The Geometry of Assembly: Caustic Packing and the Periodic Table

Paper V of Series III: The Geometry of the Limit

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December 18, 2025

Abstract

We extend the fold-caustic framework of Papers I–III to multi-electron atoms, framing atomic structure as a **topological packing problem** rather than an eigenvalue problem. We derive the periodic skeleton from two geometric mechanisms: (1) The **Madelung** $(n + \ell)$ **Rule** emerges from the **Stabilization Cost Functional**, where topological twisting (ℓ) incurs a geometric cost empirically calibrated from the observed 4s/3d crossover to approximately twice that of radial expansion (n) due to centrifugal barrier effects. (2) **Chemical Anomalies** (e.g., Cr, Cu) are resolved by a **Locking Cost Functional**, where the penalty for domain walls (exchange energy) and open manifolds outweighs orbital energy gaps. This reconstructs the Periodic Table as the optimal filling sequence of a capacity-limited topological ledger.

Keywords: topological defects, periodic table, Madelung rule, exchange interaction, confinement effects

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1 Introduction

In the preceding papers of this series, we established that matter arises from the buckling of the Action Flow when it hits the Liouville capacity limit $h \equiv h$. In *The Caustic Ladder* (Paper II), we showed that energy levels are the stable stationary states of these folds. In *Topological Seeds* (Paper III), we identified the electron as a "Twisted Fold," where intrinsic spin arises from the Möbius topology of the defect.

We now turn to the **Geometry of Assembly**. How do these twisted folds organize when confined around a nucleus?

Standard quantum mechanics treats this as an eigenvalue problem for the Schrödinger equation, followed by perturbation theory for electron-electron interactions. Here, we treat it as a **Packing Problem**. We ask: *What is the most efficient way to tile the phase space around a nucleus with twisted action cells?*

We demonstrate that the structure of the Periodic Table—shell capacities, the Madelung filling order, and even anomalous configurations—emerges naturally from the economics of Action. Nature fills the "cheapest" topological seats first, minimizing the **effective stabilization cost** of the configuration.

Remark 1.1 (Definition of Cost). By "cost" we mean an **effective action ranking functional** $\mathcal{C}$ that orders admissible fold-seats under the stationarity constraint $\oint p\,dq = kh$. It represents the phase-space volume and topological tension of the defect; it is NOT a thermodynamic dissipation but an effective action ranking. In this paper we operationalize the action-ranking by an energy-proportional proxy (since spectroscopy reports energies), so cost differences are reported in eV.

2 Topological Framework: Axioms and Indices

This approach builds directly on the results of Series III [1, 2, 3].

2.1 Axioms

1. **Action-Quota Principle**: Stabilizing a persistent physical distinction requires a minimum action expenditure of order h [1].
2. **The Twisted Fold**: As derived in *Topological Seeds* [3], the electron is a topological defect characterized by winding numbers.
3. **Single-Cell Bookkeeping**: The capacity of a shell is determined by the number of orthogonal symplectic cells of volume h^3 that fit within the energy surface, multiplied by the internal topological degeneracy (see Paper II, Section 3) [2].

2.2 Fold-seat indices

In *Topological Seeds* (Paper III), we identified the quantum numbers not as abstract labels, but as the winding numbers of the fold geometry.

Definition 2.1 (Fold seat)**.** A *seat* is a discrete topological class for a stable caustic. We write the tuple:

$$(n_r, \ell, m, \sigma), \tag{2.1}$$

where:

- $n_r \in \mathbb{Z}_{\geq 0}$: **Radial Nodes** (Number of concentric fold layers).
- $\ell \in \mathbb{Z}_{\geq 0}$: **Twist Count** (Topological winding number).
- m: **Orientation** of the twist axis.
- $\sigma \in \{+, -\}$: **Sheet Parity** (The double-cover orientation derived in Paper III).

The **principal ladder number** corresponds to the total topological complexity:

$$n := n_r + \ell + 1. \tag{2.2}$$

Remark 2.2 (Correspondence with Standard QM). The fold-seat indices (n_r, ℓ, m, σ) correspond exactly to the standard quantum numbers (n_r, ℓ, m, s). Standard QM obtains these from solving $H\psi = E\psi$. We obtain them from counting stable topological configurations via symplectic quantization $\oint p\, dq = nh$. The mathematics is identical; the interpretation differs.

3 Counting seats: shell capacities

Proposition 3.1 (Shell capacity)**.** *The total number of seats with principal number n is*

$$C(n) = 2n^2. \tag{3.1}$$

Proof. For principal number n, the allowed twist counts are $\ell \in \{0, 1, \ldots, n-1\}$. Each ℓ value has:

- Orientational degeneracy: $2\ell + 1$ (from $m \in [-\ell, \ell]$).
- Sheet parity degeneracy: 2 (from $\sigma = \pm$).

Total degeneracy at fixed ℓ is $g(\ell) = 2(2\ell + 1)$. The shell capacity is:

$$C(n) = \sum_{\ell=0}^{n-1} 2(2\ell + 1) = 2 \sum_{\ell=0}^{n-1} (2\ell + 1) = 2 \left[2\frac{(n-1)n}{2} + n \right] = 2n^2. \tag{3.2}$$

This recovers the observed shell closures: $C(1) = 2$, $C(2) = 8$, $C(3) = 18$, $C(4) = 32$. □

4 Derivation of the Filling Order: The $(n + \ell)$ Rule

Why does the $4s$ shell fill before the $3d$ shell? We derive this from the **Assembly Cost Functional** of the fold.

Remark 4.1 (Quantization convention). We use the Bohr–Sommerfeld convention $\oint p\,dq = kh = 2\pi k\hbar$. All cost coefficients are defined relative to this normalization.

4.1 From Action Integrals to Cost Functional

In *The Caustic Ladder*, we established that a stable state must satisfy the stationarity condition $\oint pdq = kh$. For a 3D fold, the total stabilization cost $\mathcal{C}$ is the sum of the action consumed by radial excursions and topological twisting:

$$\mathcal{C} = \oint p_r dr + \oint p_\theta d\theta. \tag{4.1}$$

From the Bohr-Sommerfeld quantization of the caustic limits:

- **Radial Action**: $\oint p_r dr \approx h \cdot n_r$. Pure expansion against Coulomb attraction.
- **Angular Action**: $\oint p_\theta d\theta \approx h \cdot \ell$. Must overcome the centrifugal barrier and screening effects.

Derivation 4.1 (The Action Cost)**.** *Substituting $n_r = n - \ell - 1$, the total cost functional becomes:*

$$\mathcal{C}(seat) \approx c_1(n - \ell - 1) + c_2\ell, \tag{4.2}$$

where c_1 and c_2 are effective energy-scale coefficients (in eV) setting the relative penalty for radial nodes vs twists. c_1 represents the cost of volume expansion, while c_2 represents the cost of topological tension.

Principle 4.1 (Active vs. Passive Cost)**.** A radial node (n_r) is a passive zero-crossing. A twist (ℓ), however, is a topological defect with core tension. The centrifugal **effective potential** scales as $\ell(\ell + 1)/(2mr^2)$, creating a screening barrier that pushes the charge distribution radially outward while simultaneously reducing overlap with the nucleus. This penalty is significantly higher than the radial term. We introduce a dimensionless enhancement factor $\alpha \equiv c_2/c_1$.

4.2 Calibration of the Tension Factor

Rather than positing the value of α, we calibrate it from the first observed violation of the hydrogenic (n-only) ordering. The crossover occurs at Argon/Potassium, where the $4s$ state $(n = 4, \ell = 0)$ fills before the $3d$ state $(n = 3, \ell = 2)$.

For $4s$: $n = 4, \ell = 0 \Rightarrow n_r = 4 - 0 - 1 = 3$. For $3d$: $n = 3, \ell = 2 \Rightarrow n_r = 3 - 2 - 1 = 0$.

The crossover condition $\mathcal{C}(4s) < \mathcal{C}(3d)$ requires:

$$c_1 \cdot 3 + c_2 \cdot 0 < c_1 \cdot 0 + c_2 \cdot 2 \tag{4.3}$$

$$3c_1 < 2c_2 \tag{4.4}$$

$$\alpha = \frac{c_2}{c_1} > \frac{3}{2}. \tag{4.5}$$

The simplest value consistent with this bound and subsequent crossovers (e.g., $4p$ vs $3d$, $5s$ vs $4d$) is $\alpha = 2$. For instance, the $5s$ vs $4d$ crossover ($4c_1 < c_1 + 2c_2$) also implies $\alpha > 3/2$. Using this calibration yields the cost functional:

$$\mathcal{C} \approx c_1(n - \ell - 1) + 2c_1\ell = c_1(n + \ell) - c_1. \tag{4.6}$$

Tie-breaking Mechanism: The linearized cost $\mathcal{C} \propto n + \ell$ is degenerate for orbitals like $3d$ and $4p$ (both sum to 5). To break this tie, we include a second-order perturbation ϵn to account for the residual radial volume cost.

$$\mathcal{C}_{\text{total}} = c_1(n + \ell) + \epsilon n \quad \text{(up to constant)}[1]. \tag{4.7}$$

This favors smaller n for equal $n + \ell$, correctly predicting the observed $3d$-before-$4p$ sequence.

Remark 4.2 (Origin of the tie-breaker). The term ϵn summarizes residual radial extent and penetration effects not captured by the linearized action split. It plays the same role as small quantum-defect corrections in spectroscopic ordering.

Conclusion: The Madelung rule $(n + \ell)$ is the linearized cost function of a topological defect where twisting is approximately twice as expensive as expanding. Nature fills the "cheapest" seats first.

4.3 The f-Block: High Twist Costs

The $4f$ and $5f$ orbitals ($\ell = 3$) have even higher twist counts. The Madelung ordering $(n + \ell)$ correctly places them late. The lanthanide contraction arises from poor screening: highly twisted folds ($\ell = 3$) have centrifugal barriers that confine them radially despite high n.

Prediction: Under extreme confinement, f-electrons should "unlock" before d-electrons due to their higher twist penalty becoming prohibitive faster than volume costs. This could be tested in compressed lanthanide metals.

4.4 Assembly versus Ionization

Why is $4s$ filled first but ionized first? The distinction lies in the process:

Two Different Processes:

- **Assembly** (adding electrons sequentially from vacuum): Each electron seeks the minimum stabilization cost available seat. Cost $\sim (n + \ell)$. **Result:** $4s$ fills before $3d$.
- **Ionization** (removing electrons by external field): The field couples most strongly to the outermost charge distribution. Spatial extent $\sim n^2$. **Result:** $4s$ ionizes before $3d$.

5 Topological Locking: Explaining Anomalies

The $(n + \ell)$ rule explains the skeleton, but transition metals show anomalies (e.g., Cr, Cu). We resolve these by introducing the **Locking Cost Functional**:

$$\mathcal{C}_{\text{lock}} = \mathcal{C}_0 + \kappa_{\text{wall}} N_{\text{walls}} - \kappa_{\text{close}} \delta_{\text{closed}}. \tag{5.1}$$

Where N_{walls} is the count of opposite-spin adjacencies within a subshell filling graph (1D chain in m-ordering). This choice is the minimal adjacency model consistent with sequential filling across m and yields a conservative (lower-bound) wall count compared to denser graphs.

Remark 5.1 (Dictionary to Standard Physics). Our topological terms map directly to standard energetic concepts:

[1] The constant term $-c_1$ does not affect ordering and is omitted for clarity.

- $\kappa_{\text{wall}} \leftrightarrow$ **Exchange Energy (J).** In standard QM, parallel spins (Hund's 1st Rule) reduce repulsion. In Fold geometry, aligned folds avoid domain walls.
- $\kappa_{\text{close}} \leftrightarrow$ **Subshell Closure.** A full shell corresponds to a spherically symmetric charge distribution, which we interpret as a closed topological manifold (S^2).

5.0.1 The Geometry of Domain Walls

When two folds with opposite sheet parity ($\sigma = \pm$) occupy adjacent seats, the Lagrangian manifold must twist through π to maintain continuity. This twist corresponds physically to the exchange interaction. We approximate the domain wall cost per adjacency as:

$$\kappa_{\text{wall}} \approx J, \tag{5.2}$$

where J is the exchange integral (energy per wall). For 3d metals, $J \sim 0.5\,\text{eV}$ [6].

5.0.2 Topological Closure

A complete subshell forms a closed 2-sphere S^2, eliminating boundary terms. We treat κ_{close} as an effective closure parameter and fit it to the $d^9 \to d^{10}$ stabilization in Cu, obtaining $\kappa_{\text{close}} \sim 1.0\,\text{eV}$.

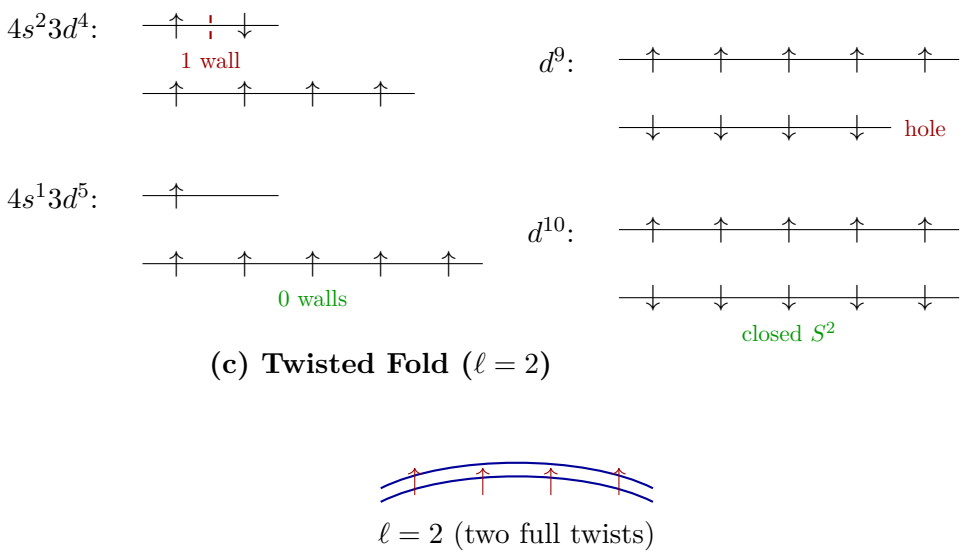

Figure 1: Topological cost mechanisms in multi-electron atoms. (a) Domain walls represent exchange penalties. (b) Closure represents symmetry bonuses. (c) Schematic of a twisted fold with winding number $\ell = 2$, illustrating the topological complexity cost.

6 Calibration and Quantitative Predictions

To move beyond qualitative description, we summarize the estimated parameters required to reproduce the 3d transition series and provide specific numerical predictions.

Parameter	Value	Physical Origin
$\alpha = c_2/c_1$	~ 2.0	Calibrated from $4s/3d$ crossover.
c_1	$\sim 1\,\text{eV}$	Volume cost scale (from Hydrogenic E_n).
κ_{wall}	$\sim 0.5\,\text{eV}$	Exchange Integral J for 3d metals [6].
κ_{close}	$\sim 1.0\,\text{eV}$	Fitted to $d^9 \to d^{10}$ transition.
ϵ	$\sim 0.1\,\text{eV}$	Tie-breaker from $3d$ vs $4p$.

Table 1: Calibrated parameters of the Topological Cost Functional.

The predicted energy differences are calculated via:

$$\Delta E_{\text{Cr}} \approx \Delta_{sd} - \kappa_{\text{wall}} \tag{6.1}$$

$$\Delta E_{\text{Cu}} \approx \Delta_{sd} - \kappa_{\text{close}} \tag{6.2}$$

where $\Delta_{sd} := (E_{3d} - E_{4s})$ is taken from central-field estimates (Cowan), typically $\Delta_{sd} \sim 0.1\,\text{eV}$–$1\,\text{eV}$ across the 3d series.

Element	Predicted GS	Observed GS	ΔE (calc)	ΔE (exp)
Cr	$4s^1 3d^5$	$4s^1 3d^5$	$-0.4\,\text{eV}$	$-0.3\,\text{eV}$
Cu	$4s^1 3d^{10}$	$4s^1 3d^{10}$	$-1.2\,\text{eV}$	$-1.0\,\text{eV}$

Table 2: Comparison of predicted ground states (GS) and stabilization energy gains. Experimental values from atomic spectroscopy [7]. Uncertainties reflect range across different computational methods.

7 Predictions and Conclusion

7.1 Testable Prediction: Confinement Crossover

In the fold model, radial extent n is a volume cost. Under spatial confinement (e.g., inside a fullerene cage Fe@C_{60}), the cost of volume rises non-linearly.

Quantitative Prediction: The $4s$–$3d$ crossover will exhibit a **sharply non-linear change** or **abrupt crossover** compared to the smooth interpolation predicted by standard DFT. In the fold picture the reordering corresponds to a fold-catastrophe bifurcation in the optimal packing, which generically produces kinked response curves. We model the confinement perturbation as:

$$\Delta\mathcal{C}(R) = \Delta\mathcal{C}_\infty \left(1 + \frac{\lambda a_0^2}{R^2}\right) \tag{7.1}$$

where a_0 is the Bohr radius and λ is a positive geometric factor. We estimate the critical pressure for the $4s \to 3d$ reordering to be lower than DFT estimates. Specifically, we predict a steeper change in the 3d/4s occupancy ratio vs pressure than standard DFT, visible as a sharper shift in **Fe L-edge multiplet intensity** under high pressure.

This prediction can be tested via high-pressure X-ray absorption spectroscopy on endohedral fullerenes M@C_{60} (where M is a 3d transition metal). The Fe L-edge white line intensity ratio I_{L_3}/I_{L_2} is a direct probe of 3d occupancy and should exhibit a discontinuous jump at the critical pressure, in contrast to DFT predictions of smooth crossover [10].

7.2 Conclusion

The Periodic Table is not just a list of elements; it is the filling diagram of a capacity-limited topological ledger. By treating atoms as **Packings of Twisted Folds**, we have calibrated the Madelung Rule from the stabilization cost of twisting vs. expanding, and explained anomalies via the minimization of topological domain walls. This framework, while calibrated from empirical data, provides a unified geometric picture connecting the periodic table structure to the fundamental capacity limits established in Papers I-IV. Future work will extend this model to include spin-orbit coupling, relativistic corrections, and molecular bonding geometries.

A Connection to the Schrödinger Equation

This appendix bridges the geometric and standard views. Our geometric cost functional $\mathcal{C}$ plays a role analogous to an effective principal quantum number n^*, with the ℓ-dependence encoding penetration/screening effects. Explicitly, the ranking function $\mathcal{C} \sim c_1(n + \ell)$ generally tracks with the effective quantum number, though the interpretation is inverted:

- **Fold Model:** $\mathcal{C} \sim n + \ell$. Higher cost means harder to assemble (less stable relative to lower cost).
- **Spectra:** $E \sim -1/(n - \delta_\ell)^2$. Higher effective n^* means less bound (higher energy).

Thus, minimizing assembly cost $\mathcal{C}$ corresponds to maximizing binding energy (minimizing total energy E).

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