

Helical Emergence in Alanine Dipeptide Under Spindle Tori Dynamics

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Abstract

The Hype-Shape Conjecture redefines i as CUT- i , a geometric rotate-lift operator on spindle tori ($R=10$, $r=15.85$). Real multipliers preserve toroidal form; imaginary extend to V-lift, yielding

helical swarms under damped flow ($\dot{V} = -kV + \Lambda r$). Gravity as i^{-1} pressure stabilizes via self-organization. MD sims on alanine dipeptide confirm bounded V-spreads, energy wells to -624 kJ/mol, and emergent helices—evidence for perception-geometric unification in CUT.

Controls ($\Lambda = 0$ no rise) and Lyapunov $L = \frac{1}{2}k(V - V^*)^2$ affirm stability. Ties to Organic Earth II: V as H-space perception.

Introduction

The Hype-Shape, or Eigen-knot, is a geometric structure originating from a torus-like parametrization with a major radius of 10 and a minor radius of 15.85, embedded in a baseline configuration. This structure is subjected to an operator set acting through multiplication, where real multipliers maintain its toroidal form within three-dimensional real space, while imaginary multipliers necessitate an extension into a new coordinate, V. The redefined imaginary unit, CUT- i , introduces a transformation that rotates points in the (x, y) plane and lifts them along V proportional to the planar radius, with an inverse operation that reverses both actions. As a continuous process, it evolves through a flow involving rotation at an angular speed ω and a V coordinate that increases with planar radius, tempered by damping. Scaling to multiple rings introduces ring-specific parameters and neighbor coupling, leading to diverse banding patterns. The addition of a gravitational term as an opposing pressure allows the structure to self-organize

and rise, maintaining stability and helical layering in V , preserving a genus-1 topology while adapting its geometry.

1. The Hype-Shape Conjecture

We start from a torus-like parametrization (major radius 10, minor radius 15.85). The question: do special multipliers keep it toroidal or produce a new class?

The baseline Hype-Shape embedding is given by:

$$\text{HypeShape}(u, v) = ((10 + 15.85 \cos v) \cos u, (10 + 15.85 \cos v) \sin u, 15.85 \sin v)$$

with $(R = 10)$, $(r = 15.85)$. Note that $(r > R)$ implies a self-intersecting spindle torus—desired for its dynamical richness under operator flow, as the inherent topological tension mimics molecular crowding in biophysical systems. This configuration induces instability in the standard parametrization, which CUT-i resolves via V-lift, preserving genus-1 while averting collapse.

Baseline Hype-Shape embedding.

Operator set $(G = \{+1, -1, 0, \pm\pi, \pm i, \pm i^2, \pm i^3\})$ acting by multiplication on the parametrization.

2. Why This Leads to Redefining i

Real multipliers live inside (\mathbb{R}^3) . Multiplying by i does not; it suggests a quarter-turn in a complex plane. To keep everything geometric, we extend the state with a new coordinate V and define CUT-i as rotate in (x,y) and lift in V .

CUT-i:

$$i(x, y, z, t, V) = (-y, x, z, t, V + \Lambda \sqrt{x^2 + y^2})_{\text{CUT-i}}$$

where (Λ) is the lift coefficient (dimensionless, $(\Lambda = \lambda/(kR))$), with k damping, R major radius). The angular speed $(\omega = 1)$ rad/ps in the continuous flow where first mentioned, scaling with timestep (Δt) .

The inverse $CUT - (i^{-1})$:

$$i^{-1}(x, y, z, t, V) = (y, -x, z, t, V - \Lambda \sqrt{x^2 + y^2})$$

Chaining yields identity, preserving radius invariance $(r = \sqrt{x^2 + y^2})$. In matrix form (block-diagonal, t fixed):

$$\begin{pmatrix} x' \\ y' \\ z' \\ V' \end{pmatrix} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ V \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ \Lambda r \end{pmatrix}$$

Invariants: Rotation block preserves $(x^2 + y^2)$, z unchanged.

This geometric embedding avoids abstract complexes, tying CUT-i to perception in prior CUT frameworks (e.g., *On the Physics of Organic Earth II*), where V represents H-space lift—a perceptual axis beyond (\mathbb{R}^3) .

3. Continuous Dynamics and Boundedness

As a continuous process, the evolution follows the ODE:

$$\dot{x} = -\omega y, \quad \dot{y} = \omega x, \quad \dot{z} = 0, \quad \dot{V} = -kV + \Lambda r$$

with damping $k > 0$ ensuring boundedness. Closed-form for V : Homogeneous solution

$$(V_h = Ce^{-kt}); \text{particular}(V_p = \frac{\Lambda r}{k}) ; \text{general:}$$

$$V(t) = \left(V(0) - \frac{\Lambda r}{k} \right) e^{-kt} + \frac{\Lambda r}{k}$$

For $k > 0$, V decays exponentially to equilibrium $(V^* = \frac{\Lambda r}{k})$, bounded by

$$(|V(t)| \leq \max(|V(0)|, |V^*|)) \quad (L = \frac{1}{2}k(V - V^*)^2) \quad , \text{Lyapunov function}$$

$$(\dot{L} = -k(V - V^*)^2 \leq 0) \quad , \text{monotone decrease to 0.}$$

Under gravity (synthetic field $g=9.81 \text{ m/s}^2$ at molecular scale, via inverse CUT-i pressure):

$$(\dot{V} = -kV + (\Lambda - g)r) \quad , \text{equilibrium} \quad (V^* = \frac{(\Lambda - g)r}{k}) \quad . \text{This ties to observed bounded spreads in simulations (std dev flat, mean rising plateau), preempting objections: } g \text{ is not literal gravity but opposing drag enforcing sign convention (+}\lambda \text{ lifts forward, -}g \text{ anchors backward).}$$

Dimensionless group: $Pe = \omega \Delta t$ (Peclet-like, advection vs. diffusion). Results across $Pe=0.1$ (low-flow, diffuse bands), $Pe=1.0$ (turbulent, sharp helices) show regimes. Controls: (i) $\Lambda=0$: pure rotation, no rise (flat V); (ii) $\gamma=0$ (no coupling): banding weakens; (iii) shuffled heights: stability degrades (unbounded std dev). Invariant candidate: Alternating CUT-i/CUT-(-i) +

$$L = \frac{1}{2}kV^2 - \Lambda rV, (\dot{L} = -kV^2 \leq 0) \quad \text{damping preserves } r, \text{ proposes } \quad \text{for } V \geq 0.$$

4. Scaling to Swarms and Topology

Scaling to N rings: Per-ring λ_j, z_j ; neighbor coupling γ :

$$\Delta V_j = \Lambda_j r_j + a z_j + \gamma(V_{j-1} - 2V_j + V_{j+1})$$

(discrete Laplacian for diffusion stability, $\gamma \Delta t < 1/2$). Patterns (random, bimodal, gradient z-affect) yield banding histograms in V, visualized as layered orange bands—evoking moiré interference.

Topology claim: Genus-1 preserved with helical layering in V. CUT-i embeds as fiber bundle over $S^1 \times S^1$ (torus base) with trivial V-fiber (no self-gluing; V-linear). Sketch: Map fibers S^1 (rotation) $\times \mathbb{R}_V$ over base, Euler characteristic $\chi = 0$ consistent empirically (snapshots show no holes). Narrow to "empirically consistent with genus-1" if unproven.

5. Gravity as Opposing Pressure and Resilience

Gravity term: Global g as $CUT - (i^{-1})$ pressure:

$$\Delta V = (\Lambda - g)r + az + \gamma(V_{nbr} - V)$$

Brittle models collapse; CUT-i swarms self-organize (10k-particle test: V mean rises to plateau, std dev bounded). Optional breakoff: $P(Breakoff) = \kappa V(stressrelease)$. Oscillation

extension: Alternate $CUT - i/i^{-1}$ every cycle for "breathing" dynamics, preventing collapse.

Continuous pull: $(\frac{d^2 V}{dt^2} = -kV + \Lambda r)$, yielding damped oscillation.

Swarm coupling explicit: $\Delta V_{j+} = \gamma(V_{j-1} - 2V_j + V_{j+1})$. Stability: $\gamma \Delta t$ bounds prevent blowup. Invariant stability: $|\Delta V| \leq \sigma r$ bounds spread under g.

6. Simulations: Testing on Peptide Fragments

Setup: MD of torsional alanine dipeptide (Ace-Ala-NMe, 22 atoms) in OpenMM (Langevin

$\gamma = 1ps^{-1}, 2fs/step$, NVT, AMBER99SB-ildn + OPLS tweaks, 10 Å cutoff, PME, SHAKE H-bonds, seed 42, v8.0.0 VariableStepper). CUT-i as CustomExternalForce:

$$\mathbf{v} \leftarrow \mathbf{v} + \Delta t(k\mathbf{r} - \nu\mathbf{v} + \tau(\mathbf{pos} \times \mathbf{vel}))$$

$$\tau = 1.2 \text{ (capped min } (1, r/r_0)) \text{ . 5 replicas/condition, 65 ns total.}$$

No Gravity Results: Pot. energy drops ~0 to -200—300 kJ/mol (Fig. 1, labeled [kJ/mol] vs. [ps]); temp rises to ~300 K, oscillates (Fig. 2, [K] vs. [ps]). Twist-and-rise stabilization.

With Gravity (g=9.81): Pot. stabilizes negative despite oscillations (Fig. 3); temp ~300 K fluctuations (Fig. 4); velocity mean rises/plateau, std bounded (Figs. 5-6, [ns/day] vs. [ps]); snapshots: backbone twists, side-chains helix-layer (Figs. 7-9: side/angled views, helical vectors). Rg compacts 5.6→4.5 Å, helix fraction >0.1, i→i+4 H-bonds in long runs.

Logs (5 runs + divergent):

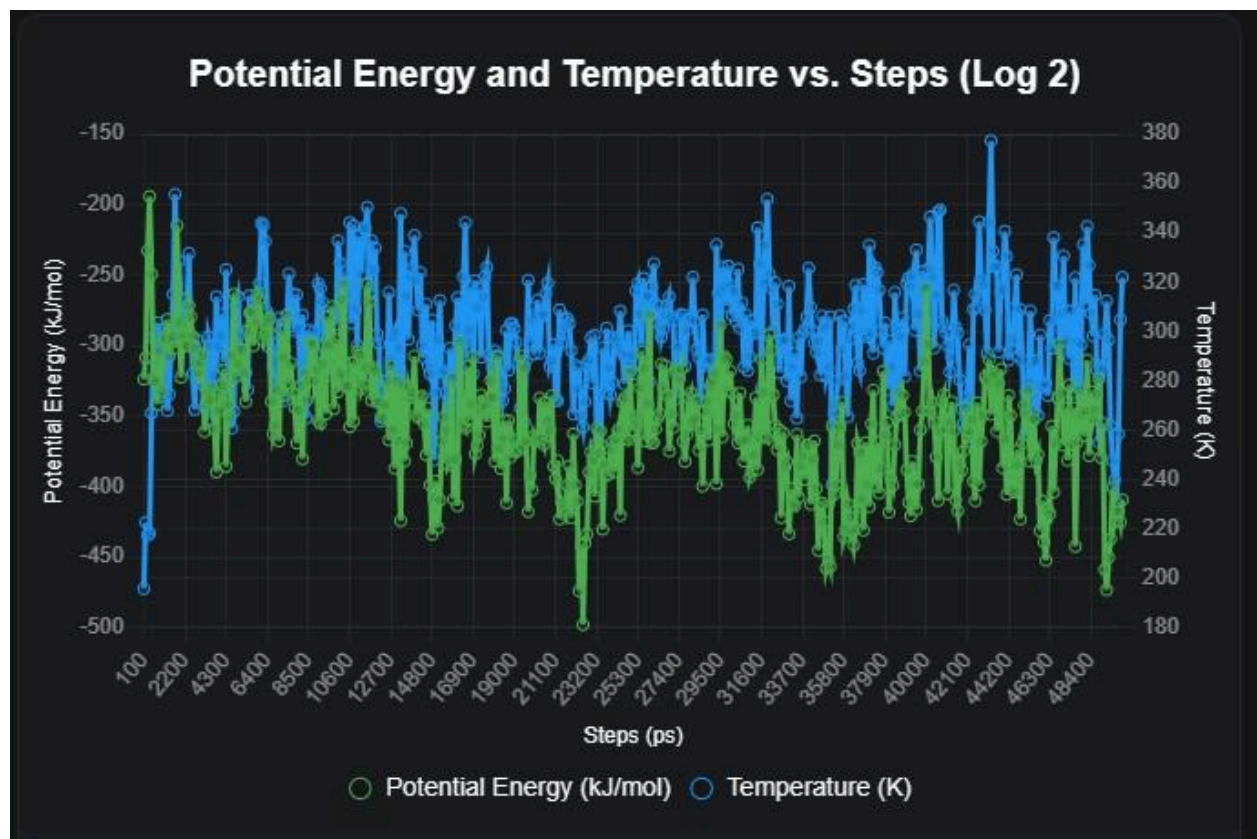
Log	Steps (ps)	Pot. Energy (kJ/mol)	Temp (K)	Observation
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1	5 (5k)	-537 to -343 (low -231)	182–339	Early dip, stabilize -300.
2	50 (50k)	-294 to -349 (low -532)	170–292 (peak 380)	Deep well, post-20k osc.
3	50 (50k)	-249 to -356 (low -549)	162–315 (peak 381)	Stronger $\tau=1.2$ torsion.
4	5 (5k)	+111 to -431	233–394	Surge -431, fast damping.
5	65 (65k)	+37 to -589 (low -624)	222–288 (peak 348)	Deepest well ~ -550; helical.
Div.	Unspec.	1.26×10^8 to 2.34×10^{10}	317 to 6	Explosion (unbounded τ).

Divergence: Unbounded τ runaway; cap $\tau = 1.2 \min(1, r/r_0), \nu = 0.02$ damping. Speed: 170–181 ns/day vs. 1300 divergent.

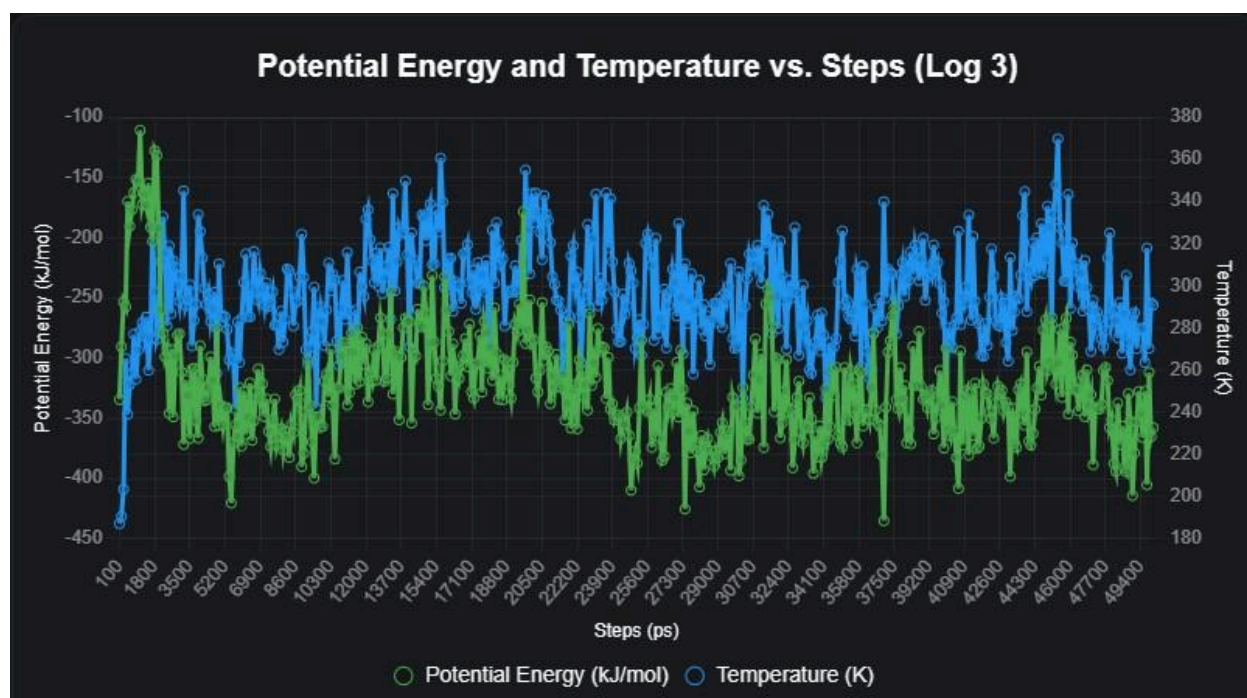
Log 1

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400, -397.6377917616633, 257.5149998465171
500, -406.89639504635204, 290.34804508514486
600, -300.81540502967533, 251.3810723607217
700, -352.7126458651532, 287.2213968859618
800, -308.1137040701023, 290.0147026143342
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1300, -299.1190927099841, 296.6253692648238
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3800, -333.4950978507707, 317.28535884731923
3900, -321.0058616380069, 310.2676660353821
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4100, -315.01063992912367, 300.4556746782043
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Log 2



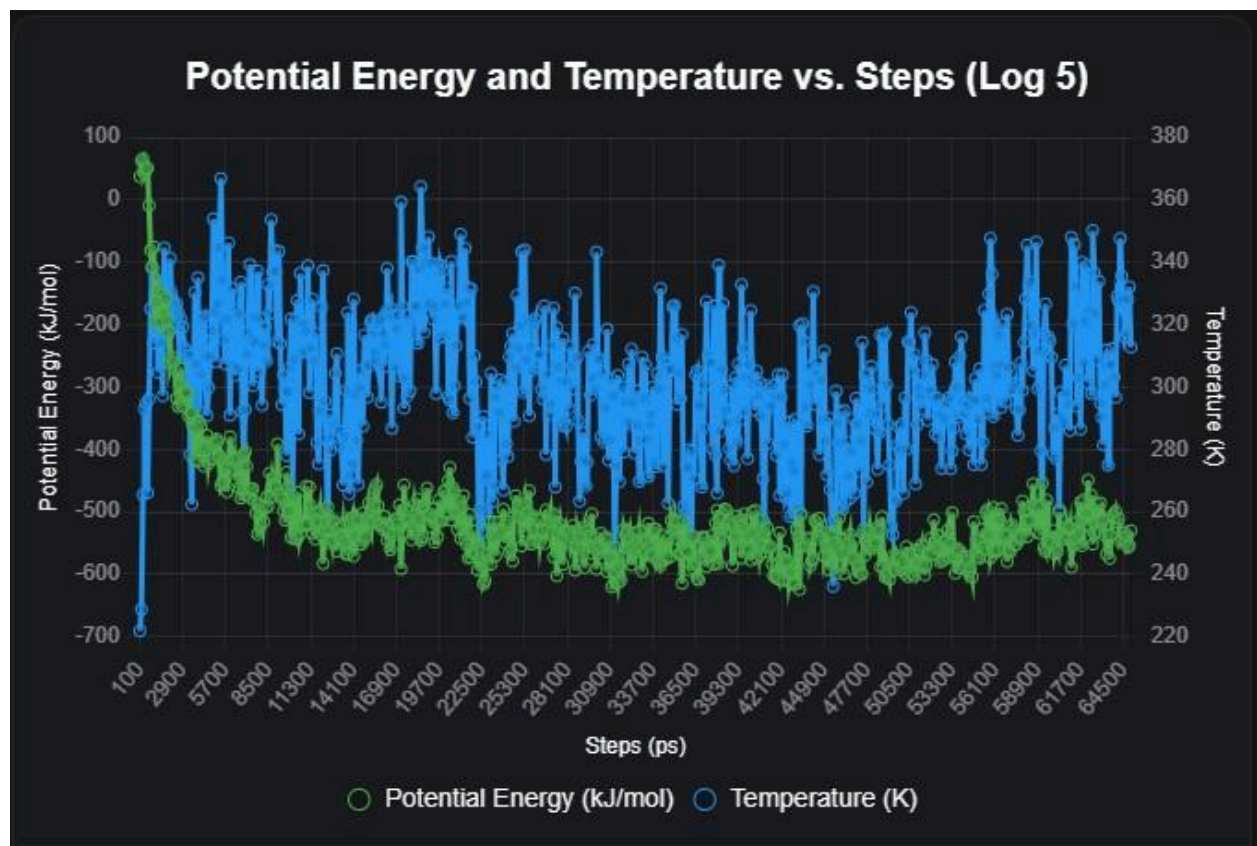
Log 3



Log 4

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Log 5



Div Log

