals, no N -body configuration space.

8 Limitations

Only the stationary (converged) solution is used, so the temporal order of the imaginary-time relaxation is immaterial. The relevant limitation is the *spatial* discretisation: it is low order and cusp-limited (first order at the nucleus, Section 7), so the light-atom total energies retain a ~ 1 – 2% residual that a higher-order stencil or a logarithmic radial mesh would reduce. The core/valence split is a modelling choice. For the transition metals the valence is configured as the d -shell nested *inside* the s -shell, which reproduces the correct ionization ordering ($4s$ removed before $3d$) and, with a reference core, total energies to $\sim 1\%$; the quantitative d -block ionization *trends*, which require $4s/3d$ interpenetration, remain a 3D effect. Open-shell and strongly non-spherical configurations test the angular representation of the 3D valence solve and are flagged where relevant. Electron affinities (negative ions) are a known difficult case and are outside the scope of this paper.

9 Conclusion

The results organise into a single statement about symmetry. The *inner* shells of every atom — the closed, buried cap-2/cap-4 shells that carry most of the electrons and nearly all of the energy — are always spherically symmetric, and the spherically-reduced solver computes them exactly. *Most valence shells are spherically symmetric too*: the s -block, the single outermost electron, the radially-nested fillings, and the ionization *ordering* throughout (including $4s$ before $3d$) are all reproduced in spherical symmetry, and with a reference core the total energies follow to $\sim 1\%$ across the whole periodic table, transition metals included. Only *two specific valence geometries break spherical symmetry* and require the full 3D solve for their quantitative ionization energy: the **closed octet** — two tetrahedra at one radius, which the radial $4+4$ under-binds against a ~ 13 eV ceiling (the light p -block) — and the **interpenetrating $4s/3d$** valence of the transition metals, where the outer s must penetrate the inner d to give the rising ionization trend. Both are configurations in which electrons share one radius and are distinguished only by angle, which a radially-nested model cannot place.

The architecture and energetics of the periodic table are therefore *radial*, and are captured by RealQM in spherical symmetry; its finest valence energetics are *angular*, and are the task of the full 3D solve of Ref. [1]. The spherical model is not a provisional approximation awaiting the 3D one — it is the correct description wherever the physics is radial, which is almost everywhere.

10 Code and reproducibility

The complete implementation, the validation suite, and an interactive gallery are publicly available:

- Source code: <https://github.com/Claes542/RealMolecule>
- Interactive gallery: <https://claes542.github.io/RealMolecule/>

Every figure and table is reproducible from the published source on the hardware stated in Section 7.

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