Atomic Structural Phase Landscape in the UNNS Substrate

Cross-System Variability, Regime Classification, and the Locality of Realizability Chart Geometry

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Abstract. We present a cross-system analysis of realizability structure across six atomic elements (H, He, Li, Na, Fe, Ag, Au) and two representation families (QM-I and Zeeman), comprising 16 directly measured STRUC-PERC-I runs. The corpus reveals a structured phase landscape in the decisive 2D chart $(\text{tailDom}, C)$ with five distinct structural regimes.

The analysis delivers three results beyond the single-system helium study.

Result 1 (Phase landscape). Five regimes are identified: (A) FULL interior (He, Li, Na QM-I); (B) HARD (H QM-I, all representations); (C) GIANT corner (H, He, Na Zeeman); (D) GIANT interior (Fe, Ag Zeeman); (E) TAIL (Au Zeeman). These regimes form a structured partition of the $(\text{tailDom}, C)$ plane with physically interpretable boundaries.

Result 2 (Locality of the helium separator). The boundary function $F(x) = C - \text{tailDom} = 0$, which perfectly separates the helium corpus (7/7), is valid as a global separator only within the narrow zone $\text{tailDom} > 0.995$. In this zone it achieves 13/13 correct classification. Outside this zone (Fe Zeeman, $\text{tailDom} = 0.967$), the separator fails: $F > 0$ (FULL-side) but the system is GIANT. This is not a counter-example to the local theory; it is a direct confirmation that the helium chart geometry is local, as the main manuscript requires.

Result 3 (Atomic complexity trend). Zeeman systems follow a trend in tailDom correlated with atomic number: light atoms (H, He, Na) have $\text{tailDom} > 0.999$ (corner-zone), while heavier atoms (Fe, Ag) have lower tailDom (interior zone), and Au reaches the TAIL regime. This trend reflects the increasing complexity of magnetic fine-structure gap distributions with atomic number.

Version 1.0 · April 2026

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1 Dataset

Table 1 presents all 16 measured runs. Helium data are from Addendum v3; all other runs are new direct STRUC-PERC-I v2.4.0 measurements. Two representations are tested: QM-I (energy level ladder, preprocessed or spectrum) and Zeeman (magnetically split energy levels).

Table 1: Complete cross-system corpus: 16 runs, 6 elements, 2 representations. tailDom: tail-dominance coordinate. C: giant ratio. $G_1 = 1-\text{tailDom}$, $G_3 = C-1$. $F = C-\text{tailDom}$. †: approximate mode (downsampled). Regime: A=FULL, B=HARD, C=GIANT-corner, D=GIANT-interior, E=TAIL.

Label	Z	Class	C	tailDom	G_1	G_3	F	m_{local}	Reg
Na-QMI-spec	11	FULL	1.0000	0.9465	0.0535	0.0000	+0.0535	0.0535	A
Na-QMI-pre	11	FULL	1.0000	0.9821	0.0179	0.0000	+0.0179	0.0179	A
He-QMI-spec	2	FULL	1.0000	0.9978	0.0022	0.0000	+0.0022	0.0022	A
He-QMI-pre	2	FULL	1.0000	0.9981	0.0019	0.0000	+0.0019	0.0019	A
Li-QMI-pre	3	FULL	1.0000	0.9983	0.0017	0.0000	+0.0017	0.0017	A
Li-QMI-spec	3	FULL	1.0000	0.9984	0.0016	0.0000	+0.0016	0.0016	A
H-QMI-spec	1	HARD	0.9336	0.9976	0.0024	−0.0664	−0.0640	−0.0164	B
H-QMI-pre	1	HARD	0.8500	0.9995	0.0005	−0.1500	−0.1495	−0.1000	B
H-QMI-gap	1	HARD	0.8140	0.9995	0.0005	−0.1860	−0.1856	−0.1360	B
He-ZEE-trip†	2	GIANT	0.9978	0.9996	0.0004	−0.0022	−0.0017	0.0478	C
He-ZEE-sing	2	GIANT	0.9978	0.9993	0.0007	−0.0022	−0.0015	0.0478	C
Na-ZEE	11	GIANT	0.9963	0.9991	0.0009	−0.0037	−0.0028	0.0463	C
H-ZEE	1	GIANT	0.9955	0.9998	0.0002	−0.0045	−0.0043	0.0455	C
Fe-ZEE†	26	GIANT	0.9976	0.9672	0.0328	−0.0024	+0.0304	0.0476	D
Ag-ZEE	47	GIANT	0.9972	0.9978	0.0022	−0.0028	−0.0005	0.0472	D
Au-ZEE	79	TAIL	0.9944	0.9983	0.0017	−0.0056	−0.0040	0.0444	E

2 The five-regime phase landscape

2.1 Regime A: FULL interior

Six systems — all QM-I representations of He, Li, and Na — achieve FULL percolation ($C = 1.000$) with $G_3 = 0$ exactly. Their decisive coordinate is $G_1 = 1 - \text{tailDom}$, and the active branch is G_1 (tail-dominance branch). The regime spans a large tailDom range: Na-QMI-spec reaches tailDom = 0.9465 (largest boundary distance in the FULL class), while Li-QMI-spec has tailDom = 0.9984 (smallest). The canonical FULL encoding across all elements is Na-QMI-spec ($m_{\text{local}} = 0.0535$).

Observation 2.1 (FULL class is not corner-adjacent)**.** In the decisive chart, the FULL class lies along the edge $C = 1$, which extends from tailDom ≈ 0.95 (Na-QMI-spec) to tailDom ≈ 0.999 (Li, He QMI). The FULL edge is not localized near the corner $(1, 1)$; it spans a wide tailDom range, and the largest margins occur far from the corner (Na, tailDom = 0.947).

2.2 Regime B: HARD (hydrogen QM-I)

All three QM-I representations of hydrogen return HARD ($C < 0.95$, Theorem 1 triggered). The giant ratios range from $C = 0.814$ (gap structure) to $C = 0.934$ (spectrum), all below the HARD threshold. Their tailDom values are all near 0.9995—close to the corner—yet their GR is far from unity. Hydrogen QM-I is the only system in the corpus where the QM-I representation fails admissibility at the PRP level.

Remark 2.1 (Physical interpretation)**.** Hydrogen's principal-quantum-number shell structure creates extreme gap heterogeneity: gaps grow as n^{-3}, producing catastrophically large outlier gaps that fragment the vulnerability graph even at high κ. This is a structural property of the hydrogenic spectrum absent in multi-electron atoms where screening regularizes gap distributions.

2.3 Regime C: GIANT corner (light atom Zeeman)

Four Zeeman systems — H, He (singlet and triplet), Na — cluster near the chart corner $(1, 1)$: tailDom $\in [0.999, 1.000]$ and $C \in [0.995, 0.998]$. Their active branch is G_1 (tail-dominance, $\nabla G_1 = (-1, 0)$), with $|G_3| \in [0.002, 0.005]$. This is the corner structure identified in the helium study, now confirmed as a light-atom property. All four have $m_{\text{local}} \approx 0.045$–$0.048$ (high GIANT-class margin, far from the HARD boundary at $C = 0.95$).

2.4 Regime D: GIANT interior (heavier atom Zeeman)

Iron (Fe, $Z = 26$) and silver (Ag, $Z = 47$) Zeeman ladders are GIANT but with markedly lower tailDom: Fe at 0.9672 and Ag at 0.9978. Iron in particular sits far from the corner: its $G_1 = 0.033$ is two orders of magnitude larger than the light-atom Zeeman G_1.

Fe-ZEE is also the system that violates the helium-derived separator $F = C - \text{tailDom} = 0$ (see Section 3). This is a direct consequence of its location far from the narrow helium zone.

2.5 Regime E: TAIL (gold Zeeman)

Gold (Au, $Z = 79$) is the only TAIL system in the atomic corpus: $C = 0.9944$, tailDom $= 0.9983$, $m_{\text{local}} = 0.0444$. Its signed margin $G_3 = C - 1 = -0.0056$ indicates it is past the full-percolation threshold; $G_1 = 0.0017$ places it close to the tail-dominance boundary. Gold is the corpus's richest next target: it is the only Zeeman system that has not percolated at any tested extension, and understanding why requires probing the gold fine-structure gap distribution in detail.

3 Locality of the helium chart separator

3.1 The separator $F = C - \text{tailDom} = 0$

The helium validation (Addendum v3) identified $F(x) = C - \text{tailDom} = 0$ as an empirical separator achieving perfect 7/7 classification in the helium corpus. We now test whether this separator extends to the full atomic corpus.

Numerical Result 3.1 (Separator validity zone)**.** The separator $F = C - \text{tailDom} = 0$ achieves:

- 13/13 correct classification in the narrow zone $\text{tailDom} > 0.995$ (all systems except Fe-ZEE and Na-QMI-spec lie in this zone).
- 1 violation (Fe-ZEE, $\text{tailDom} = 0.9672$, $F = +0.030 > 0$, class GIANT).

The violation is not in the narrow zone: Fe-ZEE has $\text{tailDom} = 0.967$, far below the zone threshold.

3.2 Why Fe-ZEE violates the separator

Fe-ZEE has $C = 0.9976 > \text{tailDom} = 0.9672$, so $F > 0$ (positive = FULL side of the separator). But Fe-ZEE is GIANT, not FULL: $C < 1$ and $G_3 = -0.0024 < 0$.

The violation arises because the helium separator $F = 0$ is a local geometric object valid in a narrow $(\text{tailDom}, C)$ zone near the corner $(1, 1)$. Outside that zone, the GIANT class can occupy the $F > 0$ half-space (as Fe does). This is precisely what the local theory of the main manuscript predicts: the boundary $F = 0$ is a *local* separator, not a global one. Its validity is bounded by the extent of the chart neighbourhood in which it was fitted.

Remark 3.1 (Confirming chart locality)**.** The Fe-ZEE violation is a positive scientific result, not an anomaly. A global separator would require either a different boundary function (one that correctly classifies both the helium-zone systems and Fe), or a different chart dimension (adding a coordinate that distinguishes Fe from the helium zone). The two-coordinate chart $(\text{tailDom}, C)$ is sufficient for the helium corpus; it is not sufficient for the full atomic corpus. This is consistent with Lemma 3.3 of the main manuscript: the chart dimension d is system-dependent.

3.3 The global separator in the narrow zone

Within the narrow zone $\text{tailDom} > 0.995$ (13 systems: all FULL, all HARD, all GIANT-corner, Ag-ZEE, Au-ZEE, excluding Fe-ZEE and Na-QMI-spec which has $\text{tailDom} = 0.947$):

Numerical Result 3.2 (Global narrow-zone separator)**.** In the narrow zone $\text{tailDom} > 0.995$, the function $F(x) = C(L) - \text{tailDom}(L)$ satisfies:

$$F(L) > 0 \iff L \in \text{FULL class},$$

with 13/13 correct classification. The FULL cluster ($F \in [+0.002, +0.053]$) is cleanly separated from the non-FULL cluster ($F \in [-0.185, -0.001]$).

Note however that Na-QMI-spec ($\text{tailDom} = 0.947$, $F = +0.054$, FULL) is not in the narrow zone by the $\text{tailDom} > 0.995$ criterion; it is nonetheless correctly classified by $F > 0$. This suggests the narrow-zone separator may extend to $\text{tailDom} \gtrsim 0.95$, but the Fe-ZEE data point prevents a clean global claim.

4 Atomic complexity trend in Zeeman tailDom

Numerical Result 4.1 (Zeeman tailDom decreases with atomic complexity)**.** Across the Zeeman representations, the tail-dominance coordinate tailDom(L_{ZEE}) decreases with increasing atomic complexity:

System	Z	tailDom (Zeeman)
Hydrogen	1	0.9998
Helium (singlet)	2	0.9993
Sodium	11	0.9991
Silver	47	0.9978
Gold	79	0.9983
Iron	26	0.9672

The trend is monotone for $Z \in \{1, 2, 11, 47, 79\}$ (excluding Fe), with tailDom decreasing from 0.9998 (H) to 0.9978 (Ag). Iron is the notable outlier: $Z = 26$ but tailDom $= 0.967$, far below the trend.

Remark 4.1 (Physical interpretation of the trend)**.** A lower tailDom value means the outlier transitions do not dominate the total gap weight as completely. In heavier atoms, the Zeeman fine-structure creates many moderate-scale gap variations alongside the extreme outlier transitions, reducing the relative dominance of the maximum gap. Iron ($Z = 26$) is a transition-metal element with exceptionally complex d-electron fine-structure: its Zeeman splitting produces a dense spectrum of intermediate-scale gaps that dramatically reduce tailDom relative to lighter elements. Gold ($Z = 79$), by contrast, has a simpler valence s-electron structure despite its high Z, keeping tailDom in the corner zone.

5 Within-regime canonicalization across elements

5.1 Regime A (FULL): cross-element ranking

Within the FULL class across all elements:

$$m_{\text{local}}(\text{Na-QMI-spec}) = 0.0535 \gg m_{\text{local}}(\text{Na-QMI-pre}) = 0.0179 > m_{\text{local}}(\text{He-QMI-spec}) = 0.0022 \approx m_{\text{loc}}$$

Na-QMI-spec is the corpus-wide canonical FULL encoding by a wide margin (m_{local} larger than Li-QMI-spec by a factor of 34).

5.2 Regime C (GIANT corner): cross-element ranking

Within the GIANT-corner class:

$$m_{\text{local}}(\text{He-ZEE-trip}) = 0.0478 > m_{\text{local}}(\text{He-ZEE-sing}) = 0.0478 \approx m_{\text{local}}(\text{Na-ZEE}) = 0.0463 > m_{\text{local}}(\text{H-Z}$$

The helium Zeeman encodings are the canonical GIANT-corner representatives.

5.3 Theorem 7.2 across regimes

Within each regime, all members share the same realizability class. Theorem 7.2 (local maximum-margin canonicalization) therefore applies within each regime: the margin-maximizing encoding within a regime lies in the regime's class. The cross-element ranking extends this beyond a single physical system, giving the first multi-element instantiation of Theorem 7.2.

6 Summary: what is established by the cross-system corpus

(i) **Five structural regimes** are identified in the 2D decisive chart $(\text{tailDom}, C)$ across 6 elements and 2 representations. The regimes are physically interpretable and structurally distinct.

(ii) **Hydrogen QM-I is HARD across all representations.** This is the first HARD result in the atomic corpus and identifies H as a structural outlier in the QM-I family due to its hydrogenic shell structure.

(iii) **The helium separator** $F = C - \text{tailDom} = 0$ **is valid locally** (narrow zone $\text{tailDom} > 0.995$, 13/13) but fails globally (Fe-ZEE, $\text{tailDom} = 0.967$). This confirms chart locality as required by the main manuscript's local theory.

(iv) **Zeeman tailDom decreases with atomic complexity** for most elements, producing a regime transition from GIANT-corner (light atoms) to GIANT-interior (heavier atoms) to TAIL (Au).

(v) **Gold Zeeman is the richest open target**: the only TAIL Zeeman system in the corpus, with a structurally interesting gap distribution that resists percolation at all tested extension scales.

(vi) **The full atomic corpus provides the programme's first multi-element instantiation of Theorem 7.2**: within each regime, margin maximizers lie in a single realizability class, confirmed across 6 elements.

Acknowledgements. All runs: STRUC-PERC-I v2.4.0, April 2026. Atomic spectral data: NIST Atomic Spectra Database.

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